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宇宙航空研究開発機構特別資料

JAXA Special Publication

東京大学 ロケットエンジンモデリングラボラトリー（JAXA社会連携講座）シンポジウム ロケットエンジンシミュレーションの最先端、そしてその次へ 後刷集

東京大学工学系研究科
ロケットエンジンモデリングラボラトリー(JAXA社会連携講座)
宇宙航空研究開発機構 情報・計算工学(JEDI)センター

2013年3月

宇宙航空研究開発機構
Japan Aerospace Exploration Agency

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ま え が き

本シンポジウムは、東京大学工学系研究科ロケットエンジンモデリングラボラトリー（JAXA 社会連携講座）と宇宙航空研究開発機構（JAXA）の情報・計算工学（JEDI）センターの共催で開催されました。JAXA 社会連携講座は、ロケットエンジンシミュレーション技術の高度化に関する教育・研究を対象として「10 年間で世界トップクラスの技術力を取得する」ことを目標として、2008 年 4 月より 5 年間の予定で活動を始め、2012 年の 9 月でちょうど 4 年半が経過しました。本講座は極低温や高圧などの液体ロケットエンジン特有の環境下における物理・化学現象の解明、およびそれに基づいた数学モデルの構築を目指しています。今講座には(1)キャビテーション、(2)噴射・微粒化、(3)高圧燃焼、(4)物性・ミクロ現象の 4 つの研究グループがあります。この研究グループは本講座と JEDI とが主体になり、東大の航空宇宙工学専攻、機械工学専攻をはじめとして、他大学・研究機関および関連企業の研究者により構成されていて、定期的に開催されている研究会を中心として活動しております。本年度が本講座の最終年度であり、本シンポジウムは本講座の成果報告の場として企画されました。

ロケットエンジンシミュレーションの対象は極低温から高温までの、しかも高圧の「極限状況」における現象で、その科学はまさに未踏領域の科学であり、多くの挑戦的な課題を内包しています。

ロケットエンジンシミュレーションを完成させるためには、亜臨界燃焼であれば高圧噴射ー微粒化ー蒸発ー着火ー燃焼、超臨界燃焼であれば高圧噴射に続く大きな密度勾配を伴う場での物質移動（混合）と燃焼（保炎機構）といったすべての要素技術を結合したシミュレーションが必要となります。特に現在の燃焼シミュレーションは火炎帯の厚さが無限小であるとするEBU,EDC といったモデルや Flamelet モデルが主流ですが、こうしたモデルが燃焼振動、着火あるいは消炎、といった限界燃焼現象に適用できるとは限りません。こうした限界の現象には詳細化学反応機構に基づく流体シミュレーションが必要ですが、このようなシミュレーションは敷居が高く、市販のソフトはもとよりインハウスのソフトでも厳密には未だ不可能です。本研究プロジェクトで得られた結果を結合して、詳細反応機構に基づく反応性流体シミュレーション技術を確立することが今後の課題であると考えています。本講座の活動を通してロケットエンジンシミュレーションがどの程度進展したか、ご参加いただいた皆様のご批判を仰ぎたいと思います。

本シンポジウムの開催に絶大なご協力をいただいた JEDI センターの皆様、招待講演、一般講演をお引き受けいただいた皆様、ご参加いただいた皆様にこの場をお借りして深く御礼申し上げます。

東京大学工学系研究科　JAXA 社会連携講座
特任教授　越　光男

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東京大学工学系研究科

ロケットエンジンモデリングラボラトリー（ＪＡＸＡ社会連携講座）

シンポジウム 「ロケットエンジンシミュレーションの最先端、そしてその次へ」

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東京大学・JAXA 社会連携講座　シンポジウム
「ロケットエンジンシミュレーションの最先端、そしてその次へ」
プログラム

【平成２４年９月２６日(水)　9:30-17:30】

9:30 -　9:40 9:40 - 10:00	開会挨拶　原田　昇（東京大学大学院工学系研究科長） 講座紹介　嶋　英志（宇宙航空研究開発機構　情報・計算工学センター長）
10:00 - 12:30 極低温キャビテーション &極低温物性	極低温キャビテーションモデリングの多面的研究と開発への応用に向けて 谷　直樹（宇宙航空研究開発機構）
	モーメント法に基づいた多重プロセス型キャビテーションモデル 津田 伸一（信州大学）
	インデューサーに発生する液体窒素・水キャビテーションの可視化 伊藤　優（東京工業大学）
	企業におけるキャビテーション研究事例の報告 能見 基彦（荏原製作所）
	水素と酸素の極低温物性分子シミュレーション 越　光男（東京大学）、津田 伸一（信州大学）
14:00 - 17:30 招待講演	Modeling and Computational Challenges to Study Combustion Instability in Rocket Engine Model Simulations Prof. Suresh Menon, Georgia Institute of Technology
	Recent Advancements in Fully Implicit Numerical Methods for Hypersonic Reacting Flows Dr. Benjamin S. Kirk(NASA/JSC)
	The Direction of Fluid Dynamics for Liquid Propulsion at NASA Marshall Space Flight Center Dr. Lisa W. Griffin(NASA/MSFC)

【平成２４年９月２７日(木)　9:30-17:10】

9:30-11:30 高圧噴射・微粒化	低ウェーバー数下の衝突微粒化促進方法とその機構 井上　智博（東京大学）
	液体燃料噴霧における乱流微粒化・蒸発混合・初期着火現象 新城　淳史（宇宙航空研究開発機構）
	超臨界圧における極低温流体混合現象の高精度数値モデリング 寺島　洋史（東京大学）
	液酸・液水高圧燃焼試験における燃焼不安定現象 布目　佳央（宇宙航空研究開発機構）
13:00-14:30 高圧燃焼	ロケットエンジンの化学反応機構 越　光男（東京大学）
	液体ロケットフルスケール燃焼器再生冷却性能予測手法の提案 大門　優（宇宙航空研究開発機構）
	ロケットエンジン燃焼に関するＬＥＳ燃焼解析 松山　新吾（宇宙航空研究開発機構）
15:00-16:30 ロケットシミュレーション の実際	宇宙輸送機の推進薬挙動予測に関する研究 姫野　武洋（東京大学）
	二液スラスタに関する基礎試験および数値解析 高和　潤弥（株式会社　ＩＨＩ）
	液体ロケットエンジン設計への流体解析技術の適用 渡邉　大輝（三菱重工業株式会社）
16:30 - 17:00 今後の展望	ロケットエンジンシミュレーションにおける今後の展望 山西　伸宏（宇宙航空研究開発機構）
17:00 - 17:10	閉会挨拶　堀　浩一　教授（東京大学）

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発 表 内 容

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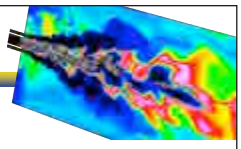
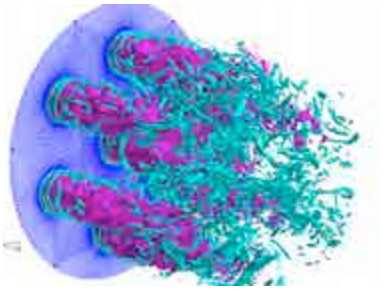


Modeling and Computational Challenges to Study Combustion Instability in Rocket Engine Model Simulations

Suresh Menon
Georgia Institute of Technology

University of Tokyo
September 26, 2012



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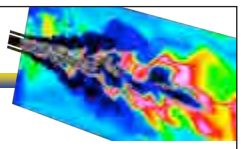

Outline

- Liquid Rocket Engines – Challenges
- Modeling Challenges
- Numerical Algorithm Challenges
- Implementation and Computational Challenges
- Results and Observations
  - Trans-critical mixing studies
  - Trans-critical reacting studies
  - Combustion Instability studies
- Conclusion and future outlook

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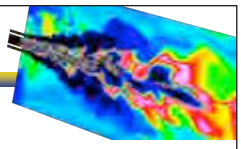

Liquid Rocket Engine

- LREs have been operational since 1950s but are still not fully understood for a variety of challenges
  - High pressure supercritical combustion
  - Many small injectors, different types of injectors, complex geometries including pre-burners and manifolds
- "Perfect storm" events lead to ***combustion instability***
  - ***Enormous heat release (> 10 GW/m^2) in confined volume***
  - ***Coupling between acoustics-heat release- shear turbulence***
  - ***Catastrophic pressure oscillations can grow rapidly***
  - ***Small design changes can have large consequences***
- Expensive testing needed to develop new engines
  - Vulcain: 280+ test firings, 85,000 s of operational tests

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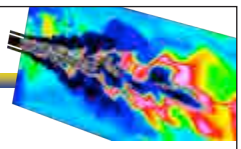

Experimental Challenges

- High pressure environment makes measurements difficult to obtain data inside the thrust chamber
  - Typically, only wall heat transfer is obtained
  - Some flow visualization, CH, OH-PLIF for some cases
- Laboratory LREs are not properly scaled real system
  - Typically single injector in large combustor leads to different kinds of flow physics – slow/large recirculation
  - Limited understanding of injector-to-injector interactions
  - Limited multi-injector studies at subcritical pressures
  - **Typically gas-gas or liquid-gas systems far from LRE**
- Flight systems therefore still require extensive empirical testing with limited in-situ assessment of combustion

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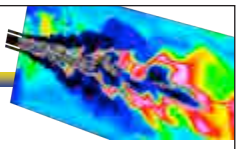
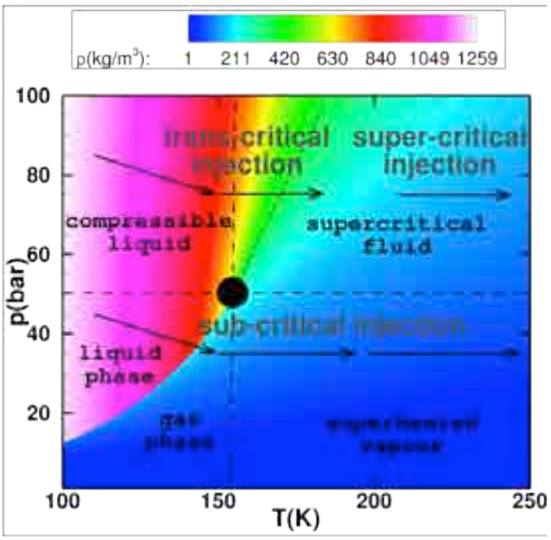


Modeling Challenges

- High pressure conditions
  - Supercritical conditions
  - Real Gas Equation of State
  - Trans-critical events
- 3D unsteady features
  - Simple geometry but complex physics in small narrow regions
- RANS cannot capture turbulent fluctuations and interactions
- DNS is too expensive
- Perhaps LES or something else?
- How to validate?



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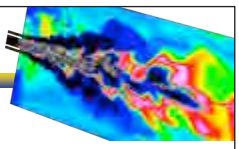

Turbulence Modeling Approaches

- Direct numerical simulation (DNS)
  - Transient, 3-D, resolve all fluctuations, no modeling
- Moment formulation (RANS/URANS-Models)
  - Mean, variances, co-variance predicted
  - Model the complete spectrum
- Large-Eddy-Simulation (LES or VLES)
  - Transient, 3-D, resolve large-scales, model ‘unresolved’ scale effect on the ‘resolved’ scale
  - Only ‘energy-containing’ scales resolved in VLES
  - Energy-containing and inertial scales resolved in LES
- Hybrid Schemes: Detached Eddy Simulation, RANS-LES
  - **New hybrid terms appear that require new closure**

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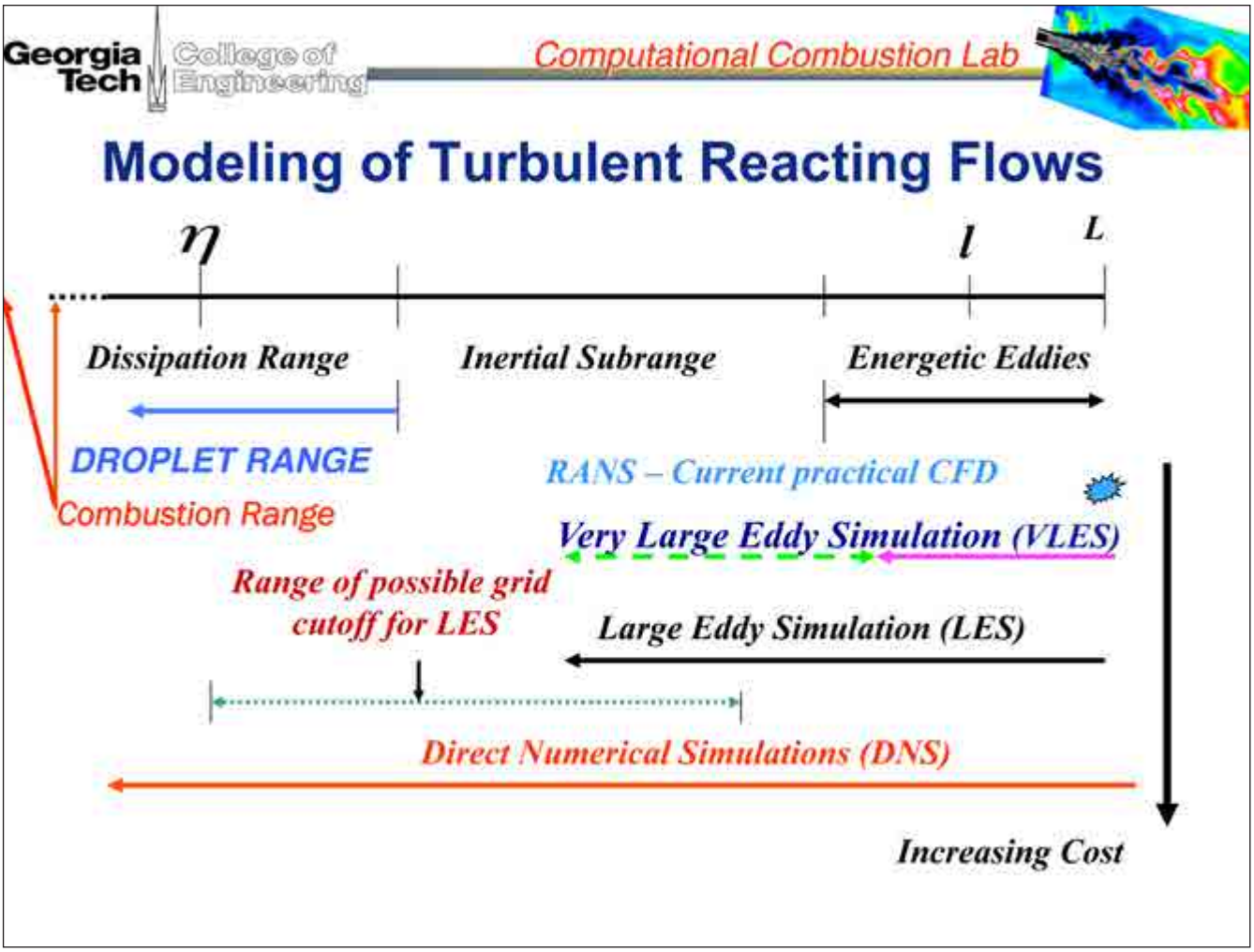

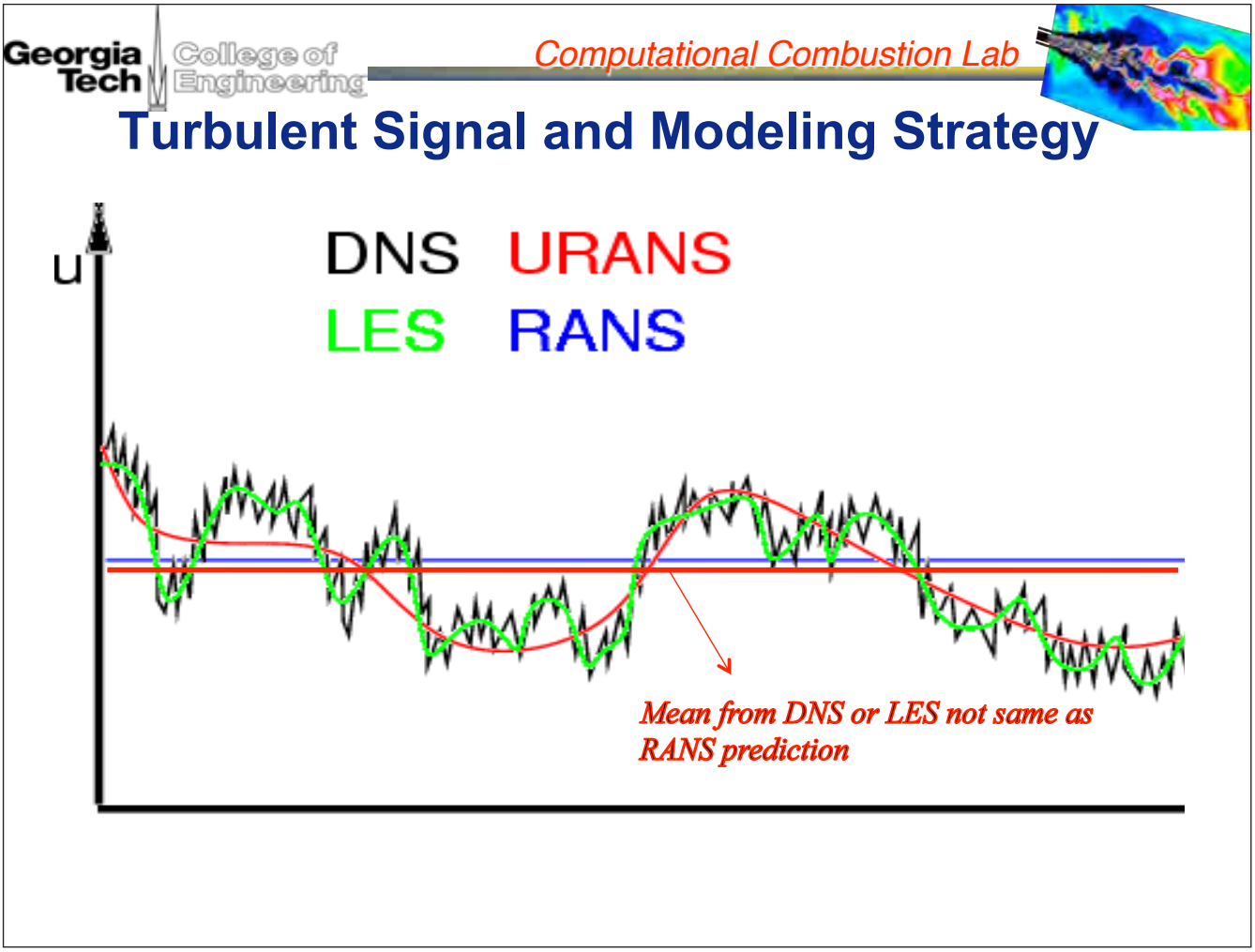

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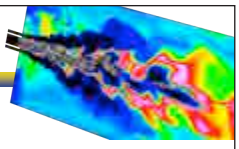

Modeling Strategy

- Compressible conservative formulation needed to capture acoustic-vortex-flame interactions, shocks etc.
- Favre-filtered equations (with many assumptions)
  - Gradient – filter commute, top-hat filter, etc.

$$\frac{\partial \overline{\rho}}{\partial t}+\frac{\partial \overline{\rho}\tilde{u}_i}{\partial x_i}=0$$

$$\frac{\partial \overline{\rho}\tilde{u}_i}{\partial t}+\frac{\partial}{\partial x_j}\left(\overline{\rho}\tilde{u}_i\tilde{u}_j+p(\overline{\phi})\delta_{ij}-\overline{\tau}_{ij}+\tau_{ij}^{sgs}+p^{sgs}\delta_{ij}\right)=0$$

$$\frac{\partial \overline{\rho}\tilde{e}_T}{\partial t}+\frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{e}_T\tilde{u}_i+p(\overline{\phi})\tilde{u}_i+\overline{Q}_{i,IK}-\tilde{u}_j\overline{\tau}_{ji}+H_i^{sgs}+\sigma_i^{sgs}+p^{sgs}\tilde{u}_i\right)=0$$

$$\frac{\partial \overline{\rho}\tilde{Y}_k}{\partial t}+\frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{Y}_k\tilde{u}_i+\overline{J}_{i,k}+Y_{i,k}^{sgs}+\theta_i^{sgs}\right)=\overline{\dot{\omega}}_k \quad \text{for } k=1\ldots N_S$$

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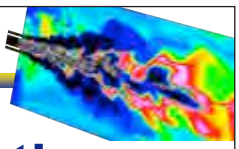

Compressible, conservative formulation

- Filtered Mass and Heat Flux (without cross-diffusion):
  - **Heat flux:**

$$\overline{Q}_{i,\mathrm{IK}} = -\overline{\lambda}\frac{\partial \tilde{T}}{\partial x_i}+\overline{\rho}\sum_{k=1}^{N_S}\tilde{h}_k\tilde{Y}_k\tilde{\mathcal{V}}_{i,k}+\sum_{k=1}^{N_S}Q_{i,k}^{\mathrm{sgs}}$$

  - **Mass flux:**

$$\overline{J}_{i,k} = \overline{\rho}\tilde{Y}_k\widetilde{\mathcal{V}_{i,k}} \qquad \tilde{\mathcal{V}}_{i,k}=-\frac{\overline{\mathcal{D}}_{k,m}}{\tilde{Y}_k}\frac{\partial \tilde{Y}_k}{\partial x_i}$$

- Filtered Real Gas Equation(s) of State (EOS)
  - Peng-Robinson (PR)
  - Soave-Redlich-Kwong (SRK)
  - Redlich-Kwong (RK)

$$p(\overline{\phi})=\overline{\rho}\tilde{Z}\tilde{R}\tilde{T}+p^{sgs}$$

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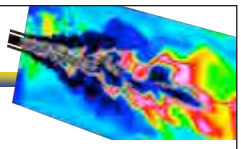
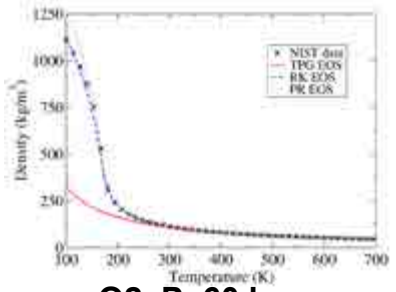
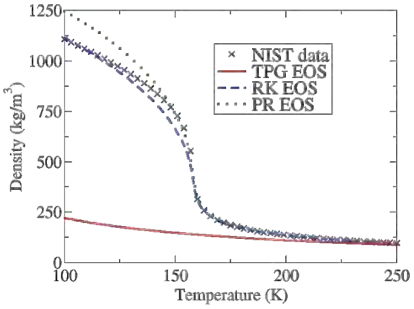


Thermodynamics and Transport properties for Real Gas Applications

- Corresponding state principles:
  - Peng-Robinson EOS
  - Chung's method for viscosity, thermal conductivity
  - Fuller's method for diffusion coefficient
- Proven good compromise cost/accuracy[1,2]
- Fully conservative formulation requires optimized non-linear solver
  - Use density and internal energy to obtain pressure and temperature



O2, P=60 bars



CH4, P=100 bars

[1]J. C. Oefelein. *Combustion Science and Technology, 178:229–252, 2006.*
[2]A. Congiunti, C. Bruno, and E. Giacomazzi. *AIAA 2003-478, 2003.*

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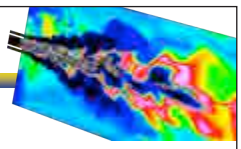

Subgrid Closure Terms

Reynolds Stress	$\tau_{ij}^{sgs} = \overline{\rho}\,(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j)$
Enthalpy Flux	$H_i^{sgs} = \overline{\rho}\,(\widetilde{E u_i} - \widetilde{E}\widetilde{u}_i) + (\overline{p u_i} - \overline{p}\widetilde{u}_i)$
Viscous Work	$\sigma_i^{sgs} = \widetilde{u_j \tau_{ij}} - \widetilde{u}_j\overline{\tau}_{ij}.$
Convective-Species	$Y_{i,k}^{sgs} = \bar{\rho}[\widetilde{u_i Y_k} - \tilde{u}_i\tilde{Y}_k]$
Heat Flux	$q_{i,k}^{sgs} = [\overline{h_k D_k \partial Y_k/\partial x_i} - \tilde{h}_k\tilde{D}_k\partial\tilde{Y}_k/\partial x_i]$
Species-Diffusive Flux	$\theta_{i,k}^{sgs} = \bar{\rho}[\widetilde{V_{i,k} Y_k} - \widetilde{V}_{i,k}\widetilde{Y}_k]$
Filtered EOS	$p^{sgs} = \bar{\rho}\left(\widetilde{ZRT} - \tilde{Z}\tilde{R}\tilde{T}\right) = \bar{\rho}R_u\sum\frac{1}{MW_k}\left(\widetilde{ZY_kT} - \tilde{Z}\widetilde{Y_kT}\right)$

- Typically gradient transport for momentum and energy subgrid transport is used
  - Isotropic scalar eddy viscosity
  - Need length scale and velocity scale(s)

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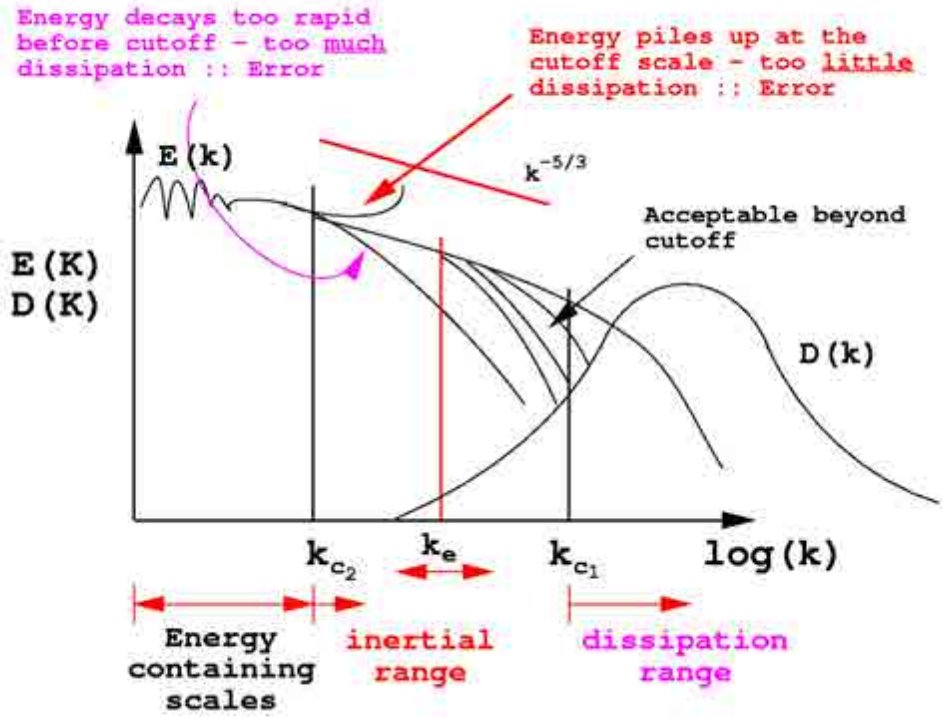
Impact of Filtering on Turbulence



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Localized Dynamic Kinetic Energy

- SGS Stress: $\tau_{ij}^{sgs} = -2\overline{\rho}\nu_t(\widetilde{S_{ij}} - \frac{1}{3}\widetilde{S_{kk}}) + \frac{1}{3}\tau_{kk}\delta_{ij}$
- Characteristic length provided by the local grid spacing
- Smagorinsky algebraic model for the subgrid stress

$$\nu_t = C\Delta^2|\widetilde{S}| \qquad |\widetilde{S}| = \sqrt{2S_{ij}S_{ij}}$$

- One-equation model for subgrid kinetic energy (Schumann)

$$\nu_t = C_\nu\sqrt{k^{sgs}}\,\overline{\Delta}$$

$$H_i^{\mathrm{sgs}} = \overline{\rho}\left[\widetilde{e_T u_i} - \widetilde{e}_T\widetilde{u}_i\right] + \left[\overline{pu_i} - \overline{p}\widetilde{u}_i\right] \approx -\overline{\rho}\frac{\nu_t}{\mathrm{Pr}_t}\frac{\partial\widetilde{h}}{\partial x_i}$$

$$Y_{i,k}^{\mathrm{sgs}} = \overline{\rho}\left[\widetilde{u_i Y_k} - \widetilde{u}_i\widetilde{Y}_k\right] \approx -\overline{\rho}\frac{\nu_t}{\mathrm{Sc}_t}\frac{\partial\widetilde{Y}_k}{\partial x_i}$$

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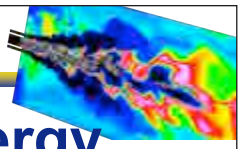

Compressible Subgrid Kinetic Energy

$$\frac{\partial \bar{\rho} k^{sgs}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i k^{sgs}}{\partial x_i} = \mathrm{T}_{k^{sgs}} + pd_{k^{sgs}} + P_{k^{sgs}} - D_{k^{sgs}} - B_{k^{sgs}}$$

- Production $P_{k^{sgs}} = -\tau_{ij}^{sgs} \frac{\partial \tilde{u}_j}{\partial x_i}$
- Dissipation $D_{k^{sgs}} = \left(\overline{\tau_{ij} \frac{\partial u_i}{\partial x_j}} - \bar{\tau}_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} \right)$
- Pressure-Dilatation Correlation $pd_{k^{sgs}} = \overline{P \frac{\partial u_i}{\partial x_i}} - \bar{P} \frac{\partial \tilde{u}_i}{\partial x_i}$
- Diffusion/Transport

$$\mathcal{T}_{k^{sgs}} = -\frac{\partial}{\partial x_i} \left((\widetilde{\bar{\rho} K u_i} - \bar{\rho} \tilde{K} \tilde{u}_i - \tilde{u}_j \tau_{ij}^{sgs}) + (\overline{u_i P} - \tilde{u}_i \bar{P}) - (\overline{u_j \tau_{ij}} - \tilde{u}_j \bar{\tau}_{ij}) \right)$$

- Pressure gradient – density gradient $B_{k^{sgs}} = \frac{\partial \ln \bar{\rho}}{\partial x_i} \frac{\partial \bar{p}}{\partial x_i}$

Génin and Menon (AIAA-2009, Comp. Fl., 2010; J. Turb., 2010)

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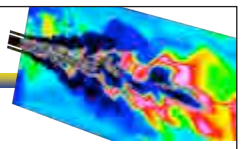

Localized Dynamic Closure

- Scale similarity is extended to test filter level and a model is assumed for

$$\tau_{ij}^{test} = C_l L_{ij}$$

- Does not employ Germano's identity

$$\mathcal{L}_{ij} = -2C_\nu \sqrt{k^{test}} \widehat{\bar{\rho}} \widehat{\Delta} \left(\frac{\widehat{\bar{\rho} \tilde{S}_{ij}}}{\widehat{\bar{\rho}}} - \frac{1}{3} \frac{\widehat{\bar{\rho} \tilde{S}_{kk}}}{\widehat{\bar{\rho}}} \delta_{ij} \right) + \frac{1}{3} \mathcal{L}_{kk} \delta ij$$

$$C_\nu = -\frac{\mathcal{M}_{ij} \mathcal{L}'_{ij}}{2 \mathcal{M}_{ij} \mathcal{M}_{ij}} \qquad \mathcal{M}_{ij} = \sqrt{k^{test}} \widehat{\Delta} \left(\widehat{\bar{\rho} \tilde{S}_{ij}} - \frac{1}{3} \widehat{\bar{\rho} \tilde{S}_{kk}} \delta_{ij} \right) \qquad \mathcal{L}'_{ij} = \mathcal{L}_{ij} - \frac{1}{3} \mathcal{L}_{kk} \delta_{ij}$$

- Denominator is well defined at the test filter level and non-zero
- Approach is stable and robust without averaging in complex flows
- Model is available in many commercial codes (e.g. FLUENT, OF)

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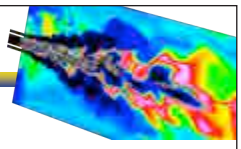

The Filtered Reaction Rate Closure

- Most difficult to close even without real gas effects
- Many alternate strategies developed to avoid the closure
- Critical to understand the application requirements
  - Assumptions valid in one flow may not work in another
- Mixed premixed-partially premixed-non-premixed regimes
- Scale Separation implicit or explicit in ALL closures
  - Turbulence and combustion scales separated in the inertial range
  - Mixing process in the inertial range independent of chemistry and simplify modeling considerable
  - Kolmogorov scaling laws are not modified by molecular mixing and heat release at the (even) smaller scales.
  - Reasonable but is this true at high Re or for Real Gas?

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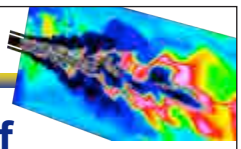

Turbulent Combustion Models in Terms of Chemistry and Mixing (Modified from Peters, pg 64)

	Premixed Combustion	Nonpremixed Combustion
Infinitely Fast Chemistry	Bray-Moss-Libby Coherent Flame	Conserved Scalar Equilibrium Model
Finite-rate w/o Molecular mixing	PDF Transport	PDF Transport
Finite-rate with filtered or modeled reaction rate	Flamelet Model G-equation, G-Z, ATF EBU, FSD, PaSR…	Flamelet Model Z, ATF, CMC, PaSr…
Finite-rate with Molecular mixing	Linear-Eddy Model	Linear-Eddy Model

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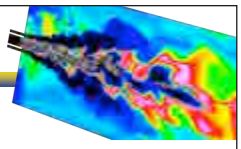

Flamelet or Finite-Rate?

- Flamelet concept is cost effective but may not be valid in LRE everywhere in the thrust chamber
- Non-premixed burning requires proper treatment of turbulent and Molecular (including differential) mixing
- Combustion instability can change flame structure
- Unsteady heat release coupling may require proper estimate of partially burned effects and radical chemistry
  - Multi-component diffusion needed
  - Finite-rate kinetics needed
- Flame structure may be much more complex

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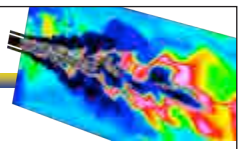

Turbulence-Flame Interactions

- Localized dynamic closure for subgrid kinetic energy
  - Scale similar closure that is stable in complex flows
- Grid-within-grid approach
  - Simulate large-scales on the LES grid
  - Simulate molecular processes: subgrid turbulent mixing, molecular diffusion and finite-rate at the SUBGRID level

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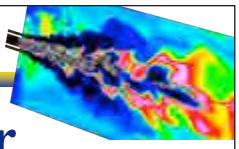

Species Equation: Two Scale Solver

- **Resolved Species Equation**

$$\frac{\partial(\rho Y_k)}{\partial t} + \underbrace{\frac{\partial(\rho u_i Y_k)}{\partial x_i}}_{\text{(Resolved+Unresolved) scale convection}} - \underbrace{\frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right)}_{\text{Molecular diffusion}} = \underbrace{\dot{\omega}_k}_{\text{Chemical source term}} + \underbrace{\dot{S}_k}_{\text{Spray source term}}$$

- **Two scale procedure is used:** $u_i = \left(\tilde{u}_i + u'_{sgs}\right)_R + u'_{UR}$
  - **Unresolved Scale**
  - **Resolved Scale**

$$\frac{(\rho Y_k)^* - (\rho Y_k)^n}{\Delta t_{LES}} = \underbrace{-\frac{\partial(\rho^n u'_{UR} Y_k^n)}{\partial x_i}}_{\text{Convection}} + \underbrace{\frac{\partial}{\partial x_i}\left(\rho^n D_k \frac{\partial Y_k^n}{\partial x_i}\right)}_{\text{Molecular diffusion}} + \underbrace{\dot{\omega}_k^n}_{\text{Chemical source}} + \underbrace{\dot{S}_k^n}_{\text{Spray source}}$$

$$\frac{(\rho Y_k)^{n+1} - (\rho Y_k)^*}{\Delta t_{LES}} = \underbrace{-\frac{\partial}{\partial x_i}\left[\rho^*\left(\tilde{u}_i^* + u'_{sgs}\right)_R Y_k^*\right]}_{\text{Convection}}$$

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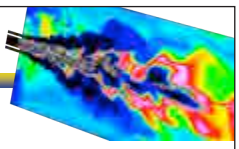

LEMLES Processes

- NO filtering of the species equations
  - Eulerian-Lagrangian solver for species equation
- Reaction-Diffusion processes
  - Evolves in a “grid” inside the LES grid
  - Full multi-component and differential diffusion included
  - Finite-rate kinetics included without needing closure
- Turbulent stirring by eddies smaller than LES grid
  - Stochastic process that is based on Kolmogorov scaling
- Volumetric expansion of subgrid field due to heat release
- Computational more expensive than flamelet but no need for a priori choice of flame type
  - Parallel optimization techniques can reduce cost

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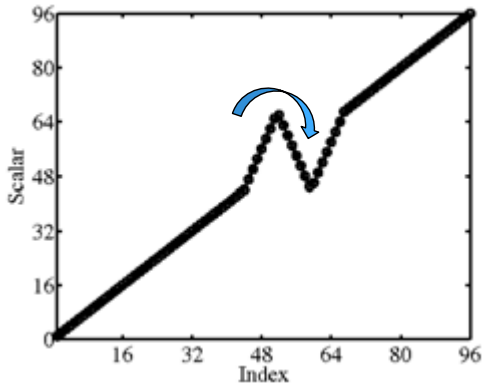
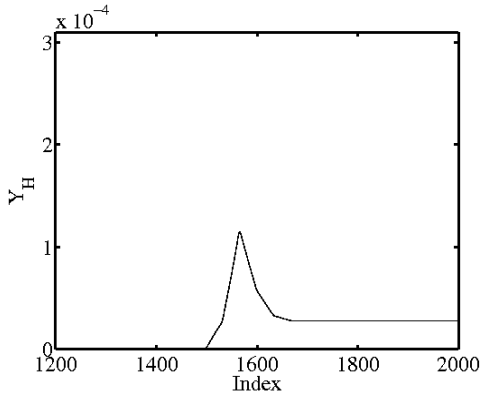
Subgrid Turbulent Stirring Example

- **Stirring in a freely propagating premixed flame**



Schematic



Y_H in freely propagating premixed turbulent CH_4/Air flame

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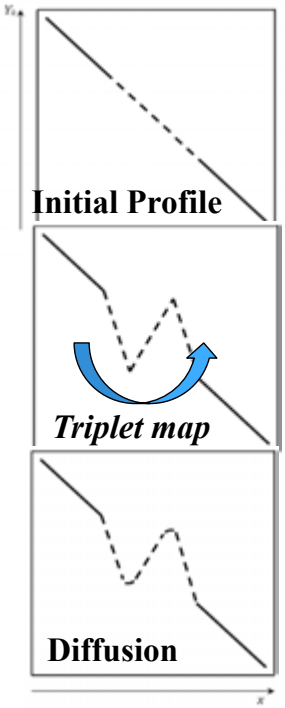
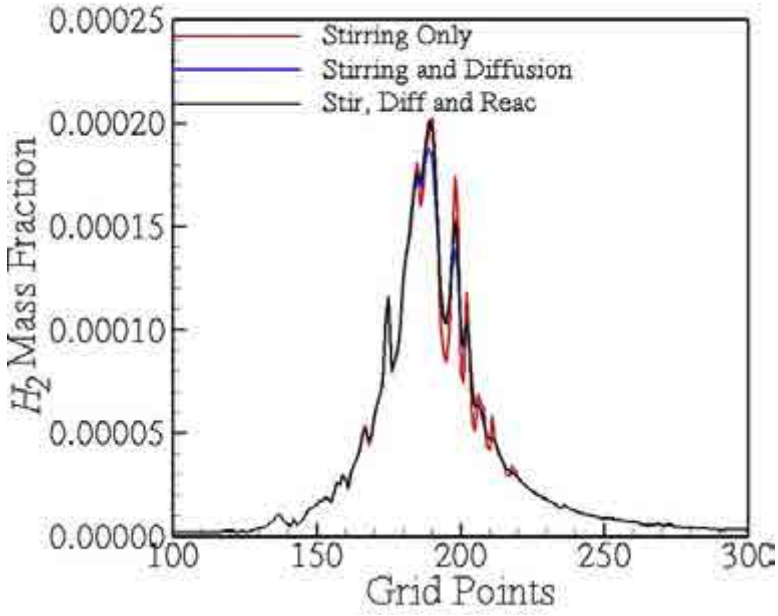
Interaction between Stirring, Diffusion and Reactions





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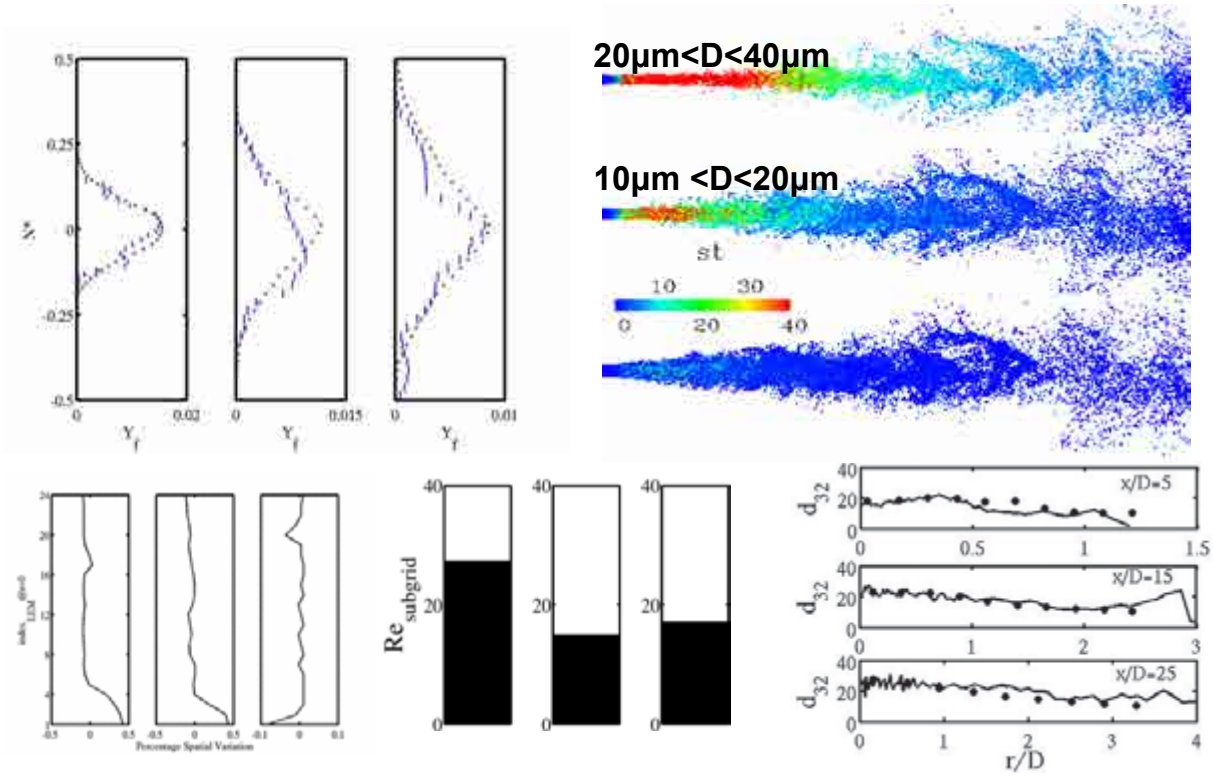
LEMLES of Vapor & Droplet Distribution*



* Acetone spray Chen et al., 2006; Srinivasan et al. (DLES, 2010)

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Numerical Challenges

- Many solver strategies in existence but not all will work for Real gas and supercritical combustion
  - Very large density gradients and shear turbulence both need to be captured in a complex geometry
- Central and compact schemes require local or explicit artificial filtering or dissipation to stabilize
- DNS high order algorithms will not work in stretched and body conforming grid
- Hybrid solvers are being developed to capture both large-gradient interface and shear turbulence
  - Hybrid WENO – Central
  - Hybrid HLLC/E – Central/Predictor-Corrector

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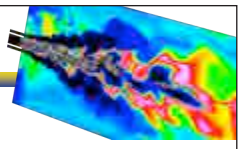
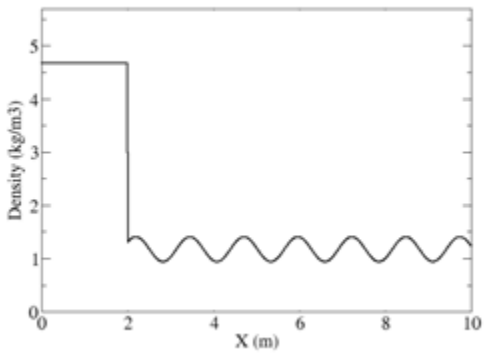
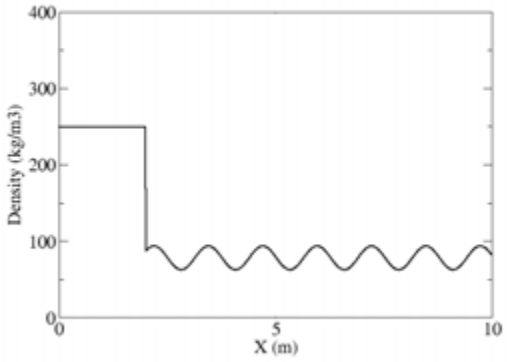


Hybrid central-HLLC scheme

- Locally adaptive sensor switches between schemes
- Shu-Osher test at Mach 3 with and without Real Gas



Standard air Z = 1



Compressed air,
Z = 0.85 pre-shock,
Z = 1.15 post-shock

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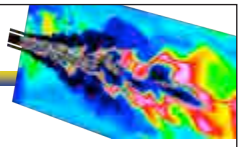
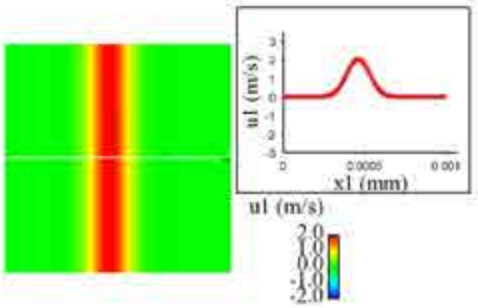
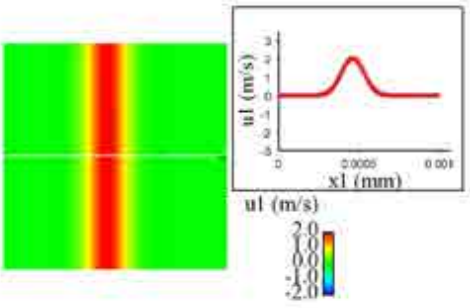


Other Numerical Challenges

- Influence of boundary conditions very critical
  - Characteristic based inflow and inflow turbulence
    - Constant mass, reflected, semi-reflected?
  - Choked outflow or characteristic outflow?
  - Wall heat transfer – coupled fluid-structure interactions



Perfect Reflecting Inflow



Non-Reflecting Inflow

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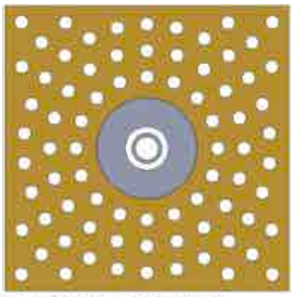
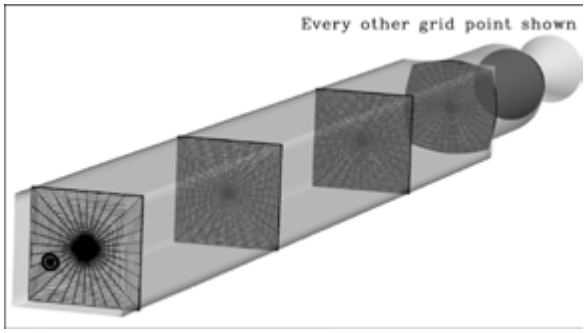
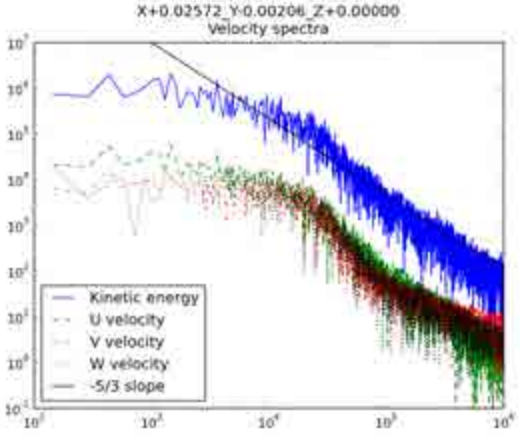
PSU LOXGOX coaxial injector at 57.5 bar

- Trans-critical injection with a single species
- Grid independence study with 3 grids:
  - coarse (600K), baseline (3.5M), refined (5.5M)





	Composition	T (K)	U (m/s)
Round jet	O2	105	23.3
Annular jet	O2	269	115
Coflow	O2	262	≈6



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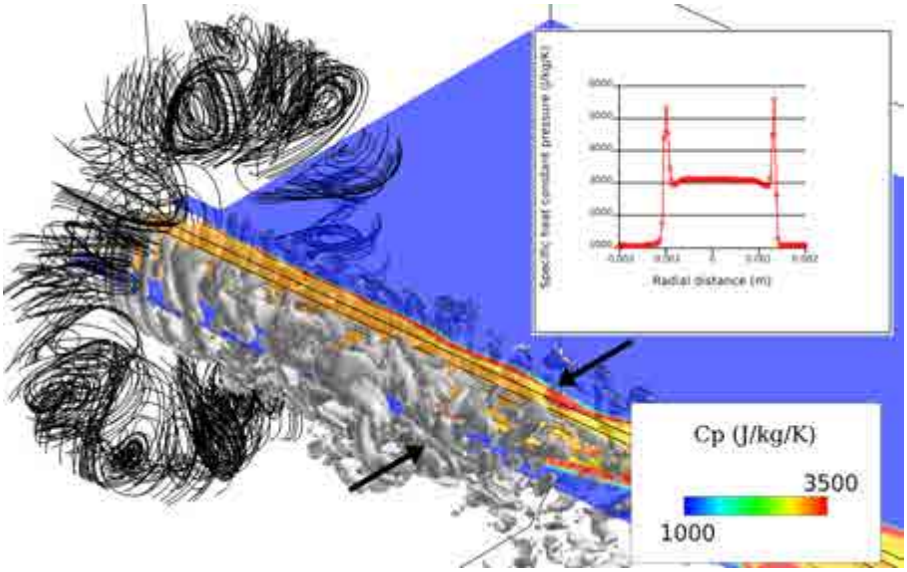
LOX-GOX Studies

- Redlich-Kwong equation of state
- Toroidal recirculation with trans-critical layer



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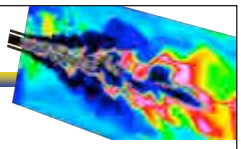
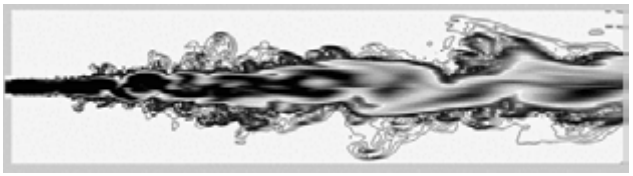
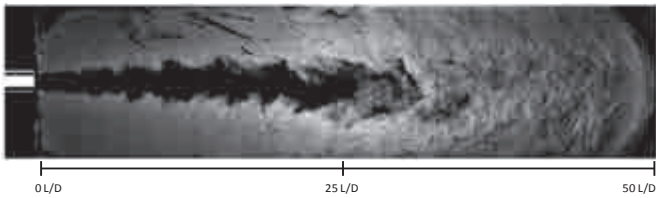


LOXGOX Jet Mixing

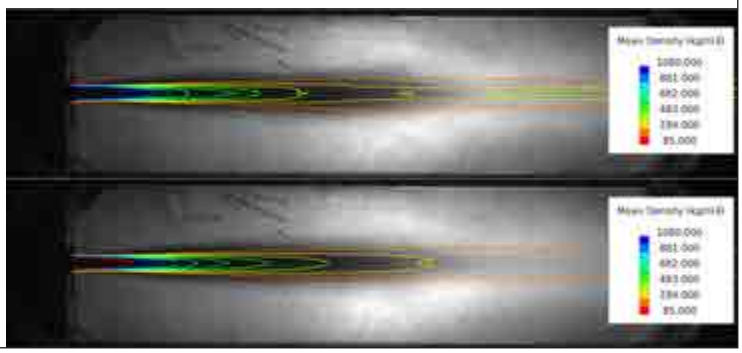
- Instantaneous comparison
  - Backlit image
  - Slice vs line-of-sight
- Time-averaged comparison
  - Processing raw data
  - Reaches stationary state in 10-15 ms





Time of averaging 1 ms

Time of averaging 10 ms



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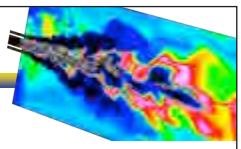
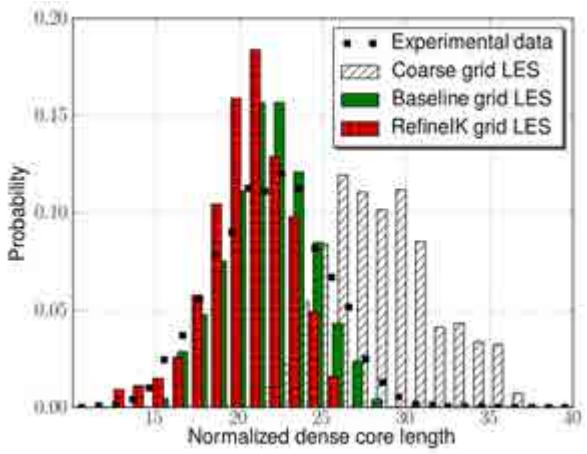


LOX-GOX Jet Mixing

- Main metric is dark core length $0.3 \le \rho^* = \frac{\rho - \rho^\infty}{\rho^0 - \rho^\infty} = \frac{\rho - 85}{1080 - 85} \le 0.6$
  - Similar to spray penetration
  - Important quantity for combustion instability [1]



[1] Chehroudi, B., “Physical Hypothesis for the Combustion Instability in Cryogenic Liquid Rocket Engines,” Journal of Propulsion and Power, 2010.

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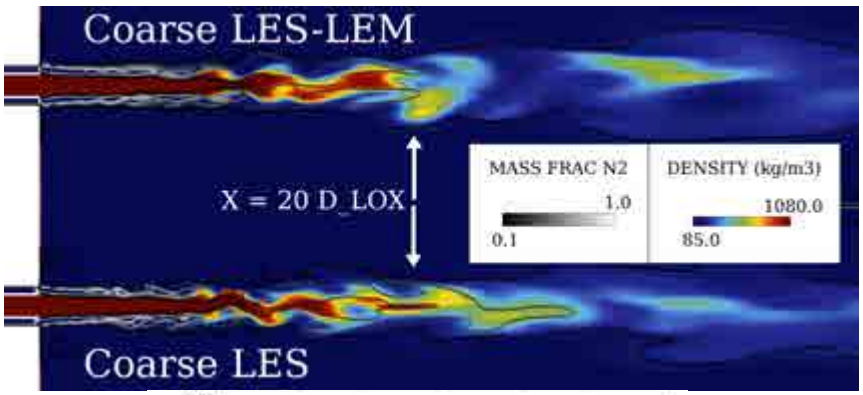
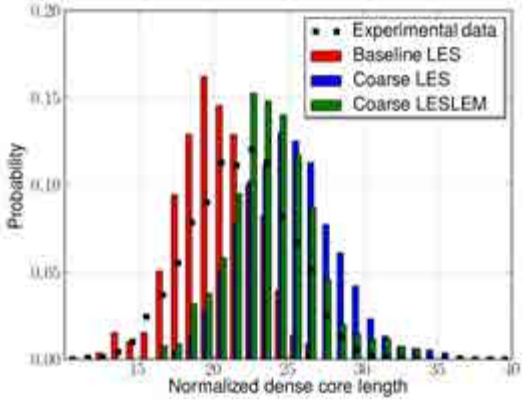
LEMLES and LES of LOX-GN2 Jet





- Similar flowfields but scalar mixing shows some differences at the small scales
- LEMLES predicts closer to gradient diffusion as expected for this non-reacting mixing case
- Reacting cases under study

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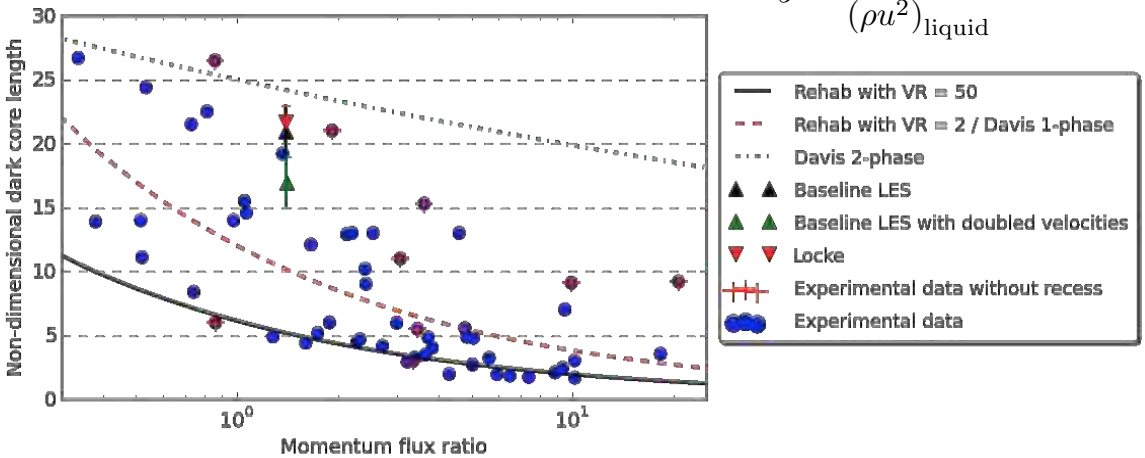
Wide Scatter in Trans-Critical Mixing Data

- LES can provide useful trends with correct physics
- LES can access flow conditions beyond sub-scale rigs
- Survey of coaxial, non-reacting supercritical flows
  - Main parameter: momentum flux ratio

$$J = \frac{(\rho u^2)_{\text{gas}}}{(\rho u^2)_{\text{liquid}}}$$



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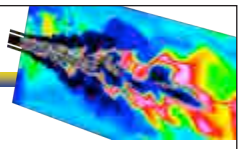

Trans-critical Combustion

- Peng-Robinson EoS instead of Redlich-Kwong
- Inflow boundary conditions and their influence
- Role of acoustics at inflow and outflow
- Turbulent combustion closure
  - Finite rate chemistry (influence of kinetic mechanism)
  - Laminar chemistry vs LEM closure
- LOX-GH2 and LOX-GCH4 combustion studies
  - Experiments at Penn State, Mascotte (France) and JAXA
- Combustion instability in high pressure subcritical GCH4-GOX combustor at Purdue

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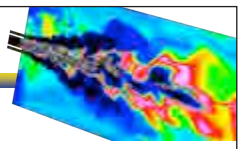

Chemistry modeling for H2-O2 combustion

- Baurle & Girimaji (2003) → reaction kinetics for H2 including 7 steps and 6 species. Radical species include OH, H and O.
- Conaire et al (2004) → reaction kinetics including 21 steps and 8 species. Addition of H2O2 and HO2 radicals.
- Shimizu et al (2011) → kinetics including 29 elementary reactions and 8 species. High-pressure effects better accounted for. (For H2-Air combustion 5 additional steps include N2, He and Ar effects)

COMPLEXITY

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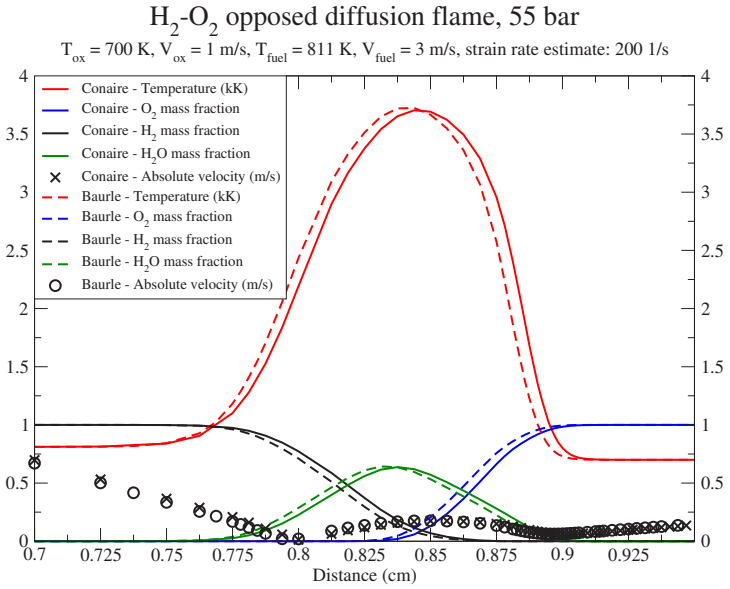
Chemistry modeling for H2-O2 System

- Opposed diffusion flame at high pressure
- Good agreement between 21-step and 7-step



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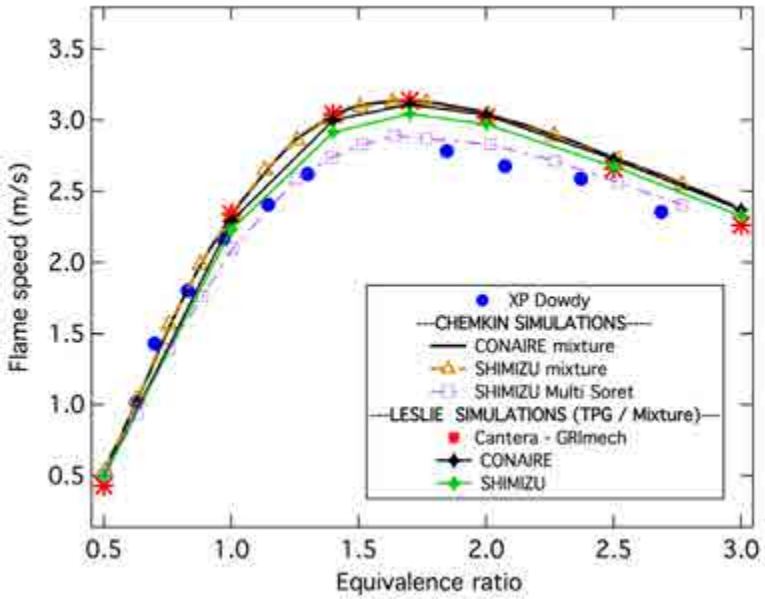
Chemistry modeling for H2-O2

- 1D-laminar flame at T=298K and p=1atm
- 21-step (Conaire et al.), 29-step (Shimizu et al.)



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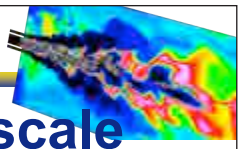

Scaling from Lab to Sub-scale to Full-scale

	Sub-Scale LOX/GCH4 PWR	Lab Scale LOX/GH2 PSU	Lab Scale LOX/GCH4 CNRS
Re (LOX)	1.38E+06	5.53E+05	6.18E+04
Re (Fuel)	4.38E+05	1.83E+05	4.87E+05
Velocity Ratio	4.99	16.93	18.06
Momentum flux ratio	3.15	1.53	11.64
Equivalence ratio	1.28	1.36	13.09
Da	2.63	1.87	58.0

- Sub-scale multi-injector test case (83 injectors):
  - Chamber pressure: 138 bar, far from p_c (O2, CH4)
  - LOX: U = 20-40 m/s, T = 100-120 K
  - CH4: U = 130-250 m/s, T = 240-300 K, ϕ=1.1-2
  - Flow speeds much higher than lab-scale single injectors
- Can LES be used to study scaling issues?

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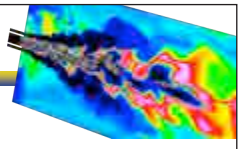
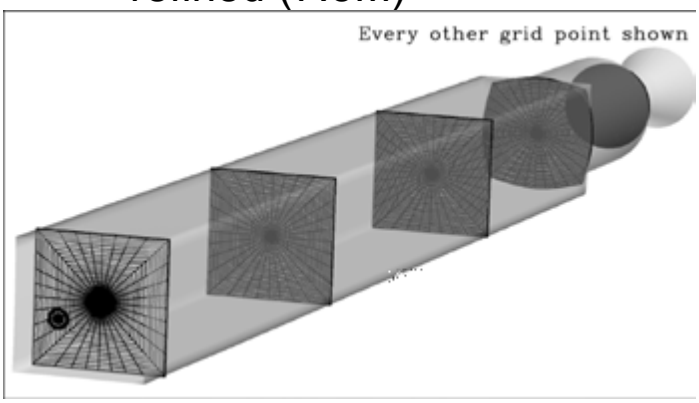
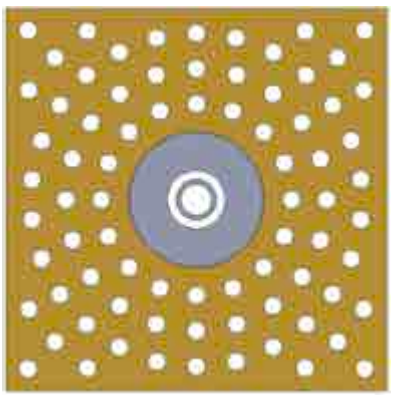


LOX coaxial injector rig

- Developed after NASA CUIP study [1]
- Square chamber for better optical access [2]
- Grid influence study with 4 grids:
- Coarse (600k), baseline (3.5M), I-refined (5M) and IK-refined (7.5M)



D_{LOX}=2.05 mm
L_{ch} = 0.35 m



[1] Tucker, Menon, Merkle, Oefelein, and Yang. In *44th JPC, AIAA 2008-522, 2008*
[2] J. M. Locke. *PhD thesis, The Pennsylvania State University, May 2011*

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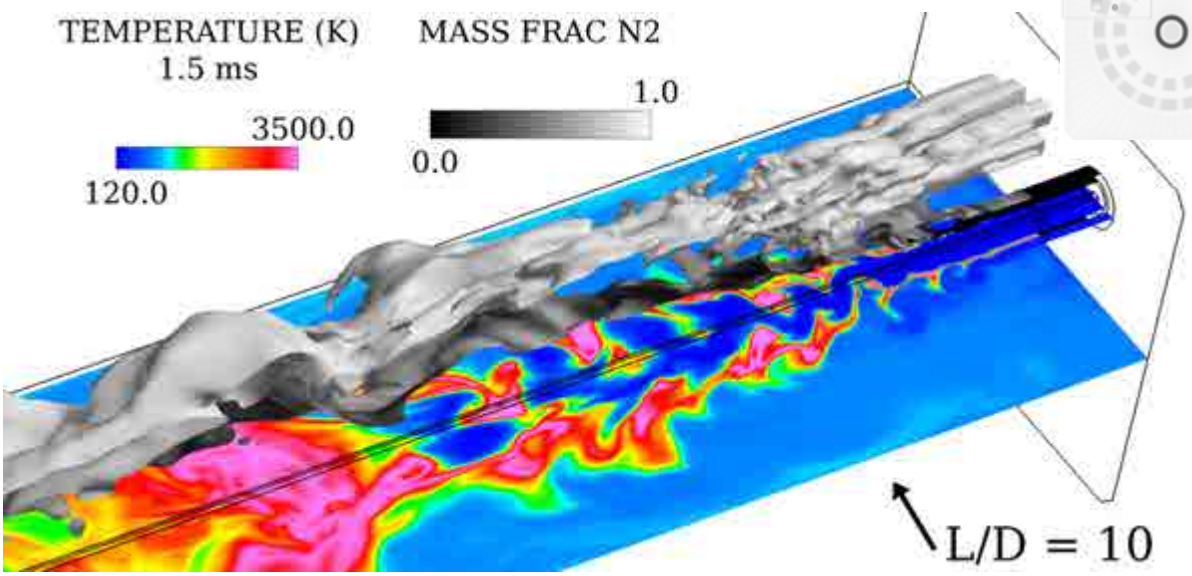
PSU rig: LOX-GH2 Reacting



- 21-step Conaire et al., 8.5 M grid points
- Strong sinuous and helicoidal modes

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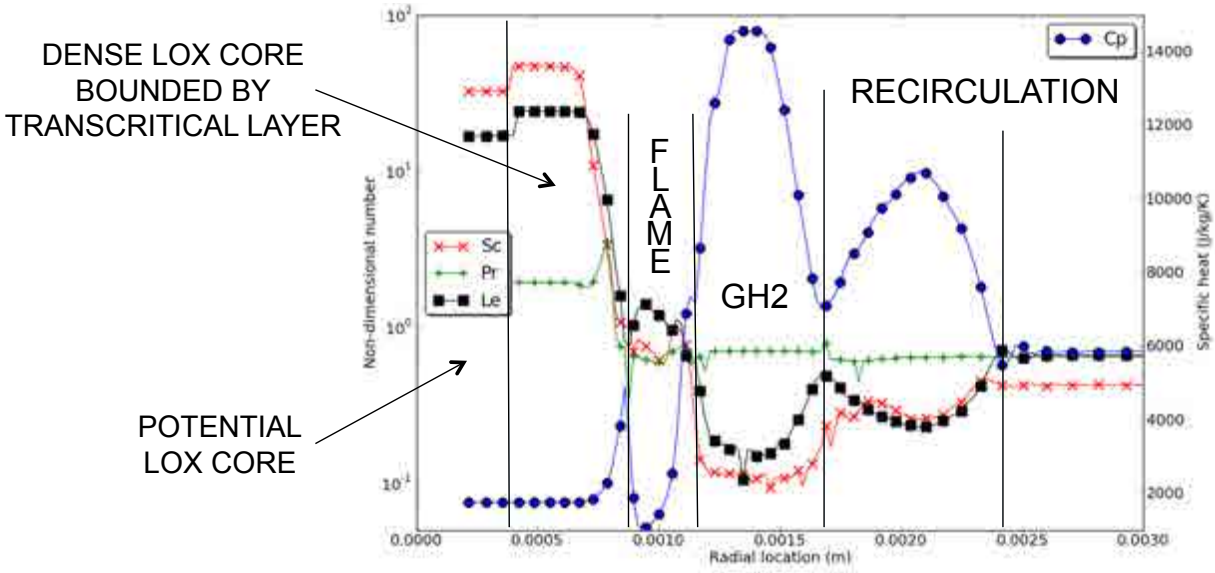
LOX-GH2 Flame Structure

- Pure diffusion flame in the near-field @ x/D = 1
- Radial profile @ x/D=1, flame structure clearly defined



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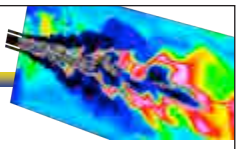
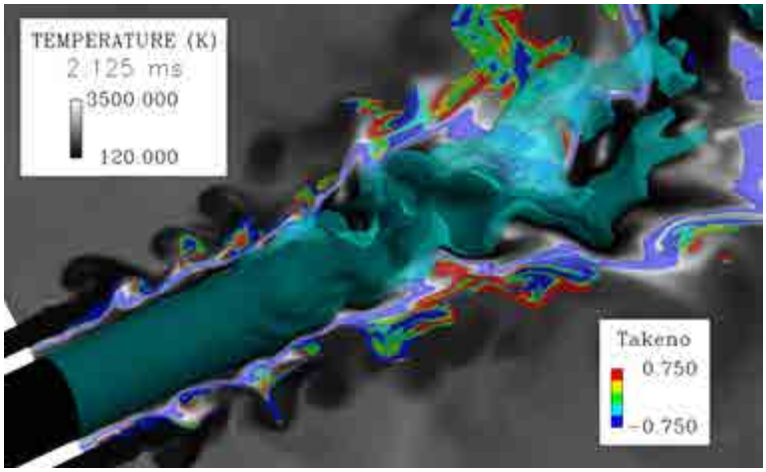


LOX-GH2 Flame Structure

- Pure diffusion flame in the near-field
- Premixing present once dense core narrows
- Another reason to use Finite-Rate Kinetics



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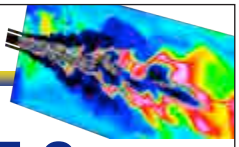

Why study CH4 combustion in LRE ?

- New interest in Liquid Rocket Engines (LRE) operating with methane as propellant.
- Important differences with hydrogen physics:
  - CH4 can be injected under both trans-critical and supercritical states[1].
  - $\rho_{CH_4} > \rho_{H2}$: large range of flux momentum ratio can be applied in LOX/CH4 injector, which allows different hydrodynamic and combustion regimes
  - Complex chemistry requires to revisit methods developed for H2/O2 combustion (mechanisms, LES closure of the reaction rate…)

[1] Singla et al. (Proceedings of the Combustion institute 2005)

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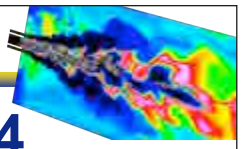

Reduced mechanism for O2/CH4 combustion

- Lack of reduced mechanism for oxy-combustion of CH4 at high pressure: at least 12 steps and 16 species[1]
  - Too expensive for real gas LES at this time!!
- Use global 1-step and 2-step kinetics with modified rates to match conditions at high pressure
- Computation of laminar premixed flames with Cantera:
  - Stoichiometric equivalence ratio
  - Pressure: 5.6 MPa
  - Real gas replaced by thermally perfect gas assumption.
  - Mechanisms: comparison of WD1[2] with GRIMECH.

[1]Sung et al. Int. Symp. Comb. (1998), [2]Westbrook & Dryer (CS&T 1982)

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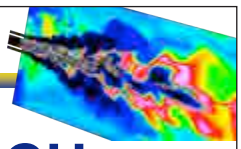
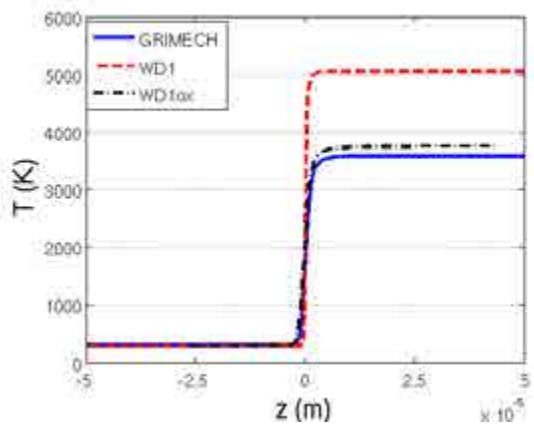
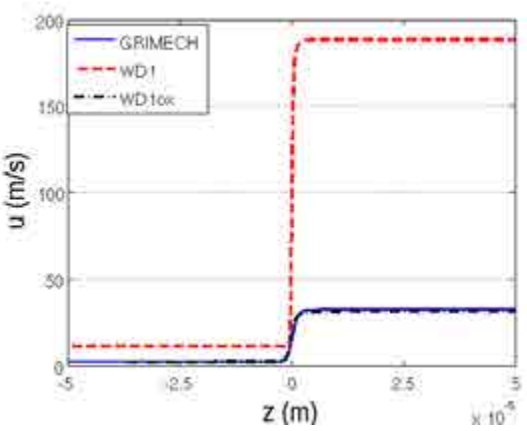


Comparison of $WD1_{ox}$ with GRIMECH





- Error on the adiabatic temperature < 5%
- Nearly perfect correction of the flame speed

	T_{ad} (K)	s_L (m/s)
GRIMECH	3584	2.317
WD1	5051	11.11
WD1ox	3755	2.283

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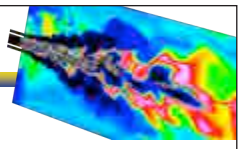
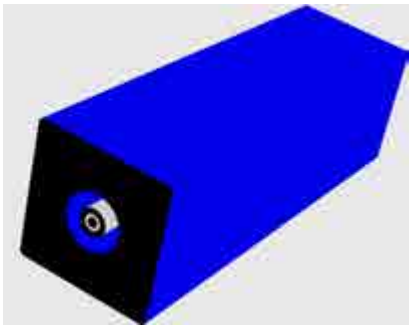
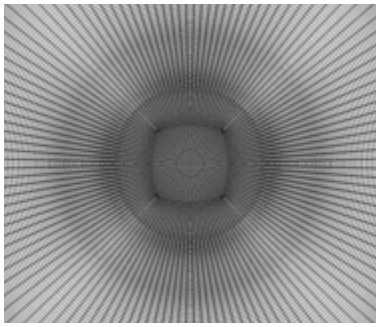


LES of Mascotte test case

- Coaxial LOX/CH4 injector (G2)[1]: P=5.6 MPa, $\phi_g = 13$
- 24 million grid points

	Composition	T (K)	U (m/s)
Round jet	O2	85	3.70
Annular jet	CH4	288	63.2





[1] Singla et al. (Proceeding of the Combustion institute 2005)

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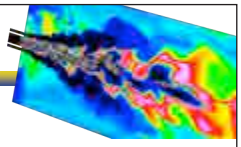
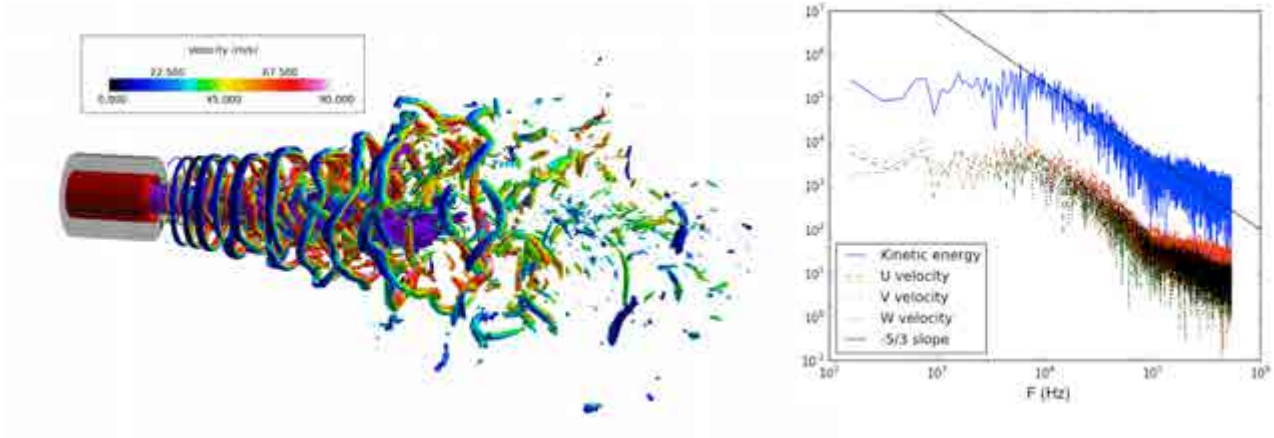


Turbulent Flow structure



- Strong coherent structures in the shear layers: entrainment of gas in coaxial jet and dense core wrinkling
- Good recovery of the Kolmogorov -5/3 spectrum

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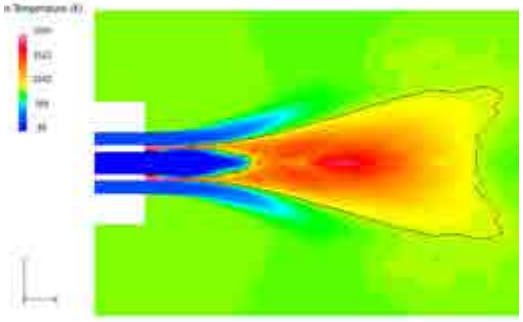
Flame structure

Experimental flame : Visualization

LES (MAX): iso surface T=1700K



- Good agreement
- Short flame: L~6 cm.
- Anchored on the LOX tip.
- Expansion angle:
  - Initial part : α<10°
  - Blooming angle : α~20°

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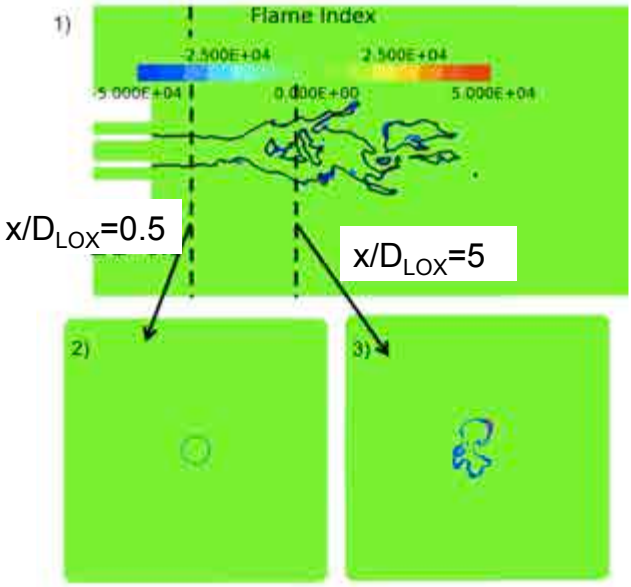
Combustion regime

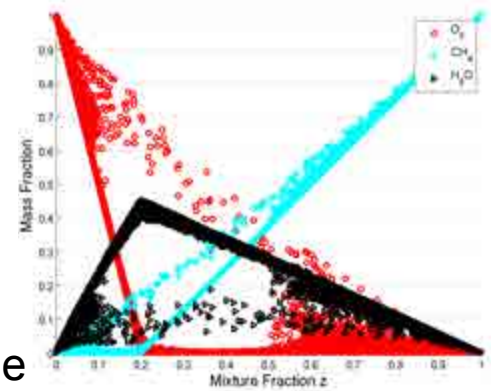


- Flame index:

$$FI = \vec{\nabla} Y_{CH_4} \bullet \vec{\nabla} Y_{O_2}$$

$FI < 0$: Diffusion flame

$FI > 0$: Premixed flame



- Diffusion flame
- Combustion regime close to the laminar infinitely fast chemistry

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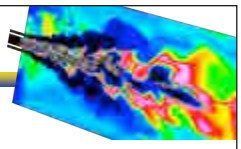

3D v/s Axi v/s 2D LOX-GH2 Studies

- 3D is essentially the only proper way to do LES but is computationally very expensive
- Strategy needed for parametric study of unsteady flame-turbulence interactions that is cost effective
  - Axisymmetric, 2D or sector 3D
  - Pros and Cons for each approach
- Axisymmetric and 3D sector with centerline injector will always result in an artificially long LOX core
  - Off-center injector may avoid centerline effects but artificial
- 2D avoids centerline issues but no 3D relieving effect, choking is artificial and energy/volume may be too high
- LES closure is invalid for axisymmetric of 2D but unsteady effects can be captured

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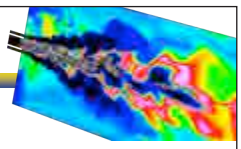
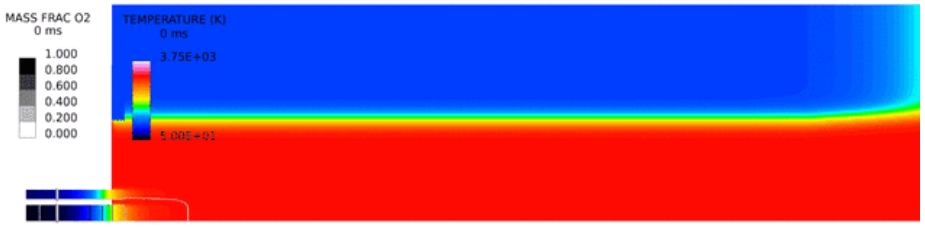
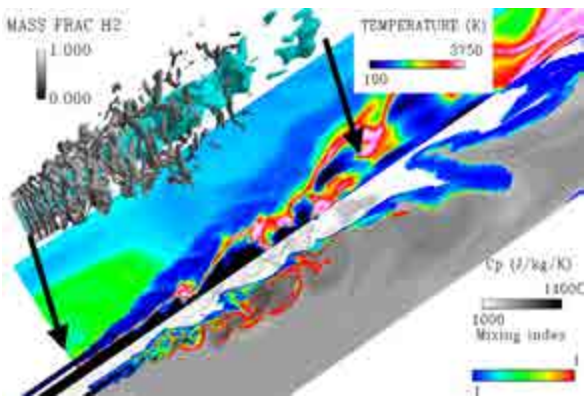


3D v/s Axisymmetric

- Liquid core length is too long in axisymmetric case



Axisymmetric



3D

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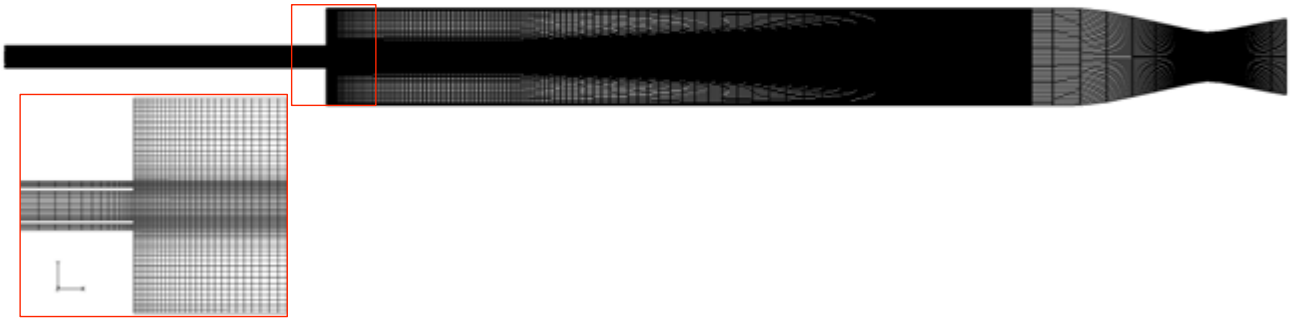
A 2D Evaluation Configuration

- 2D simplification of a shear coaxial injector including a convergent-divergent throat (injector studied by Nunome *et al.*, 2011 and Daimon *et al.*, 2011)
- Baseline mesh, total ~270,000 points, PR-EOS
- Effect of kinetics, Hydrogen temperature, recess all can be studied in a cost-effective manner
- Precursor simulations before doing full 3D



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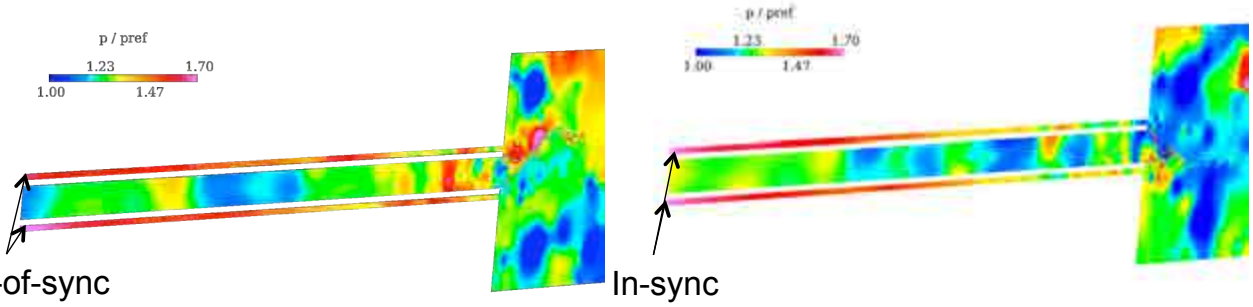
Boundary Conditions

- H_2 inlets are part of the same injector and would react identically to longitudinal pressure fluctuations
- In 2D pressure waves in inlet lines are not in phase
  - BC react differently in the two H_2 inlets
- H2 inlet BCs linked so that the same inflow conditions are applied at all times
  - The incoming waves are out-of-sync in the long inlets, the effect is limited



Out-of-sync In-sync

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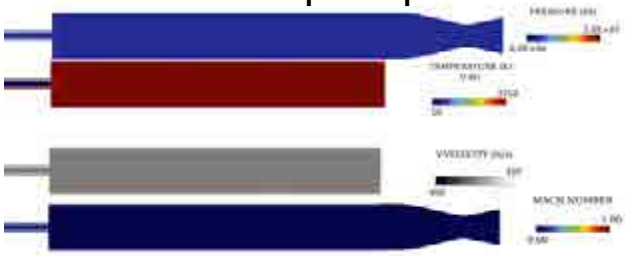
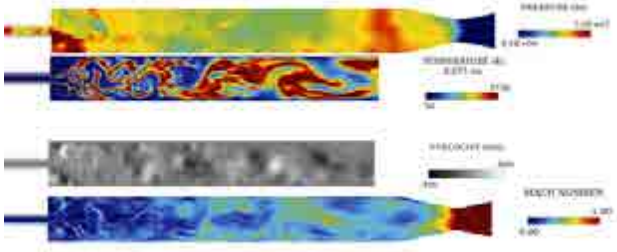
Effect of Kinetics for T_{H2} = 50 K

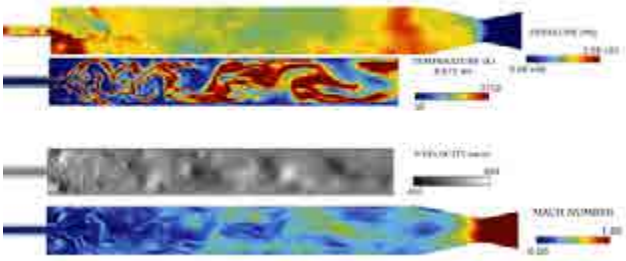
Baurle : 7-step 6-species



Conaire: 21-step 8-species



Shimizu: 29-step 8-species



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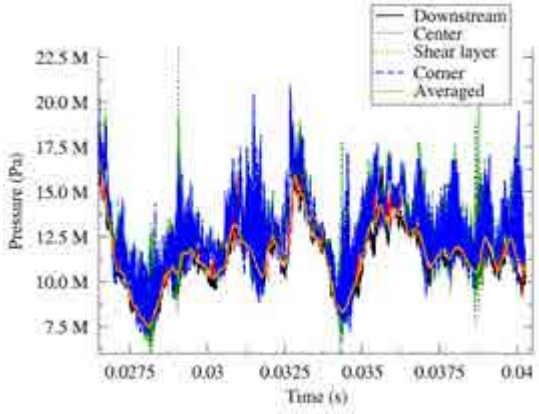
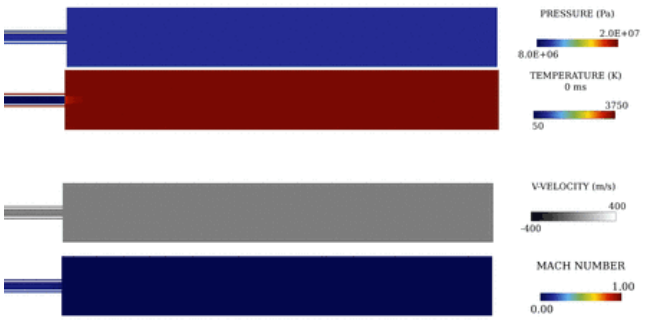
Implication of 2D Geometry

- High energy release to chamber volume ratio produces increase in mean pressure to 140 bar (design = 100 bar)
- Results similar with or without outflow choked conditions
- 2D simulations do not have the 3D relieving effect





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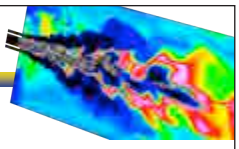
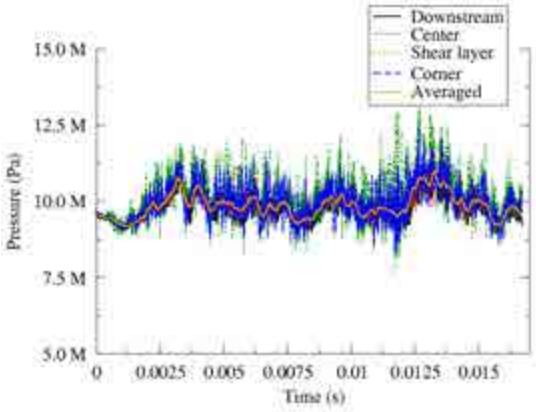


Energy/Volume ratio assessment

- Increase on chamber dimensions to reduce (energy/ volume) ratio with same injector configuration
- Pressure now at design 100 bar but flow field has larger recirculation at the corner



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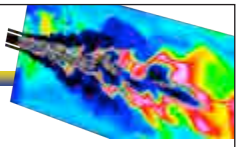
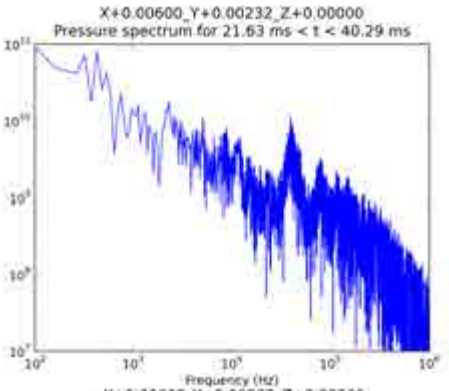
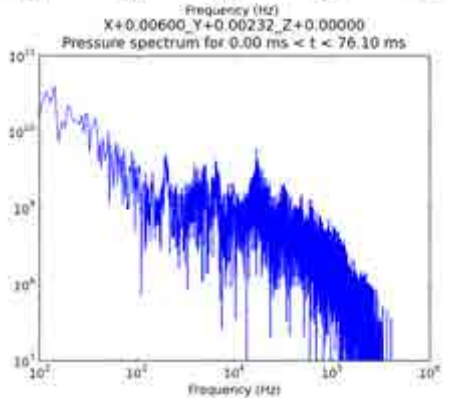


Pressure Spectra





- Both chambers show peak at the transverse mode frequency
  - Narrow case = 50 KHz
  - Wider case = 20 KHz
- Wider chamber has lower pressure amplitude

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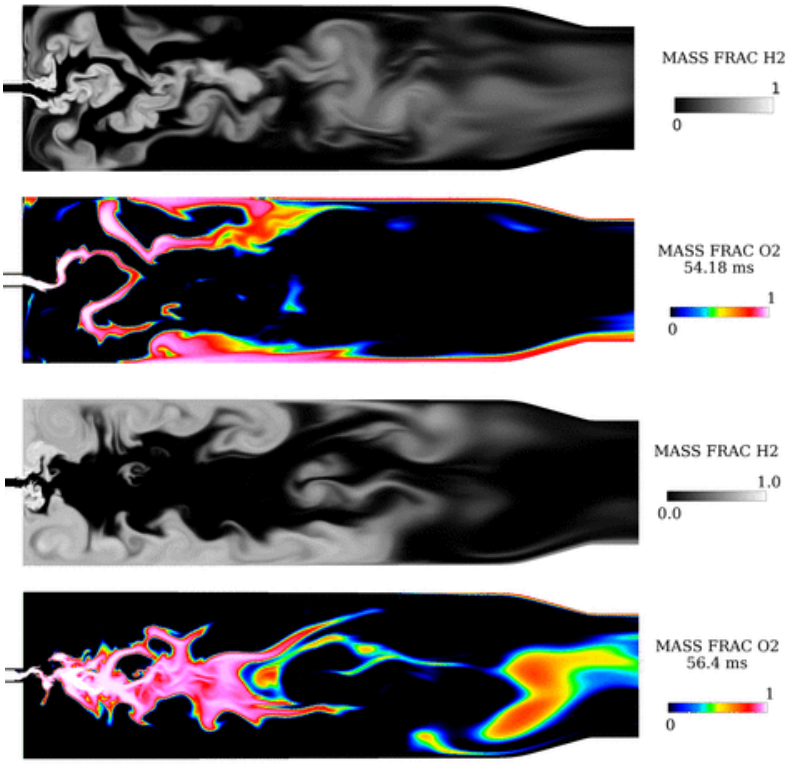
Effect of Recess



No-Recess

Recess

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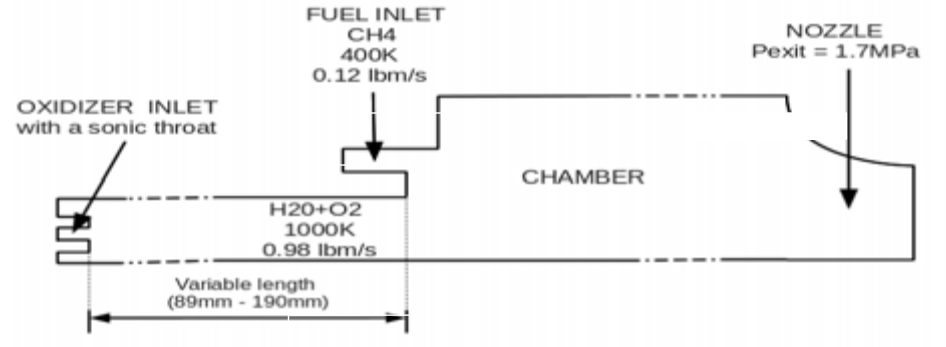
LES of Combustion Instability

- **Purdue Subcritical P=1.34MPa**

Injectors	Composition	Flow rate (kg/s)	Temperature (K)
Oxidizer	Y_{O2}=0.42 Y_{H2O}=0.58	0.32	1030
Fuel	Y_{CH4}=1	0.027	400



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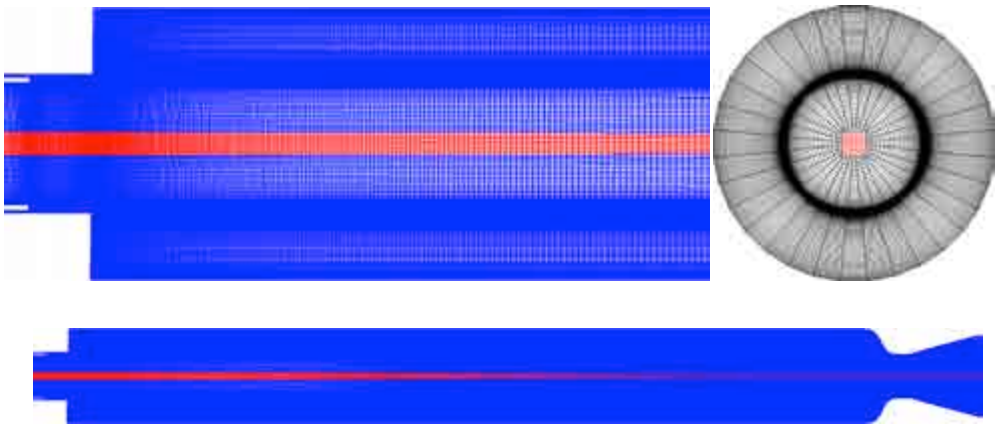
Computational Domain

- Axisymmetric and 3D studies
- Full combustor geometry with supersonic outflow nozzle
- LEMLES with two-step chemistry
  - flame speed correction for rich combustion regime.



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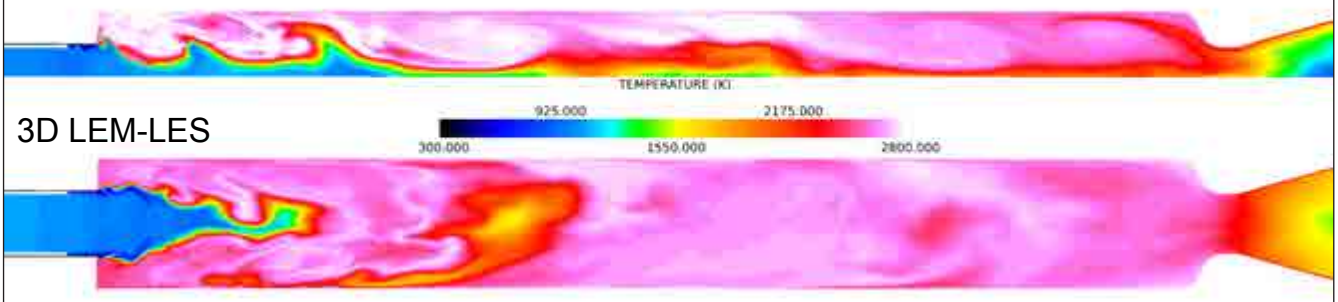
Axisymmetric v/s 3D

- Boundary condition on the axis center does not allow transverse jet flapping
- Flame anchoring identical but long oxidizer core even for gas-gas case

Axi LEM-LES

3D LEM-LES



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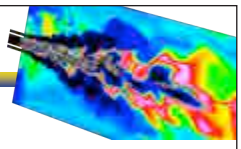
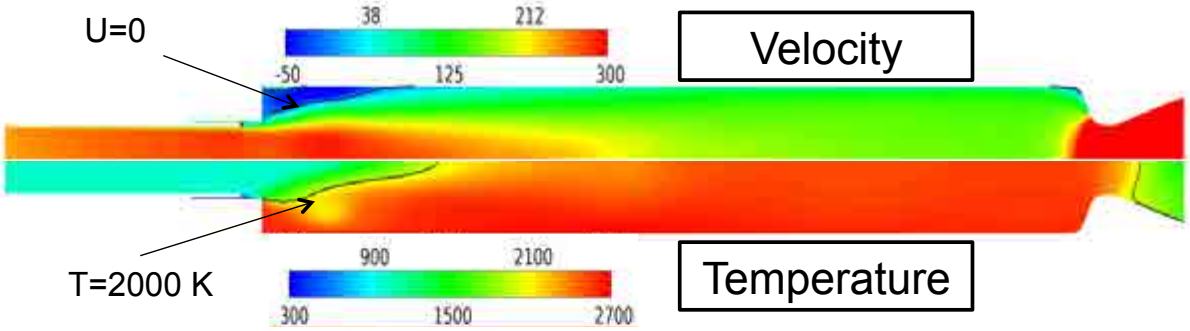


3D LES Mean Results



- Velocity field: long recirculation zone, supersonic flow in the nozzle and high velocity core along the center line
- Anchoring of the flame at the step corner.
- Stabilization of the flame in the mixing layer between the high velocity flow and the recirculation
- Distributed heat release: the flame is not compact (L_f ~8cm)

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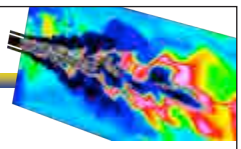
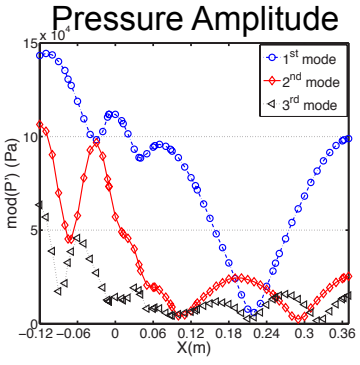
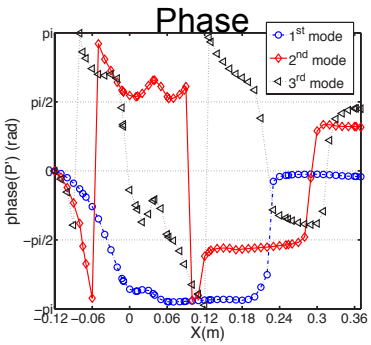
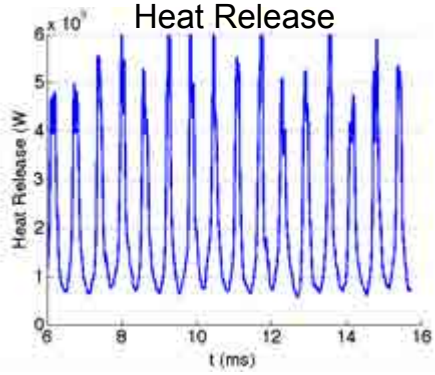


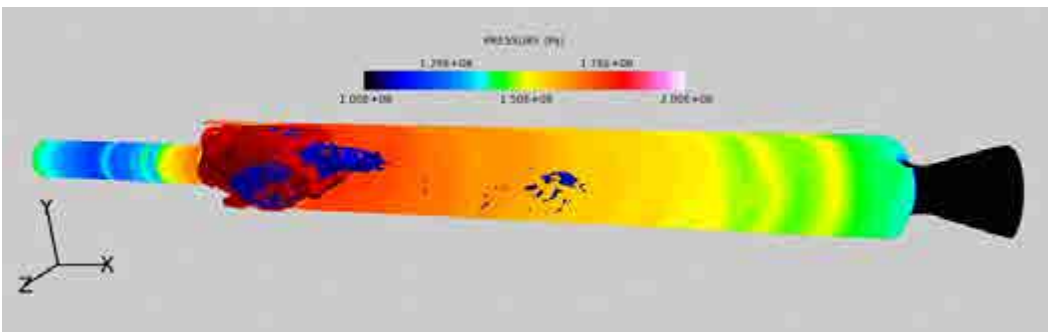
Resonant mode Structure







Two Standing Acoustic modes in the combustor



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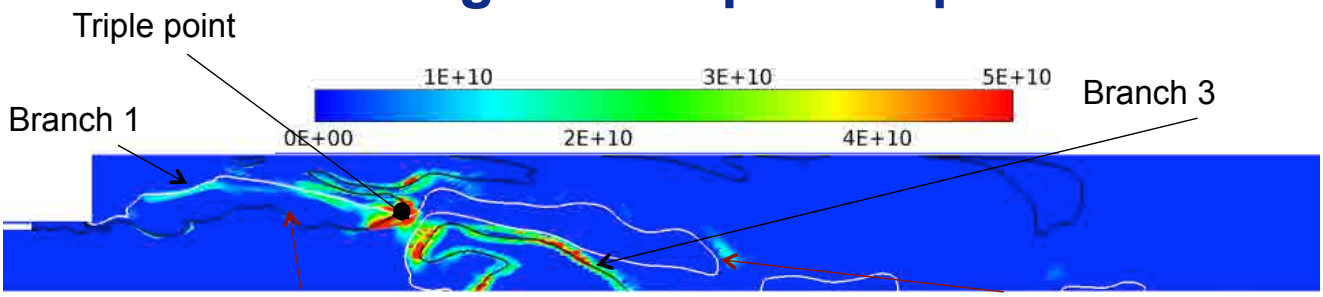
Flame Holding: A Complex Triple Flame



$z=z_{st}=0.095$ (black line)

T=2000 K (white line)

- Branch 1: rich premixed flame anchored at the step corner
- Branch 2: lean premixed flame
- Branch 3: diffusion flame (stoichiometric mixture fraction)
- Triple point : intersection of the three branches
  - Location of Maximum Heat Release

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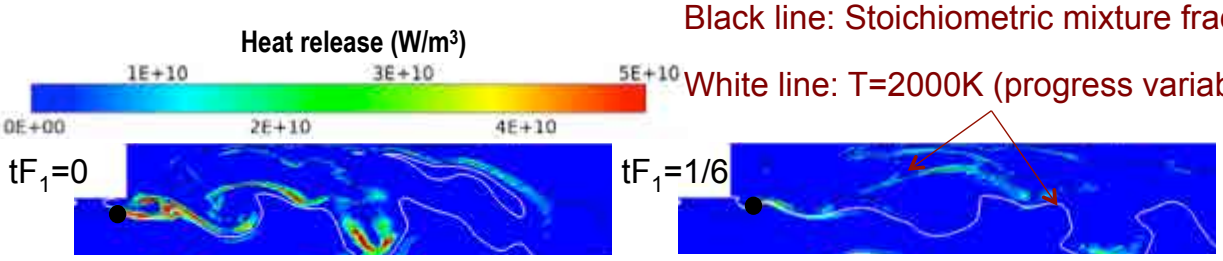
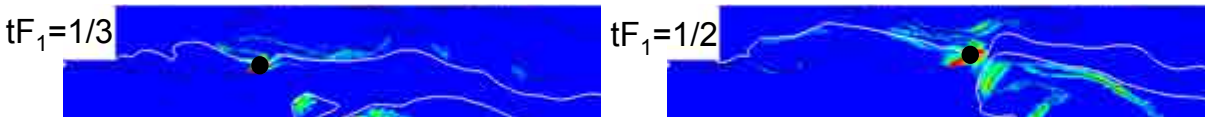
Triple Flame Structure

Black line: Stoichiometric mixture fraction

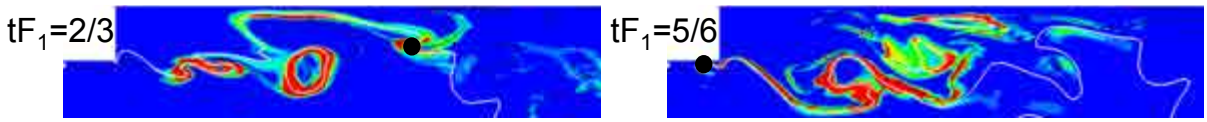
White line: T=2000K (progress variable)



1- Initiation of a triple point at the step corner: extinction of the downstream flame



2- Propagation of the triple point with the flow: weak combustion



3- Triple point is trapped in the recirculation zone: ignition of an intense rich flame. Start of a new cycle with the generation of a new triple point

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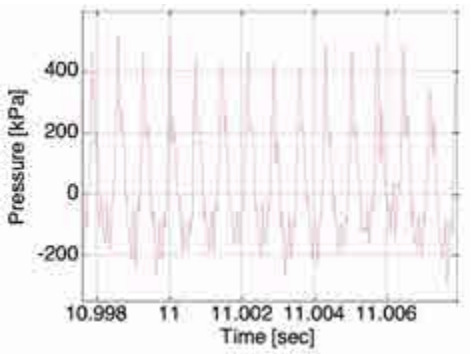
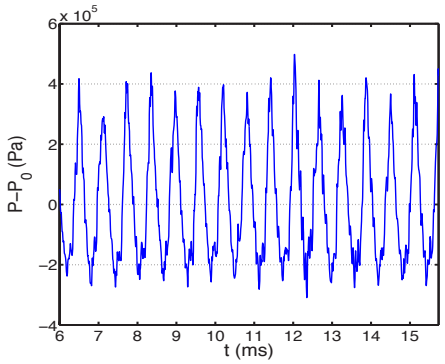
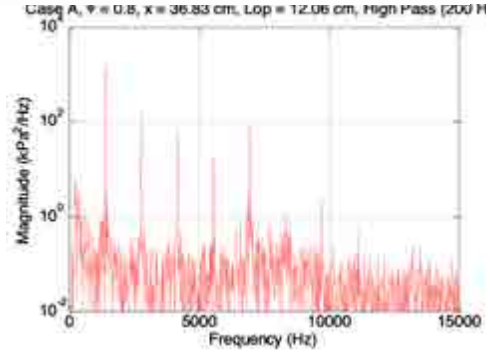
Pressure Signal and Spectra

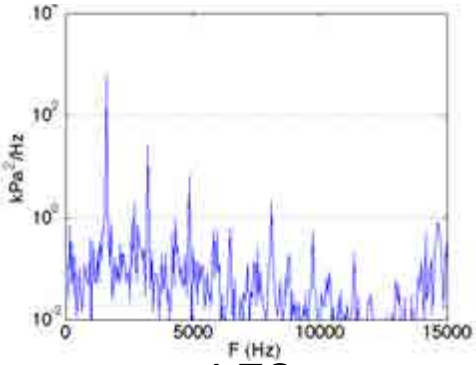


Time Trace





Frequency



Experiment LES

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Summary Comments

- LRE modeling and simulation are very challenging due to real gas effects, finite-rate kinetics, flame-turbulence-acoustic interactions and complexity of the geometry
- LES compressible solver with real gas and subgrid closures developed to address these challenges
- Application to trans-critical mixing experiments shows good agreement with data
- Application to trans-critical reacting experiments show much more is needed to reduce cost of kinetics
- Application to combustion instability in subcritical reacting cases shows ability of LES to capture dynamics
- Still a lot of studies needed to develop predictive capability for multi-injector applications

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National Aeronautics and
Space Administration

Lyndon B. Johnson Space Center

Recent Advancements in Fully Implicit Numerical Methods for Hypersonic Reacting Flows

with Application to Reentry and Arcjet Modeling

Benjamin S. Kirk†, Roy H. Stogner⋆,
Todd A. Oliver⋆, and Paul T. Bauman⋆

† NASA Lyndon B. Johnson Space Center – Houston, TX USA
⋆Institute for Computational Engineering & Sciences – The University of Texas at Austin, USA

September 26, 2012

Acknowledgments

1. This work was supported in part by the Entry, Descent and Landing Project in the NASA/ESMD Enabling Technology Development and Demonstration Program.
2. This work was supported in part by a cooperative agreement with the Predictive Engineering and Computational Sciences (PECOS) Center at The University of Texas at Austin.
3. Thanks to Dr. Dinesh Prabhu (NASA/ARC) for providing the arcjet grids.

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1 Background & Motivation
- Problem Class
- Reacting Flows
- Surface Ablation

2 Physical Modeling
- Governing Equations
- Thermochemistry
- Quasi-Steady Ablation

3 Finite Element Formulation

4 Fully-Implicit Navier-Stokes (FIN-S) Overview
- Verification
- Parallelism

5 Results
- Perfect Gas Flow over a Double Cone
- Viscous Thermal Equilibrium Chemical Reacting Flow
- Viscous Reacting Flow with Quasi-Steady Surface Ablation
- Modeling Arcjet Flows

6 Ongoing Challenges

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The physical phenomenon of interest is high-speed gas dynamics

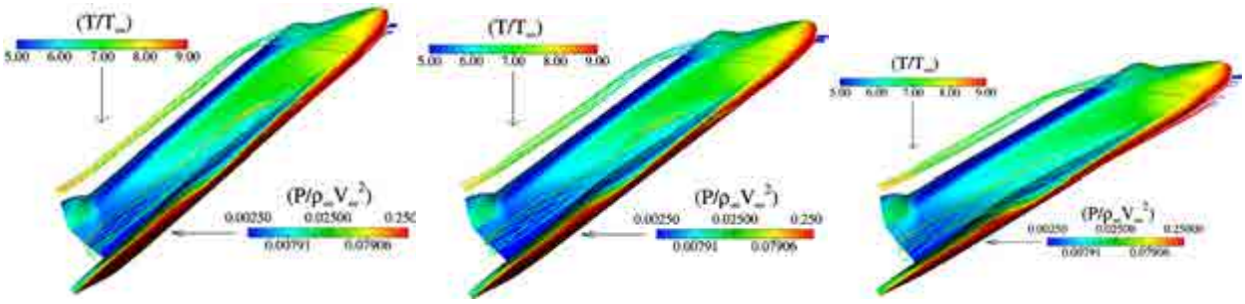
Physics

- The compressible Navier-Stokes equations describe fluid flow for all Mach numbers.
- For aerospace applications of interest the Reynolds number is almost always such that the flows are *convection dominated*.
- *Multiscale phenomena* appear in the form of shock waves, boundary layers, and shear layers.

Numerics

- Discretization of the *conservation law form* of the Navier-Stokes equations is required for convergence to physically valid solutions.
- Convective terms must be treated with some form of *upwinding*.
- Shocks are treated with some form of *limiting* or *shock capturing*, both of which amount to artificial diffusion which regularizes the problem.

Aerodynamics



. . . is concerned with predicting aerodynamic forces and moments on a vehicle which result predominantly from the surface pressure distribution, but also from viscous shear stress.

Properly characterizing the aerodynamic performance of reentry vehicles is critical for optimal trajectory design.

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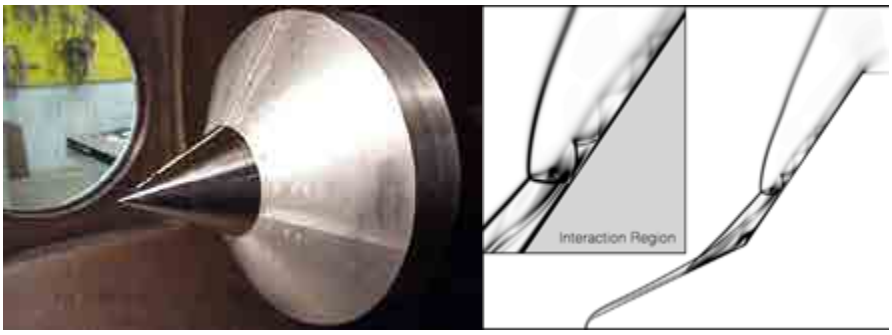
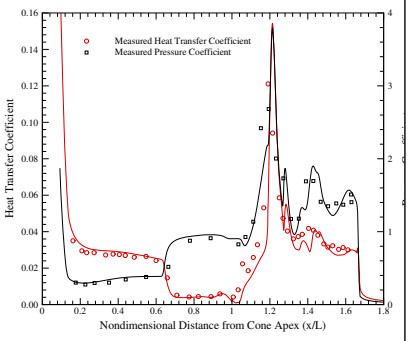
Aerothermodynamics

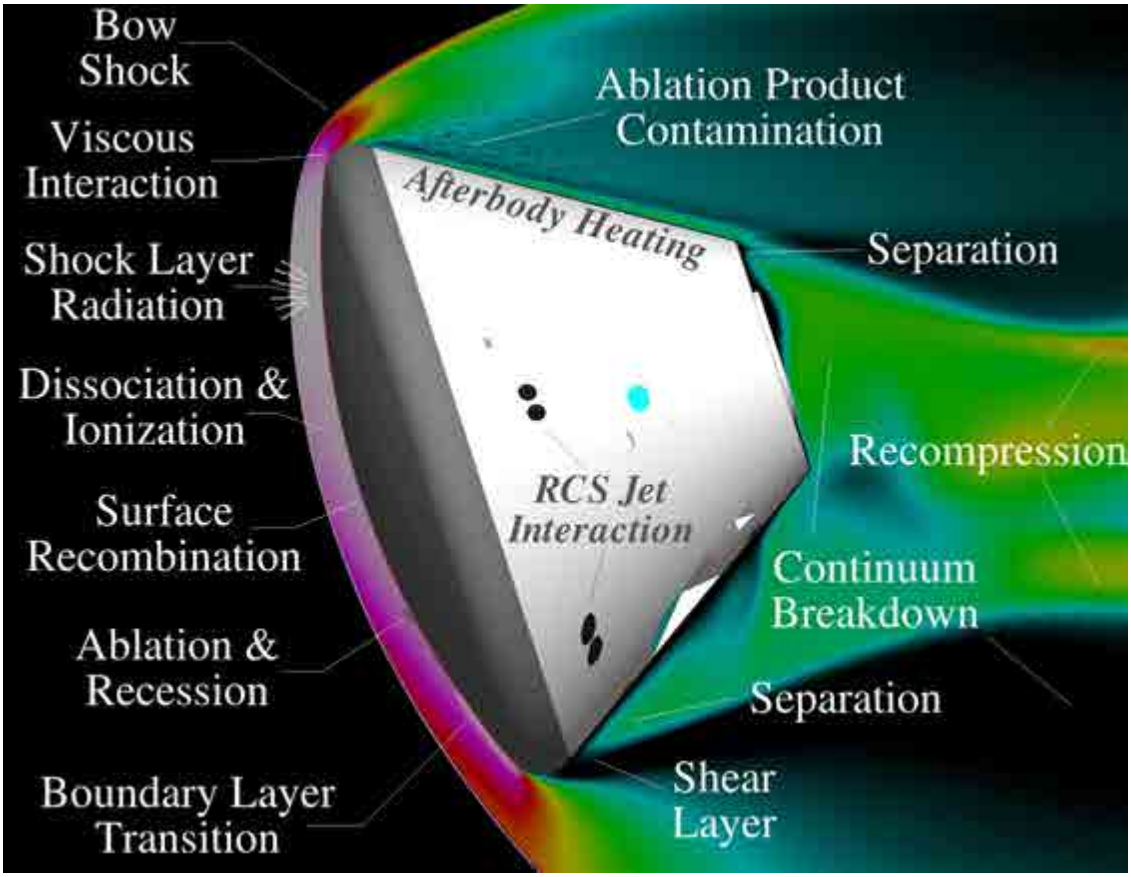




. . . is concerned with predicting the instantaneous total heat transfer rate and integrated heat load into a vehicle.

Properly characterizing this environment is crucial because it provides the design conditions for the thermal protection system:

heat transfer rate → thermal protection material selection
heat load → thermal protection material thickness



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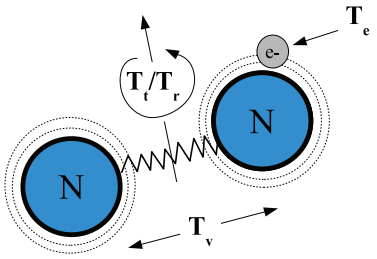
- When chemical kinetic timescales are approximately equal to flow timescales, the chemical composition of a flowfield must be determined as part of a simulation procedure. Such flows are in *chemical nonequilibrium*.



- Molecules and atoms can store energy in various *modes*.
- At hypersonic conditions these modes may not be in equilibrium, resulting in *thermal nonequilibrium*.

- The physical models and governing equations for flows in thermochemical nonequilibrium have been simulated previously with finite difference and finite volume techniques.
- In this work we review the physical models and implement a SUPG finite element scheme for hypersonic flows in thermochemical nonequilibrium.

- At hypersonic entry conditions, surface temperatures may exceed capabilities of reusable thermal protection system materials.
  - Reusable materials typically limited to $T < 2,000\,\mathrm{K}$.
  - It is necessary then to consider *ablative materials*.
- Ablative materials respond to high temperatures through pyrolysis, decomposition, blowing, and surface recession.
- Typically, ablation analysis is decoupled from the external flowfield, but we hope to do better.
- Additionally, accurately characterizing ground test facilities requires increased fidelity.

- As we will see, however, more accurate numerical modeling results in unique numerical challenges, necessitating novel numerical algorithms.

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Governing Equations

- Extension from a single-species calorically perfect gas to a reacting mixture of thermally perfect gases requires species conservation equations and additional energy transport mechanisms.

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \boldsymbol{u}) = \nabla \cdot (\rho \mathcal{D}_s \nabla c_s) + \dot{\omega}_s$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla P + \nabla \cdot \boldsymbol{\tau}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \boldsymbol{u}) = -\nabla \cdot \dot{\boldsymbol{q}} + \nabla \cdot (\boldsymbol{\tau}\boldsymbol{u}) + \nabla \cdot \left(\rho \sum_{s=1}^{ns} h_s \mathcal{D}_s \nabla c_s \right)$$

- Problem class may also require a multitemperature thermal nonequilibrium option.

$$\frac{\partial \rho e_V}{\partial t} + \nabla \cdot (\rho e_V \boldsymbol{u}) = -\nabla \cdot \dot{\boldsymbol{q}}_V + \nabla \cdot \left(\rho \sum_{s=1}^{ns} e_{Vs} \mathcal{D}_s \nabla c_s \right) + \dot{\omega}_V$$

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Turbulence Modeling

- We model the effects of turbulence using the Spalart-Allmaras one-equation turbulence model:

$$\frac{\partial}{\partial t}(\bar{\rho}\nu_{sa}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\nu_{sa}) = c_{b1}S_{sa}\bar{\rho}\nu_{sa} - c_{w1}f_w\bar{\rho}\left(\frac{\nu_{sa}}{d}\right)^2 + \frac{1}{\sigma}\frac{\partial}{\partial x_k}\left[(\mu + \bar{\rho}\nu_{sa})\frac{\partial \nu_{sa}}{\partial x_k}\right] + \frac{c_{b2}}{\sigma}\bar{\rho}\frac{\partial \nu_{sa}}{\partial x_k}\frac{\partial \nu_{sa}}{\partial x_k}$$

with closure terms

$$\mu_t = \bar{\rho}\nu_{sa}f_{v1}, \qquad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \qquad f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad \chi = \frac{\nu_{sa}}{\nu},$$

$$f_w = g\left(\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6}\right)^{1/6}, \quad g = r + c_{w2}\left(r^6 - r\right), \qquad r = \frac{\nu_{sa}}{S_{sa}\kappa^2 d^2}.$$

Turbulence Modeling

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and source term

$$S_{sa} = \Omega + S_m, \quad S_{m0} = \frac{\nu_{sa}}{\kappa^2 d^2}f_{v2}$$

where

$$S_m = \begin{cases} S_{m0}, & S_{m0} \geq -c_{v2}\Omega \\ \dfrac{\Omega(c_{v2}^2\Omega + c_{v3}S_{m0})}{((c_{v3} - 2c_{v2})\Omega - S_{m0})}, & \text{otherwise.} \end{cases}$$

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Thermodynamics & Transport Properties

- Thermochemistry models must be extended for a mixture of vibrationally and electronically excited thermally perfect gases.

$$\begin{aligned} e^{\text{int}} =& e^{\text{trans}} + e^{\text{rot}} + e^{\text{vib}} + e^{\text{elec}} + h^0 \\ =& \sum_{s=1}^{ns} c_s e_s^{\text{trans}}(T) + \sum_{s=mol} c_s e_s^{\text{rot}}(T) + \\ & \sum_{s=mol} c_s e_s^{\text{vib}}(T_V) + \sum_{s=1}^{ns} c_s e_s^{\text{elec}}(T_V) + \sum_{s=1}^{ns} c_s h_s^0 \end{aligned}$$

  Here we have assumed that $T^{\text{trans}} = T^{\text{rot}} = T$ and $T^{\text{vib}} = T^{\text{elec}} = T_V$

- Additional transport property models are required. In this work we use
  - species viscosity given by Blottner curve fits,
  - species conductivities determined from an Eucken relation,
  - mixture transport properties computed via Wilke's mixing rule, and
  - mass diffusion currently treated by assuming constant Lewis number.

Chemical Kinetics & Energy Exchange

Kinetics:

- we consider r general reactions of the form

$$\mathrm{N_2} + \mathcal{M} \rightleftharpoons 2\mathrm{N} + \mathcal{M}$$
$$\dots$$
$$\mathrm{N_2} + \mathrm{O} \rightleftharpoons \mathrm{NO} + \mathrm{N}$$
$$\dots$$

- When combined with forward and backward rates, these reactions produce the species source terms $\dot{\omega}_s$
- Presently, we use either CANTERA or an in-house library to provide these source terms.

Energy Exchange:

- Equilibration between the energy modes is modeled with a typical Landau-Teller vibrational energy exchange model with Millikan-White species relaxation times.
- Provides the vibrational energy source term $\dot{\omega}_V$

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Chemical Kinetics

- We consider r general reactions of the form

$$\mathrm{N_2} + \mathcal{M} \rightleftharpoons 2\mathrm{N} + \mathcal{M}$$
$$\cdots$$
$$\mathrm{N_2} + \mathrm{O} \rightleftharpoons \mathrm{NO} + \mathrm{N}$$
$$\cdots$$

- The reactions are of the form

$$\mathcal{R}_r = k_{br} \prod_{s=1}^{ns} \left(\frac{\rho_s}{M_s}\right)^{\beta_{sr}} - k_{fr} \prod_{s=1}^{ns} \left(\frac{\rho_s}{M_s}\right)^{\alpha_{sr}}$$

  where α_{sr} and β_{sr} are the stoichiometric coefficients for reactants and products

- The source terms are then

$$\dot{\omega}_s = M_s \sum_{r=1}^{nr} (\alpha_{sr} - \beta_{sr}) (\mathcal{R}_{br} - \mathcal{R}_{fr})$$

Energy Exchange

$$\dot{\omega}_V = \dot{Q}_v + \dot{Q}_{\text{transfer}}$$

We adopt the Landau-Teller vibrational energy exchange model

$$\dot{Q}_s^{\text{tr-vib}} = \rho_s \frac{\hat{e}_s^{\text{vib}} - e_s^{\text{vib}}}{\tau_s^{\text{vib}}}$$

where $\hat{e}_s^{\text{vib}}$ is the species equilibrium vibrational energy and the vibrational relaxation time τ_s^{vib} is given by Millikan and White

$$\tau_s^{\text{vib}} = \frac{\sum_{r=1}^{ns} \chi_r}{\sum_{r=1}^{ns} \chi_r / \tau_{sr}^{\text{vib}}}, \quad \chi_r = c_r \frac{M}{M_r}, \quad M = \left(\sum_{s=1}^{ns} \frac{c_s}{M_s}\right)^{-1}$$

and

$$\tau_{sr}^{\text{vib}} = \frac{1}{P} \exp\left[A_{sr}\left(T^{-1/3} - 0.015\mu_{sr}^{1/4}\right) - 18.42\right]$$
$$A_{sr} = 1.16 \times 10^{-3} \mu_{sr}^{1/2} \theta_{vs}^{4/3}, \quad \mu_{sr} = \frac{M_s M_r}{M_s + M_r}$$

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Vibrational Energy Production and Energy Exchange

$$\dot{\omega}_V = \dot{Q}_v + \dot{Q}_{\text{transfer}}$$

When molecular species are created in the gas at rate $\dot{\omega}_s$, they contribute vibrational/electronic energy at the rate

$$\dot{Q}_{vs} = \dot{\omega}_s \left(e_s^{\text{vib}} + e_s^{\text{elec}} \right)$$

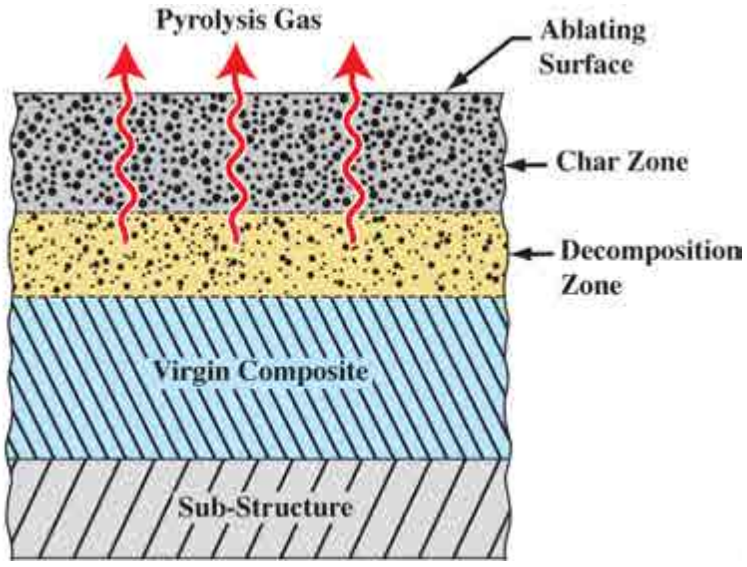
so the net vibrational energy production rate is

$$\dot{Q}_v = \sum_{s=1}^{ns} \dot{\omega}_s \left(e_s^{\text{vib}} + e_s^{\text{elec}} \right)$$

Combining terms yields the desired net vibrational energy source term

$$\dot{\omega}_V = \sum_{s=1}^{ns} \dot{Q}_s^{\text{tr-vib}} + \sum_{s=1}^{ns} \dot{\omega}_s \left(e_s^{\text{vib}} + e_s^{\text{elec}} \right)$$

Ablation Processes



Schematic of ablation processes

- Ablation is a multi-scale, multi-physics phenomenon
- Sometimes amenable to simplification for predictive simulations

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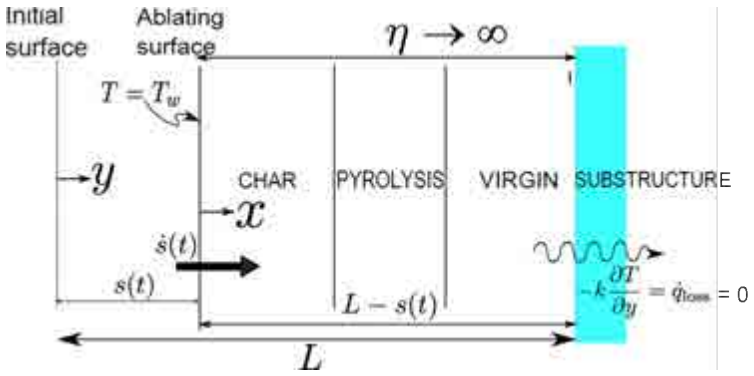
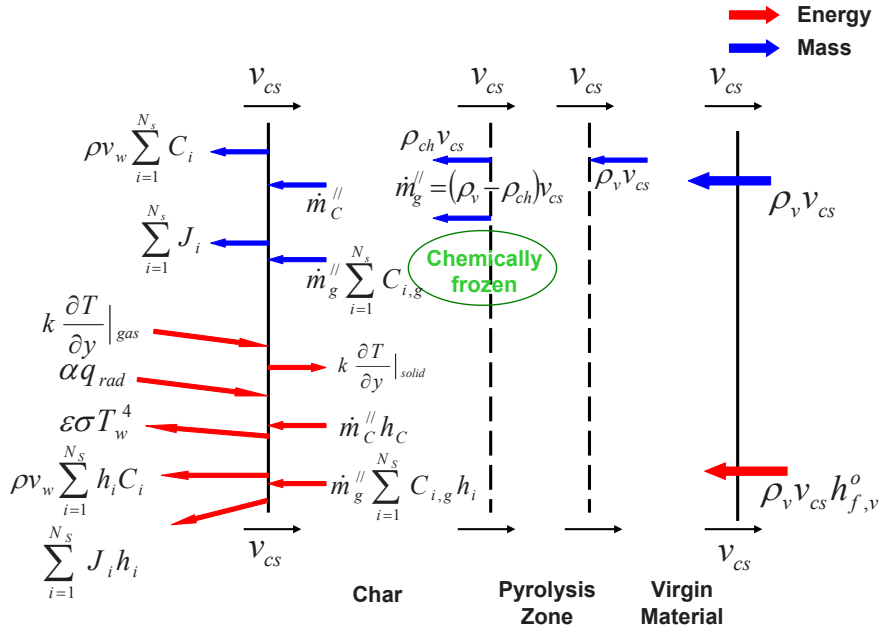
Quasi-steady State Ablation Hypothesis



1. Steady state in reference frame fixed to the receding surface
2. Time variations solely due to motion of the material domain
3. Time scale for surface motion ($\dot{s} \approx 0.1 - 1\ ^{\text{mm}}/_{\text{sec}}$) much larger than characteristic time scale of unsteady processes
4. 1-D, semi-infinite medium

Quasi-steady Ablation



- Assumes ablation timescale $\ll$ trajectory timescale
- Assumes negligible substructure conduction

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Ablation Interface Conditions

Recession:

$$\rho v_w = \dot{m}_c'' + \dot{m}_g''$$

Mass:

$$J_i|_{gas} + \rho v_w C_i = \tilde{N}_i(C_i, T) + \dot{m}_g'' C_{i,g}; (i : 1..N_s)$$

Energy:

$$-k\frac{\partial T}{\partial y}\bigg|_{gas} - \sum_{i=1}^{N_s} h_i(T_w)\, J_i|_{gas} + \dot{m}_c'' h_c(T) - \rho v_w h_w(T)$$

$$+\alpha \dot{q}_r'' - \sigma \epsilon T_w{}^4 + \sum_{i=1}^{N_s} \dot{m}_g'' C_{i,g} h_i(T_w) + k_s \frac{\partial T}{\partial y}|_{solid,w} = 0$$

- Nonlinear Robin Boundary Conditions
- Enables quasi-steady solves, restarts

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- Surface Ablation

2 Physical Modeling
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- Thermochemistry
- Quasi-Steady Ablation

3 Finite Element Formulation

4 Fully-Implicit Navier-Stokes (FIN-S) Overview
- Verification
- Parallelism

5 Results
- Perfect Gas Flow over a Double Cone
- Viscous Thermal Equilibrium Chemical Reacting Flow
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6 Ongoing Challenges

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Stabilized Finite Element Scheme

$$\frac{\partial \boldsymbol{U}}{\partial t} + \boldsymbol{A}_i \frac{\partial \boldsymbol{U}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\boldsymbol{K}_{ij}\frac{\partial \boldsymbol{U}}{\partial x_j}\right) + \dot{\boldsymbol{\mathcal{S}}}$$

Find $\boldsymbol{U}$ satisfying the essential boundary and initial conditions such that

$$\int_\Omega \left[\boldsymbol{W}\cdot\left(\frac{\partial \boldsymbol{U}}{\partial t} - \dot{\boldsymbol{\mathcal{S}}}\right) + \frac{\partial \boldsymbol{W}}{\partial x_i}\cdot\left(\boldsymbol{K}_{ij}\frac{\partial \boldsymbol{U}}{\partial x_j} - \boldsymbol{A}_i\boldsymbol{U}\right)\right] d\Omega$$
$$+\sum_{e=1}^{n_{el}}\int_{\Omega_e} \tau_{\mathrm{SUPG}}\frac{\partial \boldsymbol{W}}{\partial x_k}\cdot\boldsymbol{A}_k\left[\frac{\partial \boldsymbol{U}}{\partial t} + \boldsymbol{A}_i\frac{\partial \boldsymbol{U}}{\partial x_i} - \frac{\partial \boldsymbol{G}_i}{\partial x_i} - \dot{\boldsymbol{\mathcal{S}}}\right] d\Omega$$
$$+\sum_{e=1}^{n_{el}}\int_{\Omega_e} \nu_{\mathrm{DCO}}\left(\frac{\partial \boldsymbol{W}}{\partial x_i}\cdot g^{ij}\frac{\partial \boldsymbol{U}}{\partial x_j}\right) d\Omega - \oint_\Gamma \boldsymbol{W}\cdot(\boldsymbol{g}-\boldsymbol{f})\, d\Gamma = 0$$

for all $\boldsymbol{W}$ in an appropriate function space.

Stabilization Parameters

Discontinuity capturing operator:

$$\nu_{\mathrm{DCO}} = \left[\frac{\left\|\frac{\partial \boldsymbol{U}}{\partial t} + \boldsymbol{A}_i\frac{\partial \boldsymbol{U}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\boldsymbol{K}_{ij}\frac{\partial \boldsymbol{U}}{\partial x_j}\right)\right\|^2_{\boldsymbol{A}_0^{-1}}}{(\Delta \boldsymbol{U}_h)^T\boldsymbol{A}_0^{-1}\Delta \boldsymbol{U}_h + g^{ij}\left(\frac{\partial \boldsymbol{U}_h}{\partial x_i}\right)^T\boldsymbol{A}_0^{-1}\frac{\partial \boldsymbol{U}_h}{\partial x_j}}\right]^{1/2}$$

SUPG stabilization matrix:

$$\tau_{\mathrm{SUPG}}^{-1} = \sum_{i=\mathrm{nodes}}\left(\left|\frac{\partial \phi_i}{\partial x_j}\boldsymbol{A}_j\right| + \frac{\partial \phi_i}{\partial x_j}\boldsymbol{K}_{jk}\frac{\partial \phi_i}{\partial x_k}\right)$$

where

$$\left|\frac{\partial \phi_i}{\partial x_j}\boldsymbol{A}_j\right| = \boldsymbol{L}\,|\boldsymbol{\Lambda}|\,\boldsymbol{R}$$

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Fully-Implicit Navier-Stokes (FIN-S)

Implementation Highlights

- C++ application code built on top of the `libMesh` library.
  - `libMesh` provides all requisite finite element data, parallel domain decomposition details.
  - Inherits PETSc preconditioned Krylov iterative solvers.
  - CANTERA used for kinetic rates, in-house thermodynamics, transport properties.
  - Only $\approx$ 30K SLOC
- Fully-coupled (monolithic solves), fully-implicit discretization.
- Rigorous verification using MASA-provided manufactured solutions.
- Testbed for intrusive VV/UQ schemes applied to hypersonics.

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Manufactured Analytical Solution Abstraction Library

- Dearth of exact solutions necessitates *method of manufactured solutions*
- Some manufactured solutions exist for the calorically perfect Navier-Stokes equations
  - Developed in large part by Sandia National Labs
  - Specific solutions for field, boundary condition order-of-accuracy verification
- Existing solutions provide a necessary but not sufficient test suite
  - Will need to develop many more solutions to verify reacting flows with complex transport models
- Manufactured solutions are a valuable resource that should be accessible to anyone
- PECOS is developing the Manufactured Analytical Solution Abstraction (MASA) library to provide well-defined manufactured solutions and source terms for a range of physics applications

Manufactured solutions are being constructed and will be incorporated into the FIN-S regression test suite

Manufactured analytical solutions (used by Roy, Smith, and Ober) for each one of the primitive variables in Navier-Stokes equations are:

$$\rho(x,y) = \rho_0 + \rho_x \sin\left(\frac{a_{\rho x}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{\rho y}\pi y}{L}\right),$$
$$u(x,y) = u_0 + u_x \sin\left(\frac{a_{ux}\pi x}{L}\right) + u_y \cos\left(\frac{a_{uy}\pi y}{L}\right),$$
$$v(x,y) = v_0 + v_x \cos\left(\frac{a_{vx}\pi x}{L}\right) + v_y \sin\left(\frac{a_{vy}\pi y}{L}\right),$$
$$p(x,y) = p_0 + p_x \cos\left(\frac{a_{px}\pi x}{L}\right) + p_y \sin\left(\frac{a_{py}\pi y}{L}\right)$$

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The method of manufactured solutions applied to Navier-Stokes equations requires modifying the governing equations by adding a source term to the right-hand side of each equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = Q_\rho$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + p - \tau_{xx}}{\partial x} + \frac{\partial \rho uv - \tau_{xy}}{\partial y} = Q_u$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial \rho vu - \tau_{yx}}{\partial x} + \frac{\partial \rho v^2 + p - \tau_{yy}}{\partial y} = Q_v$$

$$\frac{\partial \rho e_t}{\partial t} + \frac{\partial \rho u e_t + pu - u\tau_{xx} - v\tau_{xy} + q_x}{\partial x} + \frac{\partial \rho v e_t + pv - u\tau_{yx} - v\tau_{yy} + q_y}{\partial y} = Q_{e_t}$$

so the modified set of equations has a known, analytical solution. Symbolic representations of requisite source terms and C-source code have recently been generated for 2D and 3D calorically perfect gas flows.

$$
\begin{aligned}
Q_\rho &= \frac{a_{\rho x}\pi\rho_x}{L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \\
&- \frac{a_{\rho y}\pi\rho_y}{L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \\
&+ \frac{a_{ux}\pi u_x}{L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
&+ \frac{a_{vy}\pi v_y}{L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
Q_u &= \frac{a_{\rho x}\pi\rho_x}{L}\sin\left(\frac{a_{\rho x}\pi x}{L}\right) \\
&+ \frac{a_{ux}\pi\rho_x}{L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2 \\
&- \frac{a_{\rho y}\pi\rho_y}{L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \\
&+ \frac{2a_{ux}\pi u_x}{L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
&- \frac{\pi a_{uy}u_y}{L}\sin\left(\frac{a_{uy}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
&+ \frac{\pi a_{vx}v_x}{L}\cos\left(\frac{a_{vx}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
&+ \frac{4a_{ux}^2\pi^2\mu_{ux}}{3L^2}\sin\left(\frac{a_{ux}\pi x}{L}\right) + \frac{a_{vy}^2\pi^2\mu_{ux}}{L^2}\cos\left(\frac{a_{vy}\pi y}{L}\right) \\
Q_v &= \frac{a_{\rho y}\pi\rho_y}{L}\cos\left(\frac{a_{\rho y}\pi y}{L}\right) \\
&+ \frac{\pi a_{\rho x}\rho_x}{L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \\
&- \frac{a_{\rho y}\pi\rho_y}{L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2 \\
&+ \frac{a_{vx}\pi u_x}{L}\cos\left(\frac{a_{vx}\pi x}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
&- \frac{a_{ux}\pi v_x}{L}\sin\left(\frac{a_{ux}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
&+ \frac{2a_{vy}\pi v_y}{L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right] \\
&+ \frac{a_{ux}^2\pi^2\mu v_x}{L^2}\cos\left(\frac{a_{ux}\pi x}{L}\right) + \frac{4a_{vy}^2\pi^2\mu v_x}{3L^2}\sin\left(\frac{a_{vy}\pi y}{L}\right) \\
Q_{e_t} &= -\frac{a_{\rho x}\pi\rho_x}{L}\frac{\gamma}{\gamma-1}\sin\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] \\
&+ \frac{a_{\rho y}\pi\rho_y}{L}\frac{\gamma}{\gamma-1}\cos\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \\
&+ \frac{a_{ux}\pi\rho_x}{2L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2+\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2\right] \\
&- \frac{a_{\rho y}\pi\rho_y}{2L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]\left[\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2+\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2\right] \\
&+ \frac{a_{ux}\pi u_x}{2L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left\{\left[\rho_x\cos\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\sin\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\frac{2\gamma}{\gamma-1}+\right. \\
&\left.+\left[3\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2+\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\right\} \\
&- \frac{a_{uy}\pi u_y}{L}\sin\left(\frac{a_{uy}\pi y}{L}\right)\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \\
&- \frac{a_{vx}\pi v_x}{L}\sin\left(\frac{a_{vx}\pi x}{L}\right)\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] \\
&+ \frac{a_{vy}\pi v_y}{2L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left\{\left[\rho_x\cos\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\sin\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\frac{2\gamma}{\gamma-1}\right. \\
&\left.+\left[\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right]^2+3\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right]^2\right]\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]\right\} \\
&+ \frac{a_{\rho x}^2\pi^2 k p_x\cos\left(\frac{a_{\rho x}\pi x}{L}\right)}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]L^2R} + \frac{a_{\rho y}^2\pi^2 k p_y\sin\left(\frac{a_{\rho y}\pi y}{L}\right)}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]L^2R} \\
&- \frac{2a_{\rho x}^2\pi^2 k\rho_x^2}{L^2R}\cos^2\left(\frac{a_{\rho x}\pi x}{L}\right)\frac{\left[\rho_x\cos\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\sin\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^3} - \frac{a_{\rho x}^2\pi^2 k\rho_x}{L^2R}\sin\left(\frac{a_{\rho x}\pi x}{L}\right)\frac{\left[\rho_x\cos\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\sin\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^2} \\
&- \frac{2a_{\rho y}^2\pi^2 k\rho_y^2}{L^2R}\sin^2\left(\frac{a_{\rho y}\pi y}{L}\right)\frac{\left[\rho_x\cos\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\sin\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^3} - \frac{a_{\rho y}^2\pi^2 k\rho_y}{L^2R}\cos\left(\frac{a_{\rho y}\pi y}{L}\right)\frac{\left[\rho_x\cos\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\sin\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^2} \\
&+ \frac{4a_{ux}^2\pi^2\mu u_x}{3L^2}\sin\left(\frac{a_{ux}\pi x}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] - \frac{4a_{ux}^2\pi^2\mu u_x^2}{3L^2}\cos^2\left(\frac{a_{ux}\pi x}{L}\right) \\
&+ \frac{a_{uy}^2\pi^2\mu u_y}{L^2}\cos\left(\frac{a_{uy}\pi y}{L}\right)\left[u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_0\right] - \frac{a_{uy}^2\pi^2\mu u_y^2}{L^2}\sin^2\left(\frac{a_{uy}\pi y}{L}\right) \\
&+ \frac{a_{vx}^2\pi^2\mu v_x}{L^2}\cos\left(\frac{a_{vx}\pi x}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] - \frac{a_{vx}^2\pi^2\mu v_x^2}{L^2}\sin^2\left(\frac{a_{vx}\pi x}{L}\right) \\
&+ \frac{4a_{vy}^2\pi^2\mu v_y}{3L^2}\sin\left(\frac{a_{vy}\pi y}{L}\right)\left[v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_0\right] - \frac{4a_{vy}^2\pi^2\mu v_y^2}{3L^2}\cos^2\left(\frac{a_{vy}\pi y}{L}\right) \\
&- \frac{2a_{\rho x}a_{\rho x}\pi^2 k p_x\rho_x}{L^2R}\frac{\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\sin\left(\frac{a_{\rho x}\pi x}{L}\right)}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^2} - \frac{2a_{\rho y}a_{\rho y}\pi^2 k p_y\rho_y}{L^2R}\frac{\cos\left(\frac{a_{\rho y}\pi y}{L}\right)\sin\left(\frac{a_{\rho y}\pi y}{L}\right)}{\left[\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_0\right]^2} \\
&+ \frac{4a_{ux}a_{vx}\pi^2\mu u_x v_x}{3L^2}\cos\left(\frac{a_{ux}\pi x}{L}\right)\cos\left(\frac{a_{vy}\pi y}{L}\right) - \frac{2a_{uy}a_{vy}\pi^2\mu u_y v_x}{L^2}\sin\left(\frac{a_{uy}\pi y}{L}\right)\sin\left(\frac{a_{ux}\pi x}{L}\right)
\end{aligned}
$$

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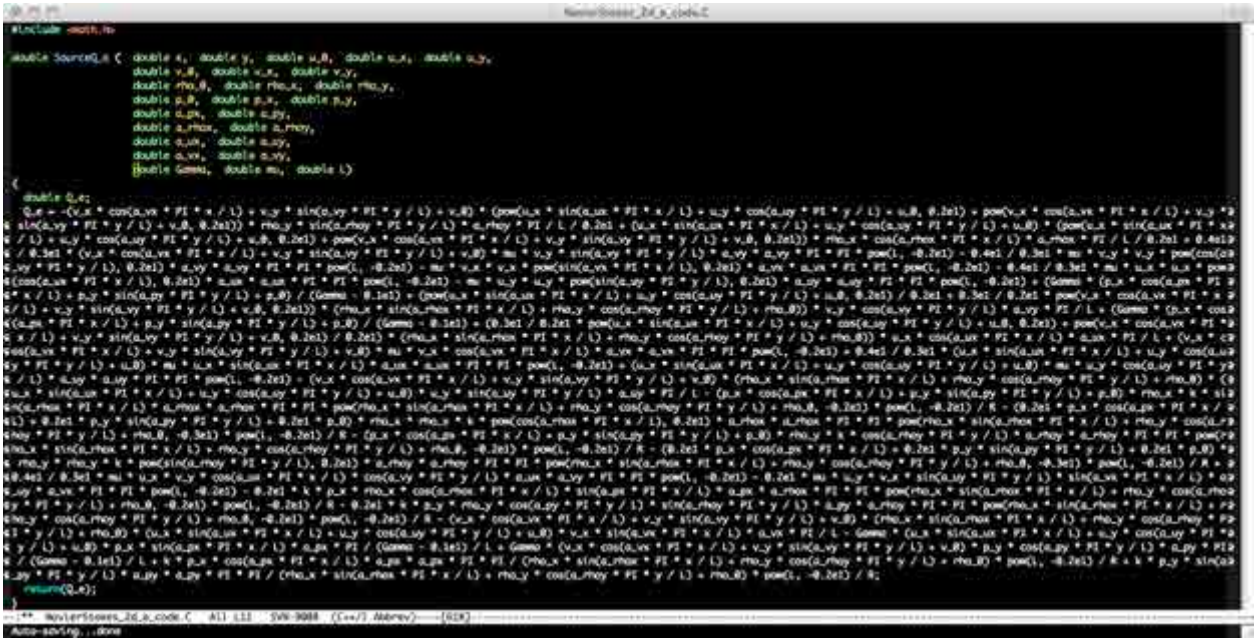
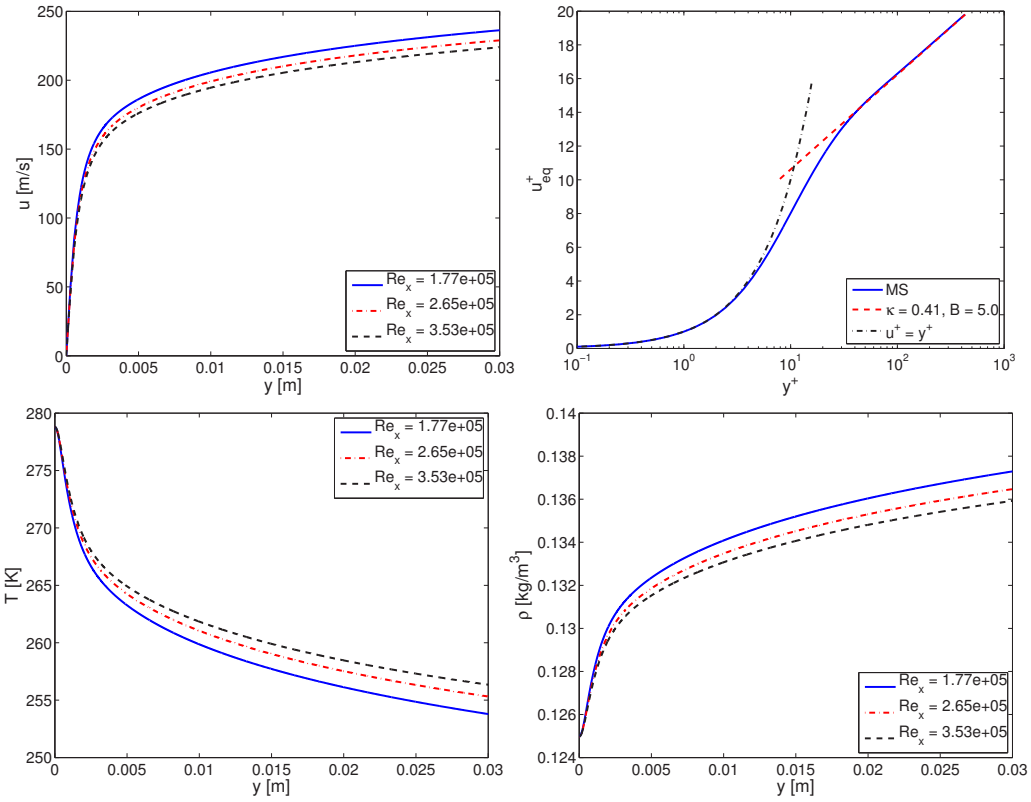


Spalart-Allmaras Perfect-Gas Verification



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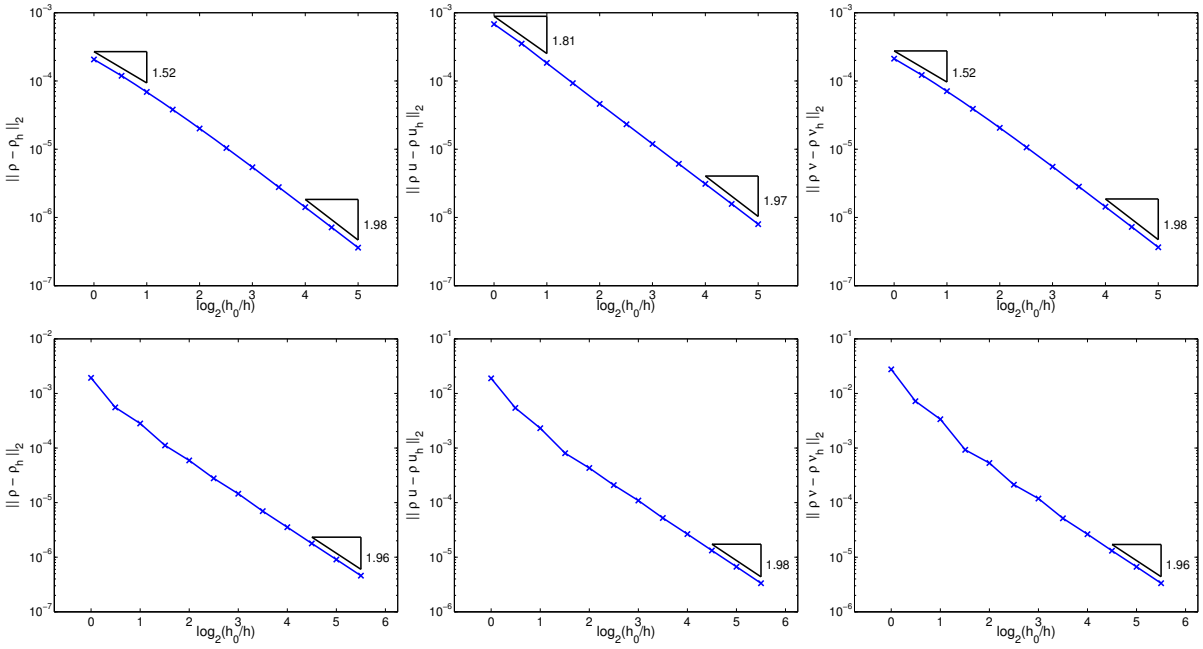
Spalart-Allmaras Perfect-Gas Verification



$\bar{\rho}$ $\bar{\rho}\tilde{u}$ $\bar{\rho}\nu_{\text{sa}}$

https://red.ices.utexas.edu/projects/software/wiki/MASA

Need for Parallelism

Large Problem Size

- Large numbers of unknowns.
  - For a Lagrange nodal basis:

$$\#\,\text{DOFS} = (\text{NS} + \text{NDIM} + \text{NE} + \text{NT}) \times \#\,\text{NODES}$$

  - Specifically, for our 13 species ablation model in 2D with turbulence

$$\#\,\text{DOFS} = (13 + 2 + 2 + 1) \times \#\,\text{NODES}$$

- For our implicit scheme, both storage and computational cost scale like $(\#\,\text{DOFS})^2$

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Need for Parallelism

Complex Physical Models

- Chemical Kinetics, transport properties for NS species inherently expensive.
- Temperature is a nonlinear function of species concentration, internal energy for a mixture of thermally perfect gases.
- Quasi-steady ablation boundary condition is also nontrivial.

Opportunities for Parallelism

Multiple Types of Parallelism

1. **Domain Decomposition:** We use a standard non-overlapping domain decomposition approach provided by `libMesh`. Local computations are perfectly parallel, and the resulting implicit system is solved using preconditioned Krylov solvers from PETSc.
2. **Multithreaded Computation:** The relatively large element matrices resulting for reacting flows are well suited for threaded assembly. `libMesh` provides a convenient interface to Intel's Threading Building Blocks which can provide further parallelization on multicore architectures.
3. **Vectorization:** Remember vectorization? While no longer the *de facto* paradigm for high-performance computing, modern microprocessors offer vectorized instructions worth exploiting. We are using Eigen for dense linear algebra and inherit its SSE optimizations.

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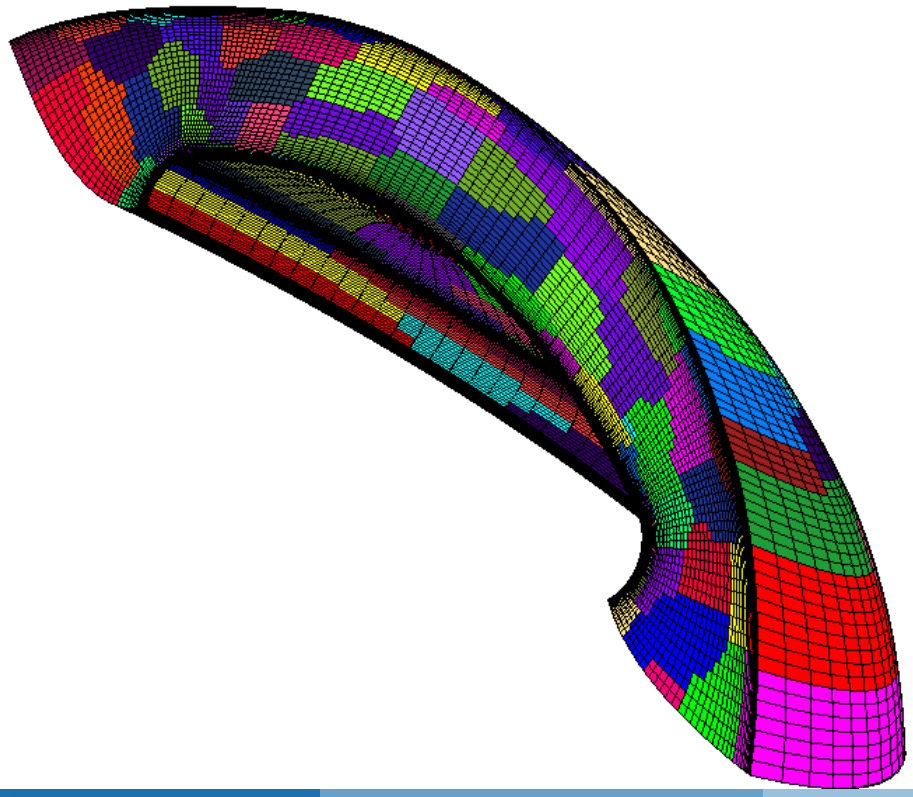
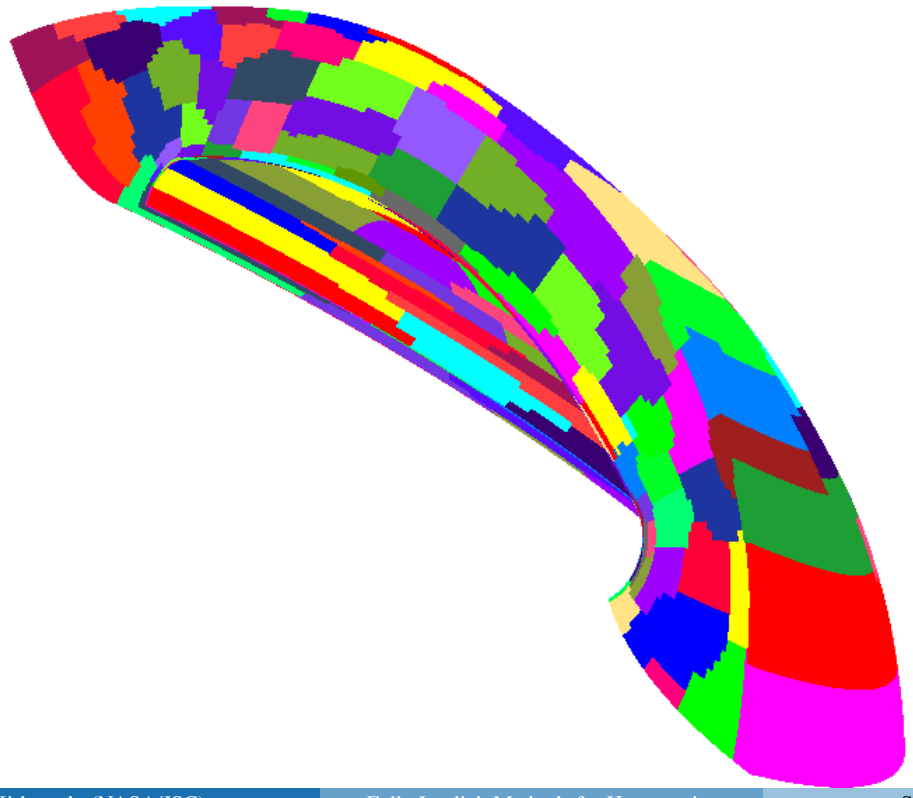
Domain Decomposition



Domain Decomposition



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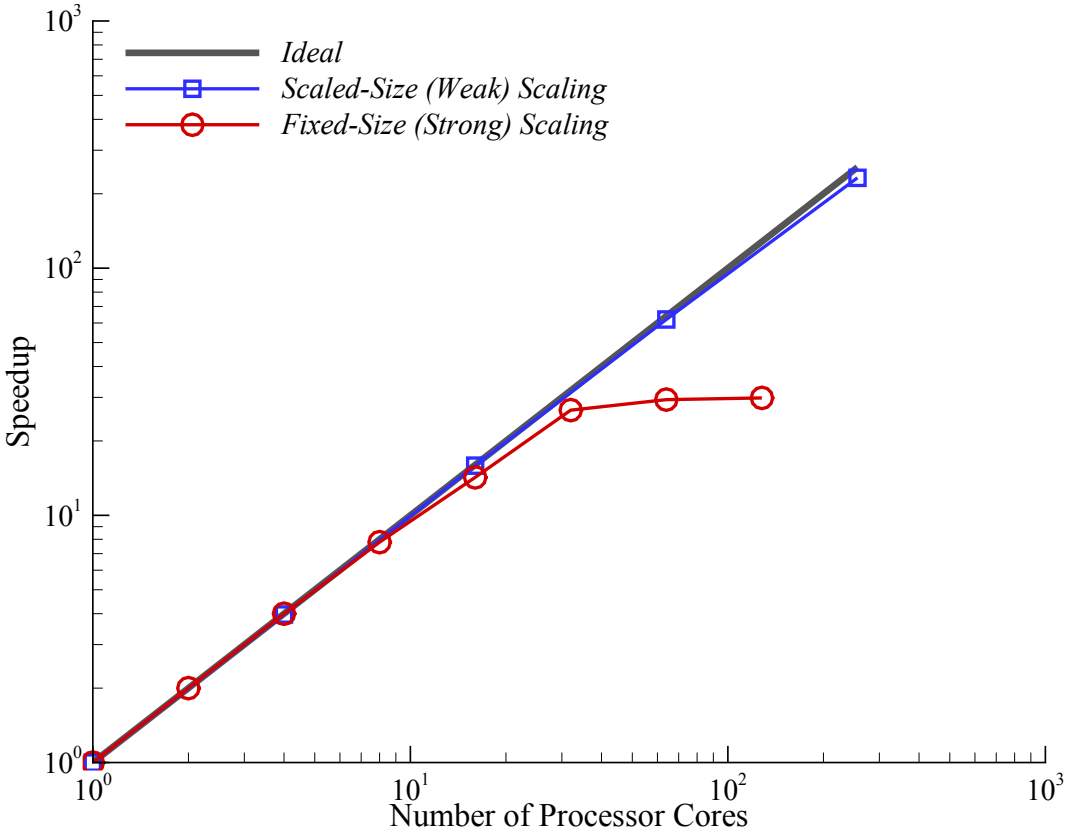
Speedup – Domain Decomposition



Multithreading

- Modern Parallel systems often contain 12–16 (or more) on-node cores connected via low-latency network.
- On-node multithreading allows an additional parallel mechanism that can extend scalability in certain circumstances.
- `libMesh` provides a clean interface to Intel®'s Threading Building Blocks (TBB) which is we have access to.
- TBB is a C++ template library consisting of
  - Algorithms
  - Containers
  - Mutexes
  - Timing routines
  - Memory allocators

  designed to help avoid low-level use of platform-specific (e.g. `pthread`) implementations.

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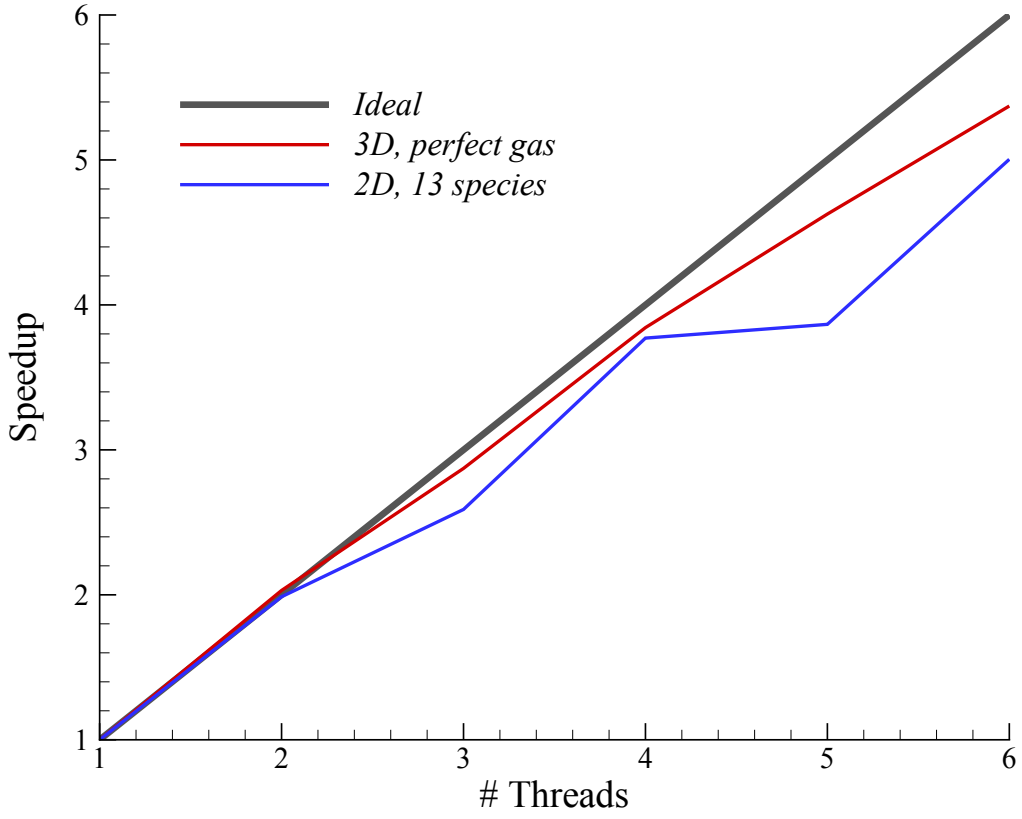
Intel®'s Threading Building Blocks

- Requires more work than OpenMP but
  - Has better type-safety
  - Easier to reuse code
  - More natural for use with C++
- Once a standard `for` loop is selected for parallelization its components are abstracted as C++ `Range` and `Body` objects
- In FIN-S we parallelize matrix assembly, primitive variable computation, and other operations in this way.
  - Some operations perfectly asynchronous – e.g. computing primitive variables.
  - Other operations require locking shared objects – e.g. inserting local contributions to a global matrix.
  - Special care needed when interfacing with 3rd party libraries.

Speedup – Multithreading



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1 Background & Motivation
- Problem Class
- Reacting Flows
- Surface Ablation

2 Physical Modeling
- Governing Equations
- Thermochemistry
- Quasi-Steady Ablation

3 Finite Element Formulation

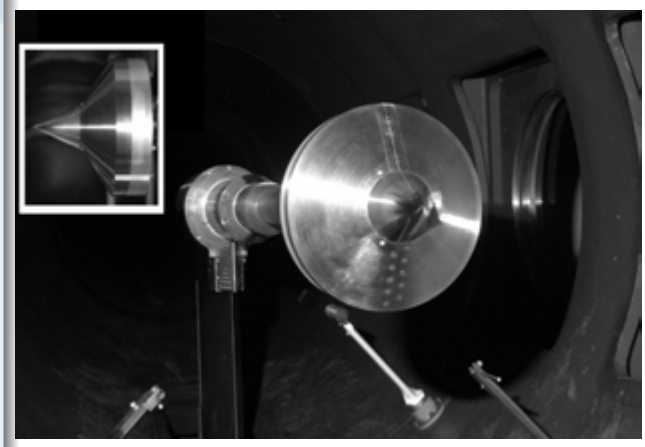
4 Fully-Implicit Navier-Stokes (FIN-S) Overview
- Verification
- Parallelism

5 Results
- Perfect Gas Flow over a Double Cone
- Viscous Thermal Equilibrium Chemical Reacting Flow
- Viscous Reacting Flow with Quasi-Steady Surface Ablation
- Modeling Arcjet Flows

6 Ongoing Challenges

Background – AEDC Sharp Double Cone

- A sharp 25°–55° double cone was tested in N_2 at CUBRC.
- It was discovered that freestream vibrational nonequilibrium must be properly modeled for CFD to match experiment (Nompelis & Candler).
- The AEDC Hypervelocity Wind Tunnel No. 9 also uses N_2 as its test gas.
- A series of tests were conducted at AEDC using the same model to investigate the presence of vibrational nonequilibrium in the freestream.



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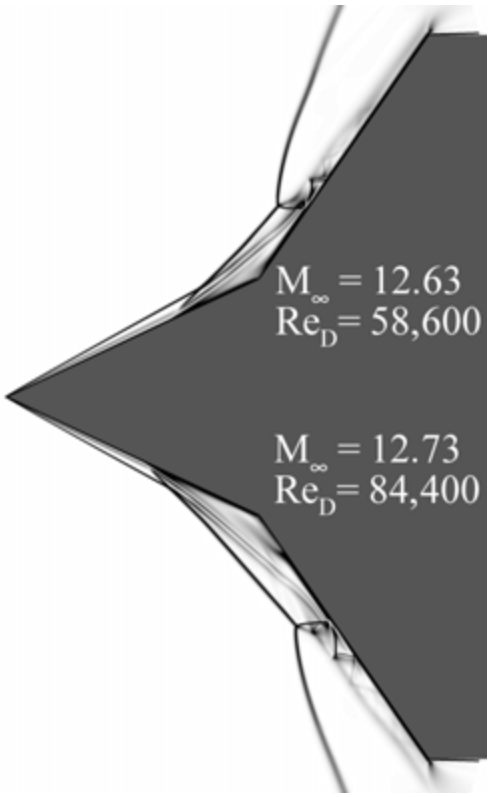
Observations

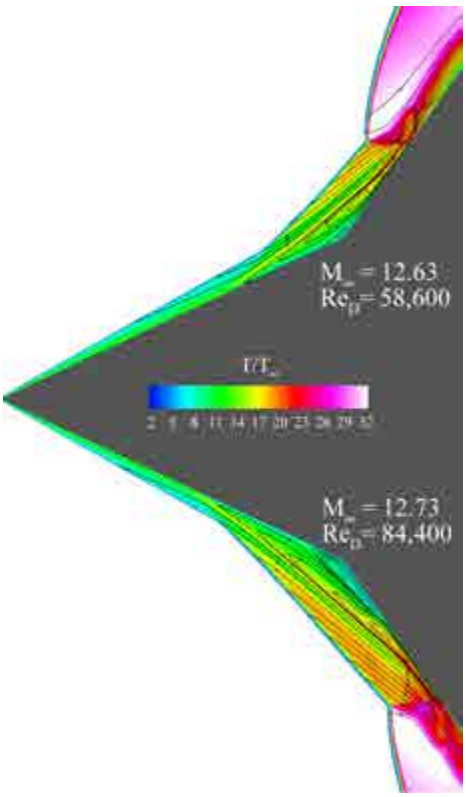
- Four Reynolds numbers were tested in the nominally Mach 14 nozzle.

Run	2890	2891	2893	2894	
M_∞	13.6	13.17	12.73	12.63	
Re_D	1.12×10^6	4.11×10^5	8.44×10^4	5.86×10^4	
ρ_∞	7.81×10^{-3}	2.96×10^{-3}	5.90×10^{-4}	3.98×10^{-4}	kg/m^3
U_∞	2006.6	1949.8	1763.5	1682.6	m/sec
T_∞	52.3	52.7	46.1	42.7	K

- No appreciable vibrational nonequilibrium effects observed.
- Highly unsteady flow observed for *all* Reynolds numbers tested.
- For a uniform freestream, CFD predicts steady flow for the two lowest Reynolds numbers.

Steady states, runs 2893 and 2894





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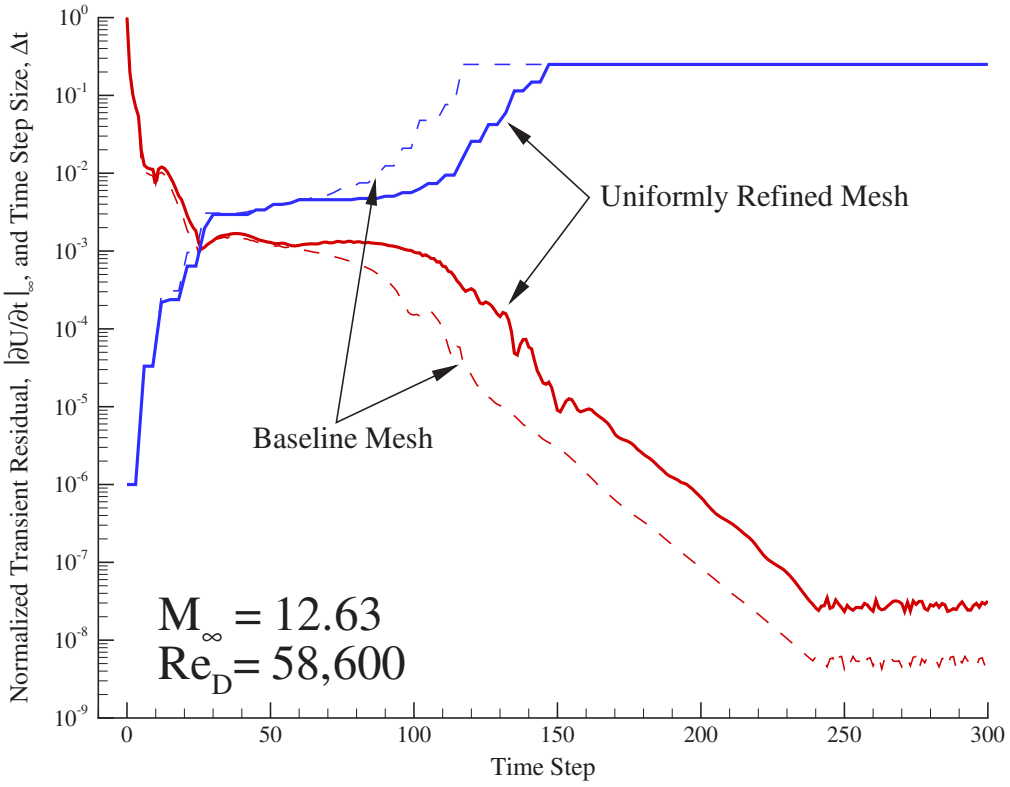
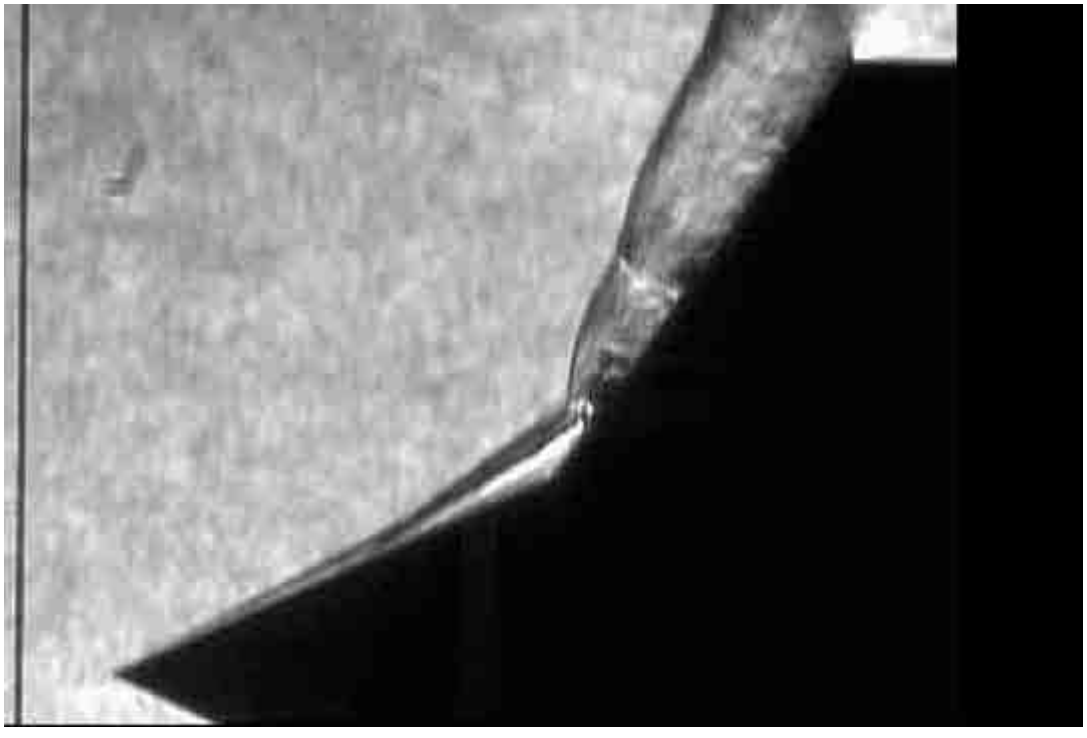
Time Convergence, run 2894



High speed schlieren, run 2890



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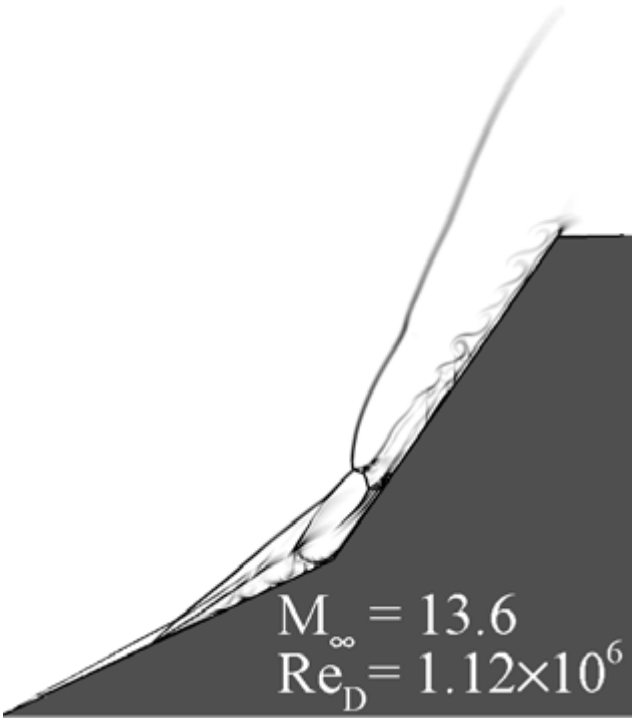
Computed schlieren, run 2890



Possible Mechanism for Observed Unsteadiness

- For a uniform inflow, CFD converges to a steady–state for the two lowest Reynolds numbers tested.
- This is in contrast to the experimental results.
- My conjecture is that freestream noise drives the unsteady behavior at these low Reynolds number.
- Remaining analysis is focused on testing this theory.

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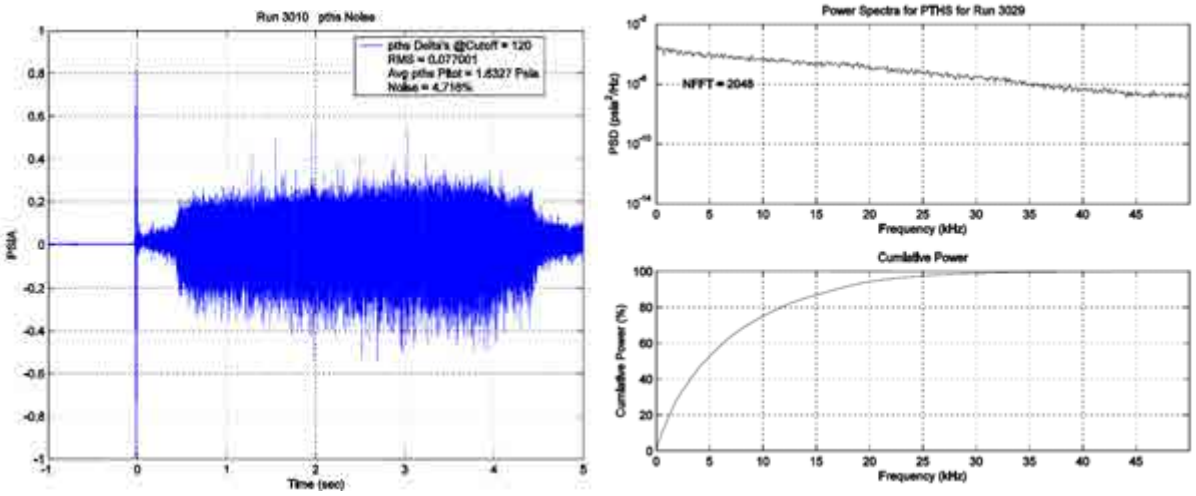
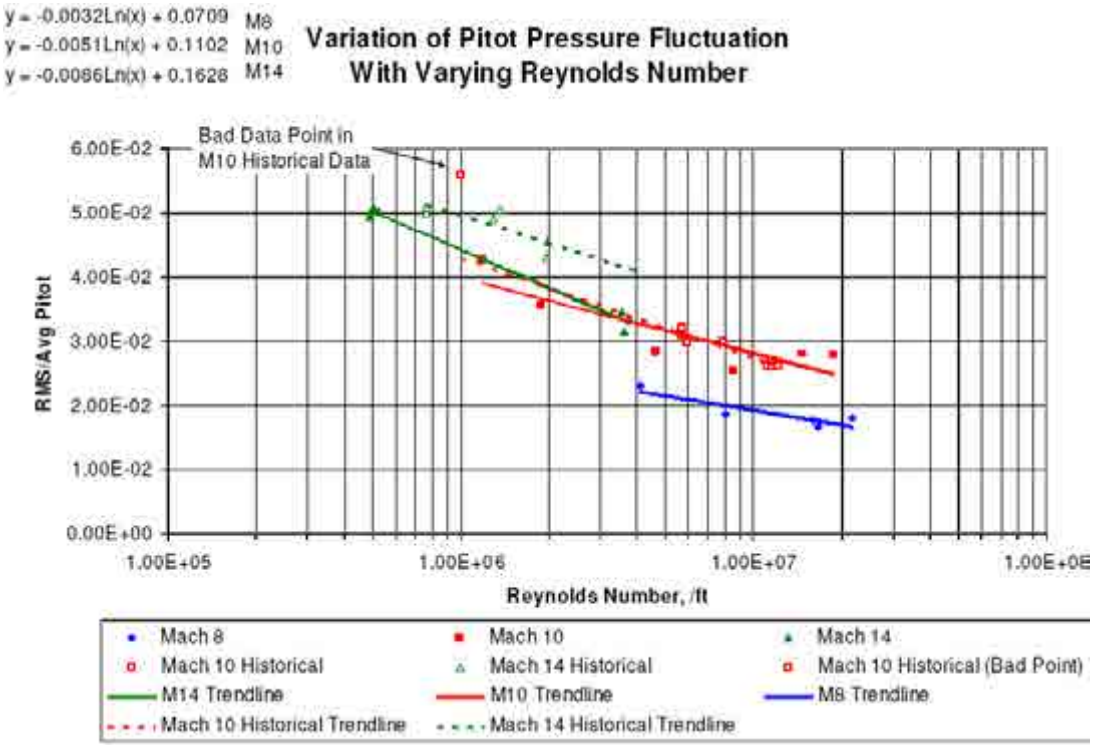
Noise Characterization



Noise Characterization



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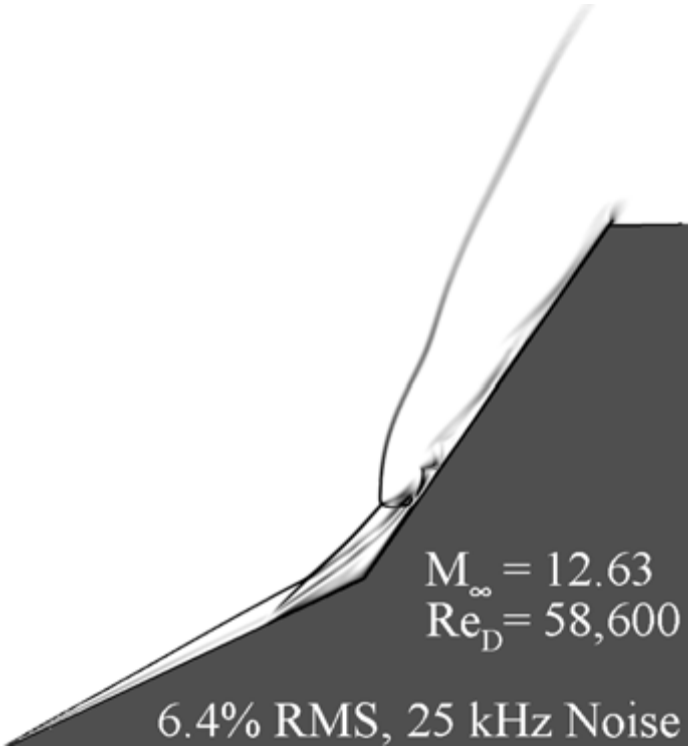
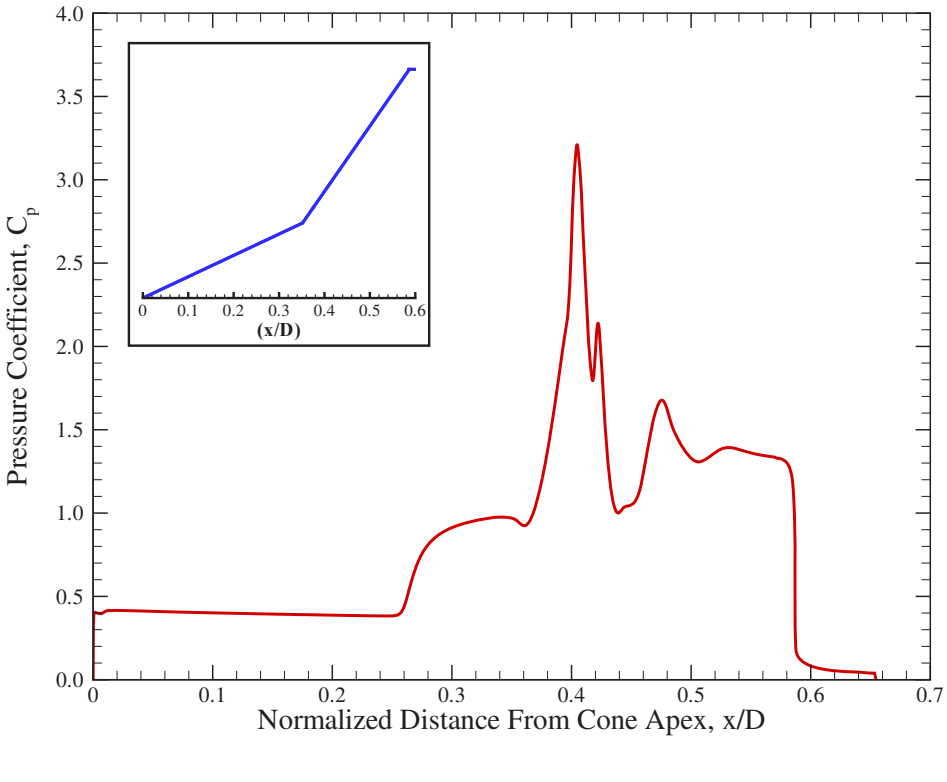
Results – Flowfield



Results – Surface Pressure



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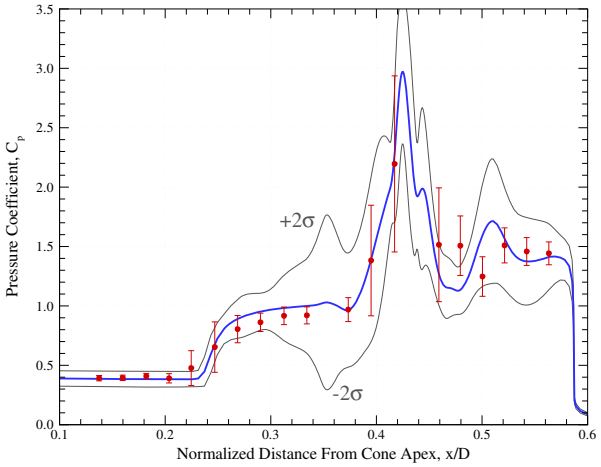
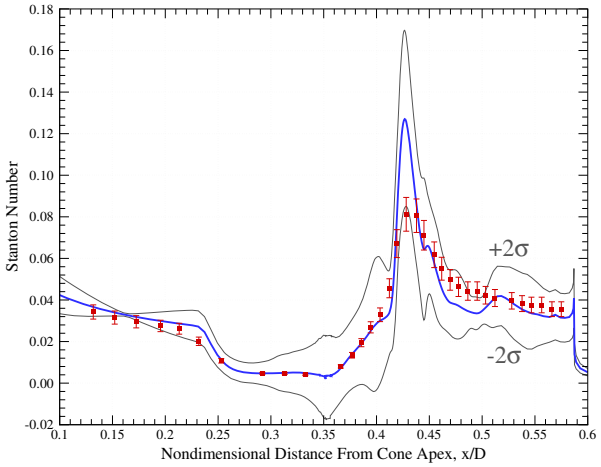
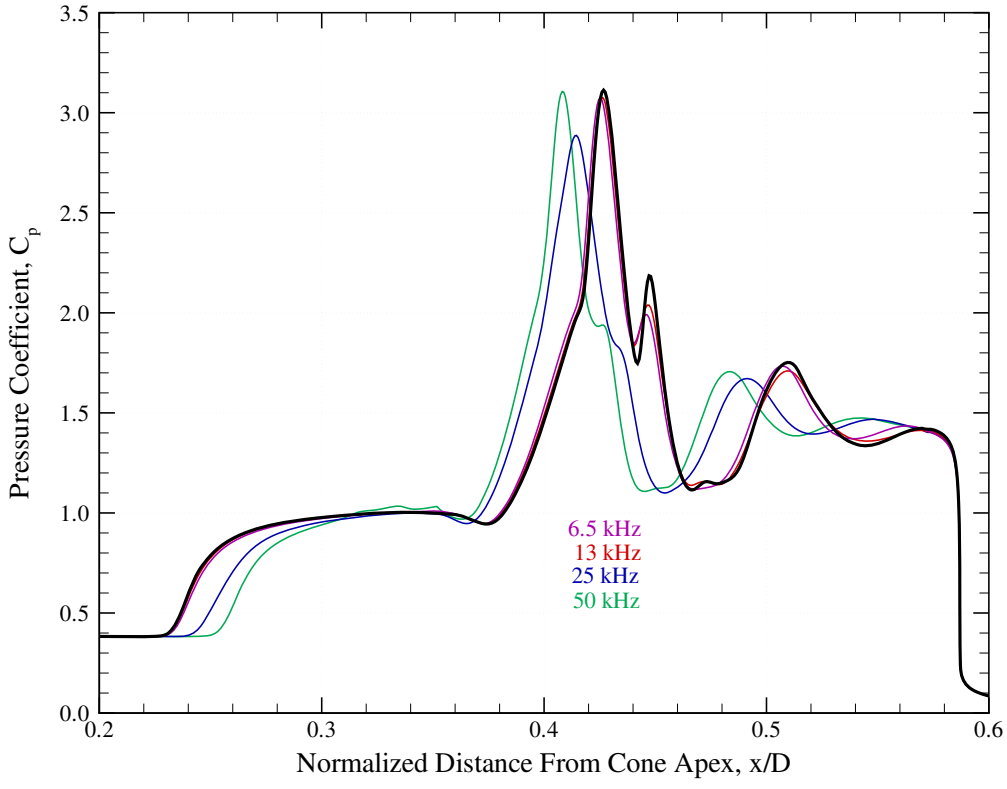
25 kHz, 6% RMS Pitot Pressure Fluctuation





Frequency Influence



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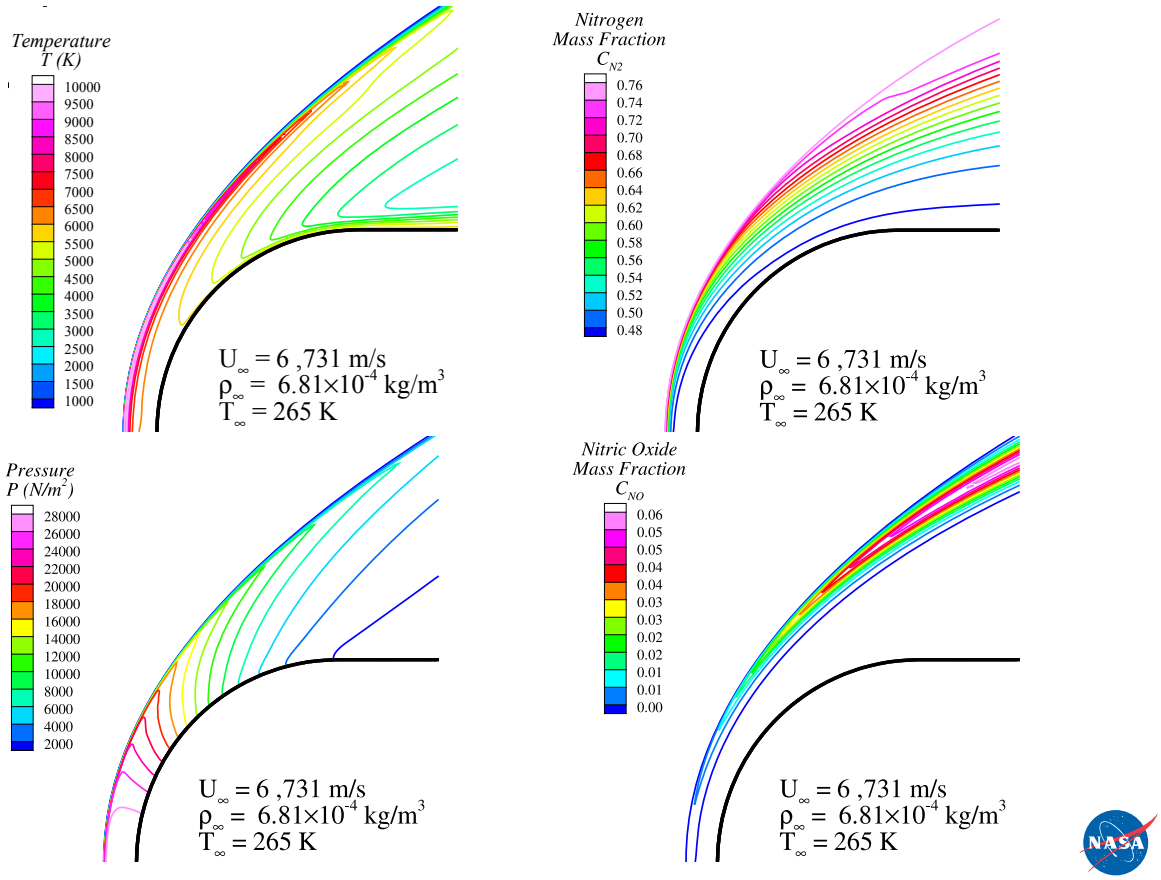
2D Extended Cylinder

- Laminar flow in thermal equilibrium
- Chemical nonequilibrium, 5 species air (N_2, O_2, NO, N, O)
- 5 reaction model with Park 1990 rates

$$cN_{2,\infty} = 0.78, cO_{2,\infty} = 0.22$$
$$U_\infty = 6,731\ \mathrm{m/sec}$$
$$\rho_\infty = 6.81 \times 10^{-4}\ \mathrm{kg/m^3}$$
$$T_\infty = 265\ \mathrm{K}$$

- Blottner/Wilke/Eucken with constant Lewis number $Le = 1.4$ for transport properties
- Mesh, iterative convergence
- FIN-S/DPLR comparison



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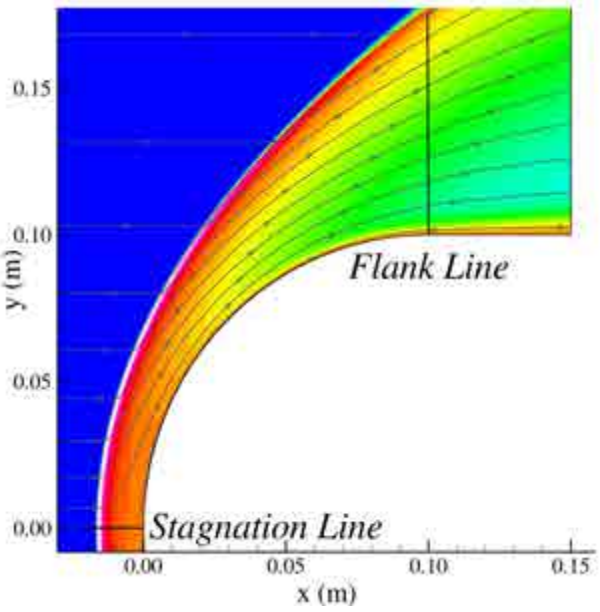
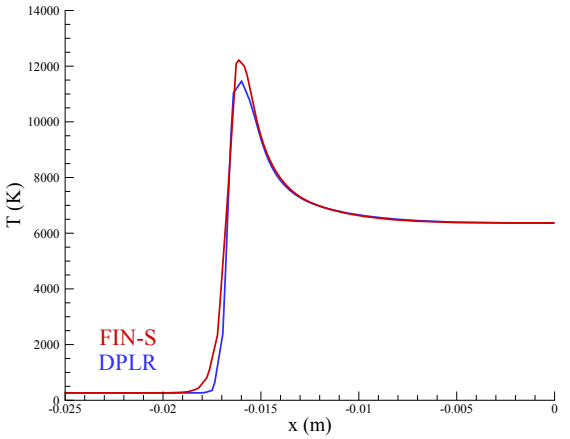
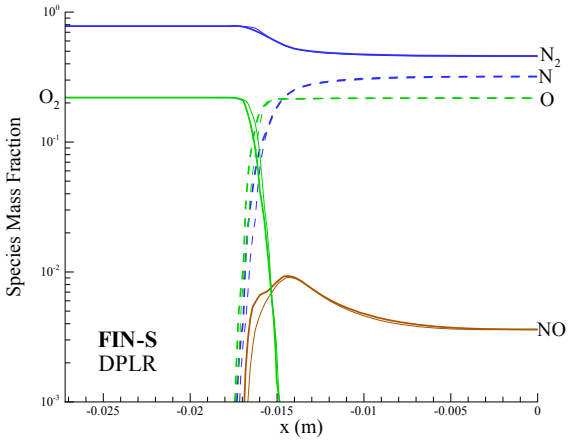
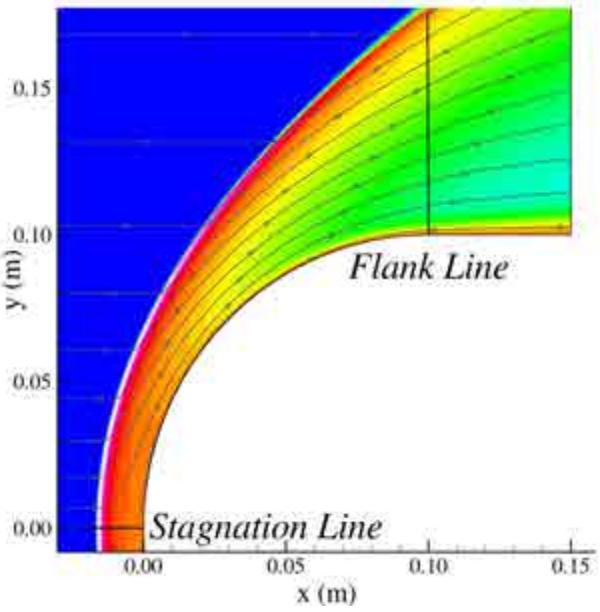
Code-to-Code Comparison – Stagnation Line

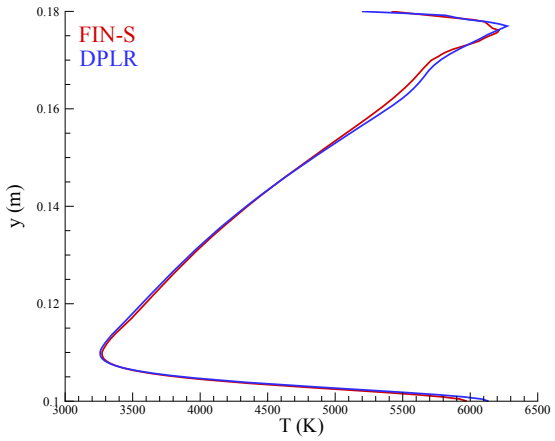


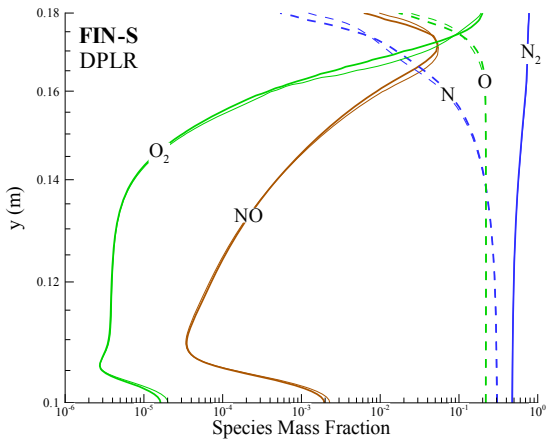




Code-to-Code Comparison – Flank Line







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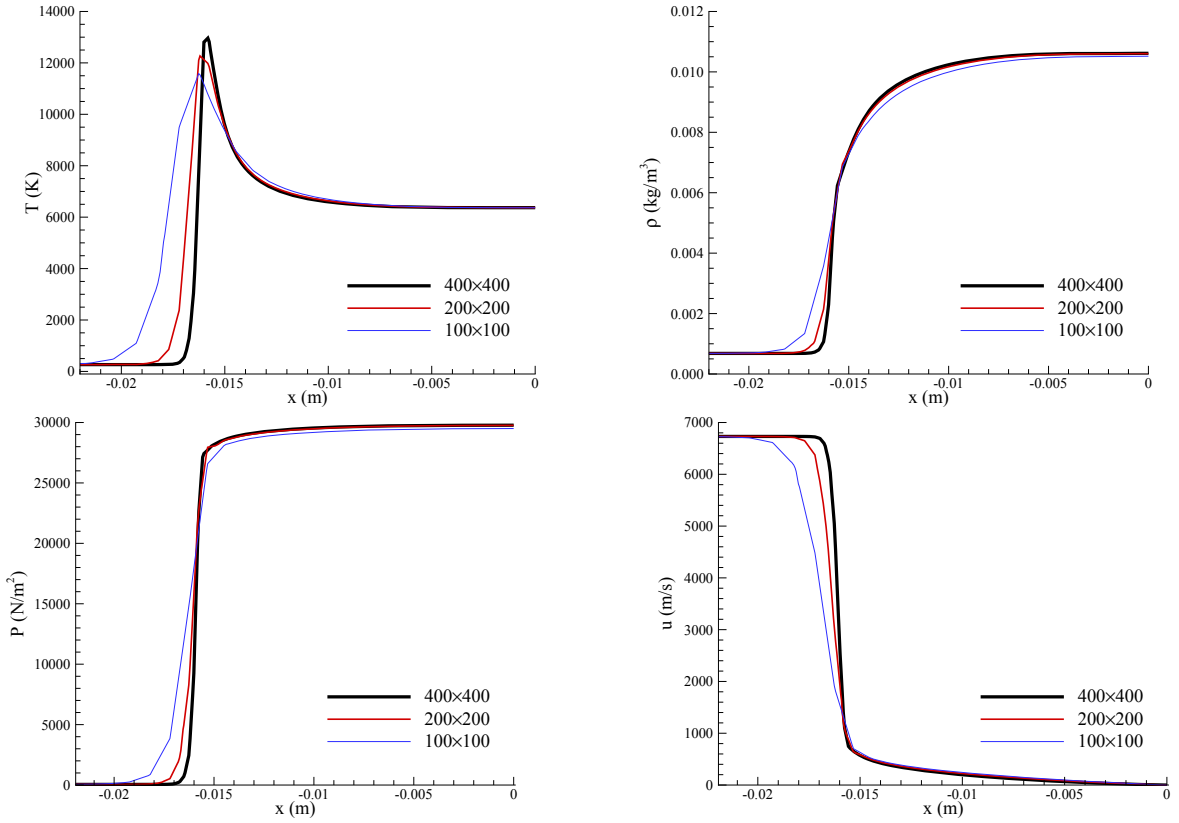
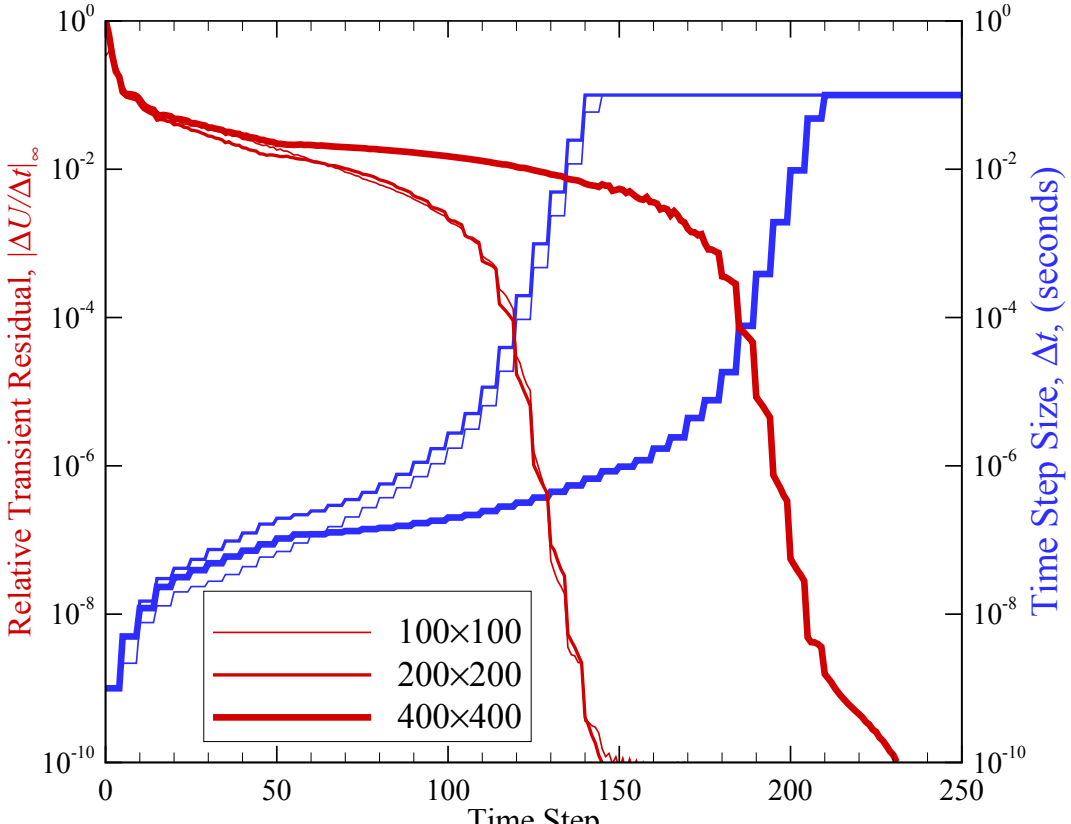
Mesh Convergence



Iterative Convergence



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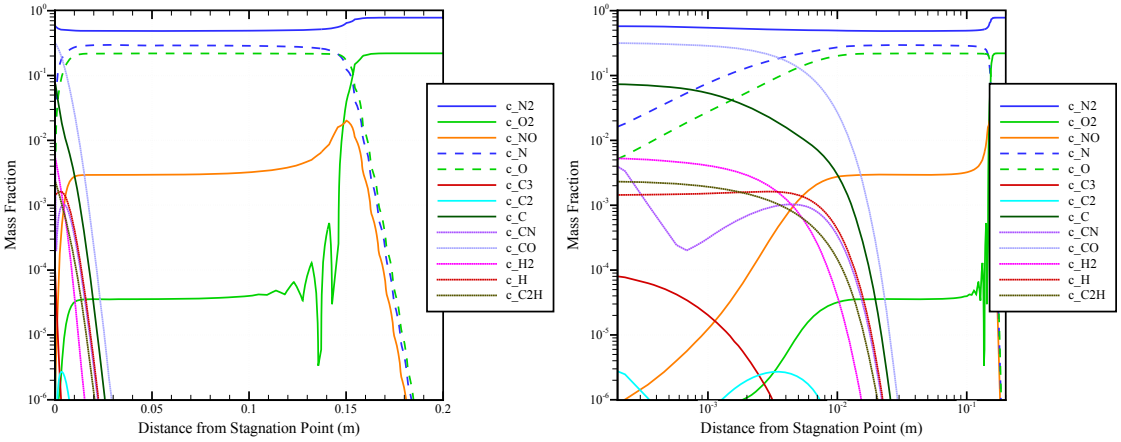
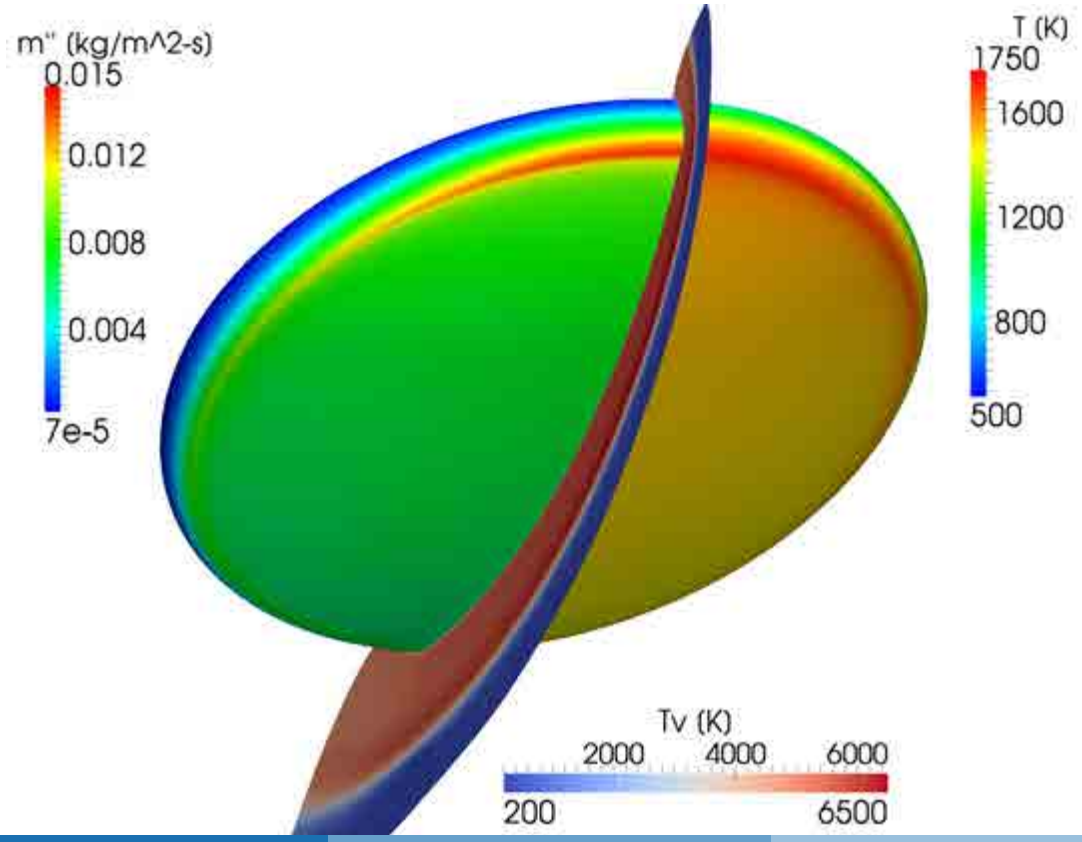
Ablating Boundary Experiments



- Turbulent flow in thermochemical nonequilibrium, 13 species air (N_2, O_2, NO, N, O, C_3, C_2, C, CN, CO, H_2, H, C_2H), 18 reaction model with Park 2001 rates
- 5 Meter-scale domain, millimeter-scale chemical boundary layer

Ablating Boundary Experiments



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Arcjet Flowfields

Motivation

- Arcjets are uniquely suited to perform high enthalpy, long duration material response testing.
- Modern computational techniques are required to adequately characterize the freestream properties.
- Analysis complicated by multitude of scales, physical phenomenon:
  - Very low speed, high pressure plenum,
  - very high speed, low pressure nozzle exit,
  - highly nonequilibrium flow about test specimen.
- Adequately treating these phenomenon simultaneously is challenging for numerical methods.

Arcjet Flowfields

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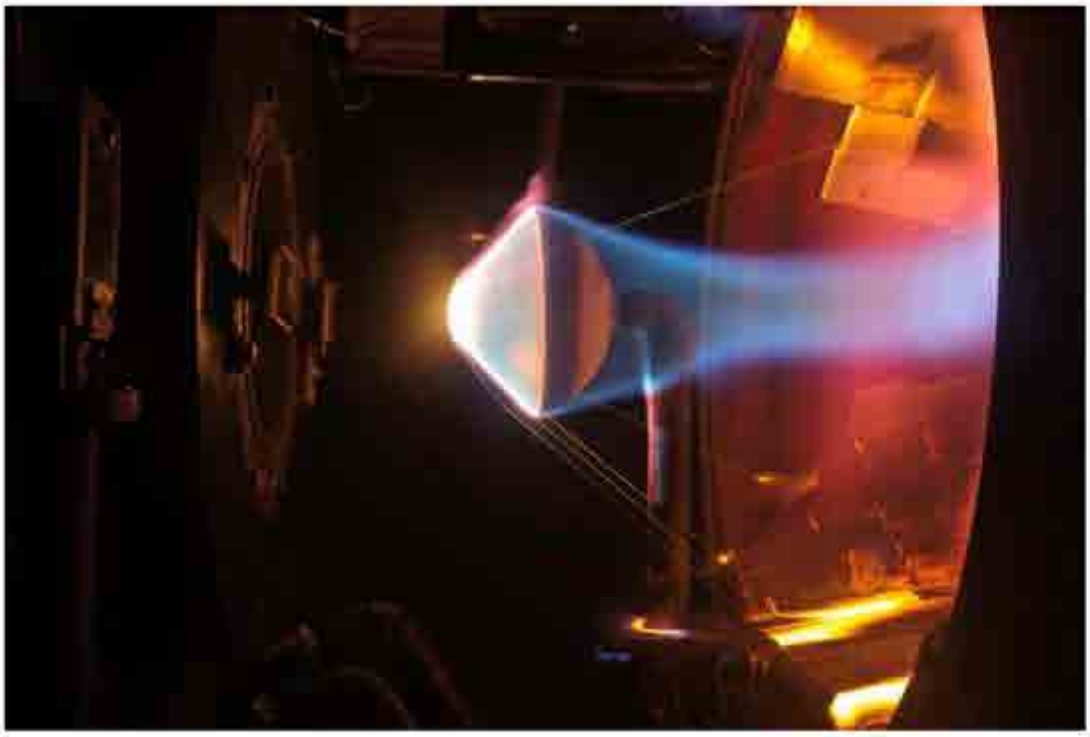
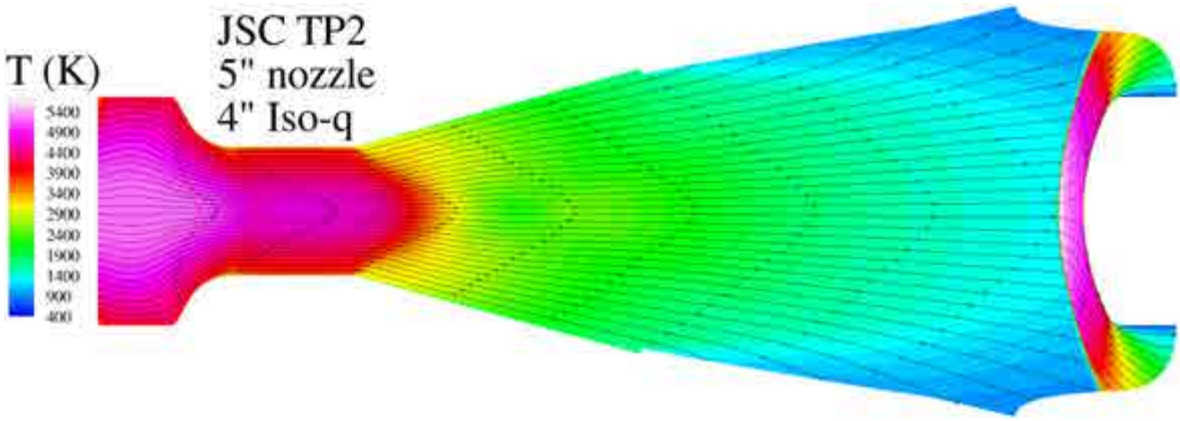
Arcjet Flowfields



Arcjet Flowfields



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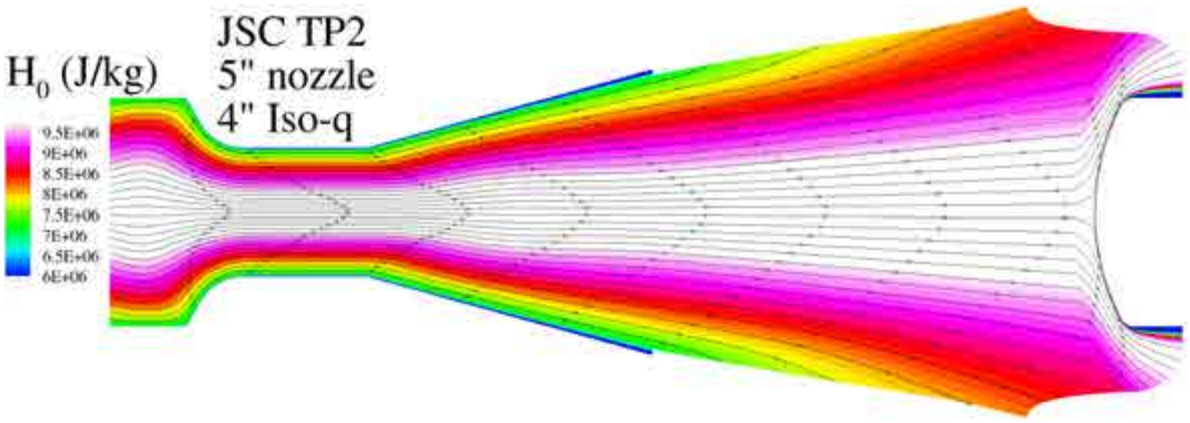

Arcjet Simulations – Enabling Boundary Conditions

Implicit, Characteristic Boundary Conditions for Thermochemical Nonequilibrium Flows

Consider the transformation from conserved variables to characteristic variables:

$$\delta\hat{\boldsymbol{U}} = \frac{\partial\hat{\boldsymbol{U}}}{\partial\boldsymbol{U}}\delta\boldsymbol{U} = \boldsymbol{M}^{-1}\delta\boldsymbol{U}$$

where $\delta\boldsymbol{U}$ is a pertubation in the conserved variables, $\delta\hat{\boldsymbol{U}}$ is a pertubation in the conserved variables, and $\boldsymbol{M}^{-1}$ is the transformation matrix given by the left eigenvectors from the inviscid flux Eigendecomposition for a specified flux direction.

We will manipulate this statement such that outgoing/incoming characteristic variables are unchanged at inflow/outflow boundaries, respectively.

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Arcjet Simulations – Enabling Boundary Conditions

Characteristic boundary conditions for reservoir-type boundaries.

Given: H_0, $\{c_s\}$, $\dot{m}_A$, $\hat{\boldsymbol{v}}$, and $\boldsymbol{U}_B$.

Let $\boldsymbol{U} = \boldsymbol{U}_B$ serve as an initial guess.
do
  Form the transformation matrix $\boldsymbol{M}^{-1} = \boldsymbol{M}^{-1}(\boldsymbol{U})$
  Define the outgoing conserved variable increment $\delta\boldsymbol{U}^+ = \boldsymbol{U} - \boldsymbol{U}_B$
  Compute the outgoing characteristics increment $\delta\hat{\boldsymbol{U}}^+ = \boldsymbol{M}^{-1}\delta\boldsymbol{U}^+$
  Define the unconstrained residual $\boldsymbol{r} = -\delta\hat{\boldsymbol{U}}$
  For each incoming characteristic, replace a row of $\boldsymbol{M}^{-1}$ and $\boldsymbol{r}$ with a
  linearized constraint derived from the reservoir conditions.
  Solve for the increment $\boldsymbol{M}^{-1}\delta\boldsymbol{U} \equiv -\boldsymbol{r} = -\delta\hat{\boldsymbol{U}}$
  Update the iterate $\boldsymbol{U} \leftarrow \boldsymbol{U} + \delta\boldsymbol{U}$
while $\|\delta\boldsymbol{U}\|_\infty > \varepsilon_{it}$
Compute $\boldsymbol{F} = \boldsymbol{F}(\boldsymbol{U})$ as the inviscid flux on the outflow boundary in the weak statement.

Arcjet Simulations – Enabling Boundary Conditions

Characteristic boundary conditions for vacuum-type boundaries.

Given: $\boldsymbol{U}_B$ and $P_{back} = \{\text{vacuum fraction}\} \times P_{exit}$.

Let $\boldsymbol{U} = \boldsymbol{U}_B$ serve as an initial guess.
do
  Form the transformation matrix $\boldsymbol{M}^{-1} = \boldsymbol{M}^{-1}(\boldsymbol{U})$
  Define the outgoing conserved variable increment $\delta\boldsymbol{U}^+ = \boldsymbol{U} - \boldsymbol{U}_B$
  Compute the outgoing characteristics increment $\delta\hat{\boldsymbol{U}}^+ = \boldsymbol{M}^{-1}\delta\boldsymbol{U}^+$
  Define the unconstrained residual $\boldsymbol{r} = -\delta\hat{\boldsymbol{U}}$
  For the single incoming characteristic, replace the row of $\boldsymbol{M}^{-1}$ and $\boldsymbol{r}$ with a
  linearized constraint derived from the back pressure condition.
  Solve for the increment $\boldsymbol{M}^{-1}\delta\boldsymbol{U} \equiv -\boldsymbol{r} = -\delta\hat{\boldsymbol{U}}$
  Update the iterate $\boldsymbol{U} \leftarrow \boldsymbol{U} + \delta\boldsymbol{U}$
while $\|\delta\boldsymbol{U}\|_\infty > \varepsilon_{it}$
Compute $\boldsymbol{F} = \boldsymbol{F}(\boldsymbol{U})$ as the inviscid flux on the inflow boundary in the weak statement.

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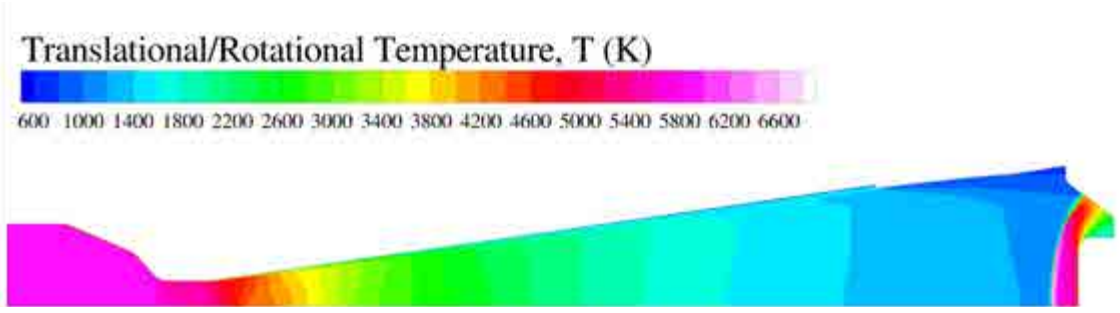
Arcjet Flowfields – NASA Ames AHF, 7in Nozzle

Arcjet Flowfields – NASA Ames AHF, 7in Nozzle



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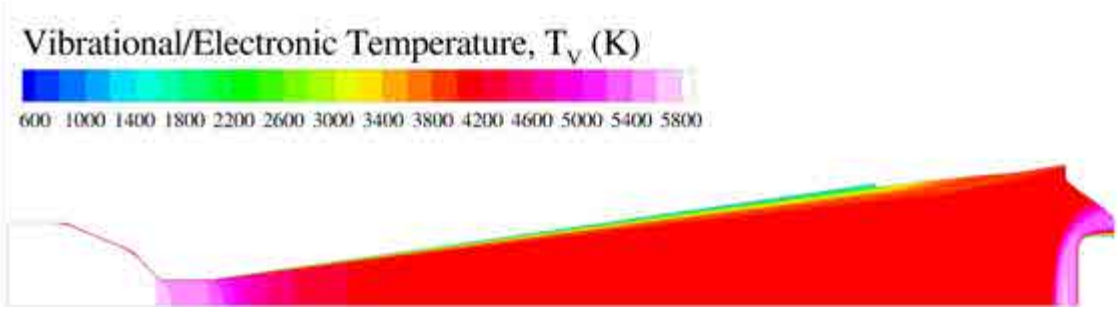
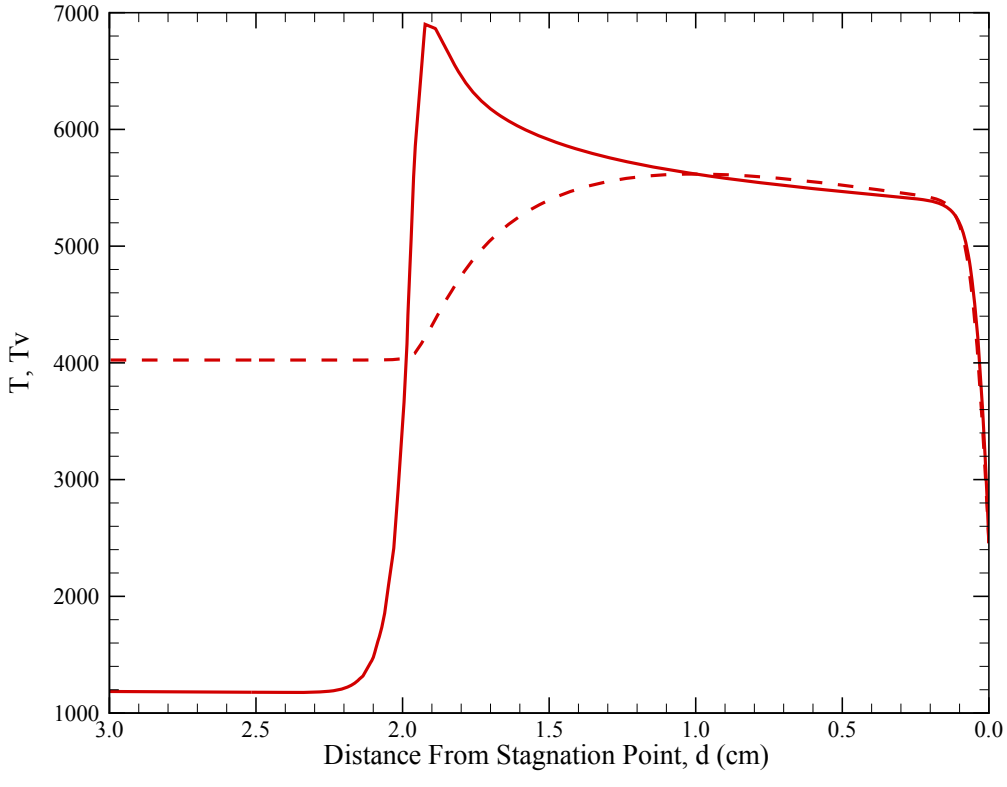
Arcjet Flowfields – NASA Ames AHF, 7in Nozzle



Arcjet Flowfields – NASA Ames AHF, 7in Nozzle



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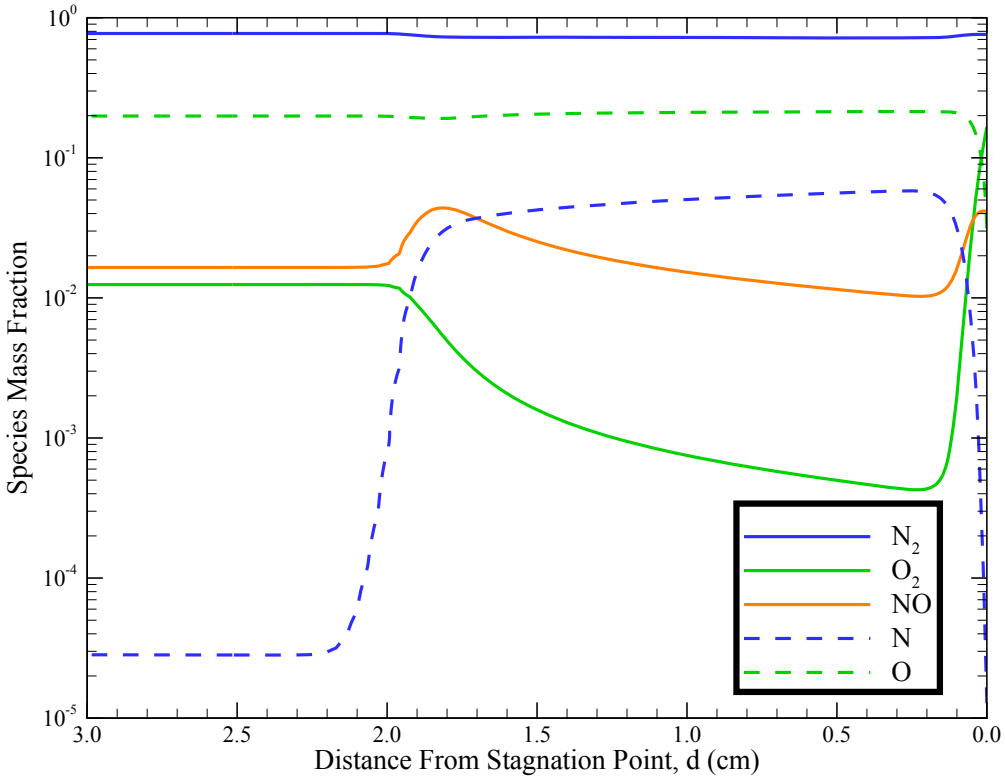
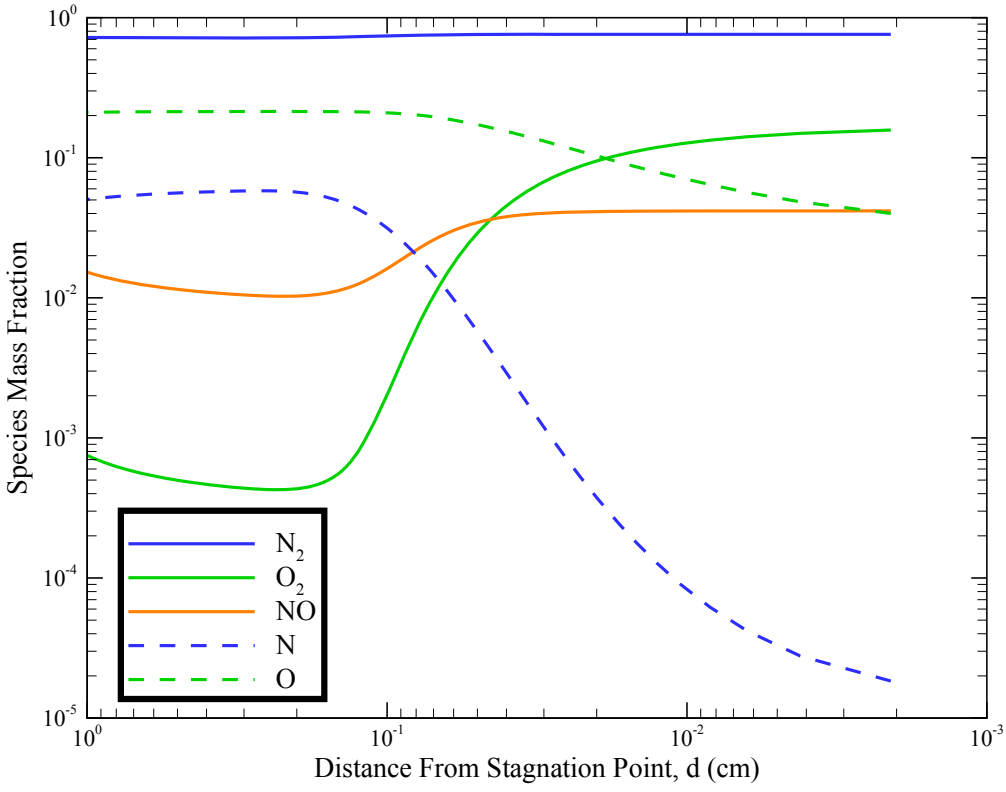
Arcjet Flowfields – NASA Ames AHF, 7in Nozzle



Results | Modeling Arcjet Flows

Arcjet Flowfields – NASA Ames AHF, 7in Nozzle



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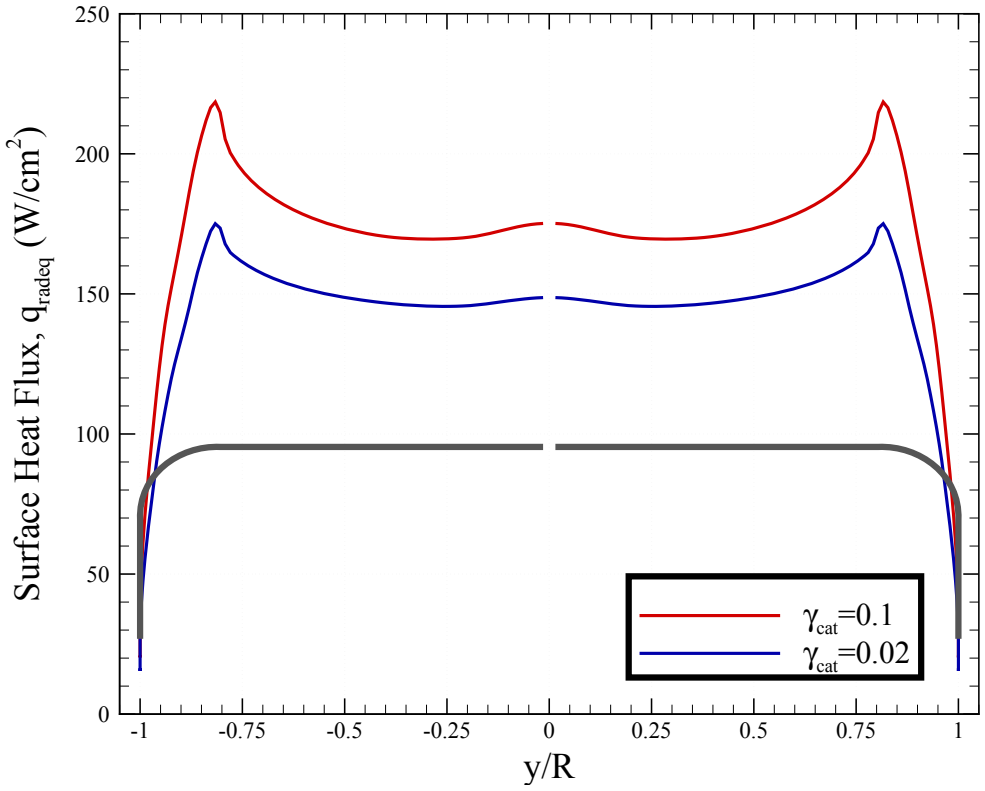
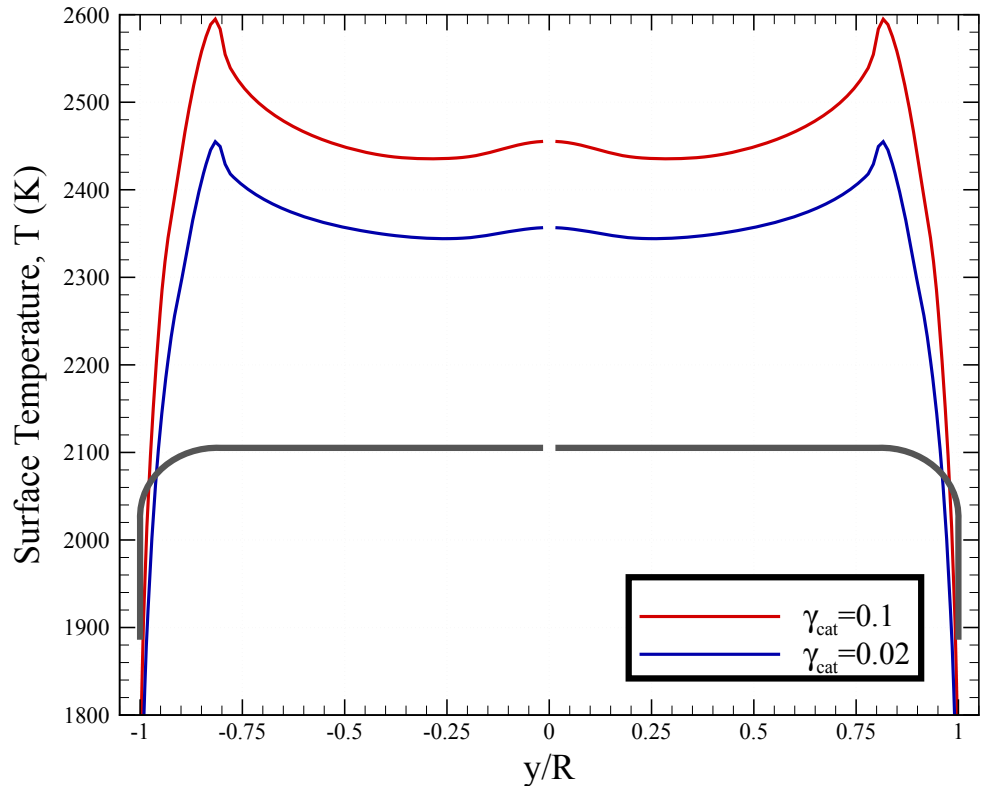
Arcjet Flowfields – NASA Ames AHF, 7in Nozzle



Arcjet Flowfields – NASA Ames AHF, 7in Nozzle



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1 Background & Motivation
- Problem Class
- Reacting Flows
- Surface Ablation

2 Physical Modeling
- Governing Equations
- Thermochemistry
- Quasi-Steady Ablation

3 Finite Element Formulation

4 Fully-Implicit Navier-Stokes (FIN-S) Overview
- Verification
- Parallelism

5 Results
- Perfect Gas Flow over a Double Cone
- Viscous Thermal Equilibrium Chemical Reacting Flow
- Viscous Reacting Flow with Quasi-Steady Surface Ablation
- Modeling Arcjet Flows

6 Ongoing Challenges

Full Disclosure

Opportunities for Further Enhancement

1. **Linear Solver Strategy:** Preconditioned GMRES is highly effective but potentially overkill for early, highly nonlinear transients. Mixed implicit/explicit schemes may provide a fast alternative.
2. **Improved Shock Capturing:** Robust shock capturing is still a challenge. Current scheme is fragile on bad meshes, and often convergence stalls.

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Additional Focus Areas

1. Physics Modeling
   - Weakly Ionized Flows
   - Additional turbulence models
   - Fully coupled radiative transport
2. Unsteady ablation coupling
3. Adjoints
   - Sensitivity analysis
   - Adaptivity

Thank you!

Questions?

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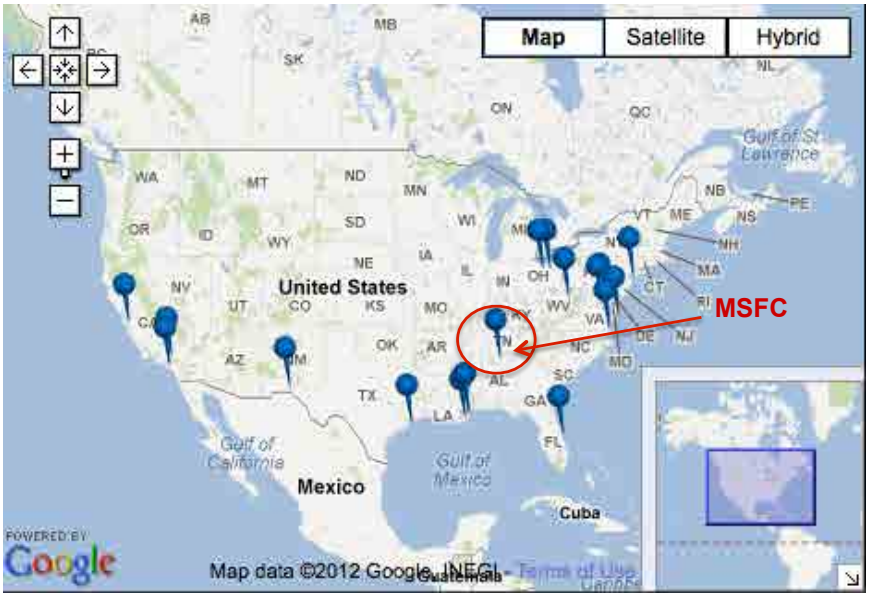
The Direction of Fluid Dynamics for Liquid Propulsion at NASA Marshall Space Flight Center

Presented by Lisa W. Griffin
Chief, Fluid Dynamics Branch – ER42
NASA Marshall Space Flight Center
Lisa.W.Griffin@nasa.gov

Advances in Rocket Engine Modeling and Simulation, and its Future
Tokyo, Japan
September 26 – 27, 2012

NASA MARSHALL SPACE FLIGHT CENTER

Marshall Space Flight Center (MSFC) is one of ten NASA field centers. MSFC supports the Agency goals of lifting from Earth, living and working in space, and understanding our world and beyond by providing propulsion, space transportation, space systems, and scientific research.



MSFC is the NASA-designated center for the development of space launch systems. The center is particularly well-known for propulsion system development

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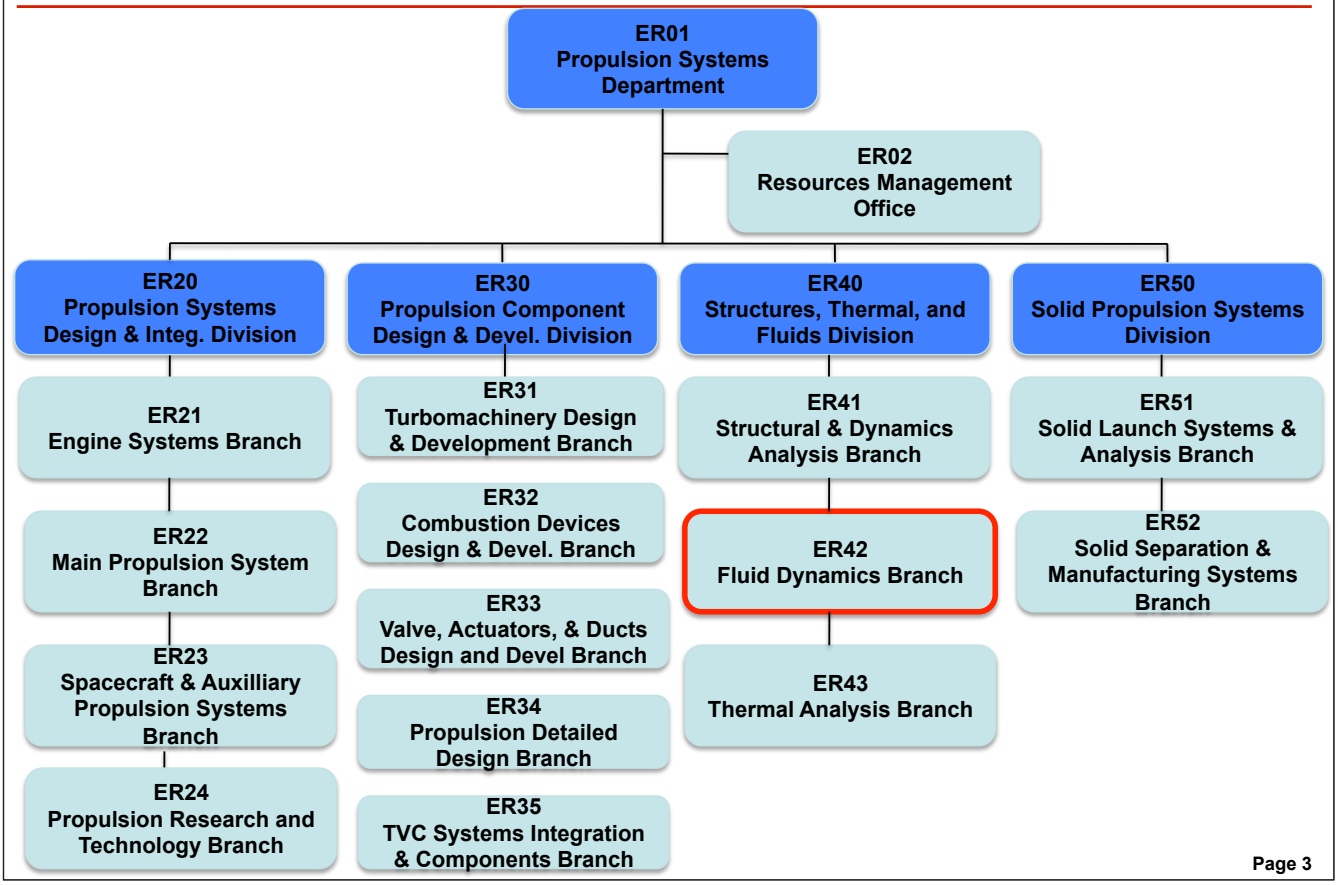
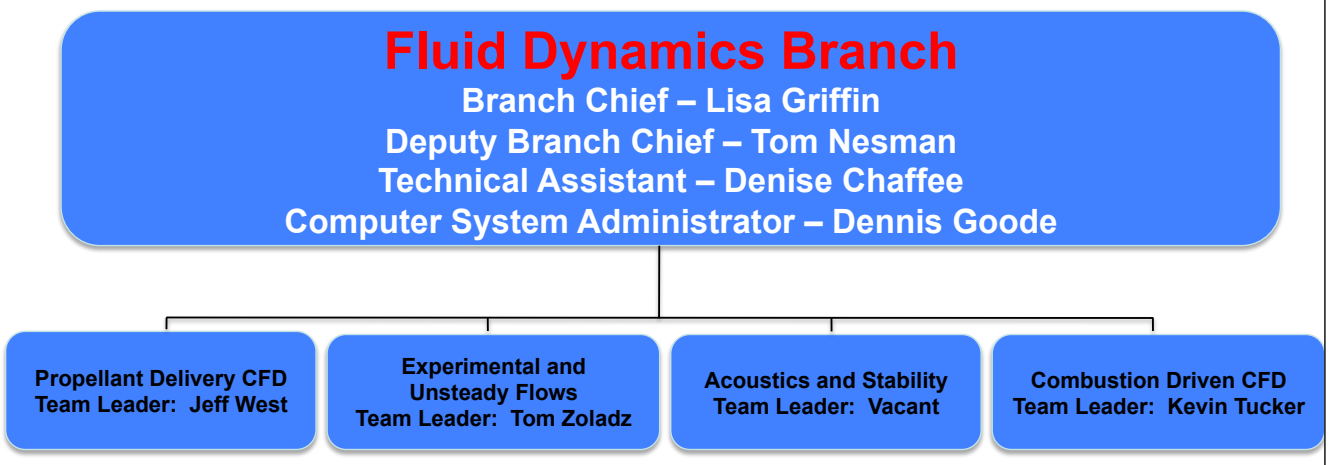
PROPULSION SYSTEMS DEPARTMENT



Page 3

FLUID DYNAMIC BRANCH STRUCTURE



ER42 is comprised of four teams of approximately forty-five employees

Page 4

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FLUID DYNAMICS BRANCH APPLICATIONS

The Fluid Dynamics Branch (ER42) is responsible for all aspects of the discipline of fluid dynamics applied to propulsion or propulsion-induced loads and environments. This work begins with design trades and parametric studies, and continues through development, risk assessment, anomaly investigation and resolution, and failure investigations. Because of the skills in the branch, ER42 also works non-propulsion items such as for telescopes and payload racks on an as needed basis.

Main Propulsion System	Turbopumps	Liquid Combustion Devices	Solid Rocket Motors
• Tank Dynamics • Cryofluid Management • Feedline Flow Dynamics • Valve Flow and Dynamics	• Pump Dynamics • Turbine Dynamics	• Injection Dynamics • Chamber Acoustics • Combustion Stability • Nozzle Dynamics	• Motor Dynamics • Nozzle Dynamics • Combustion Stability

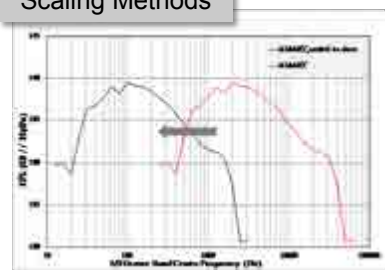
Coupled Systems	Launch, Separation, and Plume-Induced Environments and Debris
• Feed System Dynamics • Coupled Pump/MPS Dynamics, e,g,, Pogo • Thrust Oscillations and its Impact on the Vehicle •Tank Slosh and its Impact on Vehicle Stability and GN&C	• Liftoff Acoustics • Separation Acoustics • Overpressure • Inflight Plume Generated Noise • Noise Mitigation • Hydrogen Entrapment • Liftoff Debris Transport

ER42 is a Discipline-Centric branch, not analysis-centric or test-centric. Integration of all discipline methods into one branch enables efficient and accurate support to the projects.

Page 5

FLUID DYNAMICS ANALYSIS

Scaling Methods



ER42 conducts all levels of fluid dynamics analysis from scaling methods through 3D Unsteady CFD

Lump Parameter Modeling

$$P_1 = P_2; \frac{dP}{dt} = \frac{m_1 - m_2}{C_N}$$

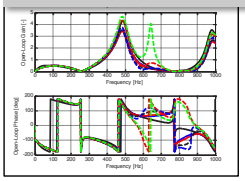
$$\dot{m}_2 = \dot{m}_3; \frac{d\dot{m}}{dt} = \frac{P_2 - R_N \dot{m} - P_3}{L_N}$$

$$x(\omega) = \frac{\bar{X}\sin\left(\omega(\bar{\tau}_{T,o} - \bar{\tau}_{T,f})\right)}{\sin(\omega\bar{\tau}_{T,f}) + \theta_g\omega\cos(\omega\bar{\tau}_{T,f})}$$

$$y(\omega) = \omega$$

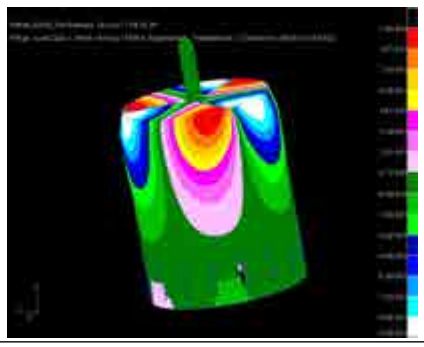
$$z(\omega) = \frac{\bar{F}\sin\left(\omega(\bar{\tau}_{T,f} - \bar{\tau}_{T,o})\right)}{\sin(\omega\bar{\tau}_{T,o}) + \theta_g\omega\cos(\omega\bar{\tau}_{T,o})}$$

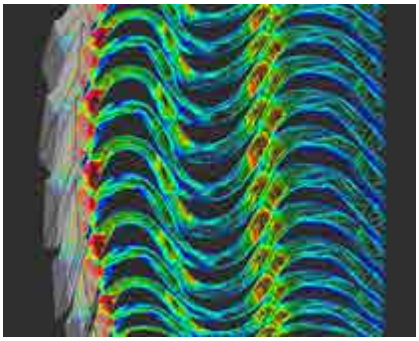
Gain / Phase Plots



System Stability Modeling

Finite Element Modeling





Computational Fluid Dynamics

Page 6

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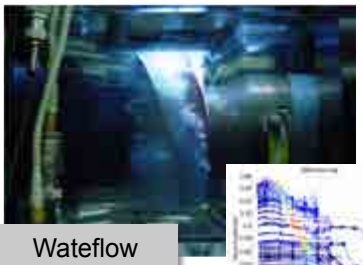
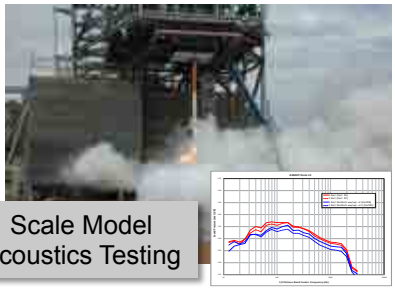
FLUID DYNAMICS TESTING

ER42 conducts and supports testing for hardware and technology development and verification, and analysis validation

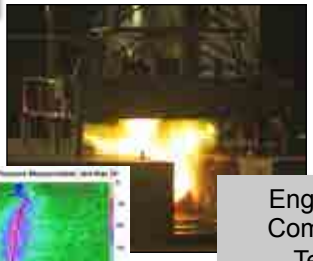
- Primary responsibility for cold flow and scale model acoustics tests
- Secondary responsibility for hot system and component testing



Wateflow Testing in Pump Facility

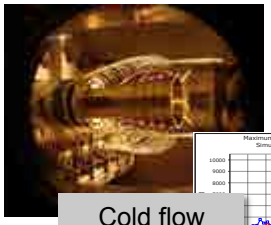


Scale Model Acoustics Testing



Engine and Component Testing

Airflow Testing in Turbine Facility



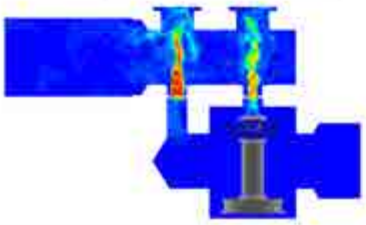
Cold flow testing in Nozzle Test Facility

Solid Rocket Testing

MAIN PROPULSION SYSTEM

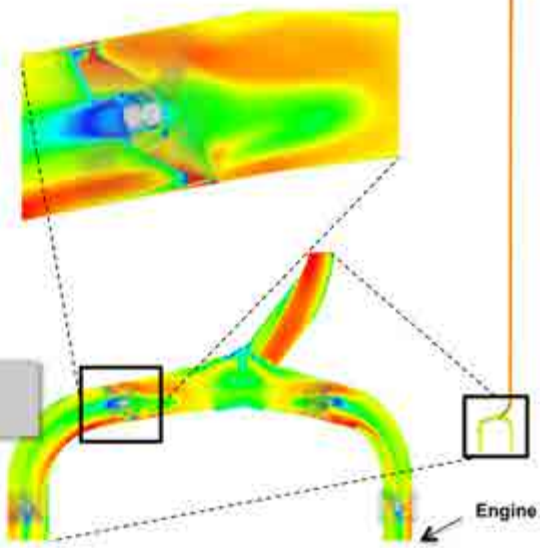
- **The Main Propulsion System (MPS) is defined as the propellant delivery system from Tank to Engine Interface.**
  - Tank with all of its internal components
  - Valves
  - Feedlines with all of its internal components
- **ER42's primary analysis tool for MPS is CFD**

Tank Ullage Pressure Valve



LOX Tank

Articulating Feedline



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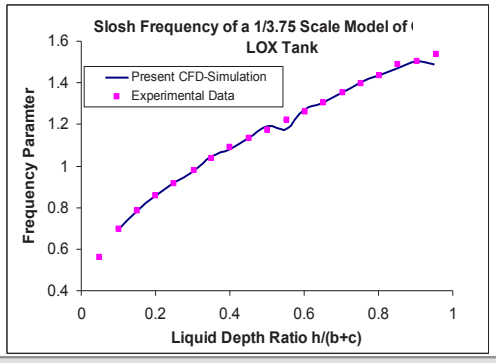
LIQUID PROPELLANT TANKS - SLOSH

ER42 performs high fidelity CFD analysis of complex geometry and/or complex accelerated propellant tank sloshing to determine slosh modes and their respective frequencies, amplitudes, and damping characteristics

Earth to Orbit Simulation



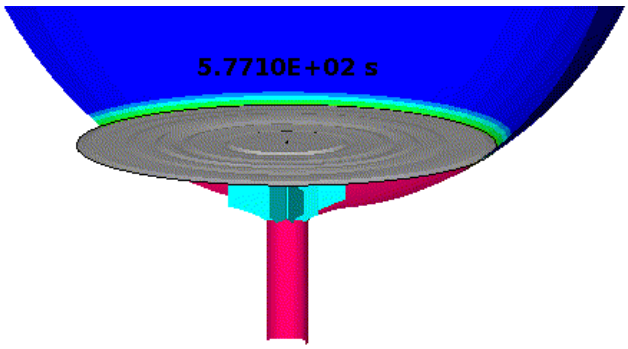
Improvement to Classic Mass-Spring Model

Next challenges with future simulations include implementation of massively parallel gas-liquid interface tracking methods and efficient hybrid implicit/ explicit methods to address disparate time-stepping requirements

Page 9

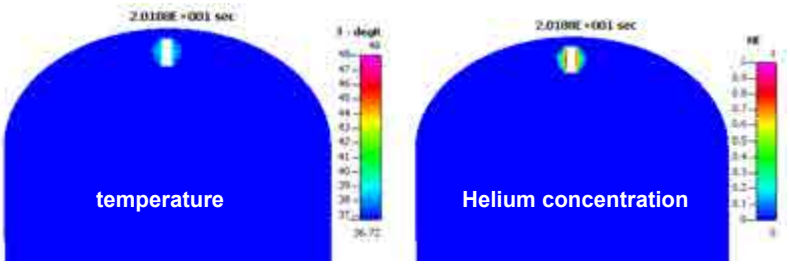
LIQUID PROPELLANT TANKS – PRESSURIZATION AND DRAIN

Assessment of Anti-Vortex Baffle Design



- **Tank Pressurization**
  - Flow through diffuser
  - Interaction of ullage gas with propellant surface (mass transfer, multiphase heat transfer, surface evaporation, chemical species)
- **Tank Drain**
  - Analysis of vortical flow in pipe
  - Assessment of anti-vortex baffle efficiency

- **Near Term Work**
  - Validation of robust method for simulating mass transfer across the gas-liquid interface



LH2 Tank Pre-press Analysis

Page 10

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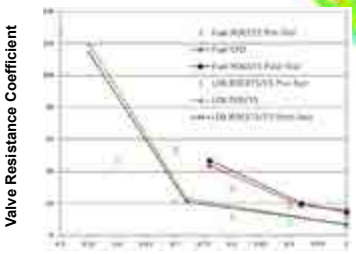
VALVES

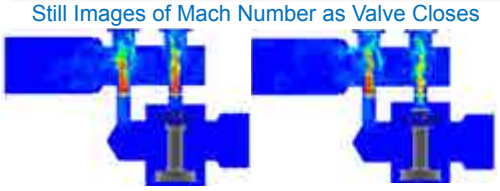
Partially Open Liquid Fuel and Oxidizer Ball Valves



ER42 conducts high fidelity CFD simulations of valves to predict fluid flow patterns, mean pressure drops, and unsteady fluid environments

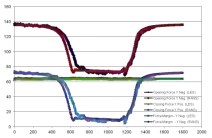
Tranisent 3D Simulation of Poppet Valve

Still Images of Mach Number as Valve Closes

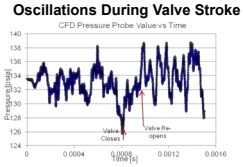


Still Images of Mach Number as Valve Re-opens

Time-accurate Forces on Poppet During Valve Stroke



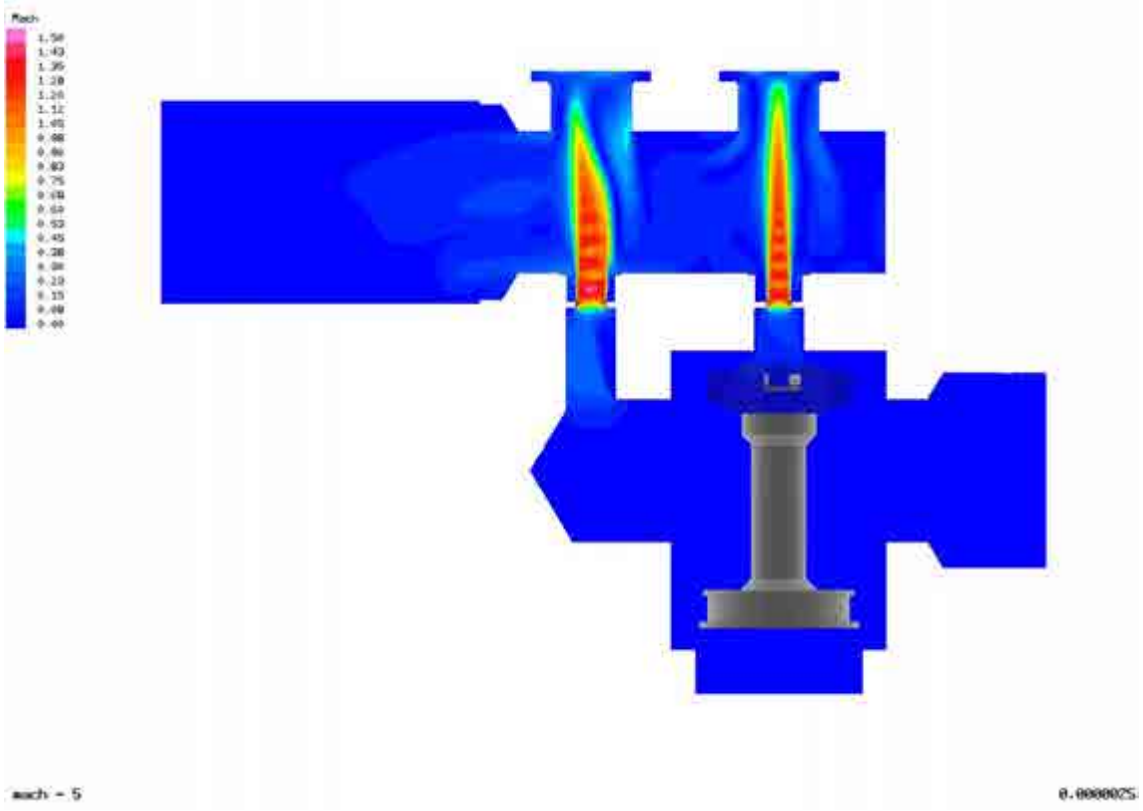
Time-accurate Pressure Oscillations During Valve Stroke



Future work aimed at implementation of valve component force and friction models

Page 11

POPPET VALVE ANIMATION



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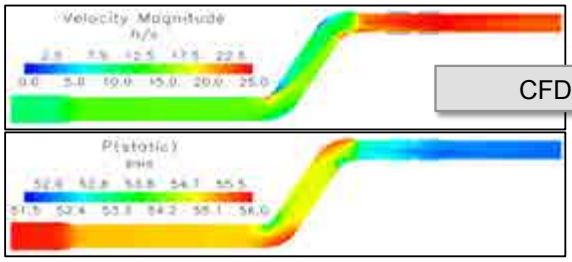
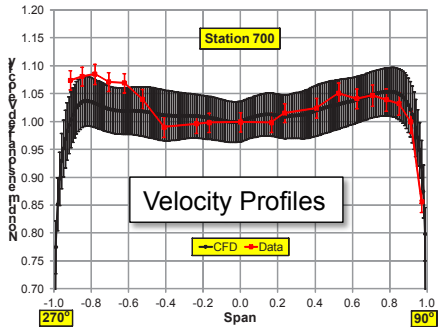
FEEDLINES

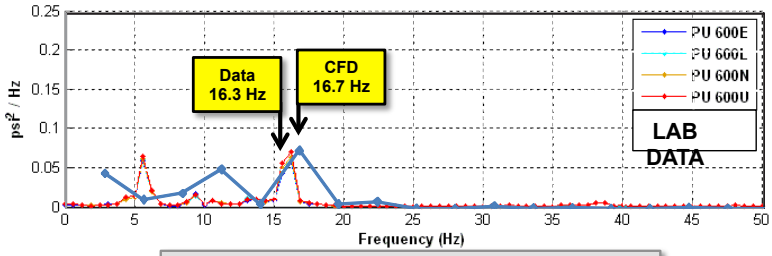
ER42 performs high fidelity CFD simulations of liquid propellant feedlines to predict pressure drops through bends, articulating joints, and splits, flow uniformity dues to bends and wakes, and unsteady pressure environments

Waterflow Test Article



CFD Predictions





Harmonic Analysis of Pressure Tap Data

Page 13

TURBOPUMPS

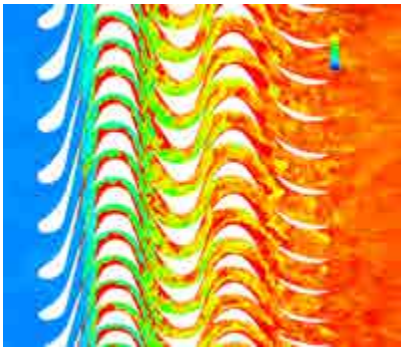
ER42 supports the design, development, and certification of high-speed turbomachinery

- Quick turnaround CFD design parametrics
- Time-accurate rotor-stator CFD analysis
- Highly instrumented pump waterflow test
- Component and engine test support

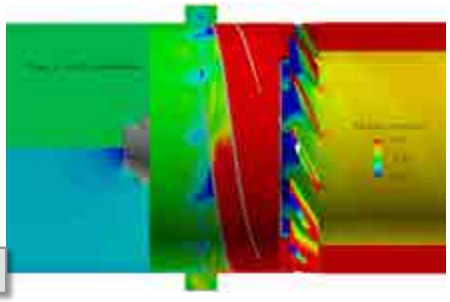
Turbine Airflow Rotating Assembly

Pump Waterflow Test Article

Hotfire Engine Test



Turbine Unsteady CFD Analysis



Pump Unsteady CFD Analysis

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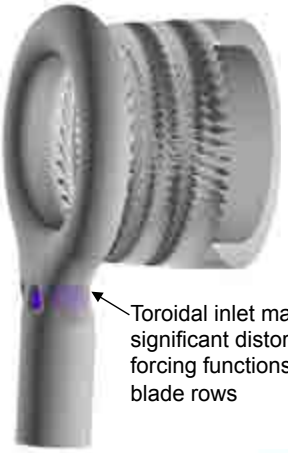
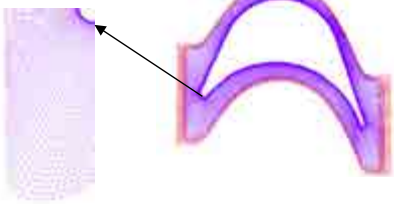
TURBOPUMPS – TURBINE ANALYSIS

Spatially Resolved First Rotor

~550 Million Grid Cells



Toroidal inlet manifold causes significant distortions of unsteady forcing functions in downstream blade rows

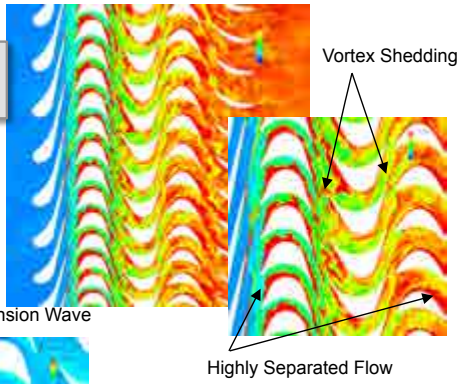


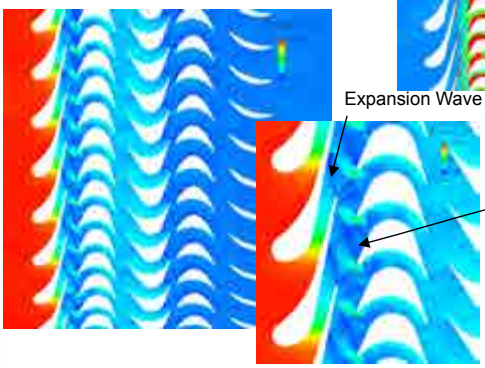
Fuel Turbine Computational Domain

Unsteady Loads Development

- All flow features which significantly modify fluid forcing functions of interest must be modeled
- Must show spatial and temporal resolution of unsteady forcing functions.
- Full 360 degrees models are necessary for most rocket turbines due to large regions of separated flow. Periodic models corrupt the unsteady forcing functions and are not sufficient.

Instantaneous Entropy Contours



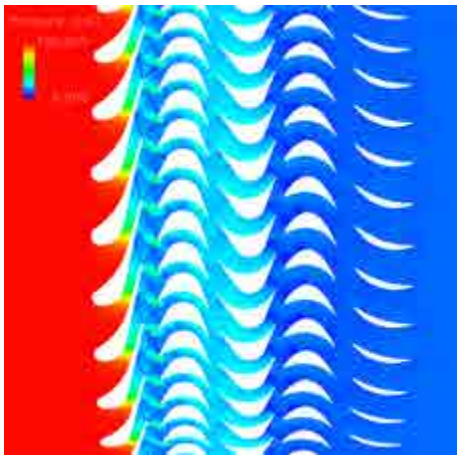


Instantaneous Pressure Contours

Page 15

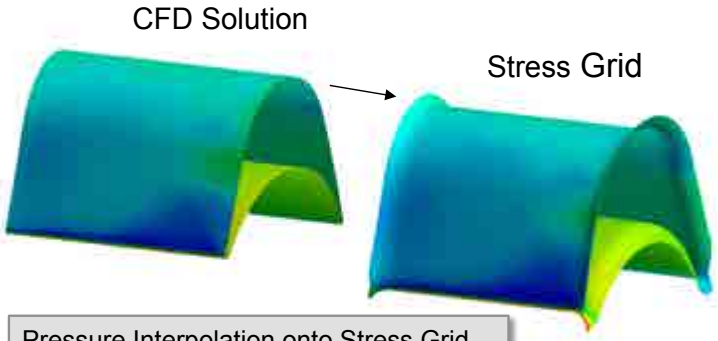
TURBOPUMPS – TURBINE ANALYSIS

Instantaneous Unsteady Pressure Fuel Turbine



Unsteady Loads Delivery

- Unsteady pressure history saved at all points of all blade surfaces Must show spatial and temporal resolution of unsteady forcing functions
- Unsteady pressure histories from blade surfaces are interpolated onto stress grids for structural analysis. All blades must be used if rotor-rotor or stator-stator effects are to be captured
- Unsteady pressures may be delivered in temporal or frequency domains



Pressure Interpolation onto Stress Grid

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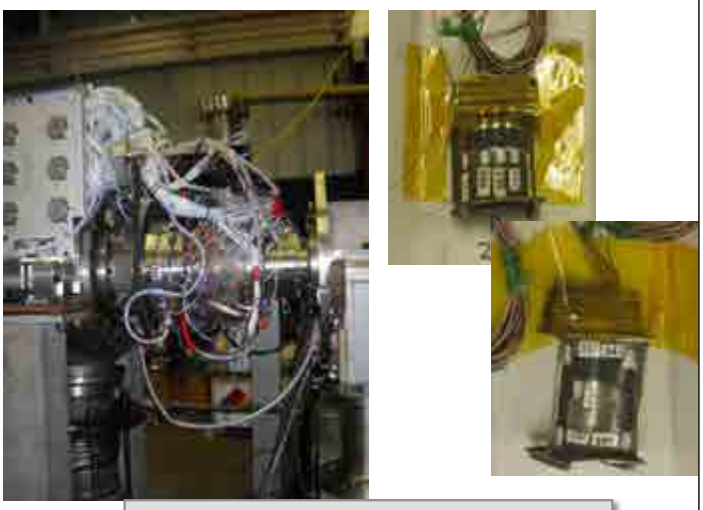
TURBINE AIRFLOW TESTING

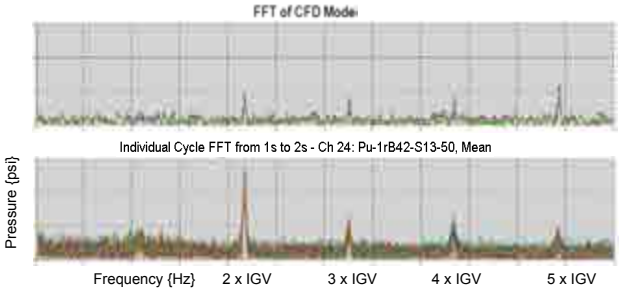
Testing of Highly Instrumented Turbine Models in Scaled Air Conditions

- Steady and unsteady pressure loadings
- Interstage cavity pressures
- Performance mapping over a wide range
- CFD validation



Highly Instrumented Turbine Test Article

Fourier Transforms of First Stage Blade Suction Side at 13% Axial Chord and 50% Span Location



On Shaft Data Acquisition System

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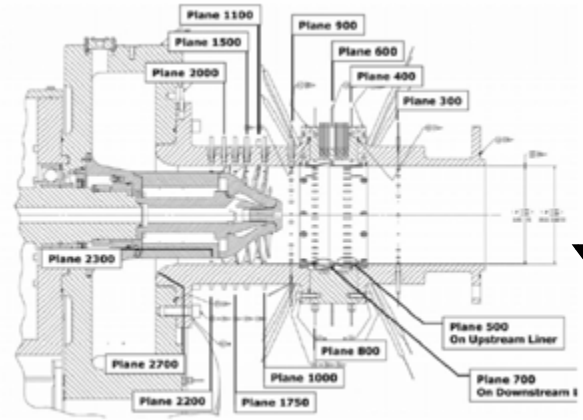
PUMP WATERFLOW TESTING



Low pressure pump with upstream main propulsion system element simulation

2-blade inducer with on-rotor dynamic force measurement system

Comprehensive steady and unsteady pump performance is evaluated at scaled engine operating conditions. Dense instrumentation suites, velocimetry, and flow visualization are utilized in mapping pump characteristics.

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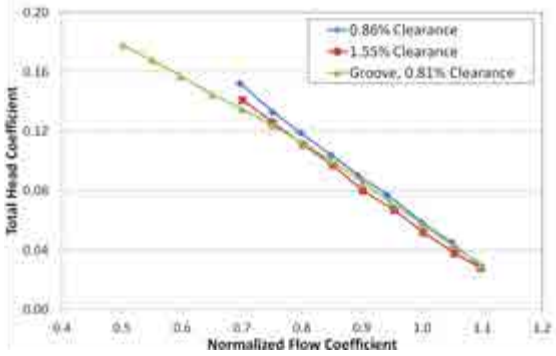
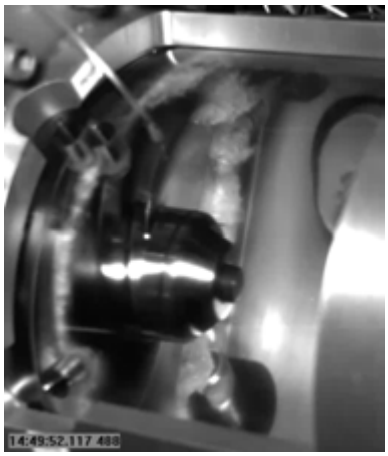
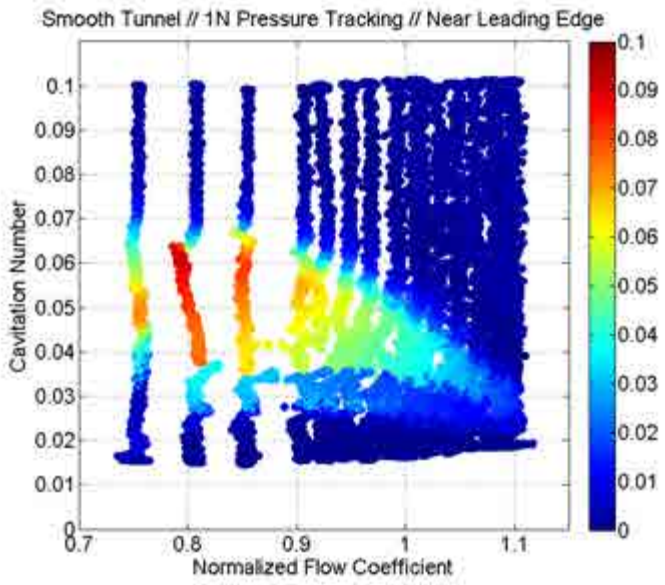
PUMP WATERFLOW TESTING

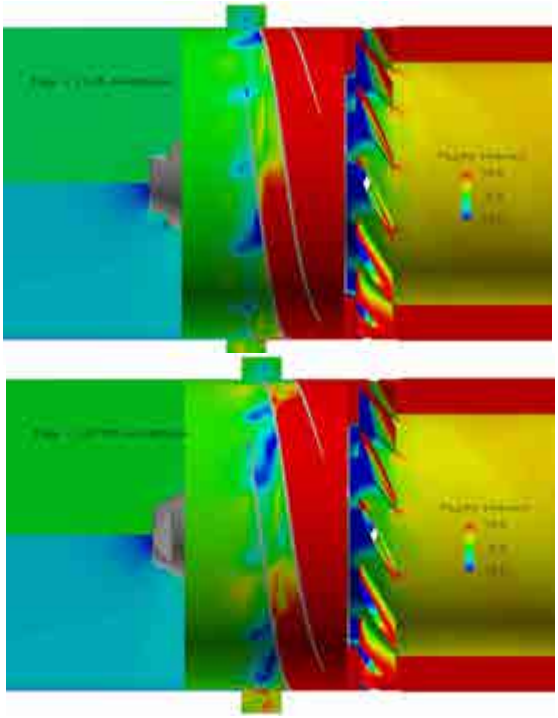






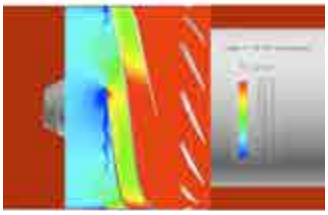
Evaluation of steady pump performance parameters, cavitation oscillation trends, and high-speed flow visualization provides early risk reduction for a turbopump during its preliminary design cycle. Sometimes, comprehensive waterflow is used to identify unsteady loadings and/or performance deficits within certified flight pumps during anomaly investigations.

PUMP CFD



Non-cavitating CFD is used to identify critical unsteady flow interactions between inducer blades and cavitation suppression grooves. These interactions are thought to promote higher order cavitation oscillations within the cavitating turbopump. The time-accurate CFD predicts slowly rotating/high cell count progressions very similar to higher order cavitation instabilities measured in waterflow test.

Time accurate CFD provides insight into the complex flow field behind higher order cavitation. Higher order cavitation is a potential forcing function for primary inducer bending modes.



CFD calculations effectively capture tip vortex dynamics for inducers operating with minimal tip clearance (without cavitation suppressor).

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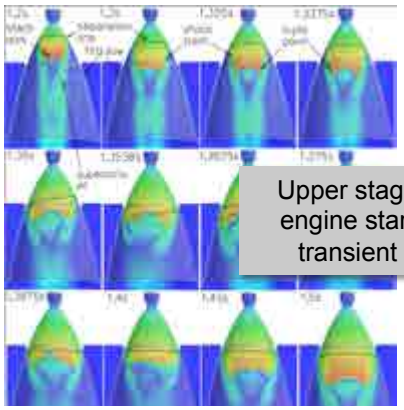
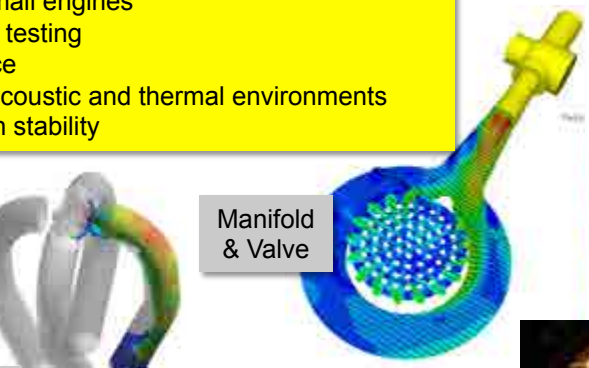
COMBUSTION DEVICES

Scope of branch responsibility in support of liquid rocket engine thrust chamber assembly design & development

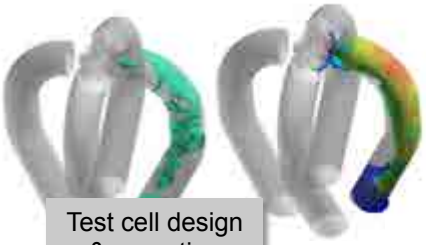
- Large and small engines
- Analysis and testing
  - Performance
  - Pressure, acoustic and thermal environments
  - Combustion stability



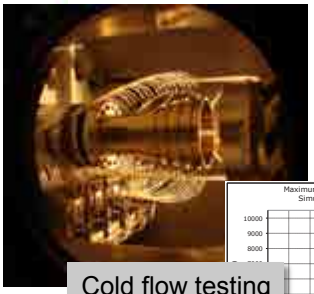
Upper stage engine start transient

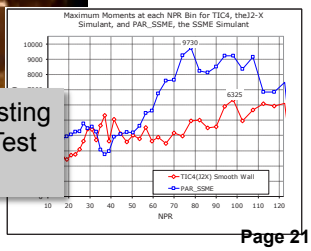


Manifold & Valve

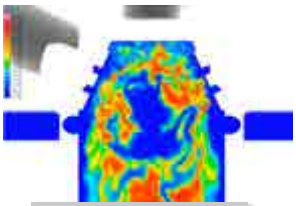


Test cell design & operation





Cold flow testing in Nozzle Test Facility



Igniter

Stability rating bomb test simulation

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COMBUSTION STABILITY ASSESSMENT APPROACH & SKILLS LEVERAGED BY ER42

- **Branch asked to assess the combustion dynamics / stability of an engine design**
  - •Chug
  - •Acoustic
  - •Other oscillation modes (e.g., buzz from upstream supply system)
- **Common to all three generic stability types are two main assessment questions:**
  - •What is the margin associated with the stability type?
    - •Requires accepted definition of stable, unstable, and marginal
  - •What margin is acceptable for a given engine design?
- **Assessment comes from a combination of two approaches:**
  - **Analytical**
    - •Linear: system stability approaches; energy based approaches
    - •Non-linear: limit cycle waveform evaluation
  - **Testing**
    - •Non-linear: waveform characterization of damp times and amplitudes

- **Skills Required**
  - Unsteady Fluid Transients and Dynamics
  - Heat Transfer and Thermodynamics
  - Acoustics
  - System Dynamics and Linear Analysis (Stability Theory, State Space, Transfer Matrix)
  - Electronics (Fluid Circuit Analogies, Linear Analysis)
  - Mathematics (DDEs, Model Development, Linear Analysis)
  - Control Engineering (System Identification, Nyquist Plots, Bode Plots)
  - Stability Theory (Nyquist Criterion, et al.)
  - Signal Analysis (Data Characterization and Reduction)
  - Instrumentation and Data Acquisition
  - Combustion Devices and Propulsion
  - Combustion Processes (Spray and Flame Dynamics, Mixing, Atomization, Vaporization, etc.)

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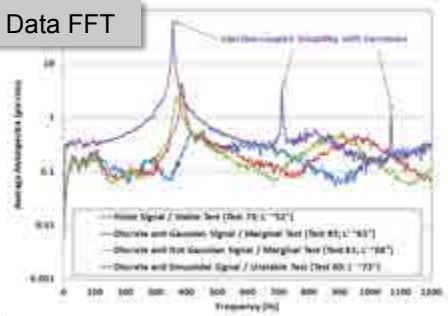
COMBUSTION STABILITY ASSESSMENT: EMPIRICAL STABILITY ASSESSMENTS

Example engine test data - 1L mode instability exhibited during testing program

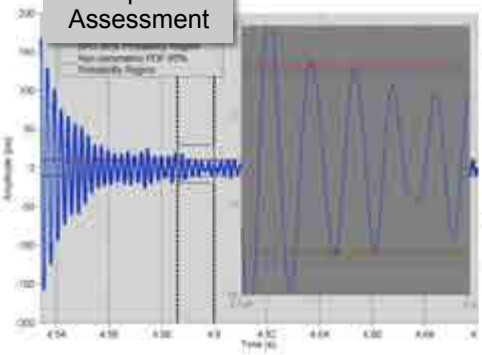
- ~300 – 400 Hz stable to unstable signal

- **New methods created to judge spontaneous stability**
  - Offered new way to approach characterizing signal via statistics and frequency variability
  - Gave metrics on how to divide stable vs. unstable
- **New methods created to judge dynamic stability**
  - Assess statistical character of data prior to bomb
  - Track when amplitudes reach back within 'statistically significant limits'

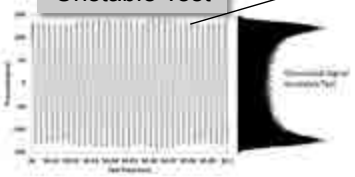
Data FFT

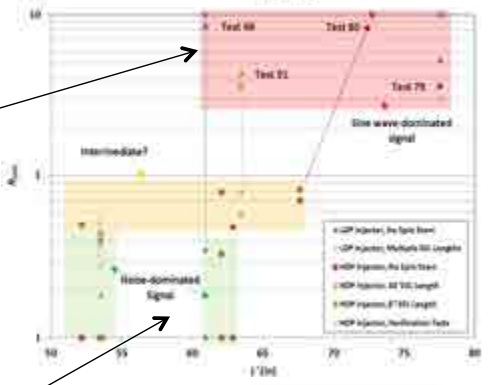


Damp Time Assessment

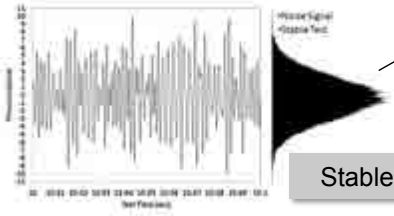


Unstable Test





Stability Map



Stable Test

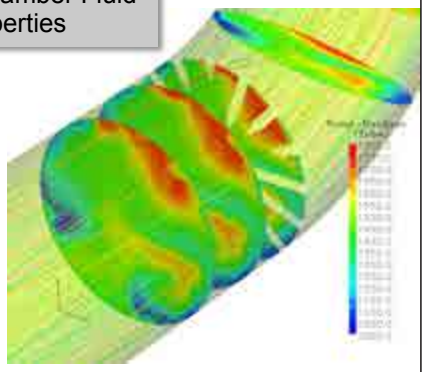
COMBUSTION STABILITY ASSESSMENT: ANALYTICAL ASSESSMENTS

Branch analytical models encompass:

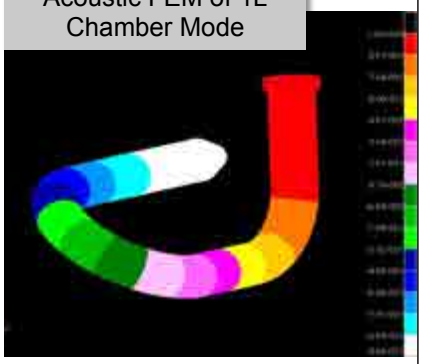
- Classical linearized stability models
- Computational Fluid Dynamics (CFD)
- Finite element modeling (FEM)

- **Linearized models are used for chug and acoustic mode evaluations**
  - State-space and impedance models
- **CFD and FEM used to better characterize complex flowfields and geometries**
  - Accounts for distribution of fluid properties
  - Coupled acoustic modes better evaluated using CAD geometries and CFD inputs

CFD of Chamber Fluid Properties



Acoustic FEM of 1L Chamber Mode

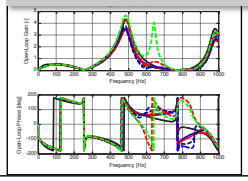


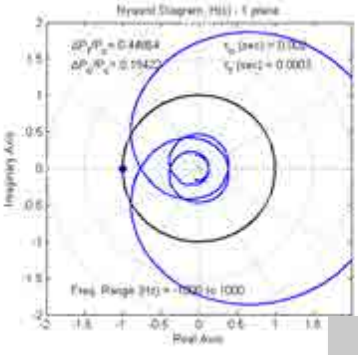
$$x(\omega) = \frac{\bar{X}\sin\left(\omega(\bar{\tau}_{T,o} - \bar{\tau}_{T,f})\right)}{\sin(\omega\bar{\tau}_{T,f}) + \theta_g\omega\cos(\omega\bar{\tau}_{T,f})}$$

$$y(\omega) = \omega$$

$$z(\omega) = \frac{\bar{F}\sin\left(\omega(\bar{\tau}_{T,f} - \bar{\tau}_{T,o})\right)}{\sin(\omega\bar{\tau}_{T,o}) + \theta_g\omega\cos(\omega\bar{\tau}_{T,o})}$$

Gain / Phase Plots





Nyquist Stability Plot

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COMBUSTION STABILITY ASSESSMENT: IMPROVING THE STATE-OF-THE-PRACTICE

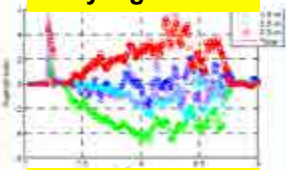
Objective of Improvements

- Advance the predictive capability of current, state-of-the-practice tools and methodologies used in combustion stability assessments
- Facilitate
  - Confident identification & characterization of combustion instabilities
  - Successful & efficient mitigation during propulsion system development
- Minimize development costs &improve hardware robustness

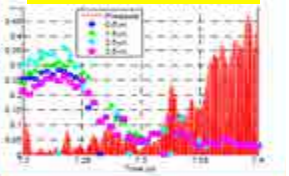
Approach to Improvements

- Improve state-of-the-practice stability assessment capability by use of higher-fidelity, physics-based information either integrated into the engineering tools or used separately in the assessment process
- Extract physics-based models/information from focused state-of-the-art CFD simulations
- Validate new capability by exercising the improved capabilities on relevant experiments

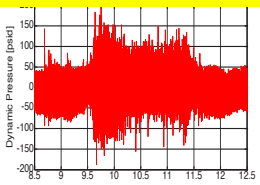
Rayleigh Index*



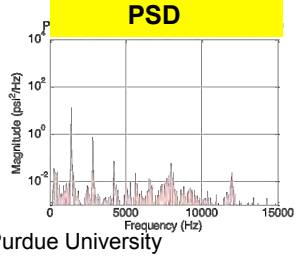
Oscillation Dec.



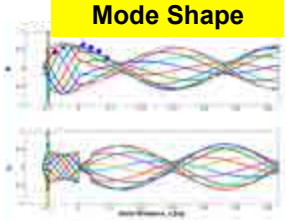
Fluctuating Pressure



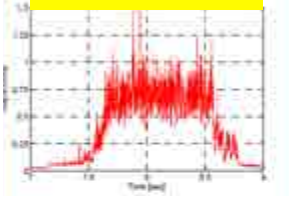
PSD



Mode Shape



Heat Release



*Courtesy of W. Anderson/Purdue University

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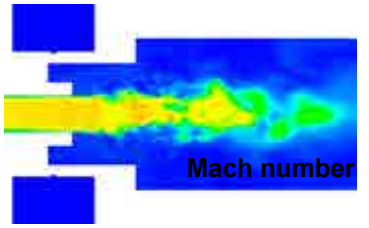
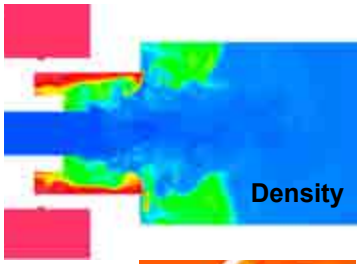
COMBUSTION STABILITY ASSESSMENT: IMPROVING THE STATE-OF-THE-ART

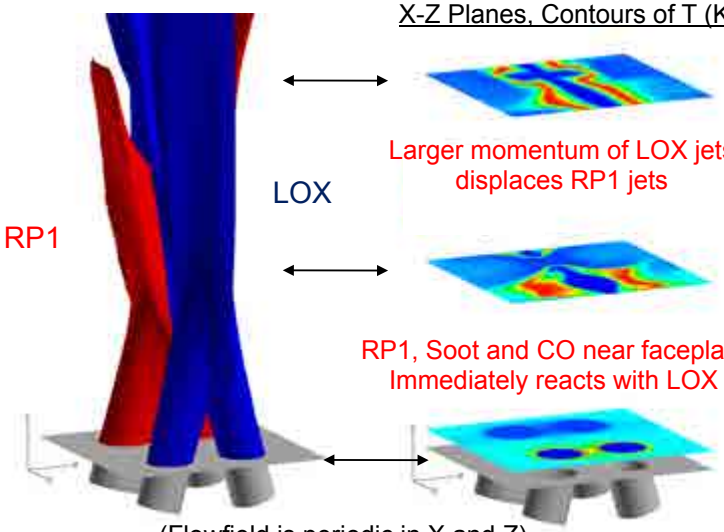
Instantaneous 2-D snapshots from a 3-D non-reacting simulation of a gas-centered swirl coaxial element





Pressure in fuel manifold

RANS simulation of a reacting like-on-like impinging doublet element



(Flowfield is periodic in X and Z)

Ongoing improvements for injector CFD
- Flamelet formulation for efficient simulation of reacting flows
- VOF & atomization for 2-phase flow
- Low dissipation schemes better resolving turbulence & acoustics

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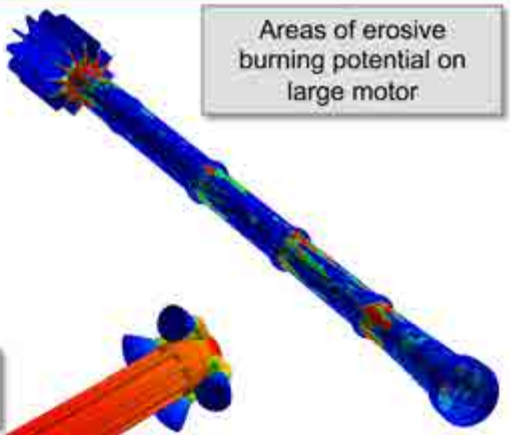
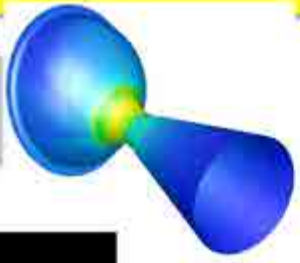
SOLID ROCKET MOTOR OVERVIEW

Scope of branch responsibility in support of solid rocket motor design & development
- Large booster-class motors
- Small motors-ullage settling, booster separation & launch abort
- Performance
- Environments-pressure, acoustic & thermal
- Stability

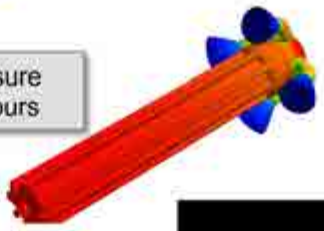


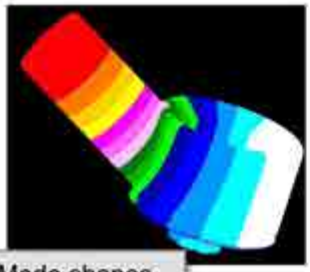
Areas of erosive burning potential on large motor

Aft dome heat transfer coefficients

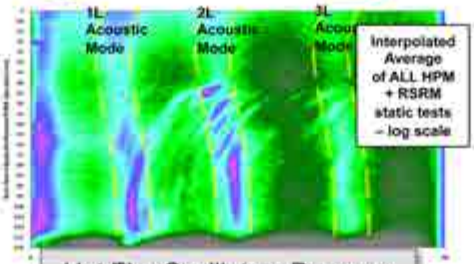


Pressure contours

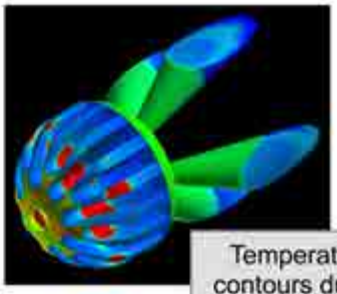




Mode shapes from finite element analysis



Hot Fire Oscillatory Pressure Characteristics



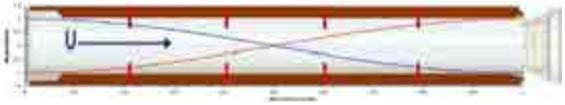
Temperature contours during ignition

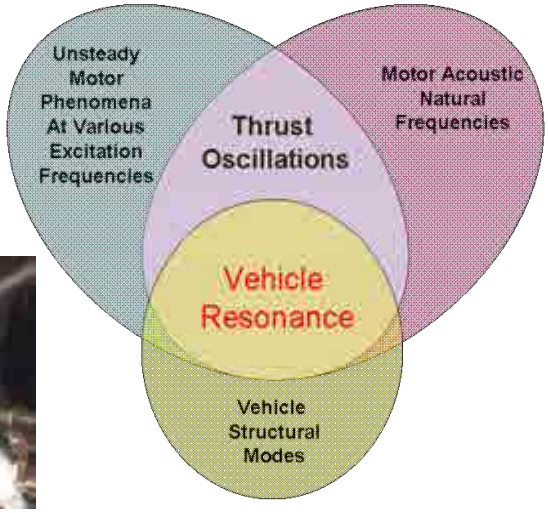
Page 27

SOLID ROCKET MOTOR THRUST OSCILLATIONS: WHY ARE THEY A CONCERN?

- **SRM thrust oscillations during flight can deliver forced accelerations to vehicle structure and acoustic mode frequencies**
  - **Space Shuttle System**
  - **Arianne 5**

- **If these forced accelerations match appropriate vehicle structural modes, then vehicle resonance can occur**
  - **Ares I**





Page 28

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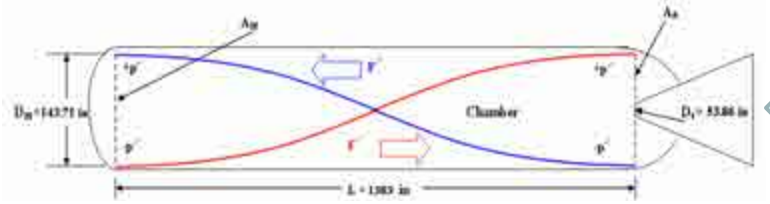
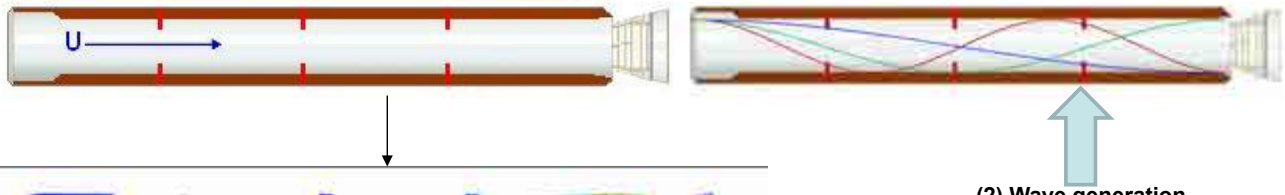
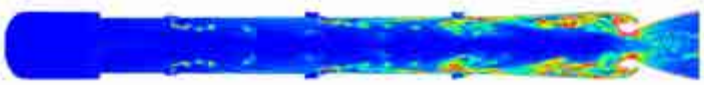
SOLID ROCKET MOTOR THRUST OSCILLATIONS: CFD INPUTS TO INCREASED UNDERSTANDING OF FLOWFIELD



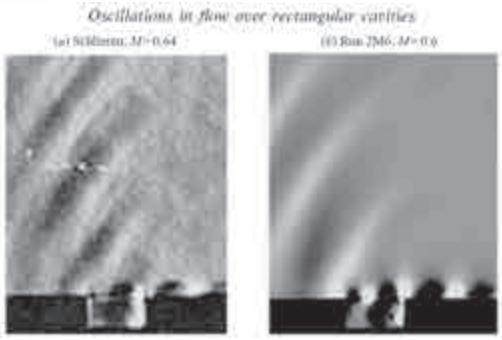
(3) 1L,2L,3L acoustic mode shapes create subsequent thrust oscillations



(2) Wave generation rate tunes with SRM 1L, 2L, 3L acoustic modes



(1) Vortex shedding within internal SRM flow field causes pressure perturbations



Ongoing Improvements
- Efficient LaGrangian particle tracking
- 2-phase capability to model slag dynamics
- Acoustic source location and mode extraction from CFD results

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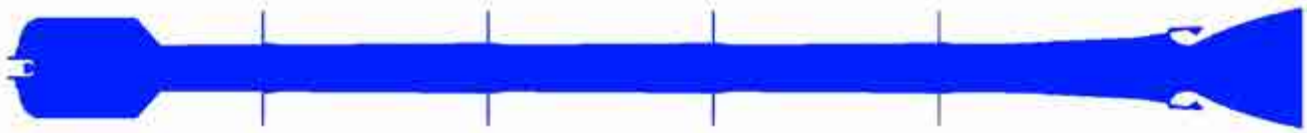
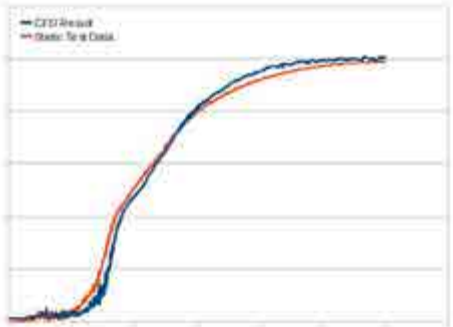
SOLID ROCKET MOTOR IGNITION

- The ignition transient is a critical part of motor operation
- Elevated thrust rise rate is too high threatens vehicle structural integrity
- CFD ignition simulation
  - As-cast motor geometry mesh with ~ 150M cells
  - Simulation execution complete on 2400 CPUs in less than 2 weeks
  - Results are being used to help understand test stand dynamics issues



Pressure field during first ~ 0.6 s of large motor ignition transient



CFD results compared to head end pressure trace from static test

Ongoing Improvement Efforts
- Efficient LaGrangian particle tracking
- Propellant grain recession capability to enable appropriate propellant geometry during longer transient simulations

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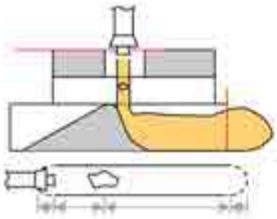
LAUNCH ENVIRONMENTS

1D Linearized Physics Models



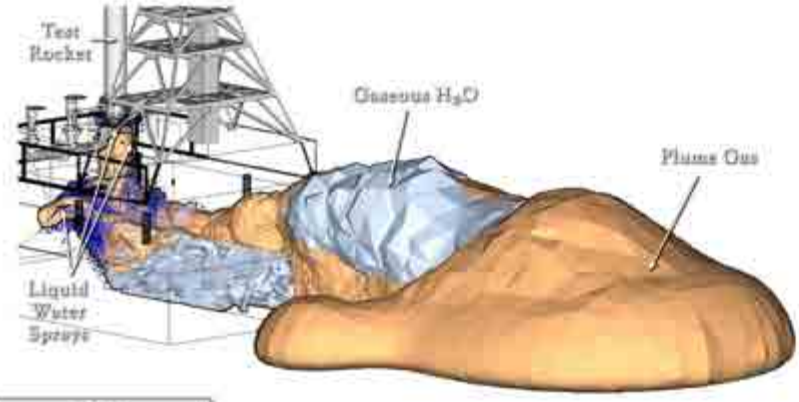
ER42 Develops the Fluid and Acoustic Environments for Launch

- Liftoff Acoustics
- Overpressure
- Sound Suppression
- Liftoff Debris Transport
- Hydrogen Entrapment

ER42 Uses Multiple Levels of Analysis and Testing to Accomplish this Work

Flight Tests

Scale Model Tests



CFD

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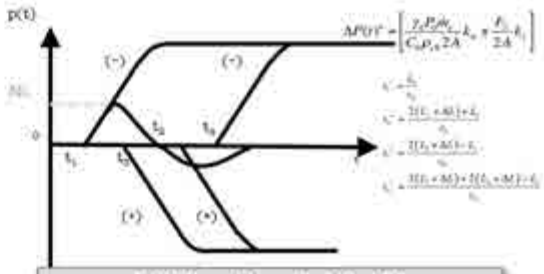
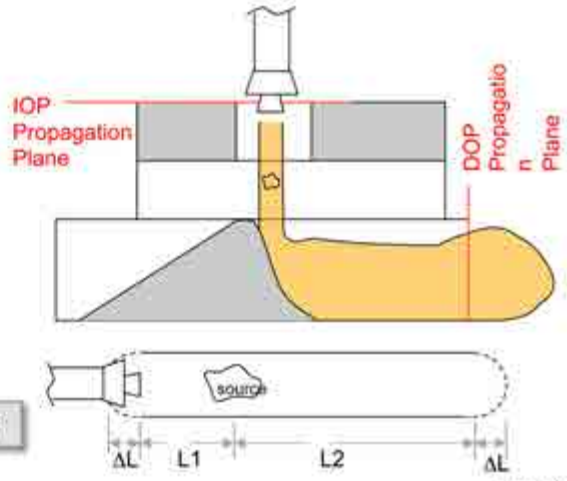
OVERPRESSURE – ANALYTICAL MODEL

Overpressure Predictions Using Analytical Models

- *Broadwell &Tsu Model*: Linearized 1-D physics-based model for overpressure in a ducted launcher
- *4-wave model*: Acoustic modification to incorporate resonant conditions
- *Attenuation Model*: Empirically based on Shuttle data or other motor/ engine correlations
- *Knockdown Factors for water suppression or pressure wave diffraction*: Empirically-based or CFD simulation-based
- *Margin*: Technical agreement based on CFD simulations and unknown
- Improvement – Continually improve models based on CFD, Test data, and Flight data



4-Wave Physics Model



Broadwell and Tsu Model Application

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OVERPRESSURE – CFD

CFD has recently shown to represent overpressure very accurately without the inclusion of water

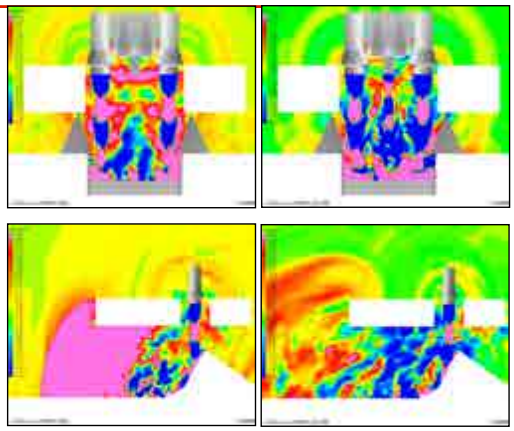
- Demonstrated ability to capture IOP and DOP waves at several locations for dry tests

Provides ability to address limitations of Analytical models

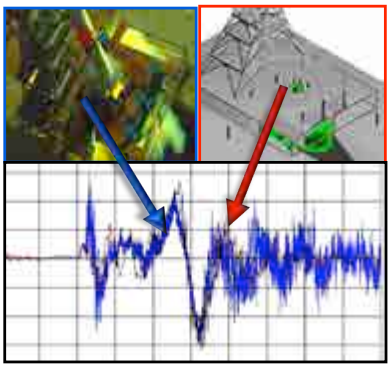
- Accounts for complex flow scenarios and three-dimensional launch pad geometry

Provides parametric studies where unknowns currently exist

Ongoing improvements include modeling water suppression systems, multiphase solid booster effluent, and capture higher frequency spectral content



CFD simulations with (right) and without (left) liquid engine plumes



Comparisons of CFD predictions with ASMAT data

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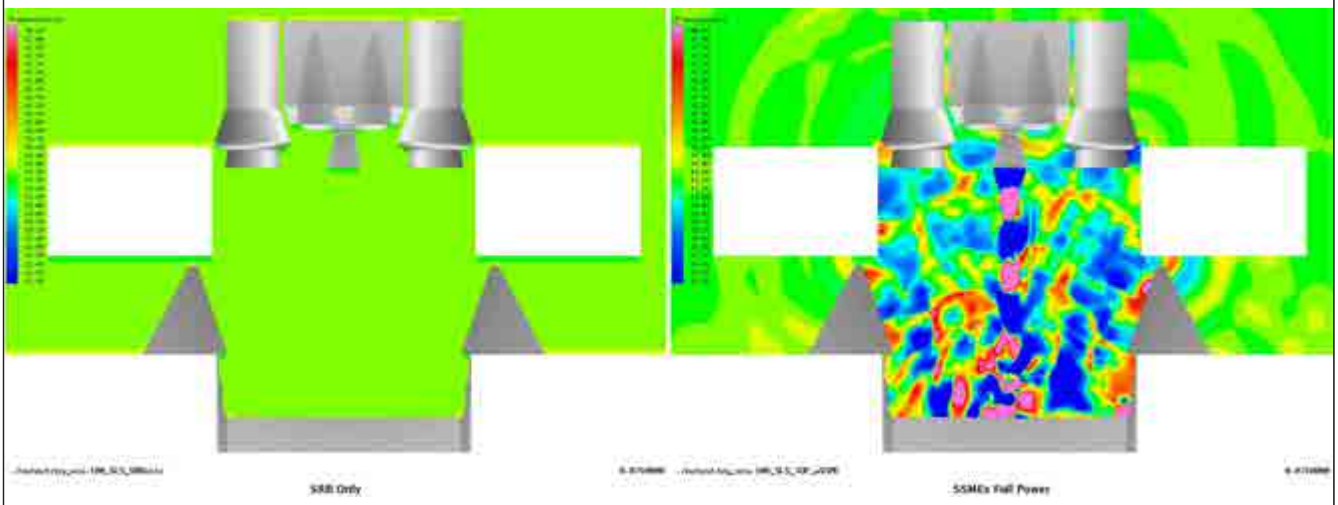
OVERPRESSURE – CFD ANIMATION



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LIFTOFF ACOUSTICS

DESIGN NEW LAUNCH VEHICLE

DERIVE LIFTOFF ENVIRONMENTS

Liftoff noise is generated by the mixing of rocket exhaust flow with the surrounding atmosphere and its interactions with surrounding launch pad structures.

ER42 creates initial liftoff acoustic environment derived from Saturn V, Space Shuttle flight data, and Ares I-X flight test data. for the development of Ares I and the proof-of-concept vehicle, Ares I-X. Parametrics and identification of sources from CFD

VALIDATESCALE MODEL ACOUSTIC TEST

Use acoustic scale model test to validate liftoff acoustic environments and water sound suppression system design.

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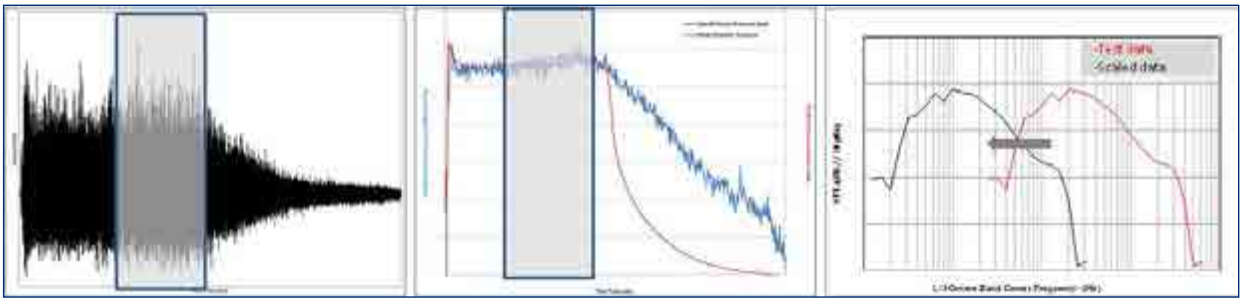
SCALE MODEL ACOUSTIC TESTING

- **Determine model scale using Strouhal Number**

$$St = \left(\frac{f_1 d_1}{V_1}\right) = \left(\frac{f_2 d_2}{V_2}\right)$$

- **Design test article to this scale; fire; acquire data.**
- **Data Processing**



Typical pressure time history with analysis window (a) and analysis window overlaid on chamber pressure measurement and RMS OASPL time history (b) and a one third octave plot for the test data compared to the scaled data (c).

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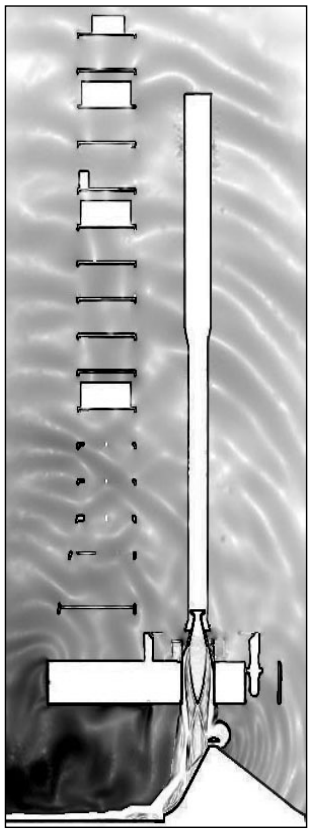
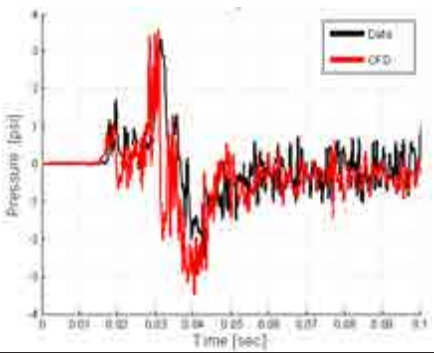
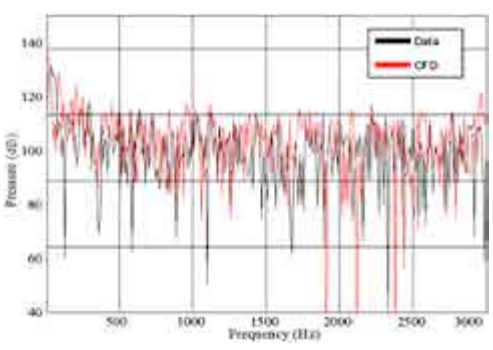
SCALE MODEL TEST MOVIE

ASMAT VALIDATION OF CFD (COMPARISONS OF FREQUENCY WITHIN DUCT)

- Simulations of 5% scale rocket to model transient startup of motor
- Validated pressure temporal/spectral accuracy of CFD vs test data.
- Simulations showed good correlation with test data.
  - Matched pressure content above deck to 1000-1500 Hz
  - Matched pressure content below deck to 2000-3000 Hz
- Provided rationale and confidence to use CFD to predict environments for full-scale vehicles (up to ~ 150 Hz)







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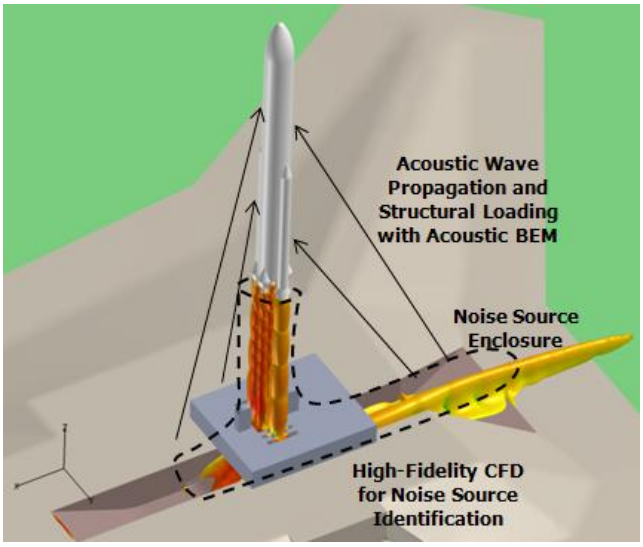
APPROACH TO ACOUSTICS PROPAGATION CHALLENGE

Solution: Implement hybrid approach of CFD + Computational Aero Acoustics (CAA) for liftoff acoustic fields

- Use high-fidelity CFD modeling to capture important plume physics (multi-phase plume, plume mixing and impingement, gas-water phase effects from deluge, etc.)
- Capture acoustic sources originating from plumes, impingement, capture water suppression effects
- Propagate using CAA from acoustic source surfaces enclosing noise source regions

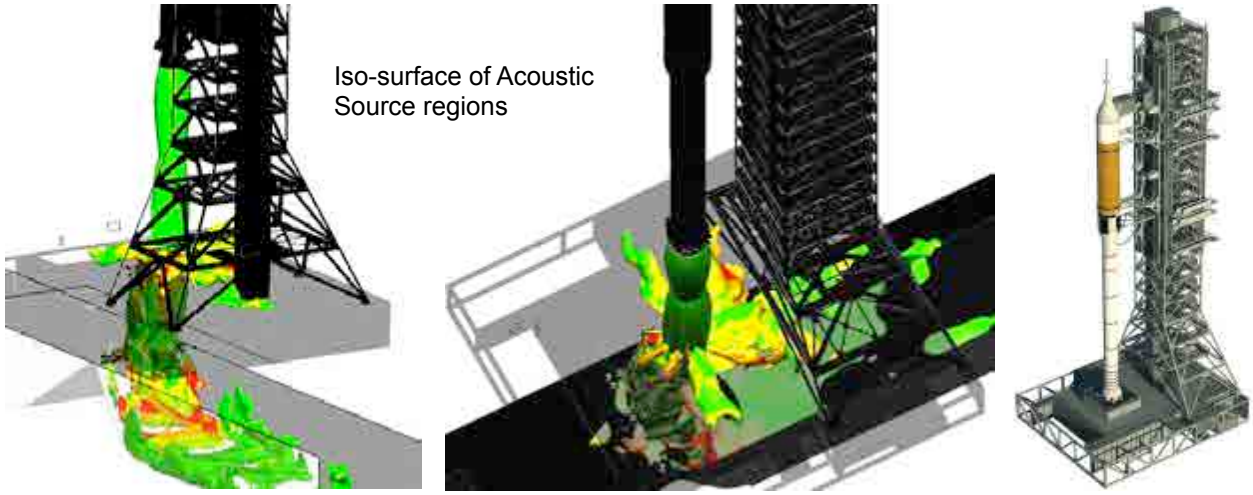


Which CAA method is best suited for this application?

- CAA acoustic field propagation method must be able to resolve reflections, refraction and attenuation from interaction with structures such as launch platform and tower
- Two approaches under evaluation:
  - Boundary Element Method (BEM)
  - Farfield high-order Euler solution

CHALLENGE: IDENTIFICATION OF THE ACOUSTIC SOURCE REGIONS

- Major challenge arises in defining envelope of source regions for handover from CFD to CAA
- Plume boundary shape is quite complex due to interaction with launch pad
- Example: Visualization of Noise Source regions for ASMAT Plume Impingement



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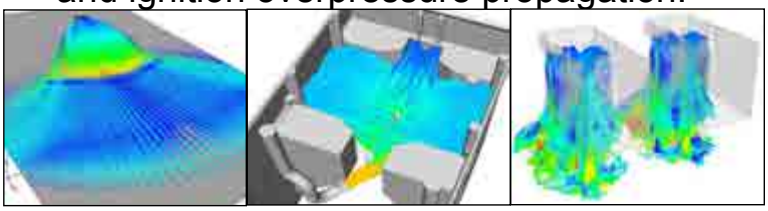
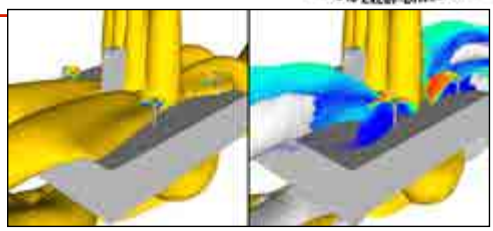
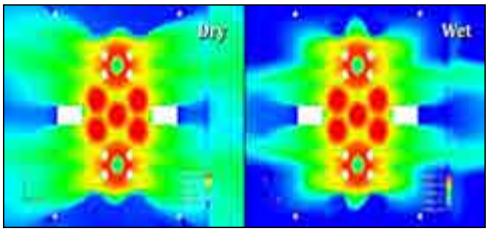
CHALLENGE: SIMULATION OF WATER MITIGATION IN CFD

- Using Lagrangian Particle model to simulate water injection into launch pad plume environment for SLS concepts, Space Shuttle, and scale tests.
- Injecting water at up to 200,000 gal/min
- Simulating up to 30M active particles
- Liquid drop emission from booster holes, trench deflectors, or from rainbird systems
- Modeling water break-up and phase change
- Considerable changes shown in turbulent kinetic energy on deck, plume temperature, and ignition overpressure propagation.

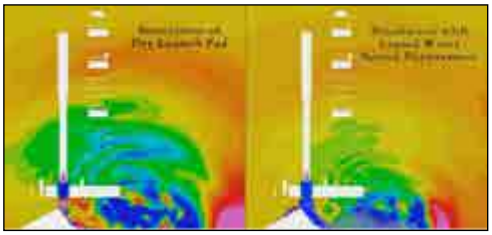




Reduction of Plume Temperature by Water Deluge



Reduction of Kinetic Energy at Deck Level



Reduction of Ignition Overpressure

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SUMMARY

- The Fluid Dynamics Branch at MSFC has the mission is to support NASA and other customers with discipline expertise to enable successful accomplishment of program/ project goals
- The branch is responsible for all aspects of the discipline of fluid dynamics, analysis and testing, applied to propulsion or propulsion-induced loads and environments, which includes the propellant delivery system, combustion devices, coupled systems, and launch and separation events
- ER42 supports projects from design through development, and into anomaly and failure investigations
- ER42 is committed to continually improving the state-of-its-practice to provide accurate, effective, and timely fluid dynamics assessments and in extending the state-of-the-art of the discipline

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極低温キャビテーションモデリングの多面的研究と開発への応用に向けて

谷直樹（JAXA）
伊藤優(東工大)
津田 伸一(信州大)
石川 勝利(東大)
姫野武洋(東大)
河津要(JAXA)
山西伸宏(JAXA)

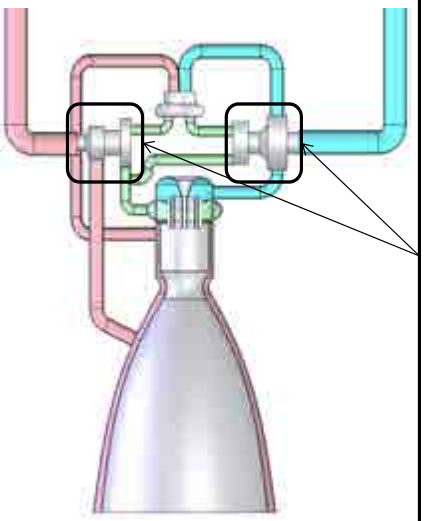
1

ターボポンプとキャビテーション

高性能ロケット推進剤

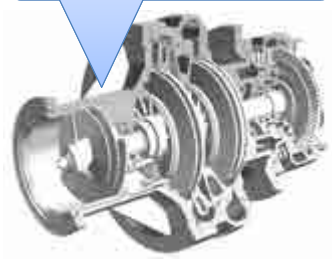
水素/酸素、ケロシン/酸素、メタン/酸素 etc.…

-100℃以下の極低温流体



ターボポンプ
小型・高速回転ポンプ
ポンプで液体が気化

極低温流体中の
キャビテーション



Advances in Rocket Engine Modeling and Simulation

2

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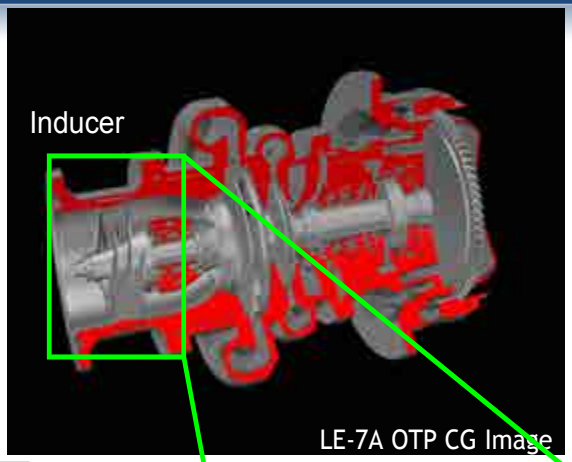
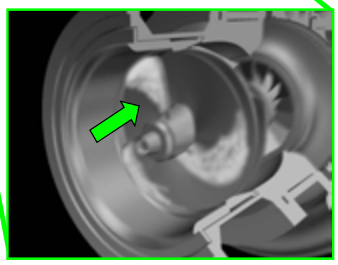
極低温流体中でのキャビテーション

キャビテーション

- •急激な性能低下
- •軸振動





極低温流体中での
キャビテーション

熱力学的効果
特徴
キャビティ縮小
性能向上

熱力学的効果

潜熱の吸収

熱力学的効果とは？

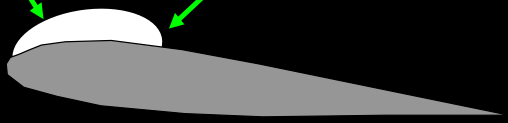
水

$T_{cavity} \fallingdotseq T_{fluid}$

極低温流体

$T_{cavity} < T_{fluid}$

$P_{cavity} < P_{sat}$



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問題点

現在のインデューサ設計時の
キャビテーション性能予測 ○○○ 水でのCFD解析

↕

実際は極低温流体中での作動

•実作動流体での試験
→開発後期の試験で初めて実施

リスクが高い

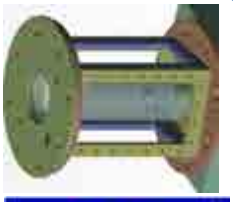
極低温キャビテーションの適切なシミュレーションの実現による
開発リスク低減

目的とアプローチ

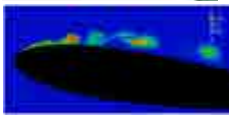
目的：極低温キャビテーションを適切に再現可能な
数値解析モデルの構築

4方向のアプローチによる総合理解

1. 極低温インデューサ可視化実験
東工大 伊藤先生
目的：実現象理解



2. 気泡流モデルによる微細現象理解
信州大 津田先生
目的：ミクロスケール現象理解



3. 気液界面追跡法による現象把握
東大 姫野先生
目的：解析モデル依存性理解

4. 巨視的キャビテーションモデルの評価
JAXA
目的：マクロスケール現象理解

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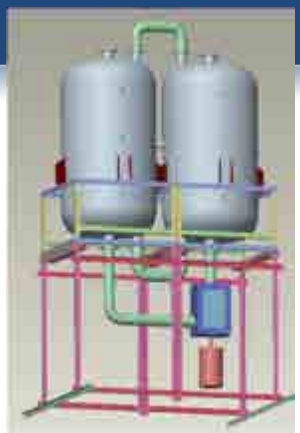
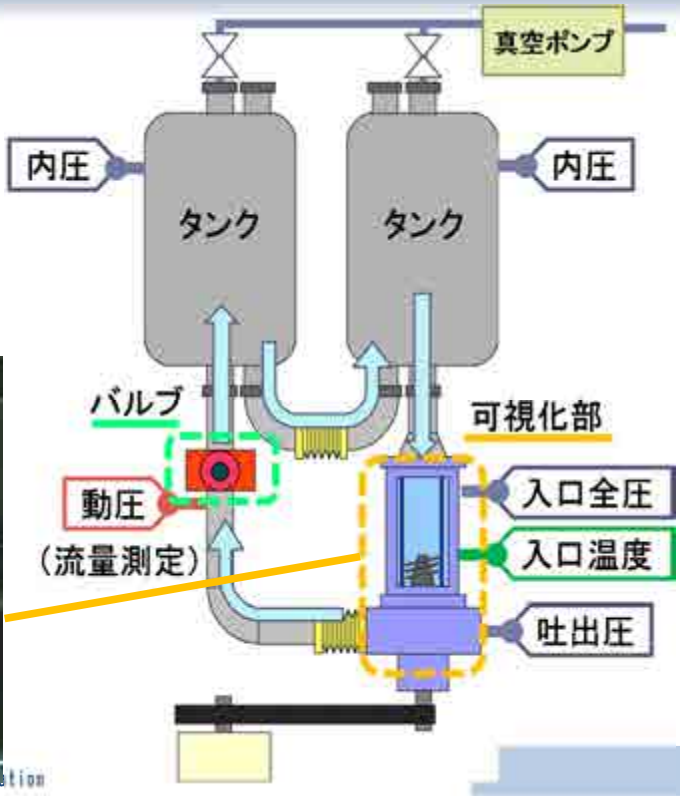
1. 極低温インデューサ可視化実験

実験装置全体図





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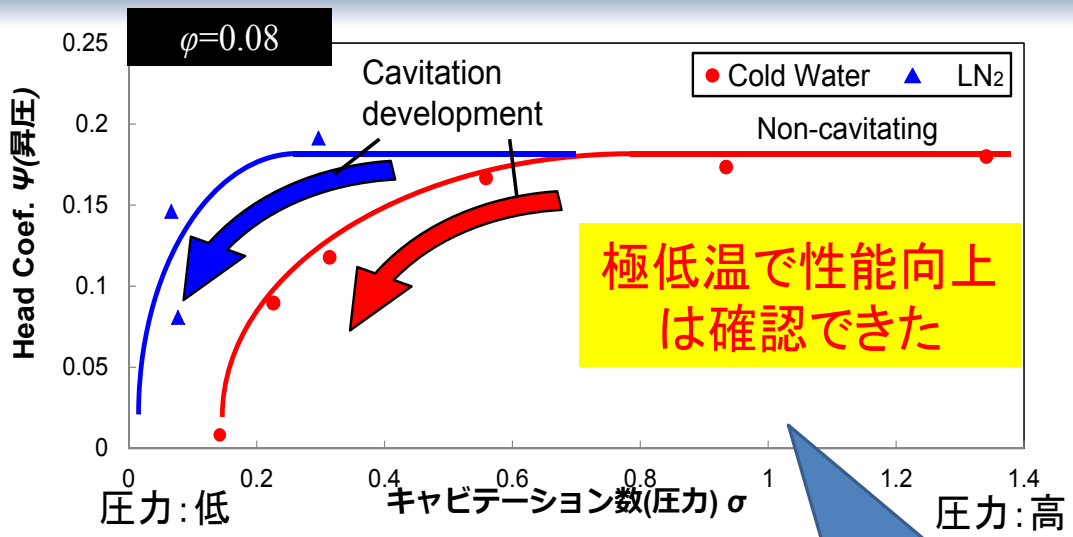
キャビテーション性能



Cavitation Number σ

σ is criterion of cavitation generation.

$$\sigma = \frac{p_1 - p_v}{\frac{1}{2}\rho_L U^2}$$

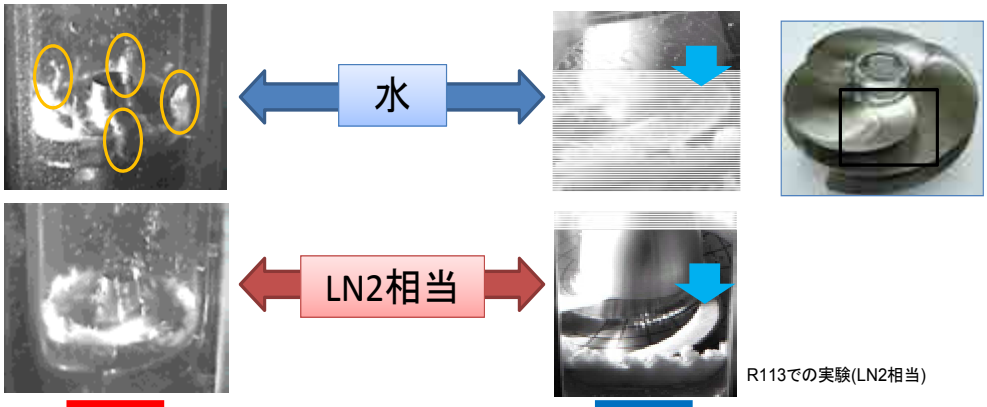
p_1 : Inlet static pressure
p_v : Saturated vapor pressure
U : Tip blade velosity ($R\Omega$)

性能がいい＝低い圧力でも昇圧性能が落ちない
青い線の方が高性能

9

実験より判明した点

逆流渦キャビテーション=気泡　　シートキャビテーション



小直径インデューサでは発生しない

発生量が小規模になるものの、必ず発生

2つの異なる物理事象を再現する必要あり

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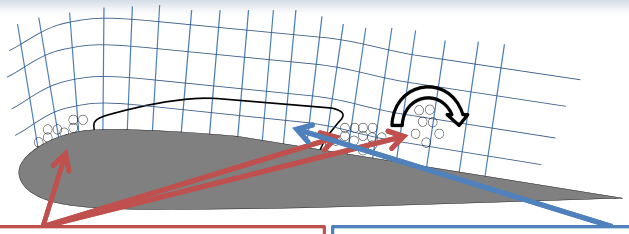
2つのアプローチ



初生・崩壊・渦部
気泡キャビテーション
熱力学的効果：スケール効果有り

発達部
シートキャビテーション
熱力学的効果：スケール効果無し

微細な物理機構をモデル化

気液界面を考慮したモデル

多重プロセス型
キャビテーションモデル

界面追跡法

特性を評価して工学的に有意な
キャビテーションモデル構築

2. 気泡流モデルによる微細現象理解

多重プロセス型キャビテーションモデルの構築と検証

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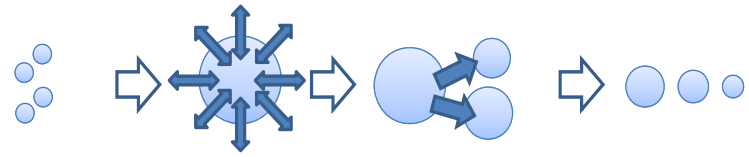
多重プロセス型キャビテーションモデル

気泡流・・・・初生、成長/収縮、合体/分裂といった多重プロセス



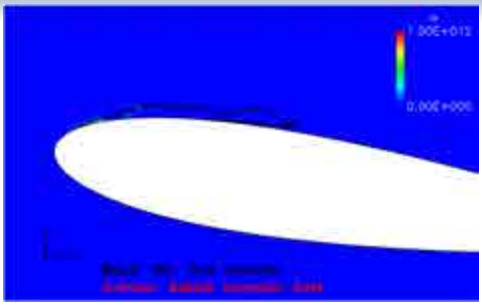
モーメント法を用いた多重プロセス型モデル

$$\frac{D}{Dt}\begin{bmatrix} M_0 \\ M_1 \\ M_2 \\ \rho_g M_3 \end{bmatrix} = \begin{bmatrix} J_s \\ G(\overline{R})\cdot M_0 \\ 2G(\overline{R})\cdot M_1 \\ \dot{m}_v \cdot M_2 \cdot M_3 + 3\rho_g \cdot G(\overline{R})\cdot M_2 \end{bmatrix}$$

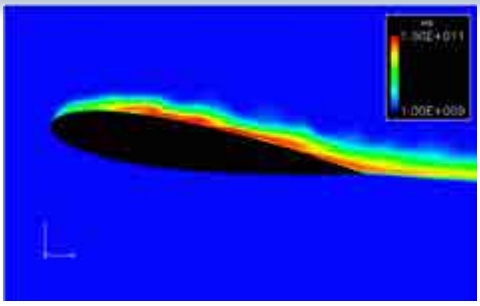
J_s ← 初生（気泡数）
$G(\overline{R})\cdot M_0$（気泡径）
相変化 → $2G(\overline{R})\cdot M_1$（気泡表面積）
$\dot{m}_v \cdot M_2 \cdot M_3 + 3\rho_g \cdot G(\overline{R})\cdot M_2$（気泡質量）

気泡の体積割合(ボイド率) $\alpha = \dfrac{\frac{4}{3}\pi M_3}{1+\frac{4}{3}\pi M_3}$ 合体・分裂を考慮したボイド率

多重プロセスモデル 定性評価



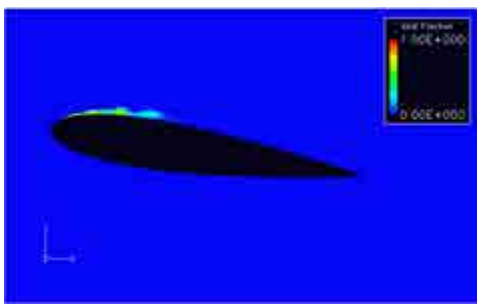
気泡発生率 [1/s/m³]



気泡数(M0) [1/m³]

黒い線は10%ボイド率

キャビティ前縁で気泡発生
キャビティが消えた後に気泡数増大



ボイド率

定性的傾向は一致

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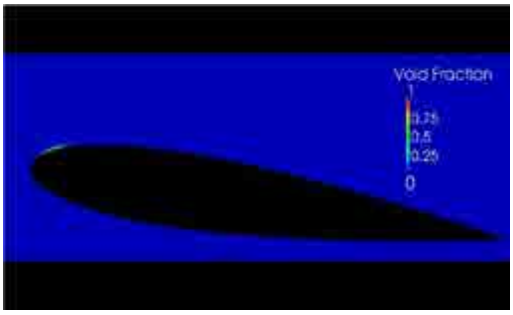
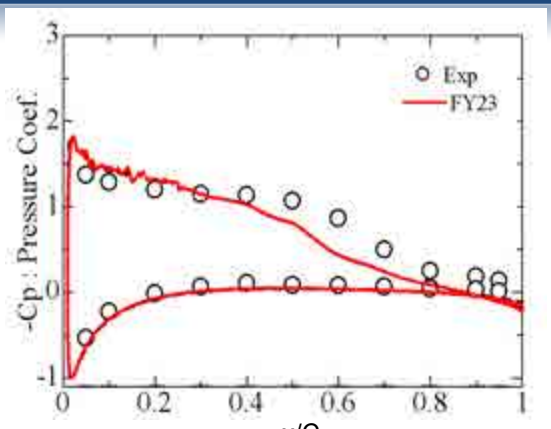
多重プロセスモデルの特性

NACA0015単独翼で検証
ｷｬﾋﾞﾃｰｼｮﾝ数：σ＝1.4



ｷｬﾋﾞﾃｰｼｮﾝの様子
(ボイド率分布)



x：流れ方向座標
C:翼コード長

前縁部での微細キャビティが大規模に成長する特徴は捉えられている
大規模不安定事象の再現は可能だが、規模が小さい

定義

ｷｬﾋﾞﾃｰｼｮﾝ数 $\sigma = \dfrac{P - P_{sat}}{\frac{1}{2}\rho_{in} u_{in}^{2}}$　　圧力係数 $C_P = \dfrac{P - P_{in}}{\frac{1}{2}\rho_{in} u_{in}^{2}}$

3. 気液界面追跡法による現象把握

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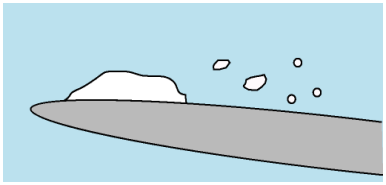
界面追跡法によるキャビテーション計算

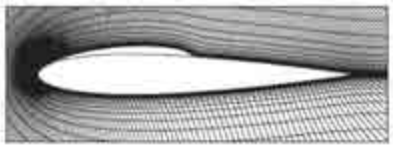
界面追跡モデル



仮定
キャビティ内は完全に蒸気

特徴
- シートキャビテーションを精度よく捉えるための アプローチ
- 研究例は少ない

研究例



re-generation-gridによるシートキャビテーション計算、Tokumasu et al.

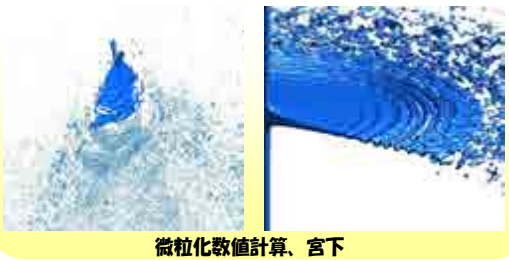
界面追跡的に計算した例は少なく、知見は少ない。
研究例としては、シートキャビテーションを一つの気膜として捉えるモデルであり、キャビテーションの詳細構造を界面追跡的に数値計算した例はない。

計算手法

キャビテーションへの解析アプローチ
- 気液界面流解析コードCIP-LSM（CIP Level Set Method）での流体計算
- 相変化を考慮したことによるキャビティ成長計算

CIP-LSMを用いた計算例

スロッシング数値計算、姫野



微粒化数値計算、宮下

相変化を考慮するときの仮定
- 相変化は界面で生じ、温度差によって駆動される
- 界面では圧力・温度が常に平衡している
- 界面を通過できない熱は全て相変化に使われる

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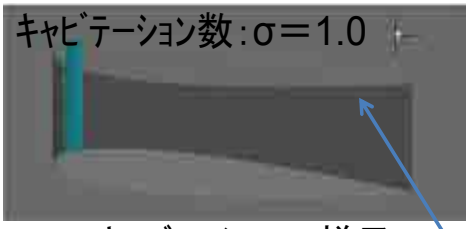
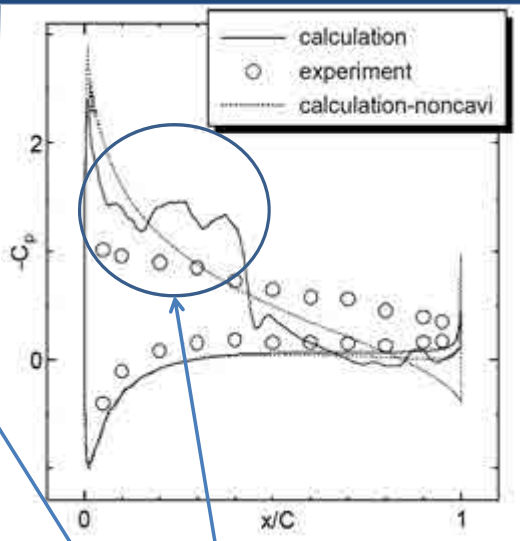
単独翼計算結果

NACA0015単独翼で検証



キャビテーションの様子
(ボイド率0.5%以上を白色)



定義

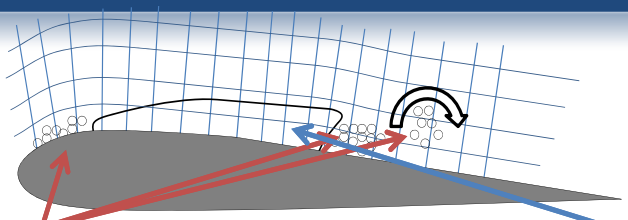
キャビテーション数 $\sigma = \dfrac{P - P_{sat}}{\frac{1}{2}\rho_{in}u_{in}^2}$

圧力係数 $C_P = \dfrac{P - P_{in}}{\frac{1}{2}\rho_{in}u_{in}^2}$

x：流れ方向座標
C：翼コード長

大規模不安定事象の再現は可能
キャビテーション発生部で相違が大きい

2つのアプローチの違い



初生・崩壊・渦部 気泡キャビテーション	発達部 シートキャビテーション
多重プロセス型キャビテーションモデル	界面追跡法
初生部に強いが非定常性が弱い	非定常性が強く発生

これらの特徴双方を包含する巨視的相変化モデルとは？

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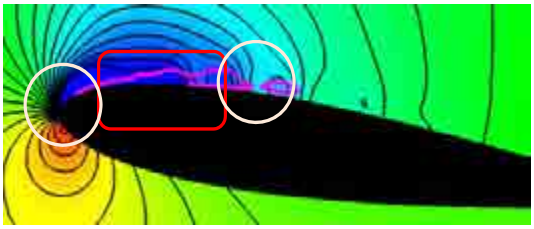
4. 巨視的キャビテーションモデルの評価

巨視的キャビテーションモデル

マクロ視点でのキャビテーション発生状況



マゼンタ色の線
ボイド率10%等値線

初生・崩壊部

気泡流

・合体/分裂の効果は局所的
・相変化量：圧力差に比例

$$\dot{m} = \frac{2a}{2-a}(4\pi M_2)\frac{P_{sat}-P}{\sqrt{2\pi RT}}$$

シート部

界面流

・相変化量：界面の温度差に比例
・飽和温度-圧力関係は局所線形

→ ・相変化量：圧力差に比例

巨視的観点では圧力差駆動の相変化考慮のみで実用上は十分

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巨視的相変化モデル

相変化量 : $m = K_f \rho_l (1-\alpha) + K_b \rho_g \alpha$

$$K_b = \begin{cases} 0 & P < P_v \\ k_b (P - P_v) & P \geq P_v \end{cases}$$

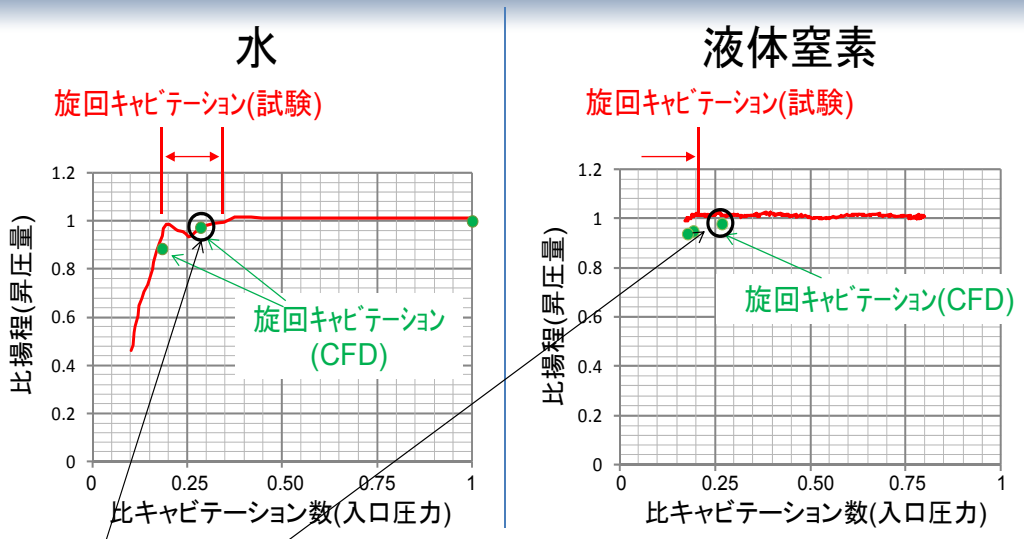
$$K_f = \begin{cases} 0 & P > P_v \\ k_f (P - P_v) & P \leq P_v \end{cases}$$

圧力差で相変化が駆動

検証

翼型より相対的に高速で大スケールのインデューサで検証

インデューサ吸い込み性能比較



双方とも試験結果と良い一致。
極低温での性能向上も捉えられている。
旋回キャビテーション発生範囲も良い一致を示す

次ページで可視化

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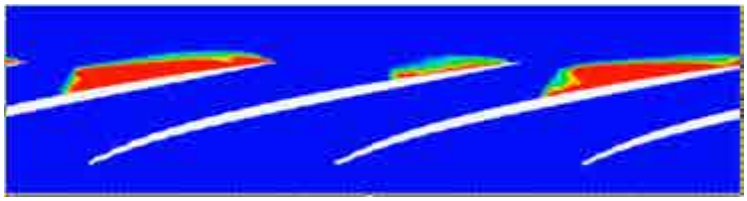
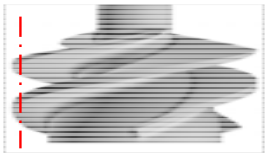
非定常特性比較

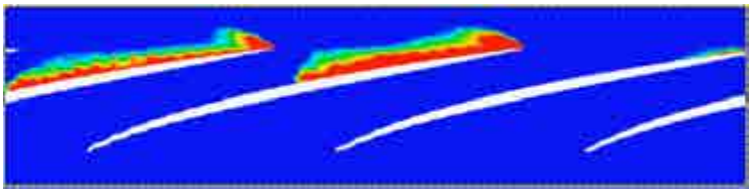
Rotation → 回転座標系上での可視化



水



90%半径での展開図



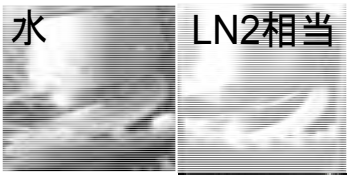
液体窒素

0 ボイド率 0.5

極低温キャビテーションの特徴
キャビティ発生が抑制=ボイド率が低くなる

実験で得られた傾向と等しい

R113での実験(LN2相当)



結論

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結論

極低温インデューサ可視化実験の結果を参考に、
キャビテーション発生状況に応じた2種のモデルを評価

・気泡流に特化した多重プロセス型ｷｬﾋﾞﾃｰｼｮﾝﾓﾃﾞﾙ

初生部に強いが非定常性再現性が弱い

・シートキャビテーション捕獲を主目的とする界面追跡法

非定常性が強く発生するがキャビティ部圧力が異なる

これらの特徴双方を包含する、圧力差で相変化が駆動される
巨視的キャビテーションモデルでインデューサを評価

・試験結果と定量的に良い一致を示し、極低温キャビテーションの特徴も適切に補足

現象理解・・・多重プロセス型 ＋ 界面追跡法ハイブリッド
実用解析・・・巨視的キャビテーションモデルの活用

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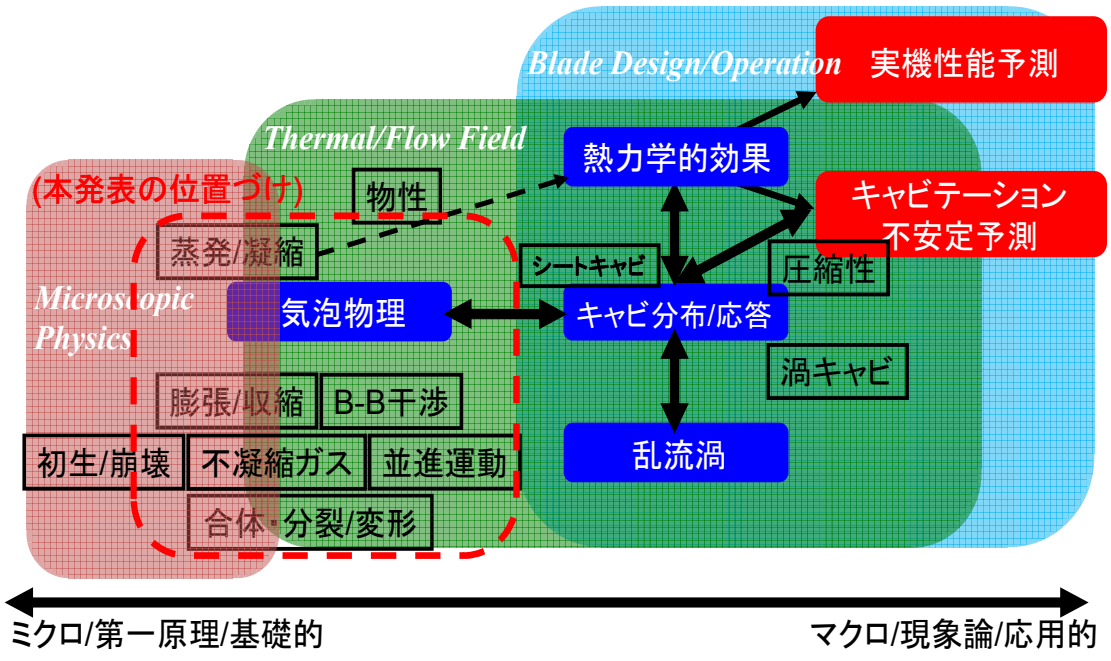
9/26/2012

モーメント法に基づいた 多重プロセス型キャビテーションモデル

津田　伸一 (信州大)

1

キャビテーションに関する相関MAP



2

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キャビテーションモデルの現状

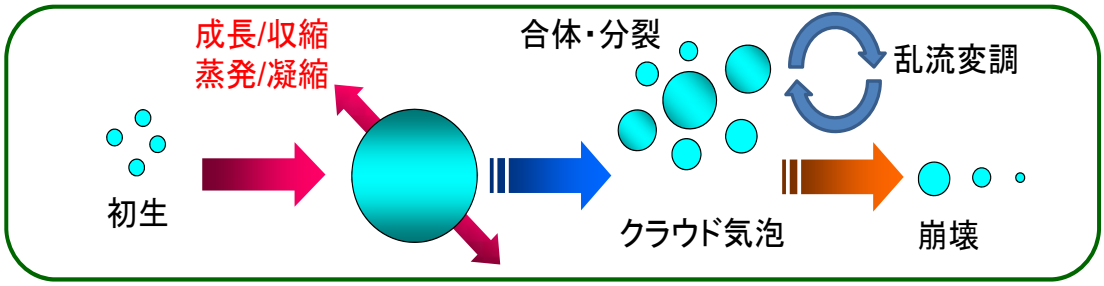
～キャビテーションモデルの分類～

大分類	中分類	小分類
1流体モデル	**状態方程式** $D_{cavi}/L_{cell}<<1$	**バロトロピー型** (混相密度は圧力のみに依存)
		非バロトロピー型 (混相密度は圧力以外にも依存)
	気泡力学 $D_{cavi}/L_{cell}<1$	**膨張/収縮モデル** (Rayleigh-Plesset方程式がベース)
		非平衡蒸発/凝縮モデル (Hertz-Knudsenの式がベース)
2流体モデル	**気泡力学** $D_{cavi}/L_{cell}<1$	Rayleigh-Plesset方程式を厳密に解く
	界面追跡 $D_{cavi}/L_{cell}>>1$	VOF, Level-Set, Front Tracking, etc. 微細な気泡群が占める領域には適用できない

3

本研究の目的

➢ キャビテーションは本質的に多重プロセス/多重スケール



既往のキャビテーションモデルは様々な素過程のほんの一端のみを表現

➢ 目的

キャビテーション現象の多重プロセス性を考慮したモデル(多重プロセス型モデル)による現象再現性の向上

4

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多重プロセス型モデル構築の方針

多重プロセス型キャビテーションモデルは以下の狙いのもとに構築

① キャビテーションの主要な素過程を陽にあらわすモデル
(初生/崩壊, 膨張/収縮, B-B干渉, 蒸発/凝縮, 合体/分裂)

② キャビテーション気泡群の単分散を仮定しないモデル

③ 今後の継続的拡張が容易なモデル

↓

モーメント法を適用

5

モーメント法の概要

"モーメント法"の適用

$$M_i = \int R^i f(R,t) dR \quad \cdots i \text{ th moment of SDF}$$

$f(R,t)$：サイズ分布関数 [m^{-4}]

↓

$for\ \ i = 0,1,2,3 \ \cdots$

M_0 気泡数
M_1 気泡径
M_2 表面積
M_3 気泡体積→ ボイド率

(全て単位体積あたりの量)

6

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モーメント法の概要

サイズ分布に対するモーメントの定義 $M_i = \int R^i f(R,t) dR$

サイズ分布関数(SDF) [m^{-4}]

4方程式モデル(or 5方程式モデル)

$$\frac{DM_i}{Dt} = iG(\overline{R})M_{i-1} + S_{p,i} \quad (for\ i = 0,1,2,3)$$

初生/崩壊, 合体/分裂

where $G(\overline{R}) = \frac{d}{dt}\left(\frac{M_1}{M_0}\right)$

代表半径 (平均半径とする) $\overline{R} = \frac{M_1}{M_0}$

ボイド率やクオリティの計算

(長所)
- SDFを間接的に取り込める(拡張性あり)
- 各素過程を見通しよく取り込める

7

膨張/収縮モデル

- Case1: 簡略化Rayleigh-Plesset方程式

$$G(\overline{R}) = sign\left(p_v - p_l - \frac{2\sigma}{\overline{R}}\right)\left(\frac{2}{3\rho_l}\right)^{1/2}\left|p_v - p_l - \frac{2\sigma}{\overline{R}}\right|^{1/2}$$

- Case2: Rayleigh-Plesset方程式
- Case3: 気泡間干渉を考慮した簡略化Rayleigh-Plesset方程式

$$\left(\frac{3}{2} + \pi\overline{d}^2 M_1\right)G(\overline{R})^2 + \left(\frac{\pi}{2}\overline{d}^2 S_{p,i}\overline{R}^2\right)G(\overline{R}) = \frac{p_v - p_l - 2\sigma/\overline{R}}{\rho_l}$$

$\overline{d}$; characteristic length for each cell (Kubota et al., J. Fluid Mech., 1992)から拡張

キャビテーションモデル

$$\frac{DM_i}{Dt} = iG(\overline{R})M_{i-1} + S_{p,i} \quad (for\ i = 0,1,2,3)$$

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非平衡蒸発/凝縮モデル

Schrageの式(古典的簡略化モデル)の適用

$$\dot{m}_v = \frac{2\alpha}{2-\alpha}\frac{p_{s,in}-p_g}{\sqrt{2\pi R_v' T}} \quad where \quad p_{s,in} = p_v(T)\exp\left(-\frac{2\sigma}{\rho_l R_v' T \overline{R}}\right)$$

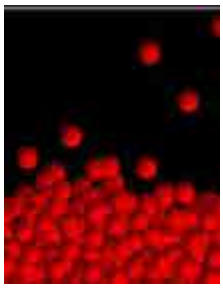
Kelvin効果

$\overline{R}$: M_1/M_0

$where \quad p_g = \rho_g R T_g$

α: 蒸発/凝縮係数

(水の場合, $\alpha = 0.4$)



9

RHS第2項(Spの項)

$$\frac{DM_i}{Dt} = iG(\overline{R})M_{i-1} + S_{p,i} \quad (for\ i = 0,1,2,3)$$

$where$

$$S_{p,i} = \int_{R_c}^{\infty} R^i \frac{D'f}{D't} dR$$

(*t*-*R*座標系におけるLagrange微分)

初生/崩壊，合体/分裂によるSDFの時間発展

$$\therefore\ S_p = \underbrace{S_{p,inception/collapse}}_{\text{初生/崩壊}} + \underbrace{S_{p,fussion/fission}}_{\text{合体/分裂}}$$

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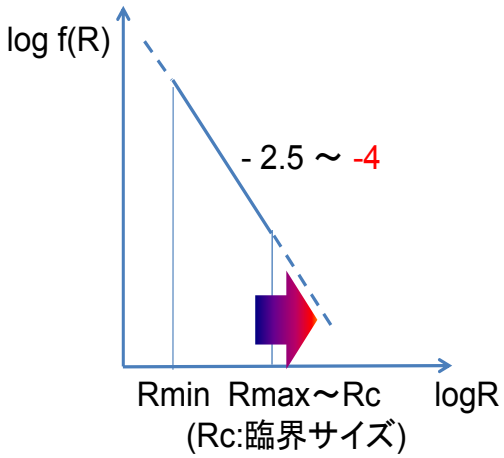
初生/崩壊モデル

➢既存気泡核のサイズ分布に対してべき乗則を仮定(多くの実験的事実と合致)

$$f_0(R)=\frac{3\phi_0}{4\pi(1-\phi_0)\ln(R_{\max}/R_{\min})}R^{-4}$$ (Wang, *J. Fluids. Eng.*, 1999)



for $S_{p,inception}$

$$S_{p,0}=\int_{R_c}^{\infty} f_0(R)\dot{R}\delta(R-R_c)dR$$

$$\therefore S_{p,0}=J_0=f_0(R_c)\dot{R}_c$$

$$(S_{p,i}(i>0)\,can\,be\,negligible.)$$

11

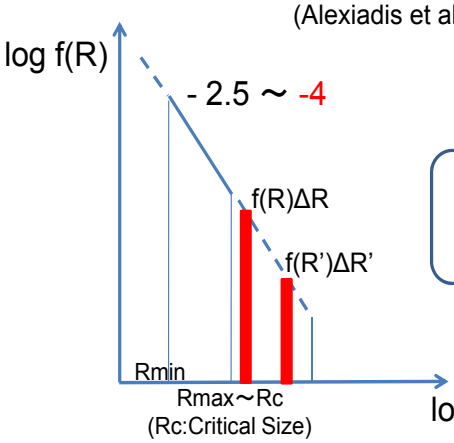
合体/分裂モデル

(合体) 理想気体における分子衝突との類似性から導出
(分裂) 気泡の変形に必要なエネルギバランスから導出

(合体) $S_c\approx\pi\varepsilon^{1/3}\left\{f(R)f(R')(\Delta R)^2\right\}(d+d')^2\left(d^{2/3}+d'^{2/3}\right)^{1/2}$

(分裂) $S_b\approx\frac{1}{d}\sqrt{8.2(\varepsilon d)^{2/3}-12\sigma/(\rho_l d)}$ $\quad where\ d=2R$

(Alexiadis et al., Applied Mathematical Modeling, 2007)などを参考に構築



仮定 (for 水)

- 気泡核のべき乗分布を気泡まで拡張
- ある2つの階層のランダム衝突-合体を仮定

12

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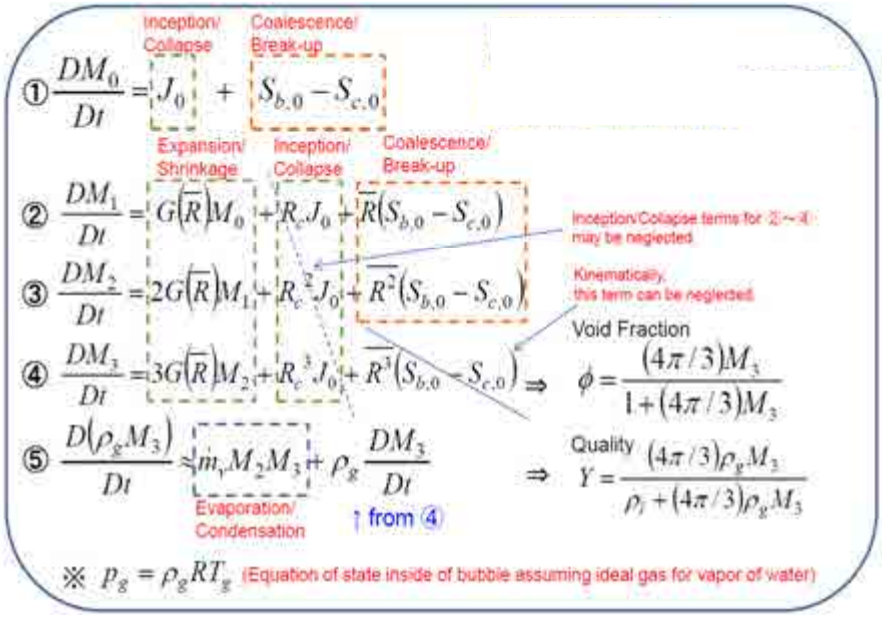
モーメント法に基づいた多重プロセス型モデル

膨張/収縮，非平衡蒸発/凝縮，初生/崩壊，合体/分裂，気泡間相互作用の五つの素過程をモデル化



(S. Tsuda et al., Int. J. Multi-phase Flow, in preparation)
※(津田・谷・山西，機論B, 2012)からの拡張形

13

CFD計算概要(2次元)

CFD計算手法(Tani & Nagashima, 2002)

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho e\end{bmatrix}+\frac{\partial}{\partial x}\begin{bmatrix}\rho u\\ P+\rho u^2\\ \rho uv\\ (\rho e+P)u\end{bmatrix}+\frac{\partial}{\partial y}\begin{bmatrix}\rho v\\ \rho uv\\ P+\rho v^2\\ (\rho e+P)v\end{bmatrix}=Viscous.Term$$

&

状態方程式：Tamman型EOS

解法：Thermo-CCUP法
乱流モデル：Baldwin-Lomaxモデル

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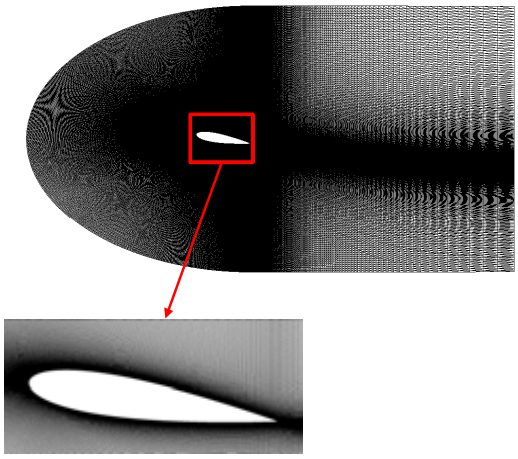
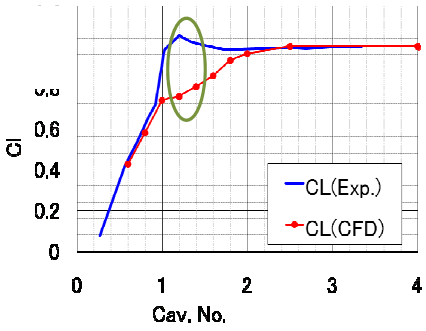
CFD計算概要(2次元)

NACA0015(迎角8deg.), Re = 1.2×10^6
σ=1.8 & 1.4



・C型格子
・格子点数 171,000

NACA0015における
予測精度は総じて低い

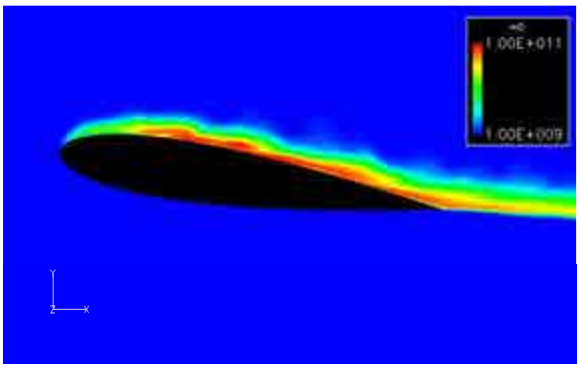


実験と計算の比較例(揚力係数)

15

気泡数密度

実験の様相
(Sakoda et al., 2001)



気泡数密度 (M_0)

気泡数密度の分布は定性的に一致

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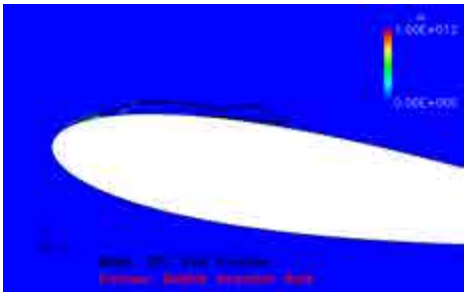
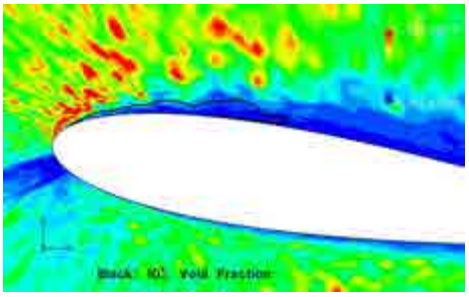
気泡数密度に対する生成項



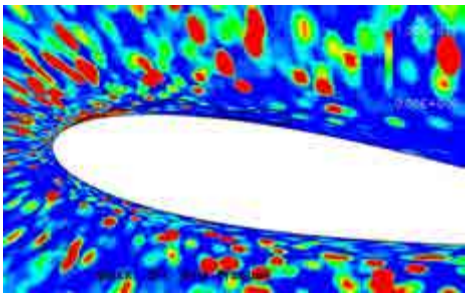
初生速度 J_s [1/s/m^3]



分裂速度 J_b [1/s/m^3]

気泡発生後にキャビティ成長
キャビティ外縁で分裂率(大)
キャビティ前縁で合体率(大)
キャビティ後縁で合体率(小)

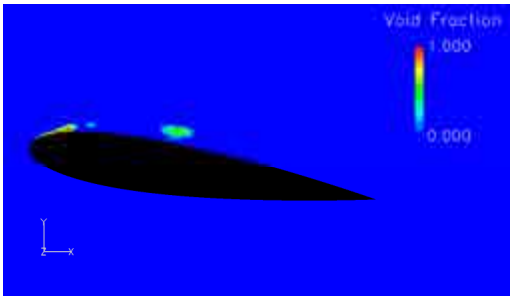
定性的な傾向は一致



合体速度J_c [1/s/m^3]

17

ボイド率分布



BTFモデル
(単分散でかつ気泡数を一定とした膨張/収縮モデル)

多重プロセス型モデル

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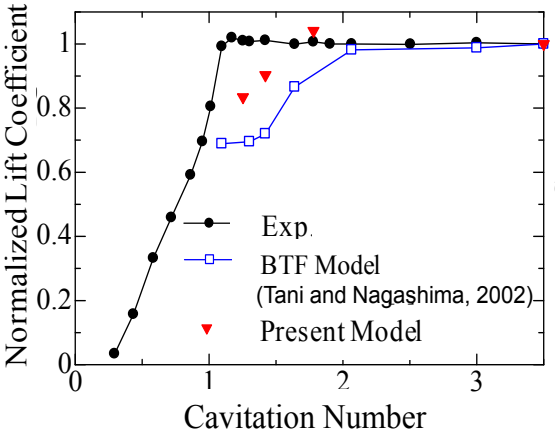
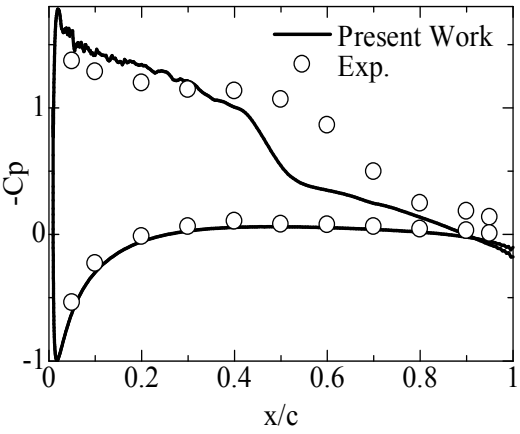
揚力係数および翼面圧力分布



揚力係数比



翼面圧力分布
(σ=1.4)

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まとめ

キャビテーションの主要な素過程を見通しよく導入した多重プロセス型モデルを構築

本モデルのCFD検証結果

- **気泡数の変化は定性的に合致**
- **クラウドキャビテーションの放出も再現(ただし規模は小さい)**
- **揚力係数の再現性は大きく向上(ただし本質的改善には課題)**

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No. 1

インデューサーに発生する液体窒素・水キャビテーションの可視化

東京工業大学
伊藤 優

No. 2

Background

Water Cavitation

In1894
English ship “Daring”

The performance of English ship “Daring” dropped unexpectedly due to water cavitation
→Research in water cavitation started especially in ship engineering field.

Cryogenic Cavitation

In 1999
Broken inducer of H-II rocket

The accident of H-II rocket was caused by unsteady LH_2 cavitation
→The clarification of behavior of cryogenic cavitation has been demanded.

Cavitation prediction method available for pump design is strongly desired associated with CFD simulation, recently.

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Manned Transportation into Space

No. 3

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Soyuz-FG, Russia

Saturn V, USA

HII-B, Japan (freight only)

Launch rocket without solid rocket boosters is ideal for manned mission.
To do this, reliable liquid rocket engines with sufficient thrust are required !!

Cavitation Performance Curve

No. 4

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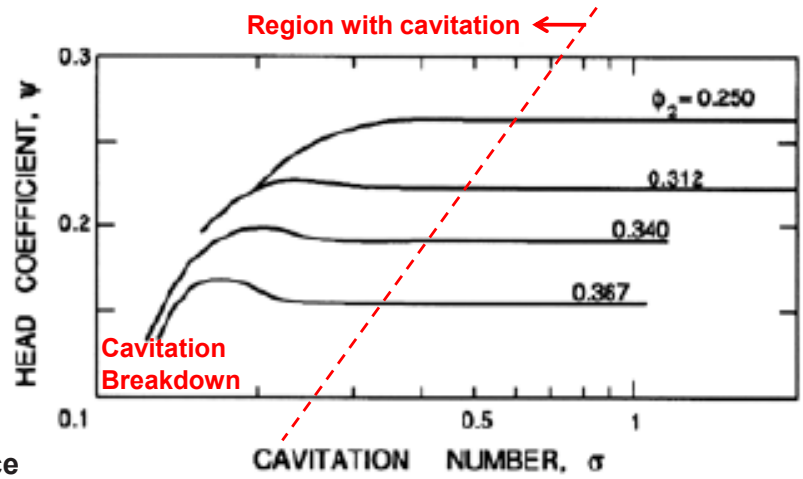
When Cavitation Number (which is a non-dimensional number for Net Positive Suction Head, or NPSH) approaches 0, Cavitation Breakdown occurs. It means that Head Coefficient (which is a non-dimensional number for Pump Head) is 0.
Just before Cavitation Breakdown,
there is a region in which Maximum Head is obtained.

Inducer of Turbo-pump
One of the most important components to decide performance in a liquid rocket engine



Establishment of a Design Method for Cryogenic Inducer Allowing Cavitation

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What is Thermodynamic Effect ??

No. 5

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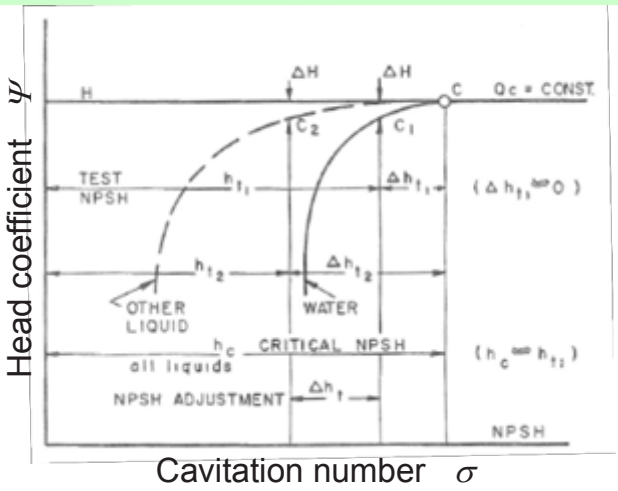
**Cavitation absorbs latent heat from ambient liquid as it grows.
Then, the ambient liquid temperature decreases.
As a result, cavitation growth is suppressed.
This phenomenon is called “thermodynamic effect”.**



**Therefore, it is well known that
fluid with greater thermodynamic effect is less subject to cavitation breakdown.**

What is Thermodynamic Effect ??

No. 6

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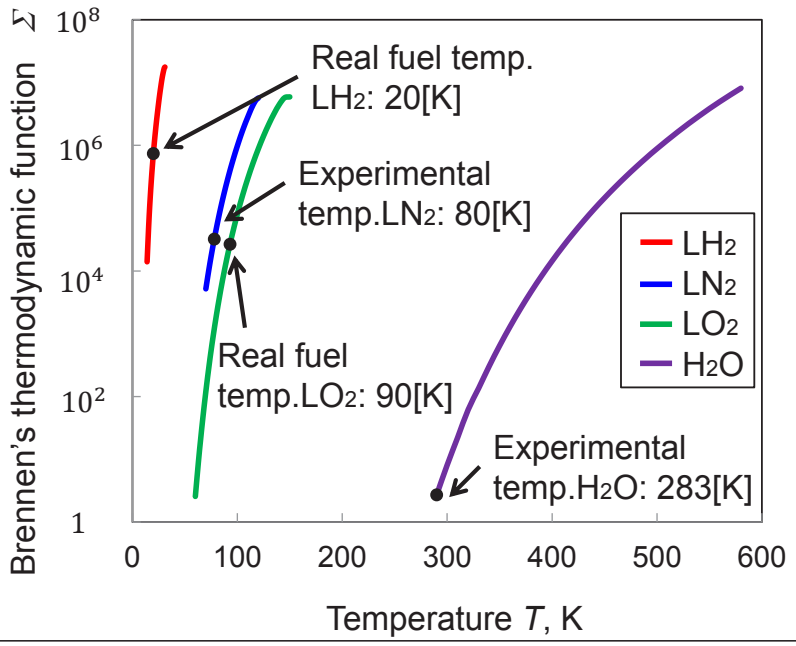
**Cryogenic fluids have greater thermodynamic effect than cold water.
→Cryogenic pump is too high safety margin by using design method for water.
→More efficient cryogenic pump may be available by using specific design method to cryogen.**

Thermodynamic Function

This parameter shows the magnitude of thermodynamic effect. It depends on a variety of fluid and fluid temperature.

$$\Sigma(T_\infty) = \frac{\rho_V^{\,2} L_{LV}^{\,2}}{\rho_L^{\,2} c_{PL} T_{\infty L} \alpha_L^{\frac{1}{2}}} [m/s^{3/2}]$$

ρ_V:vapor density
ρ_L:liquid density
$T_{\infty L}$:liquid ambient temperature
L_{LV}:laten heat
c_{PL}:liquid specific heat
α_L:liquid thermal diffisivity



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Previous Studies

No. 7

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In order to understand cryogenic cavitation in a rotating inducer, its visualization is the best.
However there have been just two examples of visualization of cryogenic rotating inducer due to experimental difficulties.

NASA test facility

It was conducted by liquid hydrogen.

It can be only for liquid nitrogen.

JAXA test facility

The both can not conduct to visualize water cavitation in a rotating inducer and can not compare cryogenic cavitation with water cavitation.

Target of Present Study

No. 8

TOKYO TECH

NASA test facility

Target of Present Study

JAXA test facility

1: Visualize a rotating inducer in liquid nitrogen.
2: Visualize a rotating inducer in water in the same flow geometry. To do this, Keep the tip clearance between the inducer tip & the shroud casing at either of liquid nitrogen temperature & water temperature.
3: Compare cryogenic cavitation results with not only water cavitation results we conducted but also water cavitation results the others conducted.
4: Clarify the thermodynamic effect for a rotating inducer.
5: Feed knowledge back to a efficient cryogenic inducer.

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Schematic View of Test Facility

No. 9

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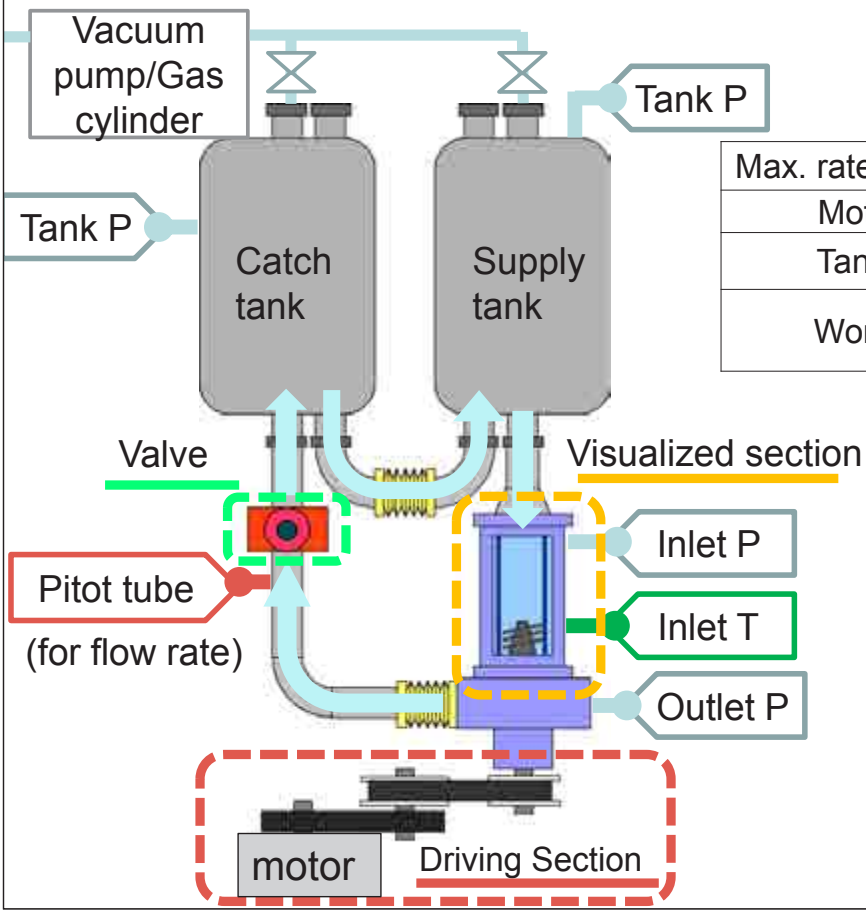

Basic specification

Max. rate of the inducer	6000rpm
Motor power	3.7kW
Tank volume	600L ×2
Working fluid	Liquid nitrogen Water

Inducer =Real LE-5 size

Tip diameter	65.3mm
Number of blade	3
Hub length	52mm
Inlet blade Angle	10°

Test Section for either LN_2 or Water

No. 10

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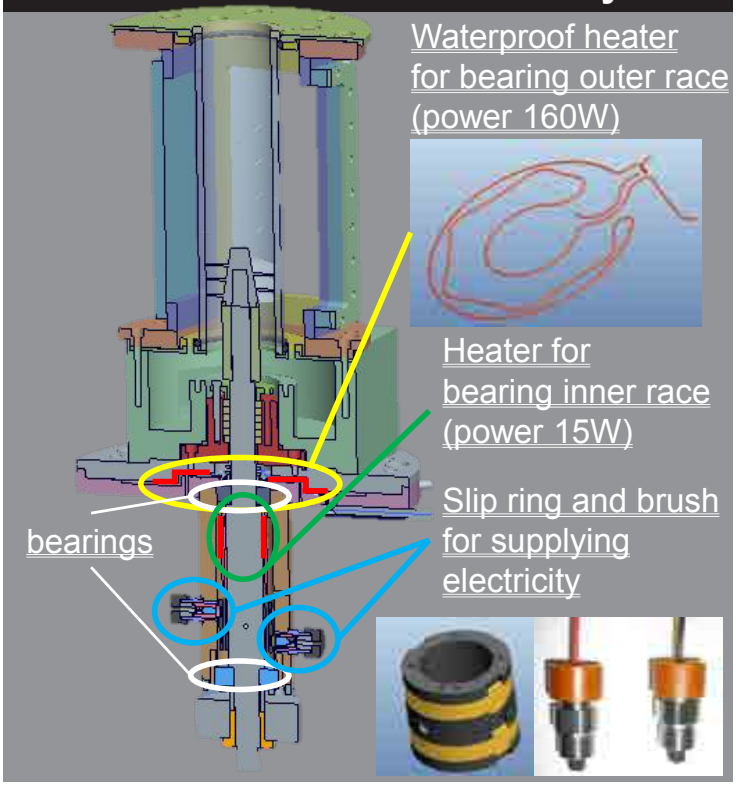
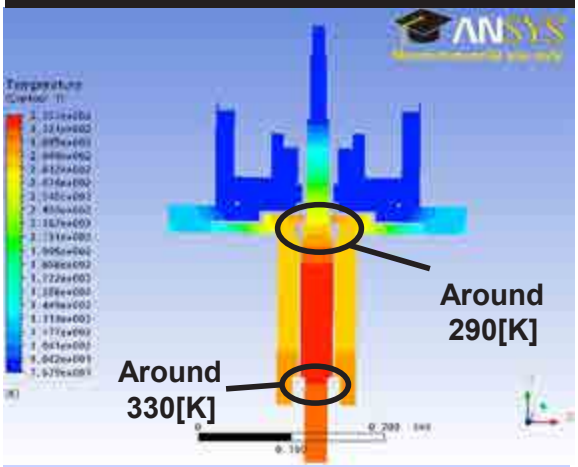
LN2 experiment was failed by ice generation inside bearing.

Section of new test facility



Simulation result of temperature profile



Boundary Condition

- Surfaces in contact with LN_2:76K (isothermal wall)
- Surfaces in contact with atmosphere: T_{atom} =300 & Heat transfer coefficient h=20 [W/m^2K]

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Schematic View of Test Section

No. 11

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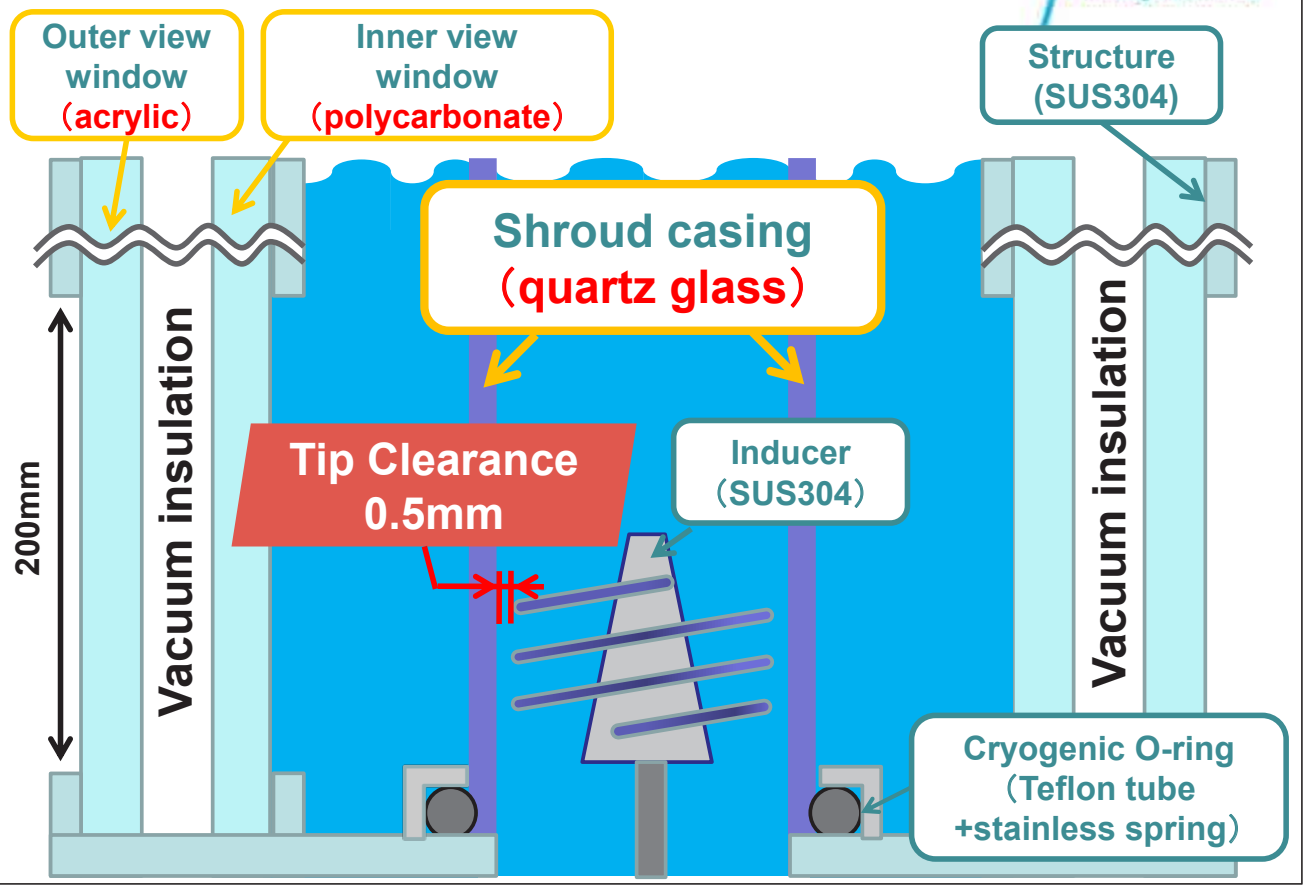

Overview of Test Facility

No. 12

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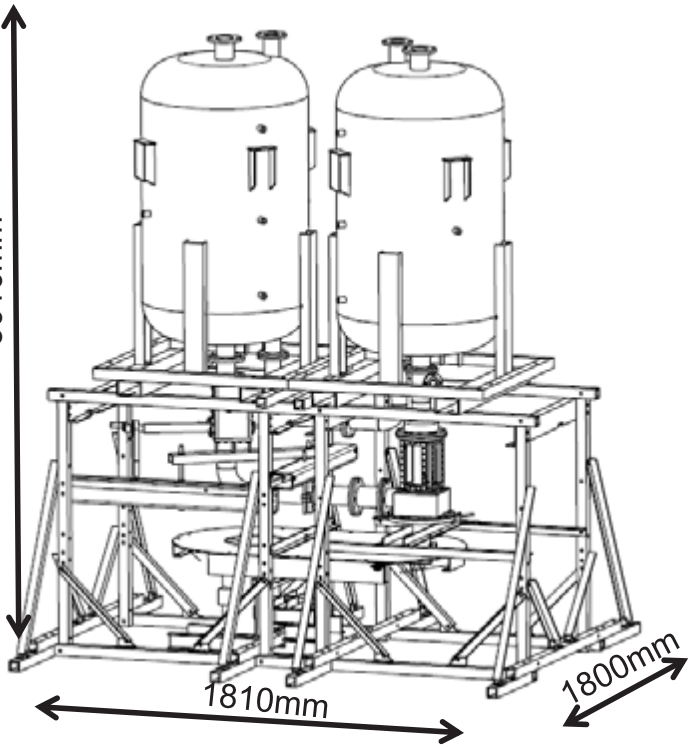
Photo of test facility

Framework drawing



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Cavitation Development with Decrease of Cavitation Number σ

No. 13

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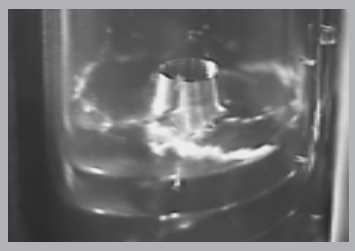
Cold Water

σ=0.49

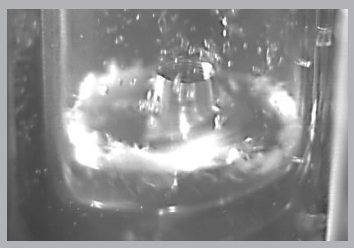
σ=0.072

σ:Large → σ:Small

Liquid Nitrogen



σ=0.075



σ=0.038

Flow coefficient ϕ=0.1

A variety of Cavitation

Tip vortex cavitation: occurs from the leading edge on the tip.

Backflow cavitation: occurs along the blade tip.

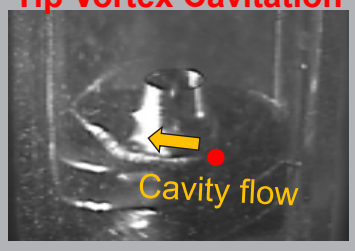
Cavitation Development with Decrease of Cavitation Number σ

No. 14

TOKYO TECH Pursuing Excellence

Cold Water

Tip Vortex Cavitation



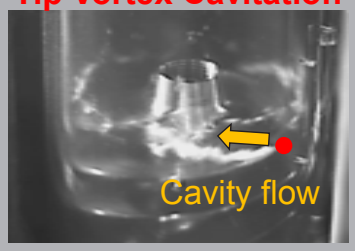
σ=0.49

σ=0.072

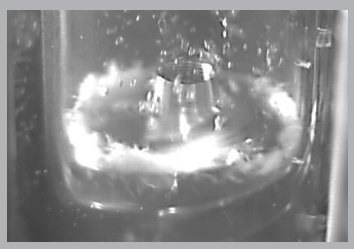
σ:Large → σ:Small

Liquid Nitrogen

Tip Vortex Cavitation



σ=0.075



σ=0.038

Flow coefficient ϕ=0.1

A variety of Cavitation

Tip vortex cavitation: occurs from the leading edge on the tip.

Backflow cavitation: occurs along the blade tip.

Tip Vortex Cavitation

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Cavitation Development with Decrease of Cavitation Number σ

No. 15

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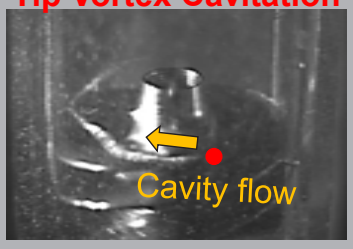
Cold Water

Tip Vortex Cavitation



σ=0.49

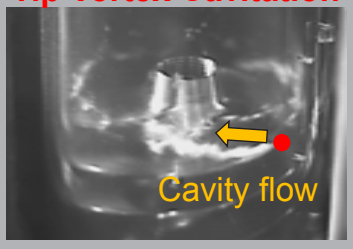
Backflow Cavitation

σ=0.072

σ:Large → σ:Small

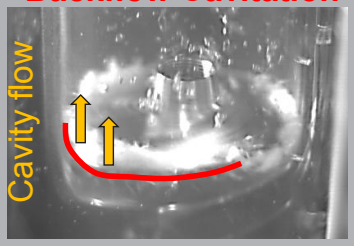
Liquid Nitrogen

Tip Vortex Cavitation



σ=0.075

Backflow Cavitation



σ=0.038

Flow coefficient ϕ=0.1

A variety of Cavitation

Tip vortex cavitation: occurs from the leading edge on the tip.
Backflow cavitation: occurs along the blade tip.

Backflow Cavitation

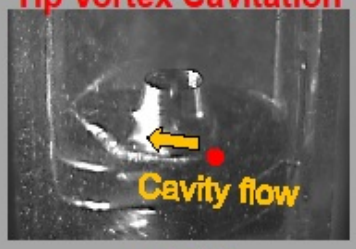
Cavitation Development with Decrease of Cavitation Number σ

No. 16

TOKYO TECH Pursuing Excellence

Cold Water

Tip Vortex Cavitation



σ=0.49

Backflow Cavitation

σ=0.072

σ:Large → σ:Small

Liquid Nitrogen

Tip Vortex Cavitation

σ=0.075

Backflow Cavitation

σ=0.038

Flow coefficient ϕ=0.1

A variety of Cavitation

Tip vortex cavitation: occurs from the leading edge on the tip.
Backflow cavitation: occurs along the blade tip.

In both fluids, cavitation develops from tip vortex cavitation through backflow cavitation to breakdown. The same trend is observed at any ϕ.

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Tip Vortex Cavitation

No. 17

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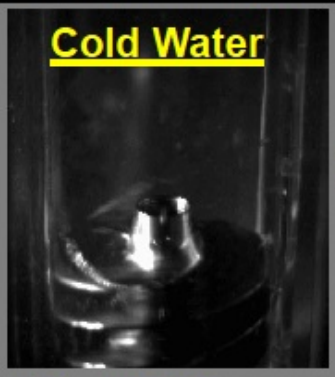
At any σ, ϕ and a variety of cavitation, the same brightness difference was observed.

Cavitation at high σ

Cold Water

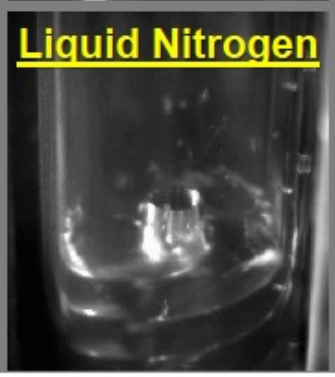


ψ=0.30, ϕ=0.099

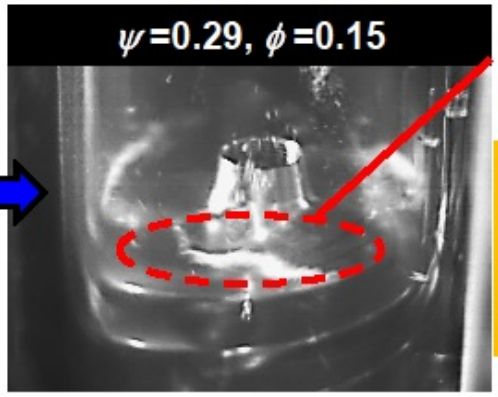
Cavitation brightness is moderate.

Cavitation consists of big bubbles, so it contains small surface area per unit volume. Light reflection is low.

Liquid Nitrogen



ψ=0.29, ϕ=0.15



Cavitation brightness is clear.

Cavitation consists of small bubbles, so it contains large surface area per unit volume. Light reflection is high.

Backflow Cavitation

Weber No. $We = \frac{\rho_L u^2 D}{\sigma}$

No. 18

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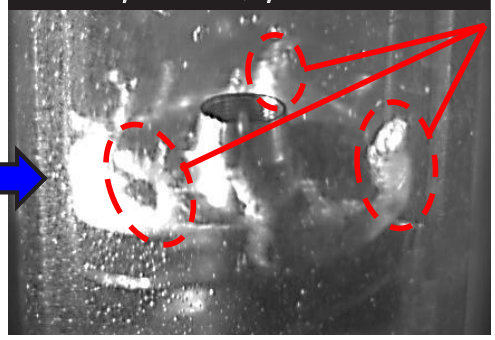
Linearly stretched backflow cavitation is not observed in cold water but in liquid nitrogen.

Cavitation at low σ

Cold Water

ψ=0.11, ϕ=0.13

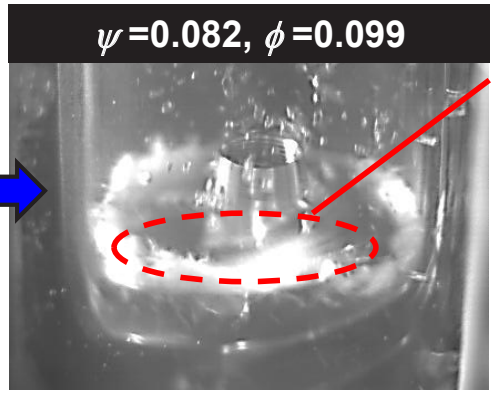


There are lots of linearly stretched backflow cavitation.

Higher Weber number of each cavitation bubble due to a bigger bubble

Liquid Nitrogen

ψ=0.082, ϕ=0.099



There is not linearly stretched backflow cavitation.

Lower Weber number of each cavitation bubble due to a smaller bubble

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No. 19

Water Pump Falls into Breakdown, But Nitrogen Pump Still Works.

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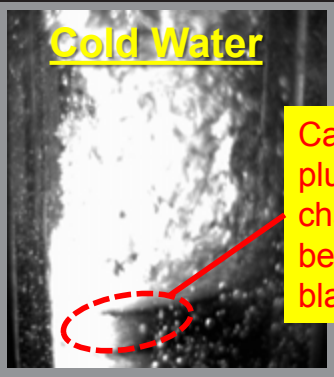
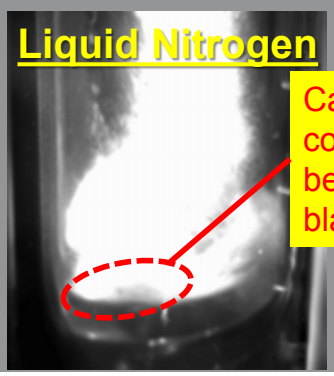
Big water bubbles can not condense, but small liquid nitrogen bubbles can condense.

Cavitation at $\sigma \approx 0$



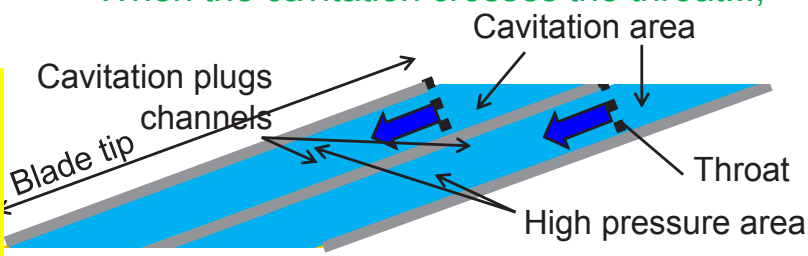
Cavitation plugs channels between blades.



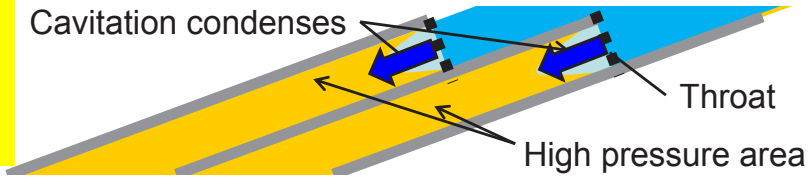
Cavitation condenses between blades.

Developed figure along blade tips

When the cavitation crosses the throat...,



Cavitation plugs channels between blades because cavitation bubbles are big.
Therefore, the pump does not work.



Cavitation condenses between blades because cavitation bubbles are small.
Therefore, the pump works.

No. 20

Cavitation on the Hub

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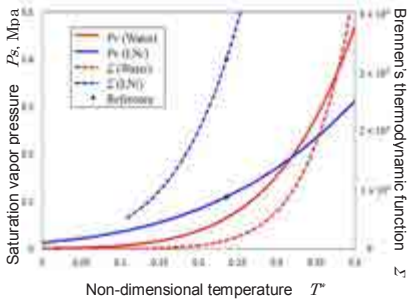
There are some cavitation on the hub in liquid nitrogen, but there no cavitation in water.

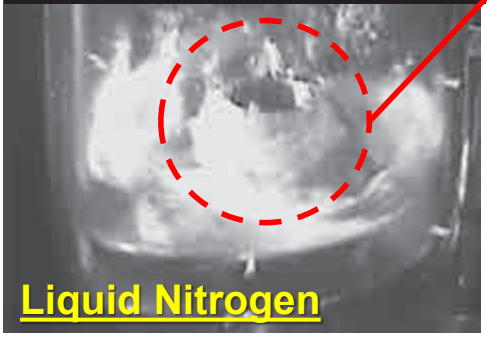
ψ=0.11, ϕ=0.11

There is no cavitation.

45.1K increase of temperature is required to genarate cavitation at stationary flow region. It is because there is the flat gradient of saturation vapor pressure curve at the lower non-dimensional temperature T^*.



ψ=0.17, ϕ=0.12



There are some cavitation on the hub.

Just 0.6K increase of temperature is required to genarate cavitation at stationary flow region. It is because there is the steeper gradient of saturation vapor pressure curve at the higher non-dimensional temperature T^*,

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Performance Curve

No. 21

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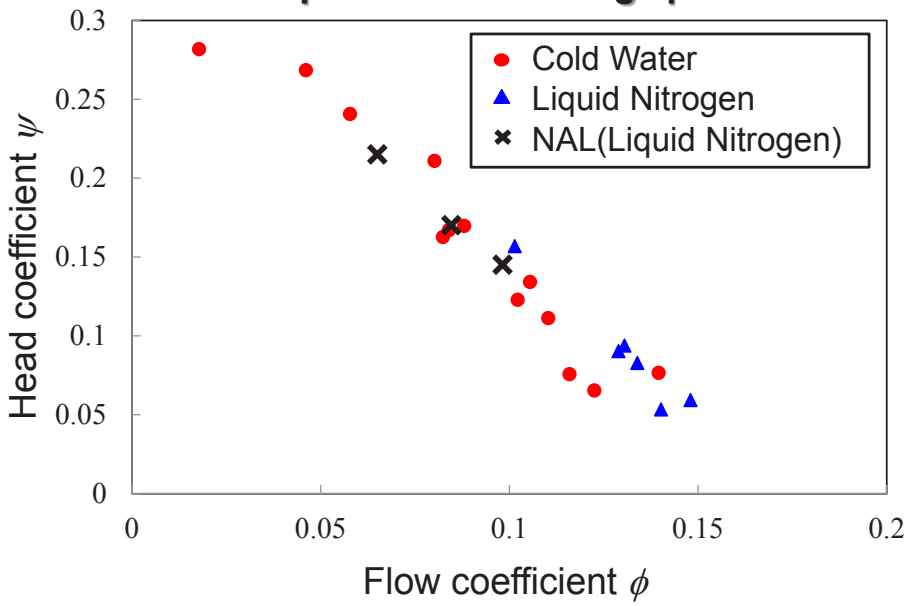
ϕ-ψ curve depends only on inducer geometry in non-cavitating condition. This curve is independent of rotating speed and a variety of fluids.



Flow Coefficient ϕ

$$\phi = \frac{Q}{AR_T\Omega}$$

Head Coefficient ψ

$$\psi = \frac{\Delta P}{\rho_L R_{T_2}{}^2 \Omega^2}$$

Q : Flow rate, m^3/s
A : Crosssectional Area, m^2
R_T : Tip radius, m
Ω : Angular speed, rad/s
ΔP : Head, Pa
ρ_L : Liquid density, kg/m^3

The data are a little bit scattering along the performance curve corresponding to the previous experiments by NAL (present JAXA). It means that the measured data are not sufficient, but not bad.

Cavitation Performance Curve at Constant Flow Coefficient

No. 22

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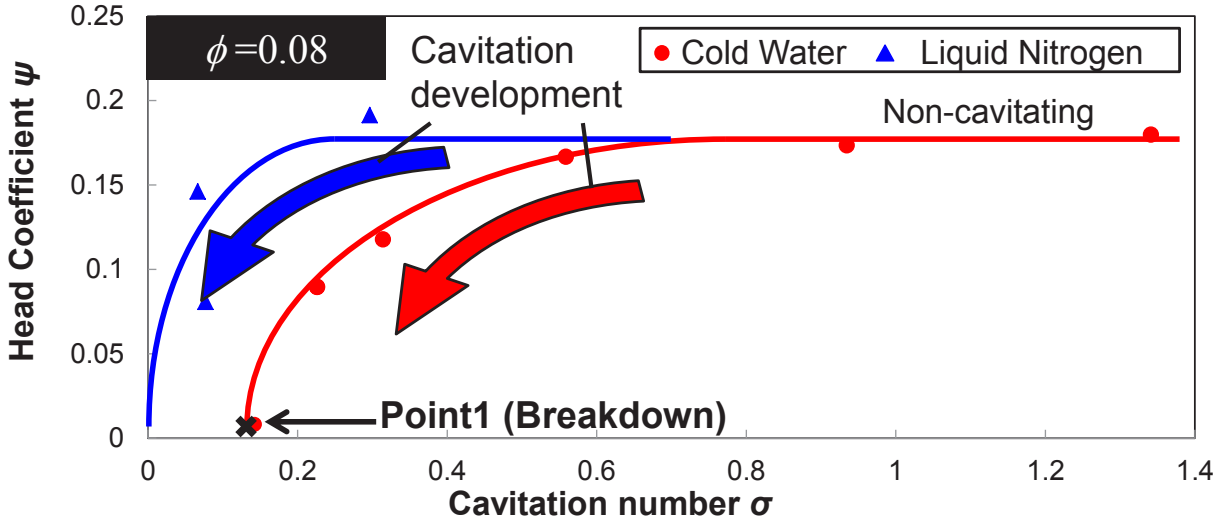

Cavitation Number σ

σ is index of cavitation possibility.

$$\sigma = \frac{p_1 - p_v}{\frac{1}{2}\rho_L U^2}$$

p_1 : Inlet static pressure
p_v : Saturated vapor pressure
U : Tip blade velocity ($R\Omega$)

By normal camera	By high-speed camera

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Conclusion

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As a result, the following three results were obtained.

- The same performance curve in liquid nitrogen and water at 6000 rpm is obtained as previous experimental results by NAL (present JAXA) using the same inducer in liquid nitrogen at 16500 rpm. It means that measured pump heads and flow rates are not bad.

- Liquid nitrogen cavitation consists of much smaller bubbles than the water cavitation bubbles. The small bubble cavitation may cause "thermodynamic effects," which decrease cavitation number or NPSH at cavitation breakdown compared with water values.

- Only in liquid nitrogen experiments, hub cavitation occurs. At the higher non-dimensional temperature T^*, there is the steeper gradient of saturation vapor pressure curve. In addition, at the higher T^*, there is the larger Brennen's thermodynamic effect function Σ, namely, fluid has the greater thermodynamic effect. Therefore, in cases of fluid with greater thermodynamic effect, hub cavitation more easily occurs due to heat inflow.

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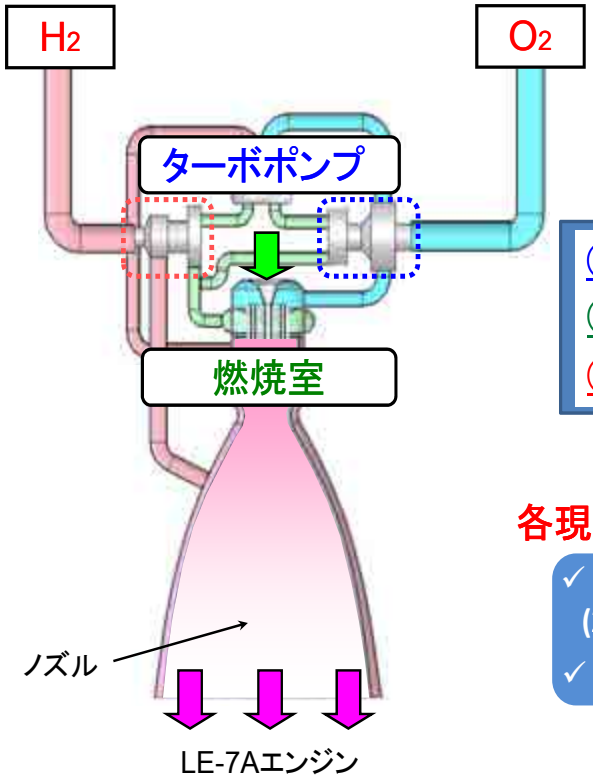
水素と酸素の極低温物性分子シミュレーション

越　光男 (東大)
津田　伸一 (信州大)

1

液体ロケットエンジン内部の熱流体現象に対する横断的特性



①極低温キャビテーション
②高圧噴射・微粒化
③高圧燃焼

各現象に対する横断的特性は？？

- ✓ 幅広い温度/圧力領域
  (20K ~ 4,000K, 0.1MPa ~ 30MPa)
- ✓ 状態方程式の適用が必要不可欠

「熱・輸送物性」

2

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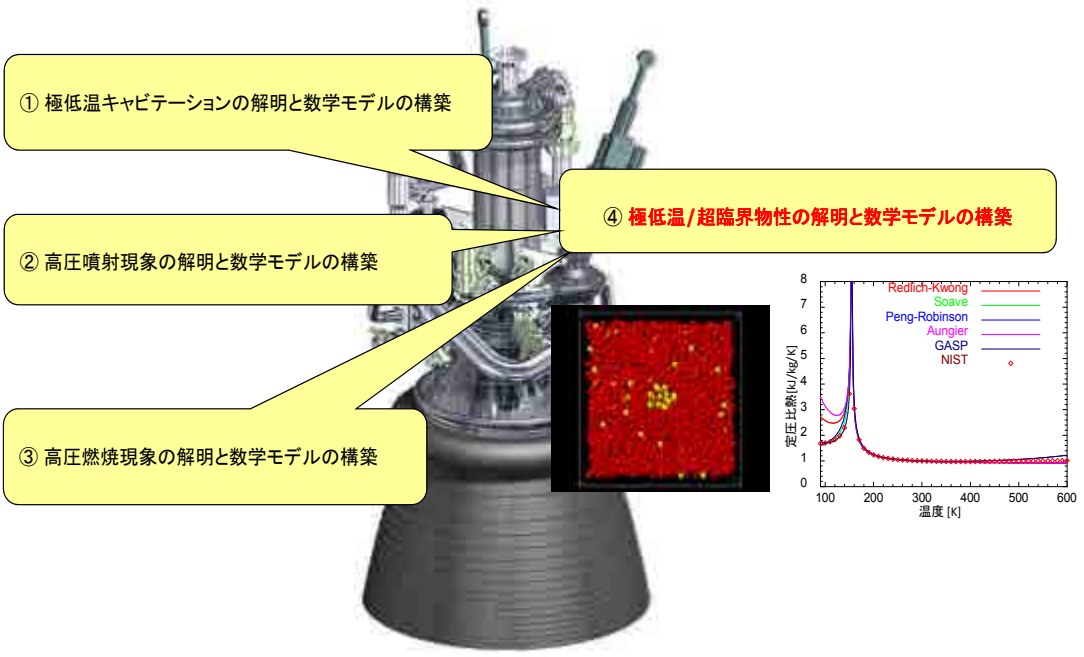
他の研究テーマとの関係性



～本研究は他の3テーマを横断的に結ぶ重要課題～
(物性解明は現象再現性の底上げに必要)

3

物性(熱物性や輸送物性)に対する研究手法

(1) 実験的アプローチ
- 位置づけ:伝統的でかつ最も有効なアプローチ法
- 現状: 極低温・超高圧のロケット推進剤(特に混合系)では実験値が非常に乏しい

(2) 統計物理学(ミクロ力学 + 確率・統計論)的アプローチ
- 位置づけ:第2のアプローチ法
  非理想性を反映する分子間相互作用モデルが重要
- 現状: 経験的モデルの使用が大多数
  様々な物性値の普遍的再現には限界

本研究では(2)のアプローチ法を採用し,
かつ非経験的手法を取り入れることで精度向上を図る

4

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研究目的・項目・方法

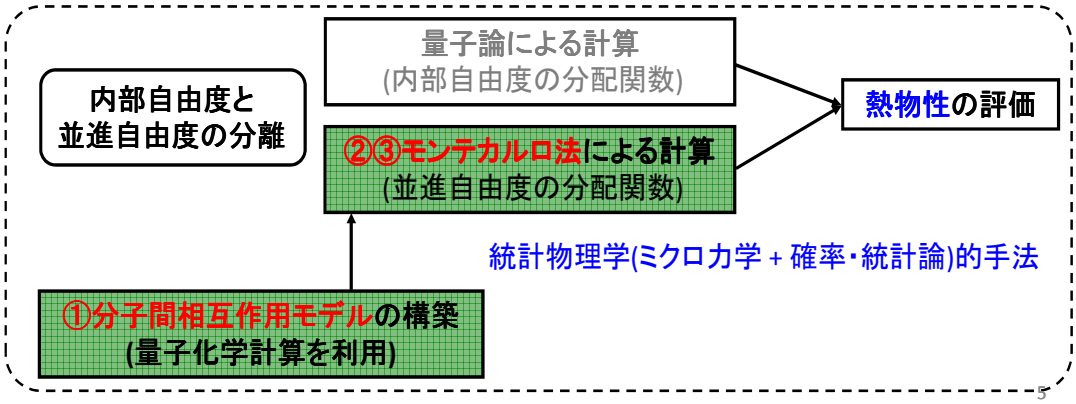
➢**研究目的**

ロケット推進剤に対する
高精度な分子間相互作用モデルによる熱物性評価手法の構築および物性解明

➢**研究項目**

① 分子間相互作用モデル(ポテンシャル)の構築
② 単成分系(水素・酸素)における再現性検証
③ 酸水素混合系の熱物性評価および課題抽出

➢**研究の流れ**



5

① 分子間相互作用モデル(ポテンシャル)の構築

6

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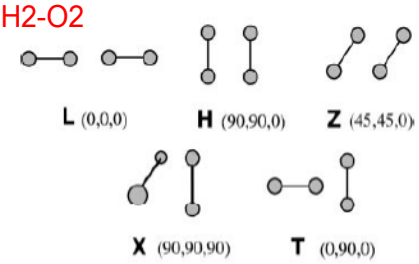
量子化学計算(分子軌道計算)

- 計算方法(GAUSSIAN03を使用)

- 計算対象 ; H2-H2, O2-O2(五重項のみ), H2-O2
- 電子相関近似; RCCSD(T)
- 基底系 ; aug-cc-PVQZ
- 配向 ; L, H, X, T, and Z型



(基底系の比較)

(Patkowski et al., 2008)

	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pV5Z
H2	2s,1p	3s,2p,1d	4s,2p,2d,1f	5s,4p,3d,2f,1g
O2	3s,2p,1d	4s,3p,2d,1f	5s,4p,3d,2f,1g	6s,5p,4d,3f,2g,1h

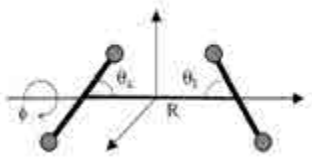
(Bartolomei et al., 2008)

7

ポテンシャル関数形(H2-H2, O2-O2, H2-O2)

(M. Koshi, S. Tsuda, K. Shimizu, Mol. Sim, 2012)

$$V(R,\theta_a,\theta_b,\phi)=4\pi\sum_{l_a l_b l} V^{l_a l_b l}(R)Y^{l0}_{l_a l_b}(\theta_a,\theta_b,\phi)$$



$$V(R,\theta_a,\theta_b,\phi)=V^{000}(R)+\sqrt{5}[V^{202}(R)P_2^0(\cos\theta_a)+V^{022}(R)P_2^0(\cos\theta_b)]$$
$$+\frac{\sqrt{5}}{12}\left[V^{220}(R)+2\sqrt{\frac{5}{14}}V^{222}(R)+\sqrt{\frac{1}{14}}V^{224}(R)\right]P_2^2(\cos\theta_a)P_2^2(\cos\theta_b)\cos 2\phi$$
$$+\frac{\sqrt{5}}{3}\left[V^{220}(R)-\sqrt{\frac{5}{14}}V^{222}(R)-4\sqrt{\frac{1}{14}}V^{224}(R)\right]P_2^1(\cos\theta_a)P_2^1(\cos\theta_b)\cos\phi$$
$$+\sqrt{5}\left[V^{220}(R)-2\sqrt{\frac{5}{14}}V^{222}(R)+6\sqrt{\frac{1}{14}}V^{224}(R)\right]P_2^0(\cos\theta_a)P_2^0(\cos\theta_b)$$

→ 5-term or 6-term potentials (V000, …, V224)

5つないし6つの代表的な分子配向に対する量子化学計算結果を球面調和関数展開により再現(分子間ポテンシャル)

8

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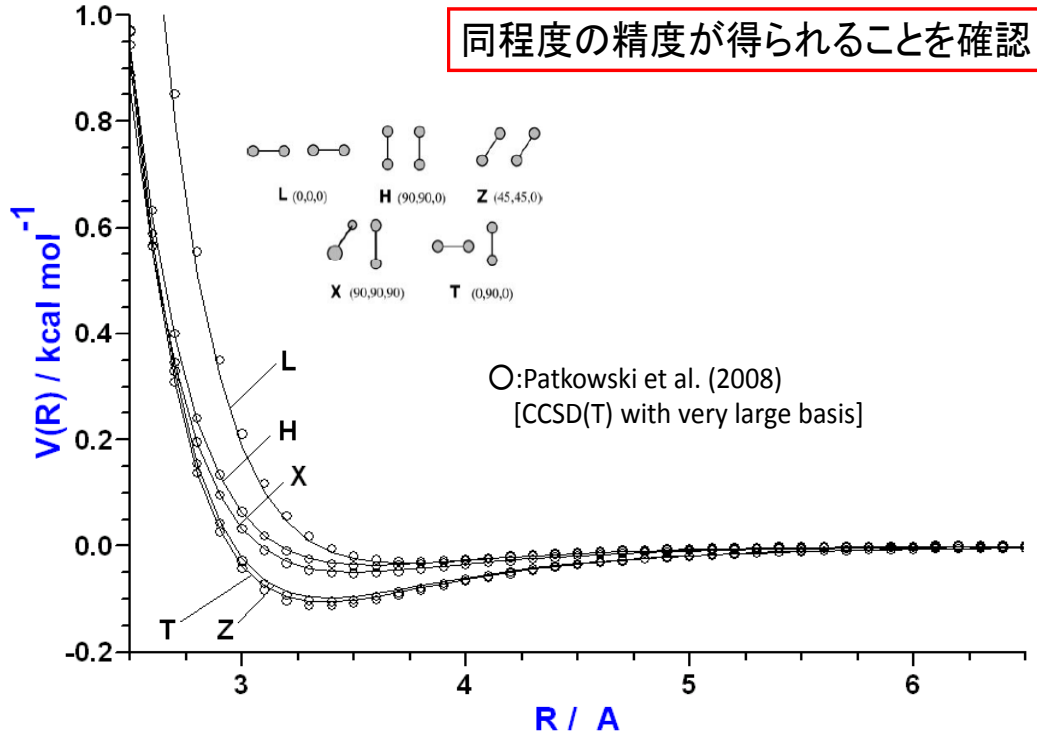
H_2-H_2ポテンシャル(先行研究との比較)

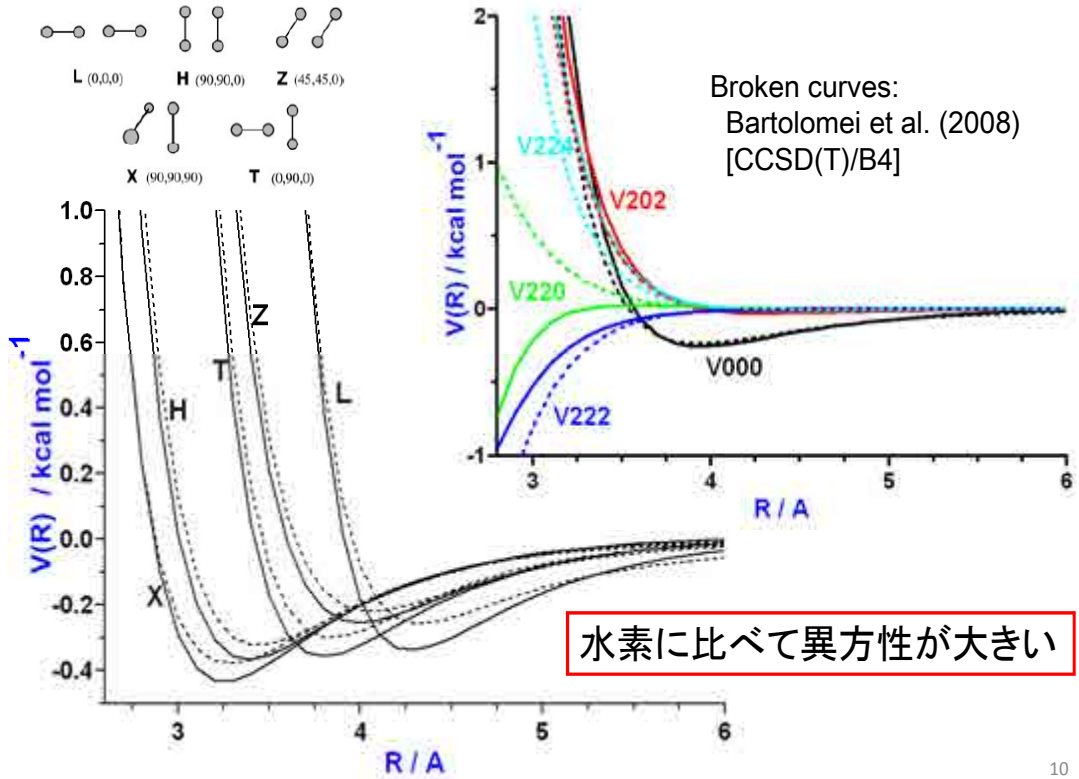
同程度の精度が得られることを確認



○:Patkowski et al. (2008)
[CCSD(T) with very large basis]

9

O_2-O_2ポテンシャル(先行研究との比較)



Broken curves:
Bartolomei et al. (2008)
[CCSD(T)/B4]

水素に比べて異方性が大きい

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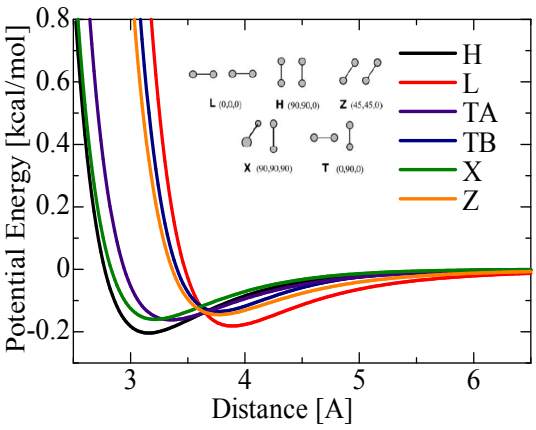
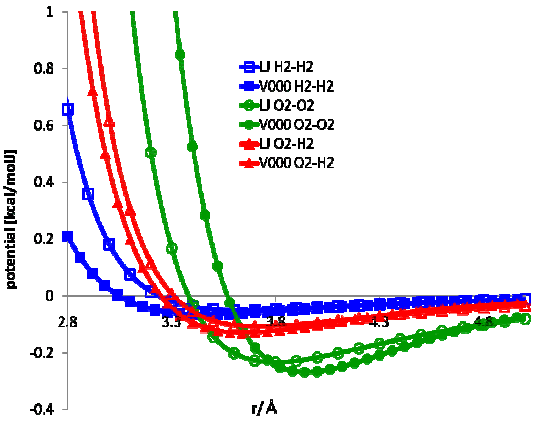
H_2-O_2ポテンシャル(aug-cc-pVQZ)



H_2-O_2ポテンシャル曲線



経験的モデルとの比較

- 水素単成分系に比べると異方性の影響が大きい
- 最もよく知られている経験的モデルの限界を示唆

11

まとめ

先行研究と同等程度以上の近似レベルによる
量子化学計算を実施

- 水素については妥当な精度が得られていることが期待
- 酸素については異方性が大きく,
  本研究で構築したポテンシャルには課題がある可能性
  ⇒Bartolomei et al.(29項展開)と比較することで検討
- 異種分子間(酸素-水素)についても異方性が大きく,
  また経験的モデルによる評価には限界があることが示唆

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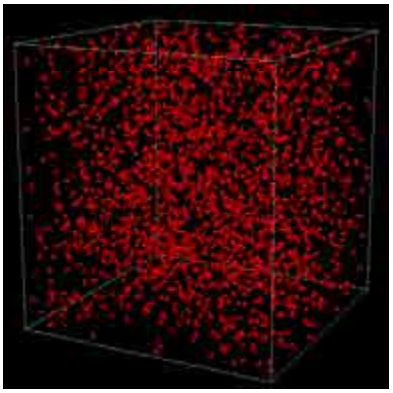
② 単成分系(水素・酸素)における再現性検証

13

熱物性の評価方法

～古典統計物理にもとづいたモンテカルロ計算を実施～

- 分子モデル; 剛体回転子モデル
- 分子間相互作用; 非経験的ポテンシャル with カットオフ距離(12Å)
- 統計集団; NVT(密度と温度を指定)
- サンプリング法; Metropolisの方法
- 境界条件; 周期境界条件
- 分子数; 500 ~ 2,048
- MCステップ数: 20,000 ~ 100,000



14

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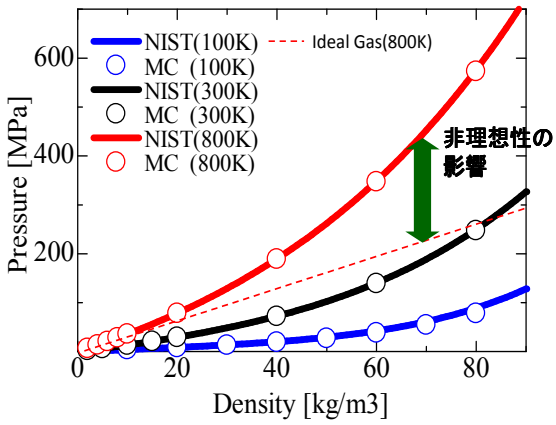
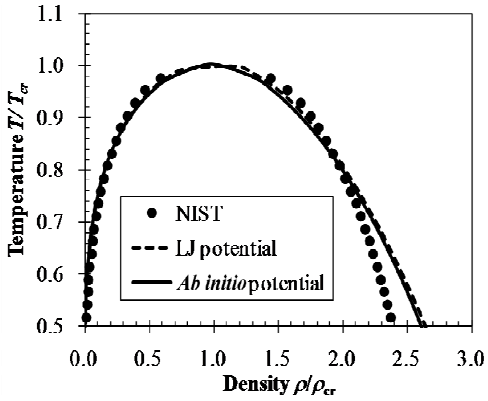
水素の熱物性評価結果





(Nagashima et al., Mol. Sim., 2012)

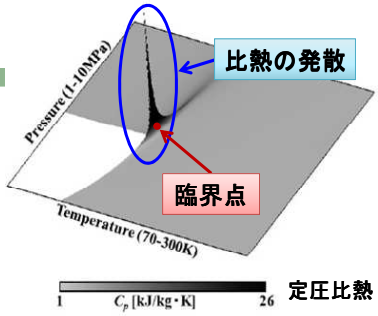
MC計算結果とNISTデータの比較

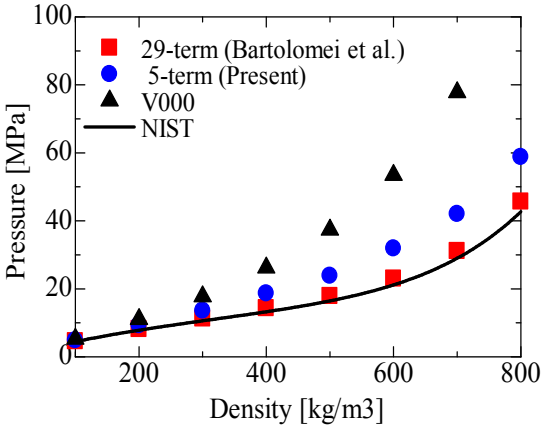
- 超臨界領域での物性予測精度は極めて良いことを確認
  (分子間ポテンシャルの精度はじゅうぶん)
- 逆に亜臨界領域での再現性は良くないことが確認
  (分子間ポテンシャルではなく，古典統計物理による手法の適用限界が原因)

15

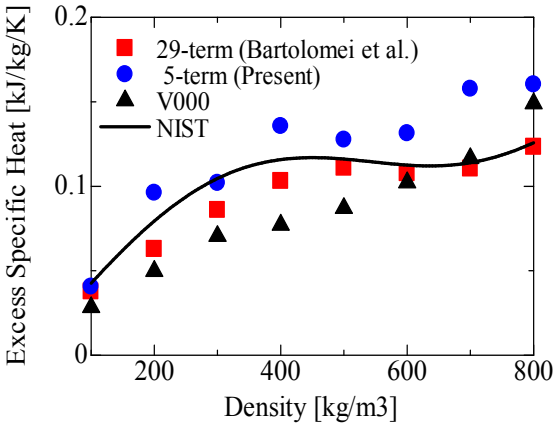
酸素の熱物性評価結果(超臨界)

再現性の確保には30項近い展開項が必要
(酸素の場合，異方性の反映が必要不可欠)





P-V-T関係



余剰比熱

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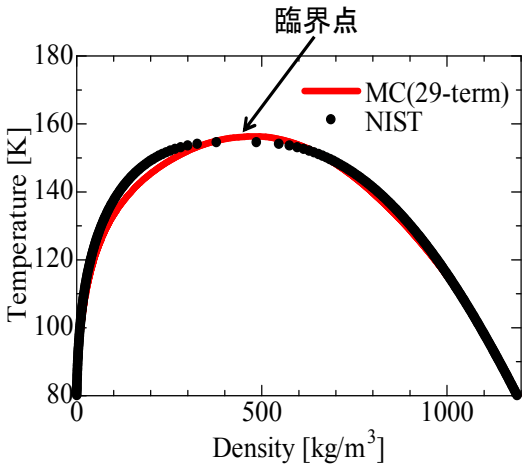
酸素の熱物性評価結果(亜臨界)



30項近い展開項を適用することで
非常によい再現性が得られる

（ただし，五重項以外のスピン多重度や
多体効果の定量的影響は不明）

[参考] 臨界点の比較

	Tc [K]	ρc [kg/m3]	Pc [MPa]
計算	156	480	6.4
実験	154.58	436.14	5.043

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まとめ

古典統計物理にもとづいたモンテカルロ計算により
熱物性値の再現性を評価

- 水素については非常に良い精度が得られるいっぽうで，
  極低温(亜臨界)では量子統計物理の適用が必要不可欠
- 熱物性値に対する酸素の異方性が大きいことを具体的に提示
  (30項近い展開項を用いることで非常に良い再現性を確保)

ただし高密度領域で重要になる五重項以外のスピン多重度や
多体効果の定量的影響は不明

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③ 混合系の熱物性評価および課題抽出

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ロケットエンジン内部流れ解析用のEOSと混合則

エンジン燃焼室内部流れの解析で使用されている
典型的な状態方程式

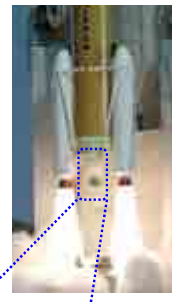
SRK(Soave-Redlich-Kwong)-EOS

- エンジン燃焼室内部流れで最も使用されているvdW型EOS
- 水素/酸素単成分系の実験データにより精度が判明
- 多成分系への適用には**混合則**が必要

＋

古典的混合則

- エンジン燃焼室内部流れで最も使用されている混合則
- 燃焼室内部を対象とした混合系の物性データが皆無のため精度検証が進んでいない



H-IIAロケット

LE-7A エンジン

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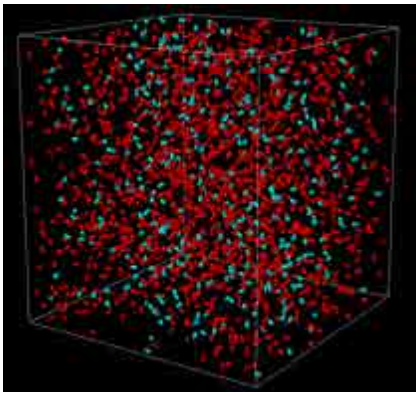
熱物性の評価方法

～評価対象はP-V-T関係および余剰比熱～

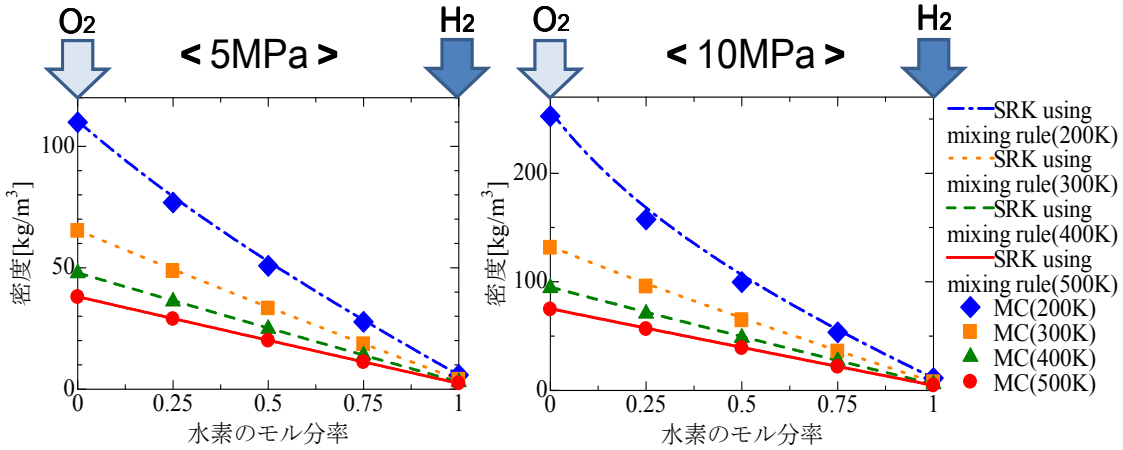
- 分子モデル; 剛体回転子モデル
- 分子間相互作用; 非経験的ポテンシャル with カットオフ距離(12Å)
- 統計集団; NPT(圧力と温度を指定)
- サンプリング法; Metropolisの方法
- 境界条件; 周期境界条件
- 分子数; 500 ~ 2,048
- MCステップ数: 20,000 ~ 100,000



21

酸水素混合系における比較

検証結果①＜P-V-T 関係＞



MC計算結果と古典的混合則を適用した
SRK-EOSの結果は良い一致

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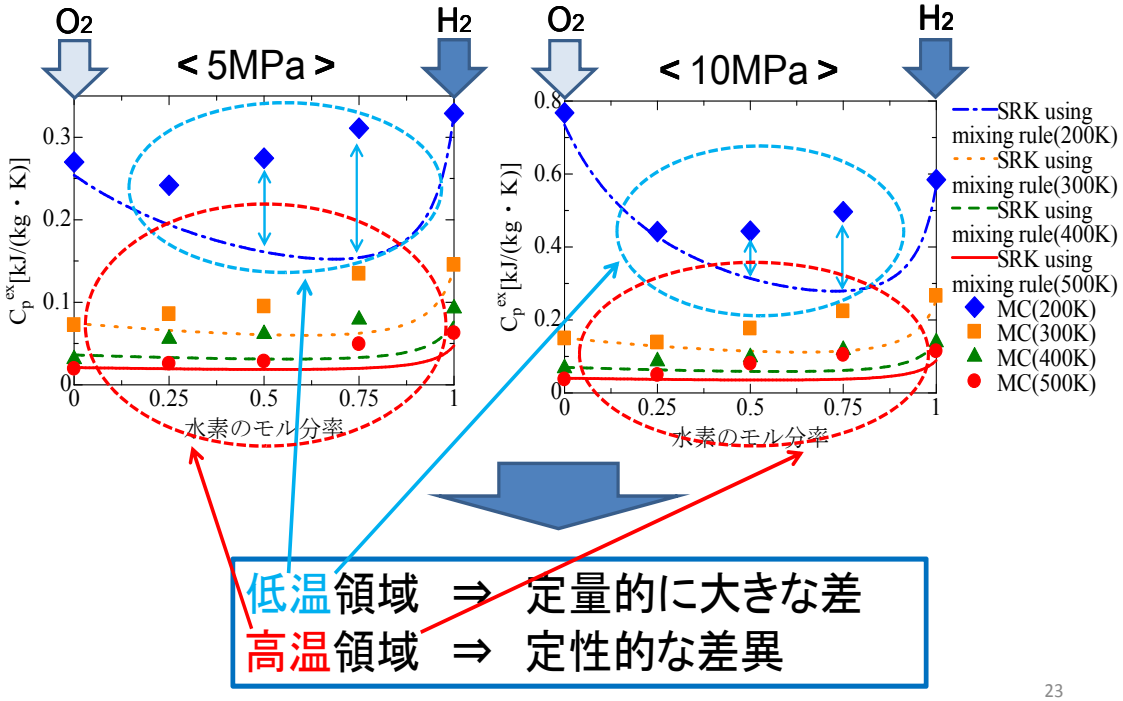
酸水素混合系における比較

検証結果②＜定圧比熱＞



低温領域 ⇒ 定量的に大きな差
高温領域 ⇒ 定性的な差異

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まとめ

ロケットエンジン燃焼室内部流れの解析で
現在最もよく使用されている古典的混合則を評価

- P-V-T関係の再現性は非理想性の顕在化する温度条件でも良好
- 比熱については大きな予測誤差があることを示唆

燃焼室内部流れで現在適用されている混合則の問題点を
具体的に指摘した最初の例

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研究成果のまとめ

～ロケット推進剤の熱物性に対する非経験的アプローチ～

① **酸水素系に対する分子間相互作用モデル**の開発

成果: **水素と酸素の分子間相互作用**の詳細理解

② **酸水素単成分系に対する熱物性値**の評価

成果: 極低温状態の水素を除いて,
単成分系の酸水素系を妥当な精度で予測可能
成果: **酸素の異方性反映**が物性評価に極めて重要であることを明確に指摘

③ **酸水素混合系に対する古典的混合則**の精度評価

成果: ロケットエンジン燃焼室内部流れの解析で使用されてきている
最も典型的な混合則を初めて第一原理的に評価 → **問題点の指摘**

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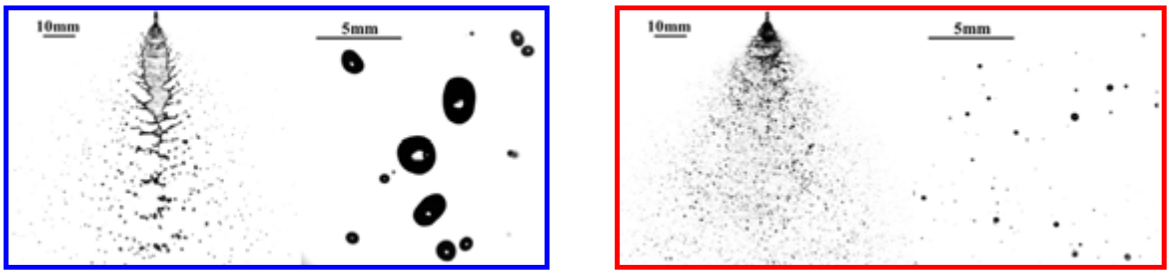
2012年9月27日連携講座シンポジウム
@武田先端知ビル

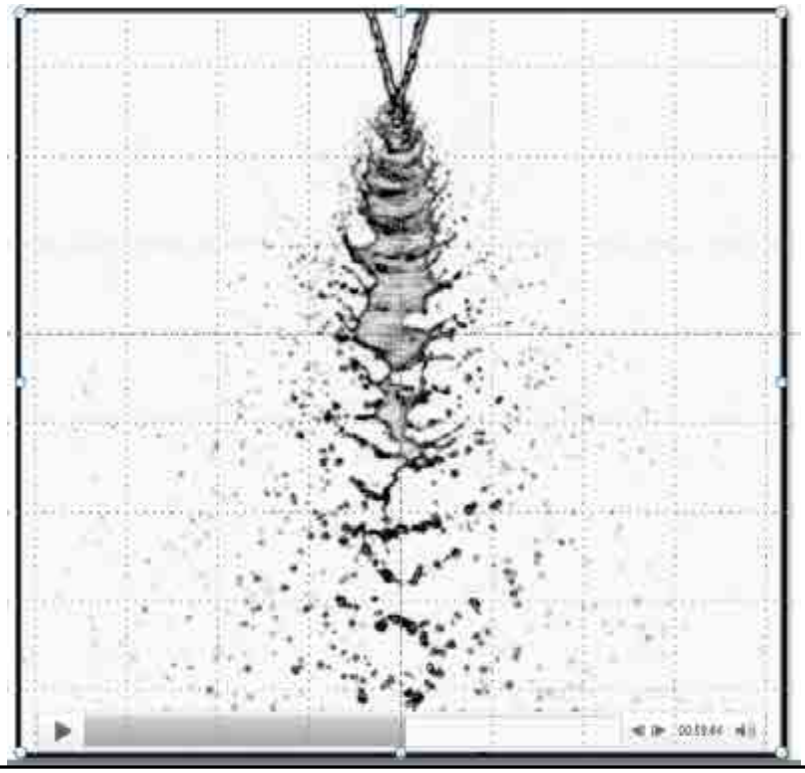
低ウェーバー数下の衝突微粒化促進方法とその機構



東京大学
井上智博　渡辺紀徳　姫野武洋　越光男

1

衝突微粒化現象



2

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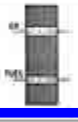
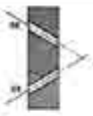
微粒化技術の適用事例

微粒化方法	噴射器	噴射器形状	用途
圧力エネルギー	単噴孔		
	衝突型		
気体エネルギー	エアーブラスト		
遠心力	回転カップ		
振動エネルギー	振動ノズル		

微粒化は、燃料噴霧形成や塗装など、多くの場面で活用されている。

3

衝突微粒化を利用したエンジン

衛星スラスター

© JAXA

© IA

- 推力レベル
  ：10^1N~10^3N
- 酸化剤：NTO
- 燃料：ヒドラジン
  ：MMH

打ち上げエンジン

© JAXA

- 推力レベル
  ：~10^5N~10^6N
- 酸化剤：酸素
- 燃料：メタン
  ：ケロシン

4

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人工衛星スラスター

衛星スラスター

- 推力レベル
  ：10^1N~10^3N
- 酸化剤：NTO
- 燃料：ヒドラジン
  ：MMH

- 人工衛星スラスター性能向上
  - 定格比推力向上
  - 噴射面および燃焼室壁面の冷却性能向上
  - パルス作動時に微粒化特性悪化
- 設計技術高度化
  - 微粒化・燃焼特性予測技術の向上

5

液体を衝突させると微粒化が促進される

6

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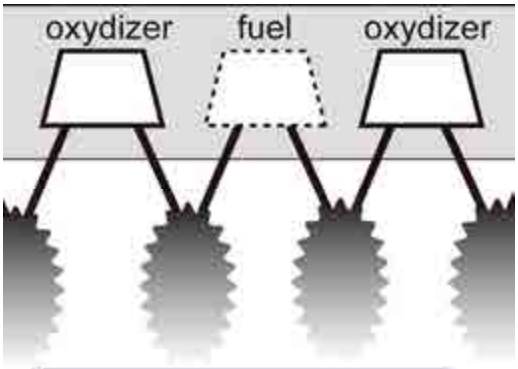
噴射器設計



①単噴射孔あたりの流量、配置を決定

②各部寸法(孔径、角度)を決定

③水流し試験を実施

④単噴射孔・サブスケール燃焼試験

⑤実機燃焼室を構成した燃焼試験を行い、燃焼特性や安定性を確認。

衝突微粒化の利点と問題点

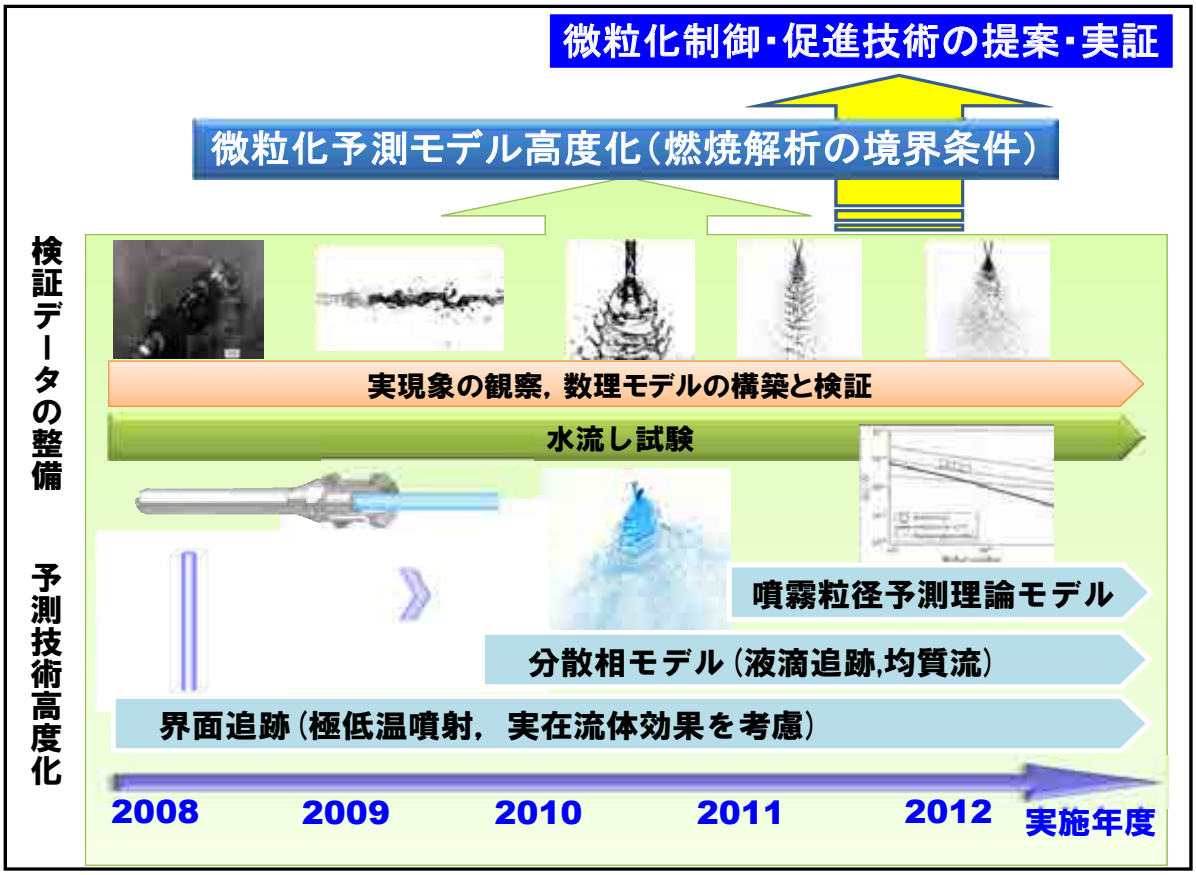
○ 数気圧程度の噴射圧でも良好な微粒化を達成可能。

○ 単純な構造

× 微粒化特性を事前に予測することが困難。例えば、粒径を予測したうえで、設計を行うことが難しい。

× エンジン始動開始やパルス作動開始・停止といった低速噴射時に、噴霧特性が必ず悪化する。

7



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主な記号

d ： 粒径 [m]

D ： 噴射ノズル径 [m](主にD=1mm)

h ： 液膜厚さ [m]

V_e ： 噴射速度 [m/s]

We ： 噴射ウェーバー数($\rho_{liq} V_e^2 D/\sigma$)

ϕ ： 気液質量流量比(気体/液体)

σ ： 表面張力係数[N/m]

9

2. 実験・数値解析方法

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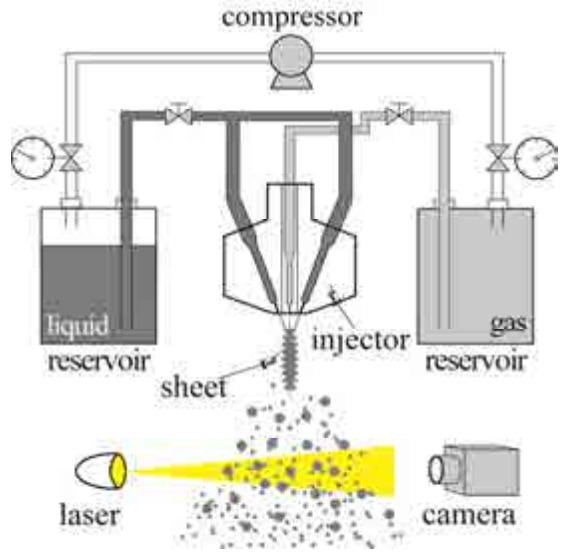
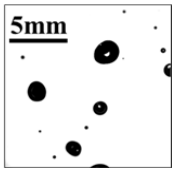
実験装置と計測法



fluid	density ρ [kg/m^3]	viscosity μ [Pa·s]	surface tension σ [mN/m]
air	1.2	1.8×10^{-5}	72.4±0.4
water	1000	1.0×10^{-3}	

【可視化】ハイスピードカメラ
- Photron FASTCAM APX-RS
- バックライトによる可視化
- 10,000fps, 1/100,000s

【粒径・速度計測】影絵撮影＋画像解析
- ダブルパルスYAGレーザー
  DANTEC DYNAMICS DualPower 135-15
- カメラ(2048×2048pix)
  DANTEC DYNAMICS FlowSense 4M MkII
- 長焦点顕微鏡レンズ
  INFINITY Model K2/SC



【表面張力】
- プレート法
  協和界面科学(株) CBVP-Z

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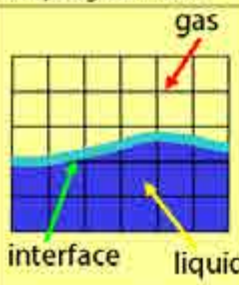
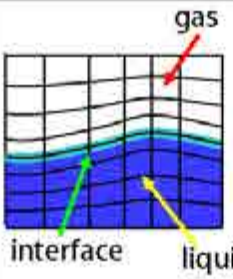
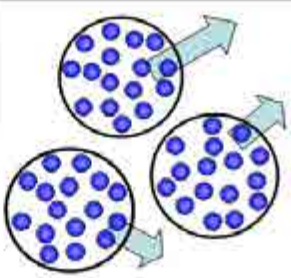
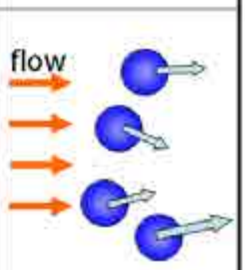
数値解析手法

Simulation of Atomization Process		Simulation of Spray	
Fixed Grid System	Moving Grid System	LHF Model	SF Model
capture and track motions of liquid/gas interface	grids move following motions of liquid/gas interface	Averaged equations of two phase flow are resolved	Track particle dynamics
			
○ breakup of liquid column, droplet ○ large transformation of interface △ computational time × analysis of spray	○ liquid and gas phase can be described by different equation × large transformation of interface × analysis of spray	○ mist flow with lots of droplets × analysis of atomization process	○ spray behavior △ analysis of atomization process with breakup model × dependence on model

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Capture Interface Precisely with Volume Conservation - HLSM(Level Set & MARS) [Himeno(2003)]-

Distance Function

Osher,S.(1988)

Distance function ϕ is generated from moving interface

Owing to distribution of ϕ

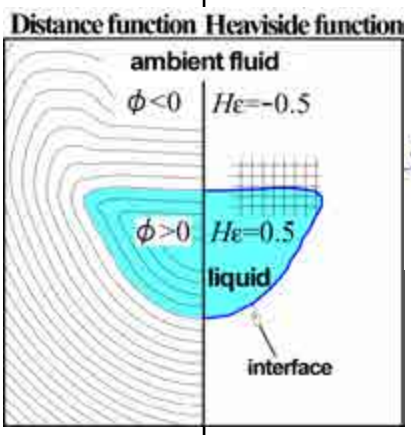
Normal Vector

$$\vec{n}_s = \frac{\nabla\phi}{|\nabla\phi|}$$

Curvature

$$\kappa = \nabla\cdot\vec{n}_s = \nabla\cdot\left(\frac{\nabla\phi}{|\nabla\phi|}\right)$$

are computed exactly

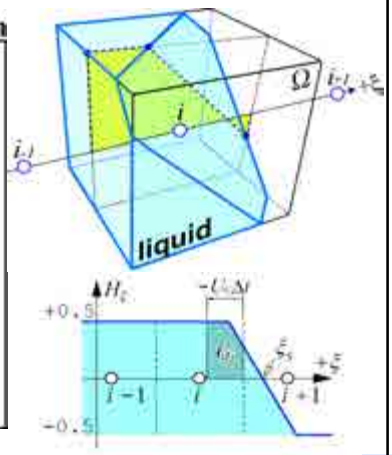


Surface tension is computed by CSF model

MARS

Kunugi,T.(2000)

VOF is interpolated with a piecewise linear function



Distribution of heaviside function

13

微粒化制御・促進技術の提案と実証

衝突微粒化促進法

・目的：低ウェーバー数環境で微粒化特性が悪化する、衝突微粒化の本質的欠点を克服し、低速噴射時にも良好な微粒化を達成する。

井上、機論**B**(掲載予定) 14

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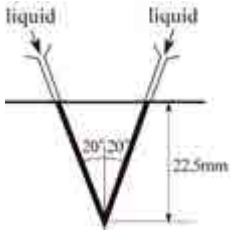
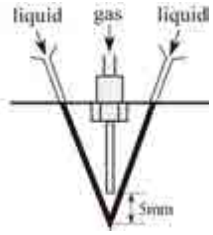
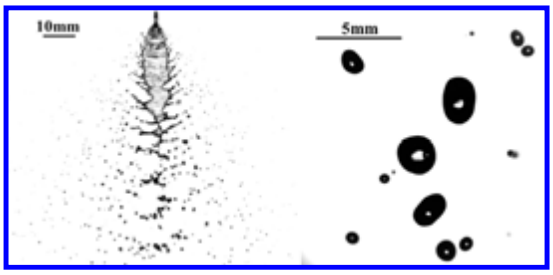
気体噴射を利用した衝突微粒化促進法

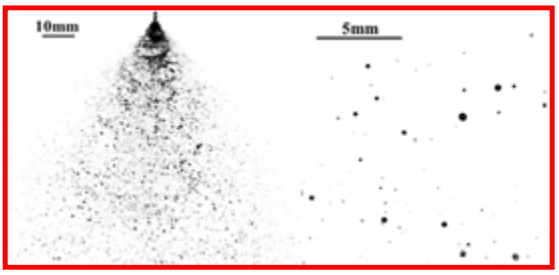
気体噴射なし
- 二液衝突
- 頂角40deg.





気体噴射あり
- 気体噴射孔–二液衝突点間距離5mm(実機相当)





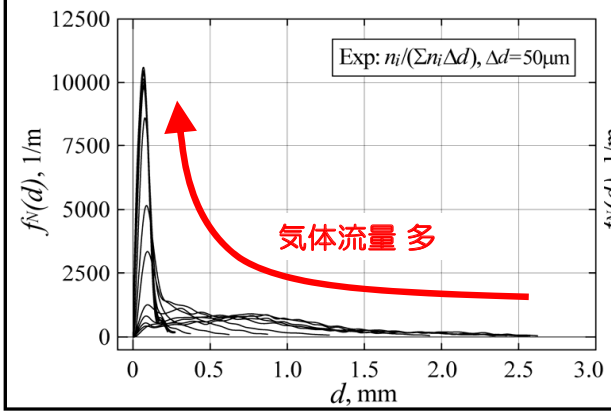
・微粒化促進効果を実証・微粒化促進機構を理解・噴射条件最適化
→可視化実験・粒径計測・数値解析を実施

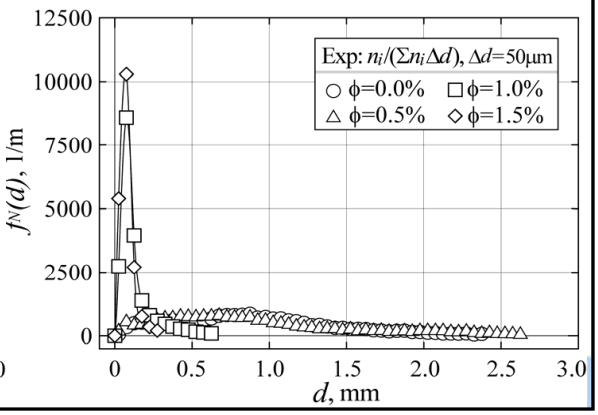
15

可視化と粒径計測結果

Φ=0% Φ=0.5% Φ=1.0% Φ=1.5%

We=500、質量流量比Φ：気体/液体





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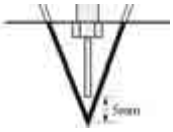
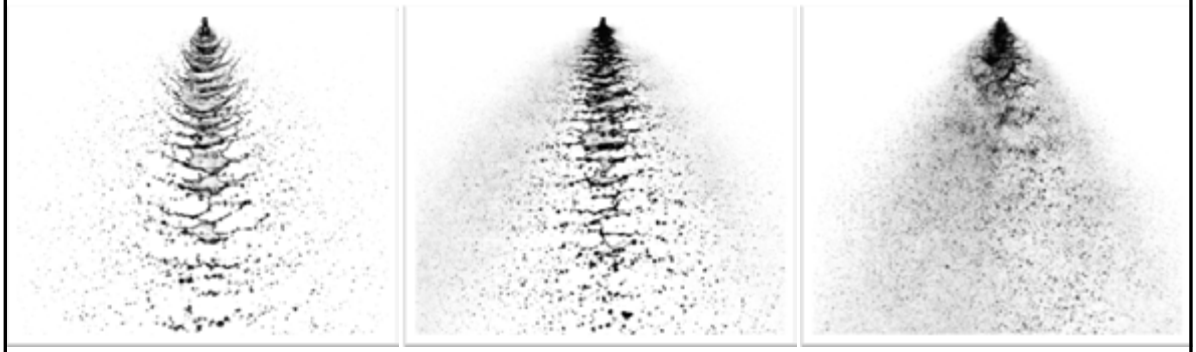
微粒化促進機構

- 液体：3~17m/s
- 気体：~315m/s

ウェーバー数
- 部分負荷相当
- We=100~4000





① Φ=0%	② Φ～0.5%	③ Φ>1.0%
• 連続液膜が存在 • 液膜→液糸→液滴	• 連続液膜が存在 • 液膜を取り囲むように液滴が形成	• 連続液膜が存在しない • 著しく微粒化が促進

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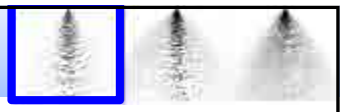
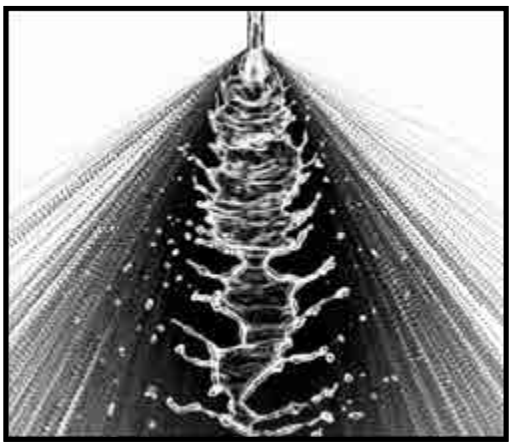
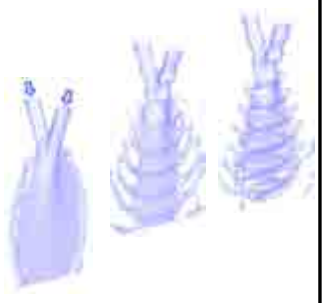
①気体噴射なしの場合

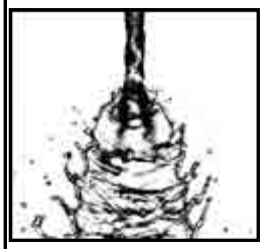


- 液膜側方に液糸成長
- 噴霧外縁は衝突点近くの液糸から分裂した液糸が形成
- 液糸は衝突点上方を起点に発生・伸長
- 液滴は直線的に飛散

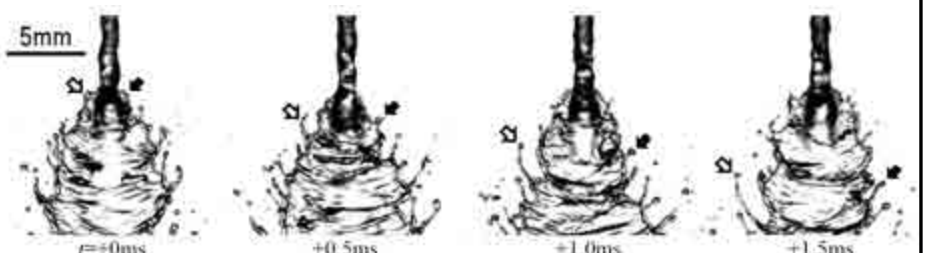




We=500



（逆再生）



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②流量比1%以下の場合

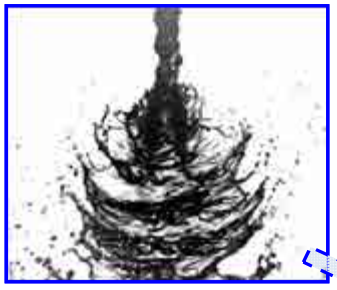
Φ=1.0%

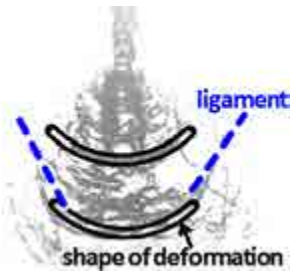
We=1800

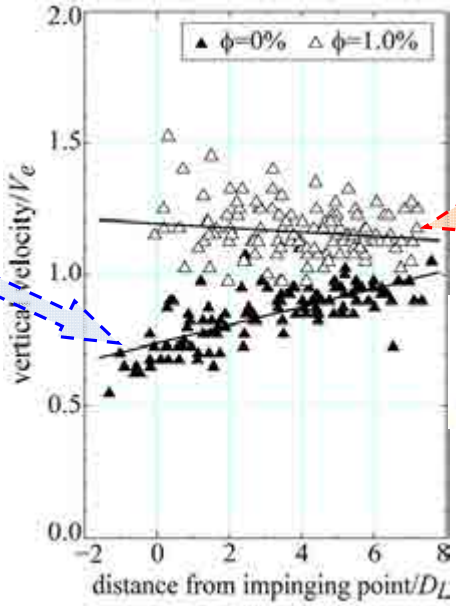
19

②流量比1%以下の場合

Φ=0%



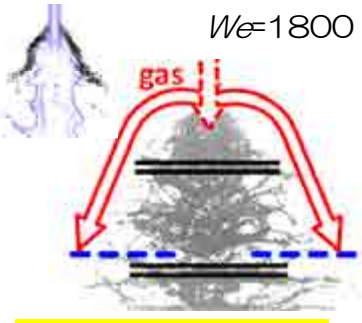




液糸先端の鉛直方向移動速度
(*We*=500)

Φ=1.0%

We=1800



液膜側方を流れる気流によって液糸分裂促進

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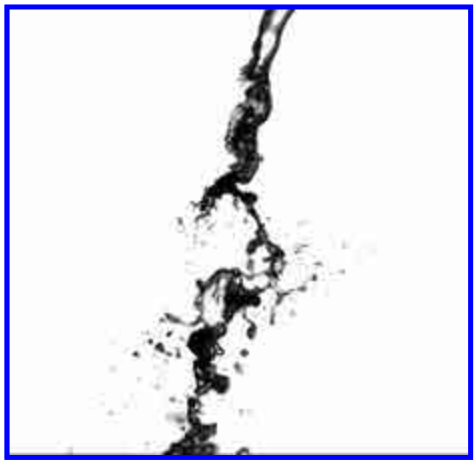
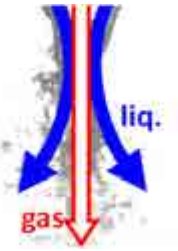
③流量比1%以上の場合





一液＋気体噴射

We=150, Φ=7.0%

- 気流が貫通
- 二液の干渉は小さい

⇒

- 二液のうち片側のみ噴射
- そこに気流を吹付ける

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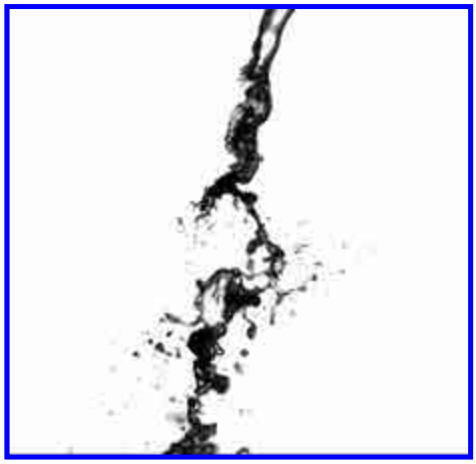
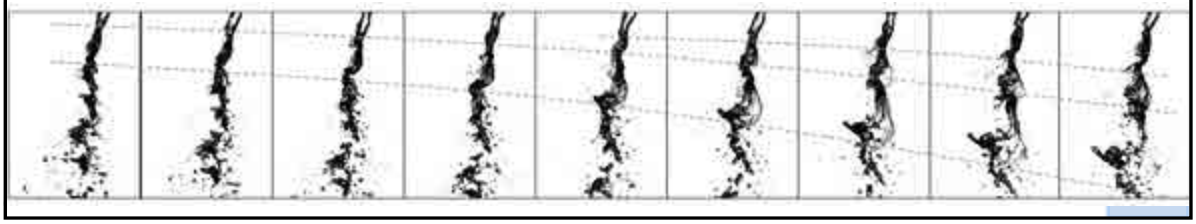
③流量比1%以上の場合

二液＋気体噴射



一液＋気体噴射



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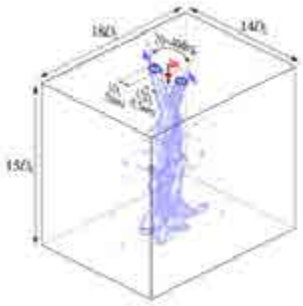
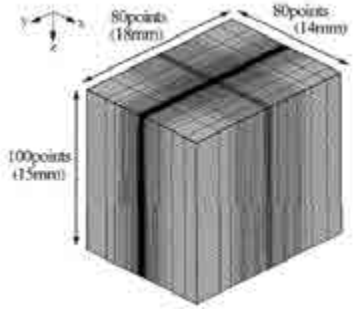
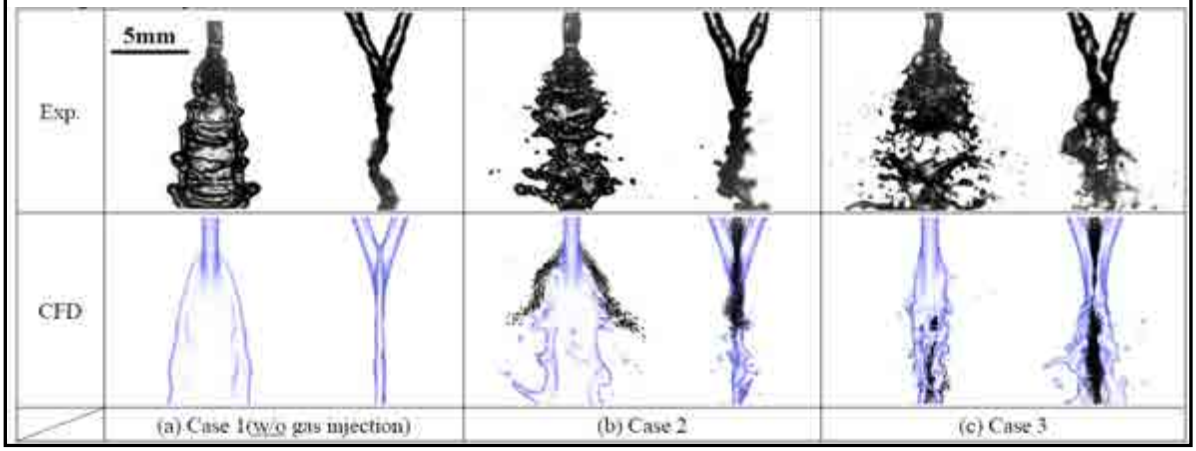
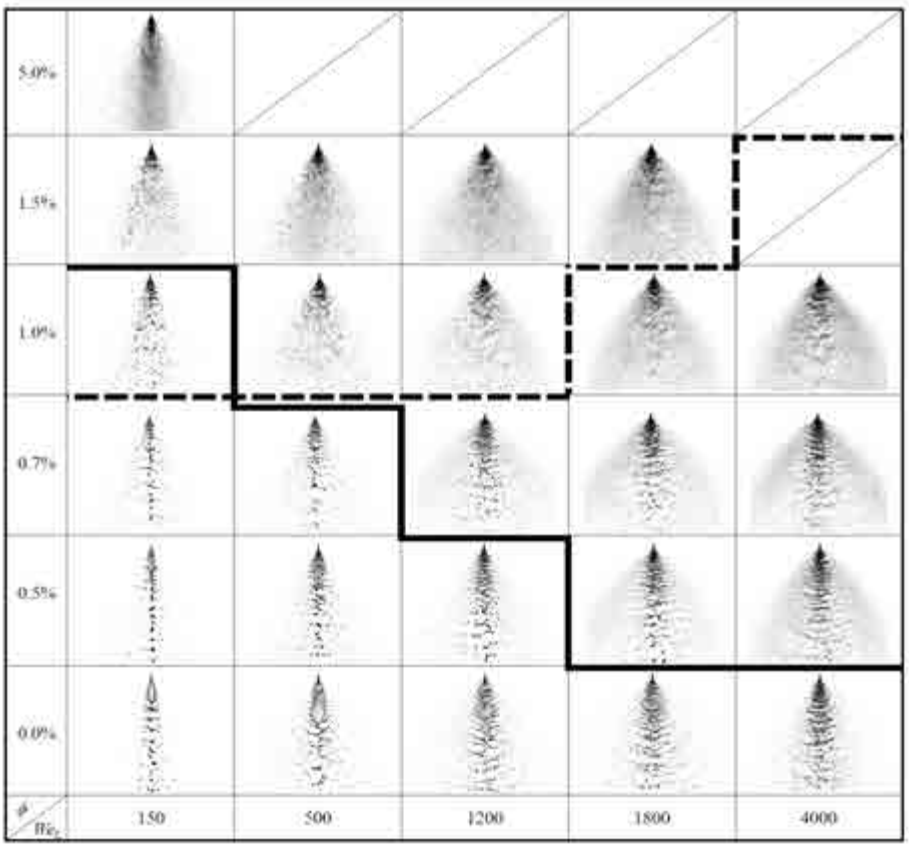
数値解析による気体流れの把握





	V_L, m/s	V_G, m/s	We_{rel}	q_{avg}
Case 1	3.3	0	0	0
Case 2		78	80	0.6
Case 3		150	190	1.3





衝突点における
気液動圧比
q=0.9

気液相対
ウェーバー数
We_{rel}=400

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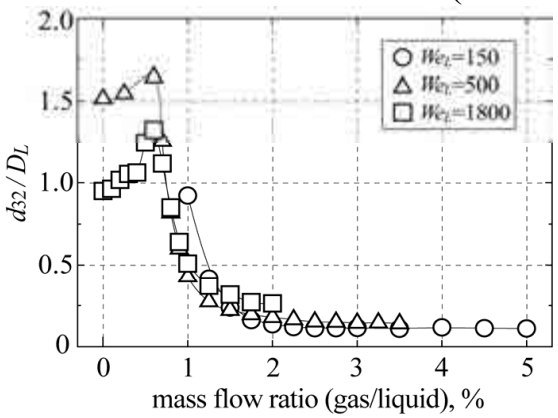
気体噴射条件の最適化

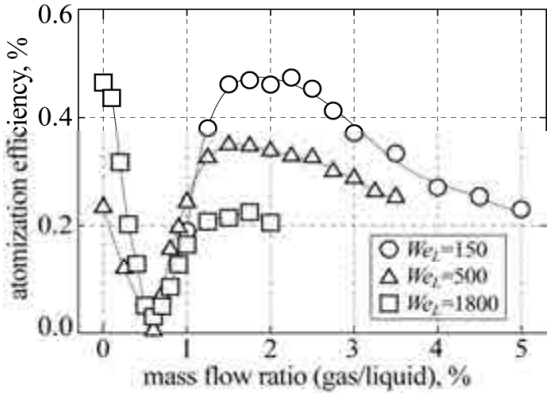
実機適用時には、少ない気体流量で効率的な微粒化促進が求められる。

微粒化効率η_σ=投入したエネルギーに対する、液体の表面自由エネルギーおよびラプラス圧の増加割合

$$\eta_\sigma \equiv \frac{40817}{2160We_L(1+0.5\dot{k}_{uni_G}/\dot{k}_{uni_L})}\left(\frac{D_L}{d_{32}}-\frac{3}{5}\right)$$



気液流量比とSMDの関係



気液流量比と微粒化効率の関係

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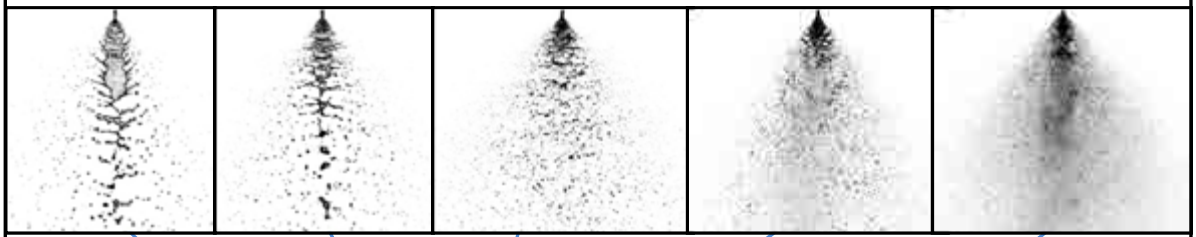
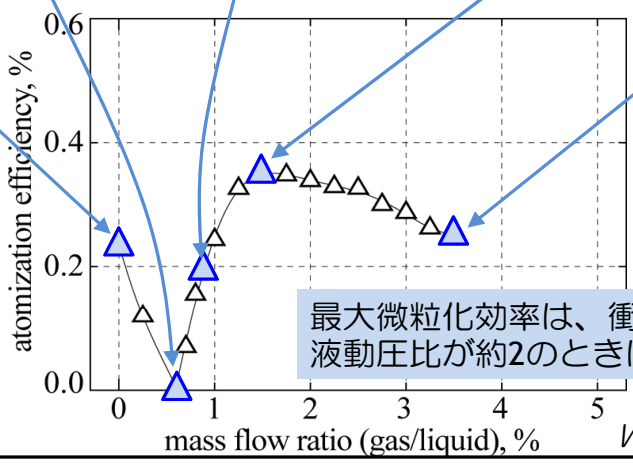
気体噴射時の微粒化効率(流れ場vs微粒化効率の関係)

ϕ=0.0%, η_σ=0.23% ($q_{imp.}$=0.0)　ϕ=0.6%, η_σ=0.004% ($q_{imp.}$=0.5)　ϕ=0.9%, η_σ=0.20% ($q_{imp.}$=1.1)　ϕ=1.5%, η_σ=0.35% ($q_{imp.}$=2.1)　ϕ=3.5%, η_σ=0.25% ($q_{imp.}$=4.8)





最大微粒化効率は、衝突点における気液動圧比が約2のときに達成される。

We=500

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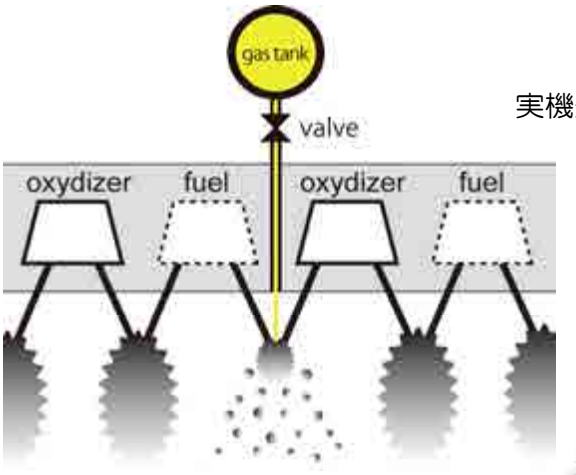
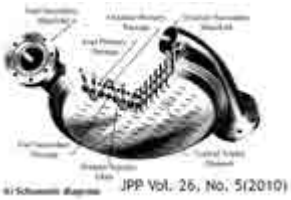
実機搭載に向けて



実機適用イメージ



【利点】
- 混合比をほとんど変化させることなく良好な微粒化を実現可能
- 他の推力制御方法と比べて構造が単純(e.g.dual manifold)
- 噴射面に遡る液滴を低減(熱的防御性能向上)

【欠点】
- 気体噴射なしの衝突型噴射器と比べて重量が増し、システムが複雑になる。
- 高圧貯気タンクが必要(専用ボンベまたは推進薬加圧Heを抽気。一部の噴射器への追加工で済めば重量ペナルティは軽減)

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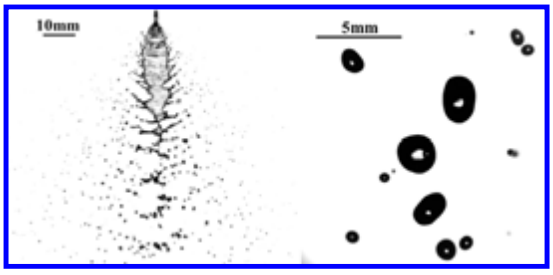
ま と め

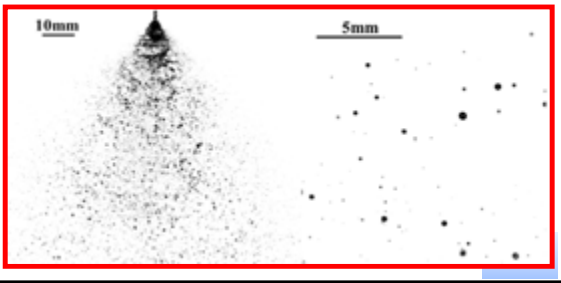
① 気体噴射を利用した新たな衝突微粒化促進技術を実証

② 1%質量流量の気体噴射で著しく微粒化促進

③ 衝突点の気液動圧比と相対ウェーバー数で現象を整理可能

④ 衝突点における気液動圧比がおよそ2のときに最大微粒化効率達成





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今後の課題

- **微粒化制御**：人工衛星スラスターのパルス作動を想定した場合の適用可能性。微粒化促進時の燃焼特性の把握は、実機への適用に向けた最重要課題。（企業・JAXAとの連携が必要）
- **微粒化の数値解析**：微粒化後の液滴挙動をラグランジュ的に追跡する手法を取り入れることで、噴射面から下流遠方までの噴霧特性予測。（界面追跡/粒子追跡ハイブリッド）
- **粒径推算法**：気流を伴う液柱あるいは液膜の微粒化に適用可能な理論解析法を構築。ロケットエンジンの同軸型噴射器や、ガスタービンにおけるエアーブラストアトマイザーにおける粒径を瞬時に予測。
- **粒径推算法**：粒径分布関数を推定する際には、指数分布やガンマ分布など、抜山-棚沢の式よりも自由度が少ない分布関数を適用することも有効である可能性。
- **その他**：パルス作動時の微粒化特性、マニホールド内の推進薬挙動、多噴射器間干渉の影響の解明。
- 人工衛星の長寿命化、液体ロケット設計に資する微粒化技術の向上

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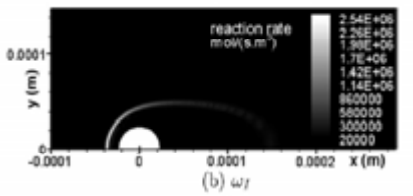
液体燃料噴霧における乱流微粒化・蒸発混合・初期着火現象

新城　淳史
宇宙航空研究開発機構　研究開発本部

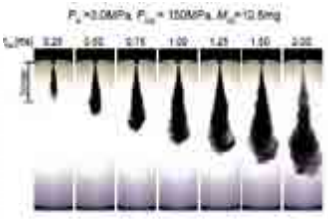
Sep 27, 2012

乱流噴霧燃焼のスケール

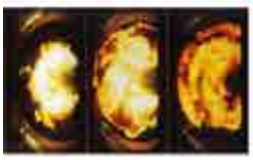


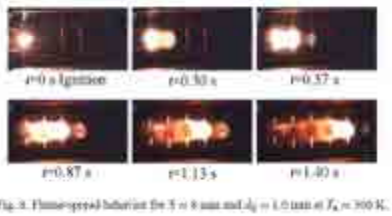
(b) ω_f

Wu et al. (CNF 2011)



Manaka et al., (ICLASS2009-234)





Mikami et al. (CNF 2005)

Sallam et al. (IJMF 2002)

単液滴・液滴列　　単噴霧　　燃焼器・実エンジン

スケール小 ⟷ スケール大

モデル化の割合 → 大

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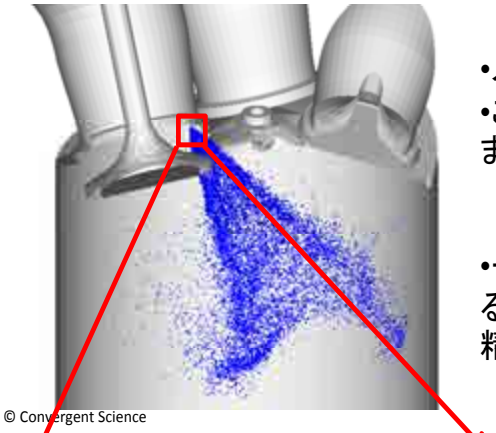
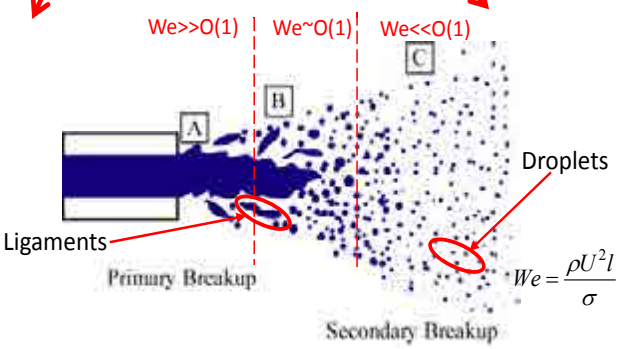
現象理解の重要性

- 実エンジンシミュレーションはDNSでは不可能
  ⇒モデル計算
- モデル：何を再現、何を無視？
  ⇒分かっていて取捨選択している場合
  ⇒そもそも現象が分かってない場合
- 現象の理解が精度向上に重要
  – 噴霧燃焼は乱流・多相・蒸発・反応流れで分かっていない現象が多いが…
  ⇒ここでは、そのなかでも特に…（次ページ）

濃い噴霧（一次微粒化）領域





- ノズル直下の濃い噴霧領域
- これまでその困難さからあまり正面から取り組まれず現象理解・モデル化が進んでいない
  - 高速小スケール、ラグランジュ的扱い不可
- 一方で、実スケール解析の流入境界条件であるので、ここの精度が実スケール燃焼器解析の精度に大きく効く

まず、物理過程を詳細に理解しなければならない

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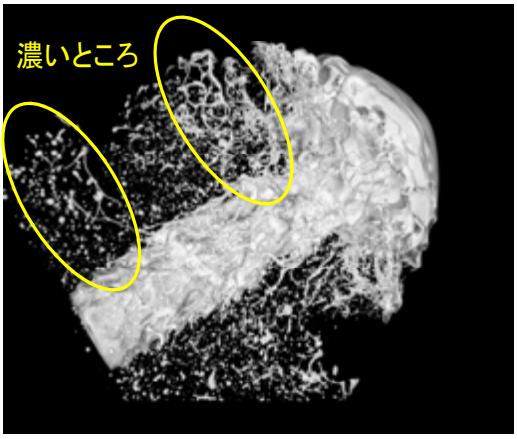
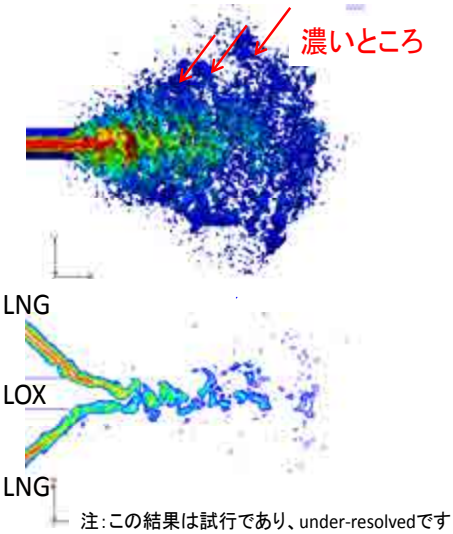
現象の特徴

- 液滴空間分布の非一様性（局所の液滴径や液滴数密度の違い）
- 流れ場の構造
  - その後の蒸発・混合・燃焼はこの履歴に影響される

⇒微粒化機構が決定。各噴霧形態での機構の理解が必要



後ほど議論します



注：この結果は試行であり、under-resolvedです

過去の研究例
（下流の薄い噴霧or気相反応）

•Euler-Lagrange計算
➢乱流スケール >> 液滴径

Fig. 1. Initial gas velocity vectors and distribution of droplet locations (only 5% of the velocity vectors are shown for clarity).

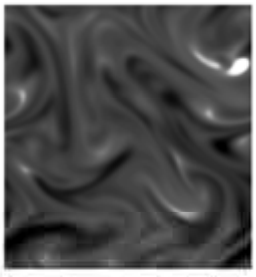


Fig. 2. Temperature contour at $t = 0.891$ ms for the $T = 1300$ K case (black = 1300 K, white = 2000 K).

Wang & Rutland
(PCI 2005)

•気相のみの自着火
➢低散逸率のところで着火

Viggiano (CNF 2010)

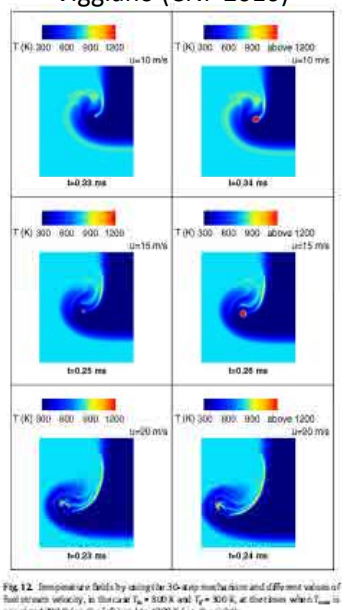


Fig. 12. Temperature fields by using the 30-step mechanism and different values of fuel stream velocity, in the case T_{ox} = 800 K and T_F = 300 K, at the times when T_{max} is equal to 1,800 K (on the left) and to 1700 K (on the right).

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過去の研究例
（単液滴）

熱・物質輸送

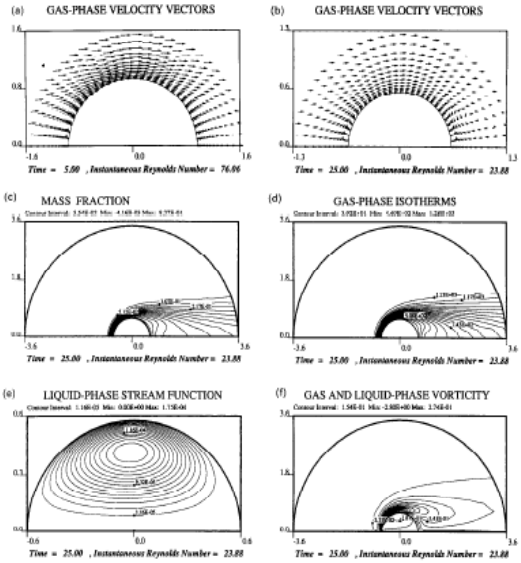
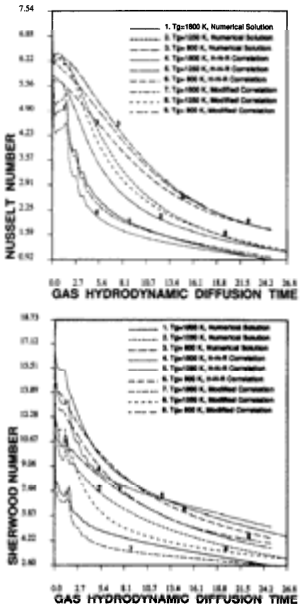


FIG. 2. (a) Instantaneous velocity of gas phase at time = 5. (b) Instantaneous velocity of gas phase at time = 25. (c) Mass fraction contour plot at time = 25. (d) Gas phase temperature contour plot at time = 25. (e) Stream function of liquid phase at time = 25. (f) Vorticity contour plot of gas and liquid phases at time = 25.

気相が燃焼器条件に近い単液滴

Chiang, Raju, Sirignano (Int. J Heat Mass Transfer 1992)



*この時間変化は液滴の減速によるレイノルズ数の低下による

目的とアプローチ

- これまでの研究ではノズル直下の直接の現象理解が抜けているので…
  - 乱流微粒化のメカニズムを解明する
  - さらに蒸発・混合・反応現象を解明する
    - 燃焼への道筋
    - 実スケールへモデルとしてフィード
  - 詳細数値計算による
    - 恣意的モデルを導入しない
    - ただし計算機資源の制約から依然として小スケールに限定

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計算手法

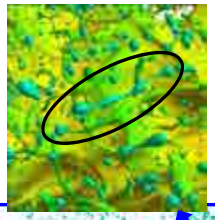
- 3次元Navier-Stokes方程式
  - 密度、速度、温度、各化学種
  - 移流はCIP法
- Level-set界面追跡
- 蒸発
  - 平衡モデル
  - 界面での跳び条件
- 化学反応
  - n-heptane総括一段反応*

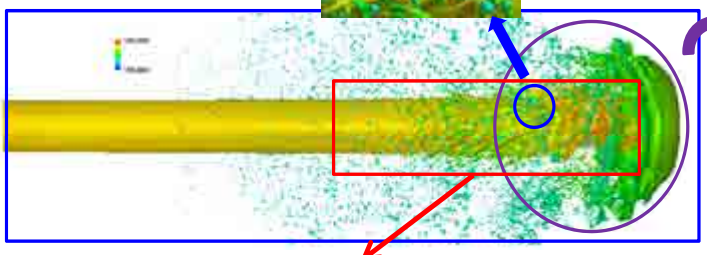
$$C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$$

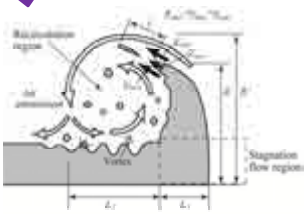
*Westbrook & Dryer, Combust. Sci. Technol. 1981

（1）コールドフロー結果

噴霧の全体挙動と液糸・液滴生成 (Shinjo & Umemura, IJMF 2010)







液柱コアの表面不安定と微粒化 (Shinjo & Umemura, IJMF 2011)

先頭部のはたらき (Shinjo & Umemura, PCI 2011)

Case	Nozzle diameter $D=2a$	Ambient pressure p	Gas density ρ_g	Liquid density ρ_l	Liquid viscosity μ_l	Surface tension coefficient σ	Liquid velocity $U_l=U$	Gas velocity U_g	Bulk liquid Reynolds number	Bulk liquid Weber number
3	0.1mm	3MPa	34.5kg/m^3	848kg/m^3	2870e-6 Pa·s	30.0e-3 N/m	100m/s	0m/s	1470	14100

最小解像度0.35μm　格子点数60億点

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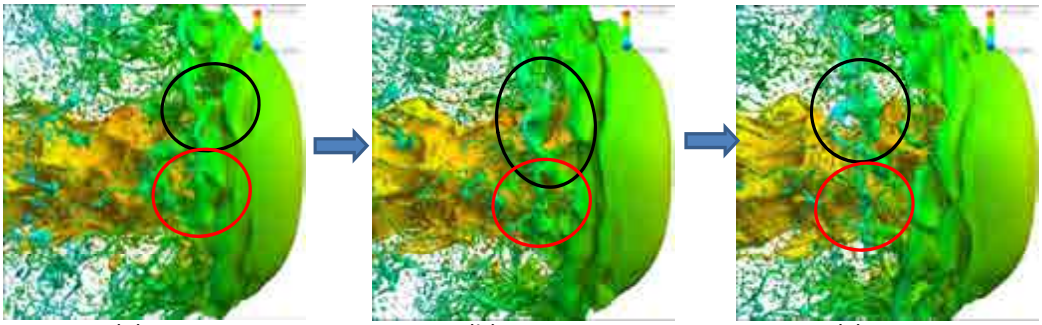
先頭部の渦挙動と微粒化

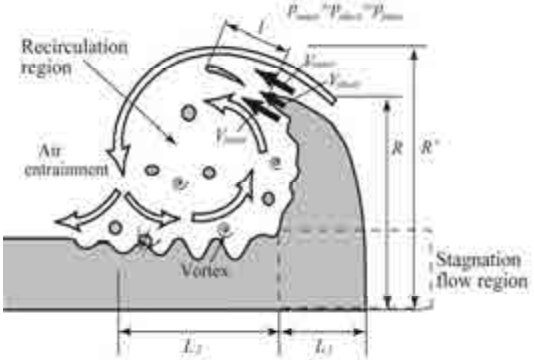


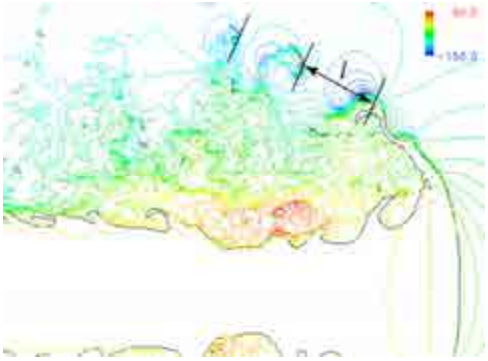
Case 3 (a) t=14.39 (b) t=15.11 (c) t=15.83

•軸対称渦の定期的放出と液糸の形成
•これにより液滴分布の空間ムラができる

•乱流化するため、渦間には縦渦も形成

先頭部での微粒化ループ





From theoretical consideration,

$$l = [\left(V_{outer(inner)} + V_{sheet}\right)/2]\tau$$

$$\left(V_{sheet} - U_c\right)\tau = \left(V_{sheet} - \sqrt{\sigma/\rho_l a_{sheet}}\right)\tau = \lambda$$

CFD result satisfies the above relations

$$\hat{V}_{outer(inner)} = 1.0, \quad \hat{V}_{sheet} = 0.5,$$
$$\hat{\lambda} = 0.37, \quad l = 0.6, \quad a_{sheet} = 0.04,$$
$$\hat{\tau} = 0.8$$

V_*: Edge velocity (fixed on spray front)
a_{sheet}: Thickness at edge
l: Spatial interval
σ: Surface tension
λ: Wavelength on edge
R: Edge radius
L_2: Recirculation zone length
τ: Time interval of atomization

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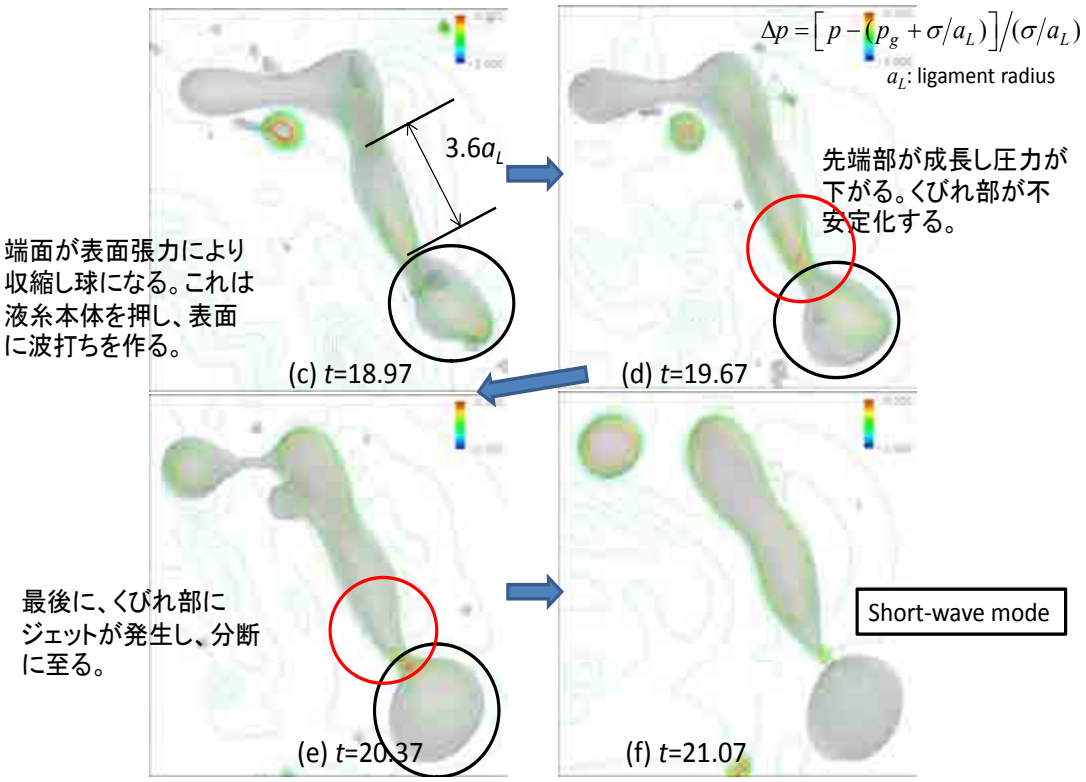
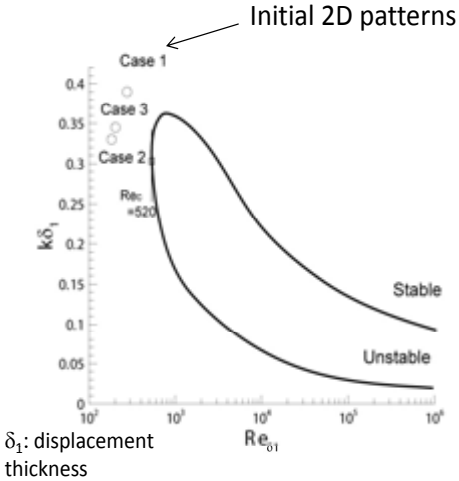
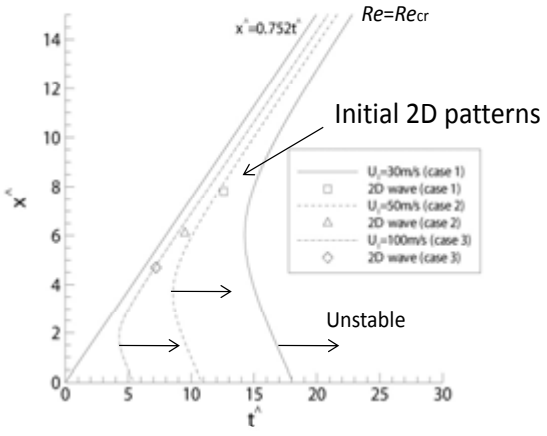
液糸からの液滴生成



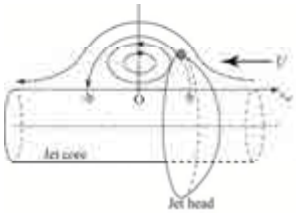
表面不安定性とTSモード



δ_1: displacement thickness



Without jet head wake effect



With jet head wake effect modification

$$\delta = K\sqrt{\nu\int_0^x \frac{dx}{U\left[1-(b/x')^2\right]}}$$

$$Re_\delta = K\sqrt{\frac{U}{\nu}\left[1-\left(\frac{b}{Ut-b-x}\right)^2\right]}\sqrt{x-\frac{1}{2}b\ln\left(\frac{Ut-2b-x}{Ut-2b}\cdot\frac{Ut}{Ut-x}\right)+Ut}$$

高速液噴射では、初期不安定波は気相境界層のTS不安定である

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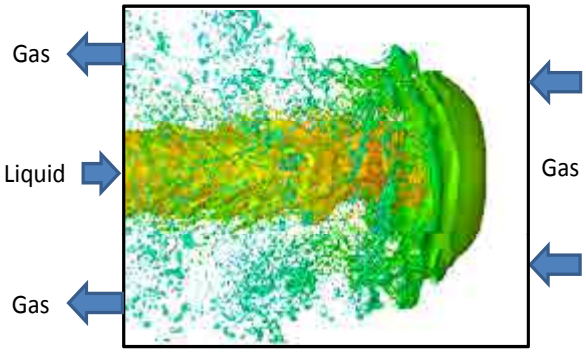
(2)蒸発・反応計算

- コールドフローの結果を利用
  - スケールの制約で火炎の完全発達は追えない
  - それでも初期挙動は追える



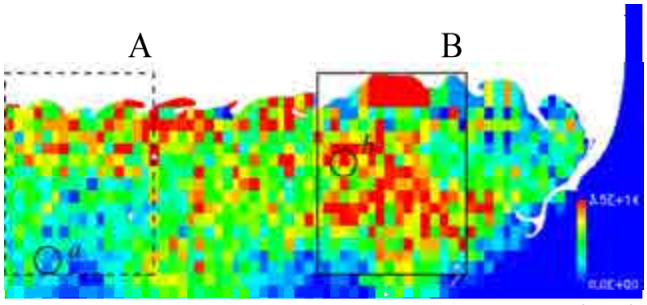
- 900K空気 （時刻 $\hat{t}=15.47$ ）
- 30atm
- 平衡蒸発
- n-heptane (C_7H_{16}) 総括一段反応 (Westbrook & Dryer, CST 1981)
- NISTデータによる物性値
- 22億点格子

Nozzle diameter D_N	Ambient pressure p	Air density ρ_g	Liquid density ρ_l	Air temperature T_g	Liquid temperature T_l	Liquid injection velocity U_l=U	Air initial velocity U_g	Liquid viscosity μ_l	Air viscosity μ_g	Surface tension coefficient σ
0.1mm	3MPa	11.5kg/m^3	848kg/m^3	900K	300K	100m/s (Lab frame)	0m/s (Lab frame)	2.87e-3 Pa·s	3.90e-5 Pa·s	30.0e-3 N/m

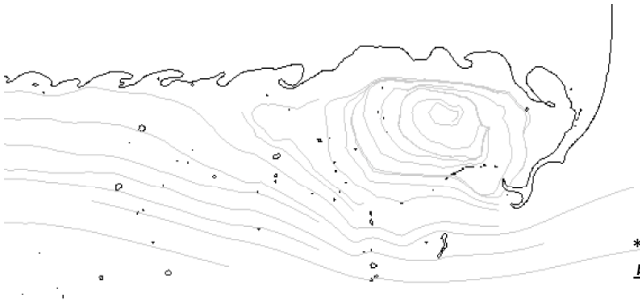
15

流れ場

- 再循環背後の液滴分布
  - 先ほどの空間ムラ



Color: droplet number density (1/m^3)



*2次元スライスは液滴が少ない印象を与えるが3次元的には多数存在している

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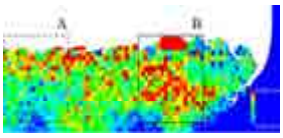
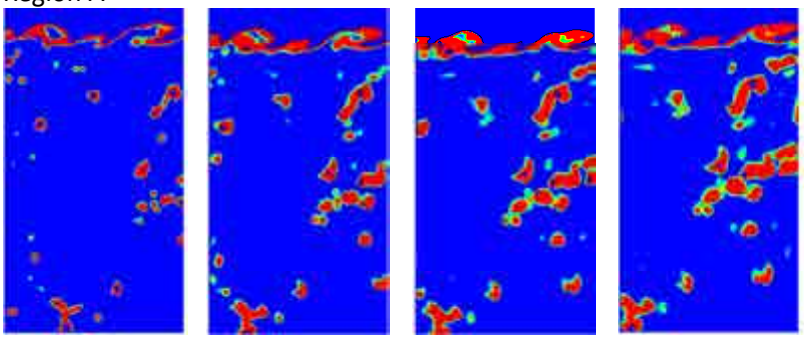
燃料蒸気の混合



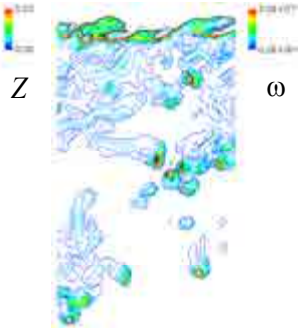
*Evaporation starts at $\hat{t}=15.47$

・数密度が高い（B）と混合がクラスター化

Region A

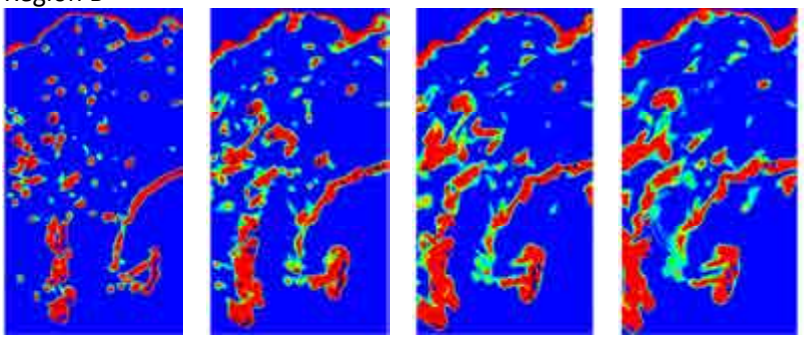


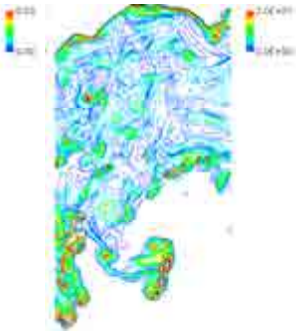
$\hat{t}=15.62$ $\hat{t}=15.81$ $\hat{t}=15.93$ $\hat{t}=16.03$



$\hat{t}=16.03$

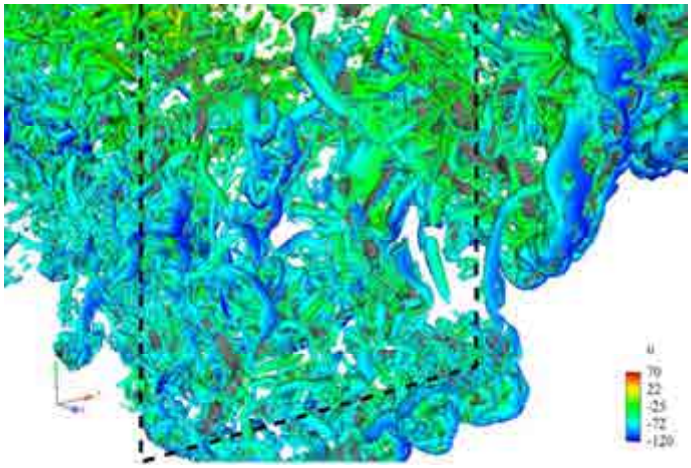
Region B



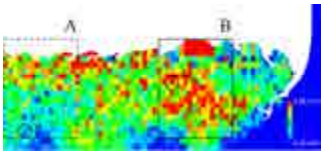


液滴/気相干渉

- 液滴/乱流スケール



Droplets (gray) and eddies (Q-isosurface) near region B



Kolmogorovスケール

$$\eta=\left(\nu^3/\varepsilon\right)^{1/4} \quad \varepsilon=\nu\overline{u'_{i,j}u'_{i,j}}$$

$$\eta\sim 1\mu m=0.23D_{32}$$

D_{32}: Sauter mean diameter

液滴Stokes数

$$S_t=\rho_l {D_{32}}^2 U/18\mu_g L$$

$$S_t\sim 22$$

•まだ気液で相対速度がある。
•渦度を生成する (eddy diameter~8-12η)：次スライド

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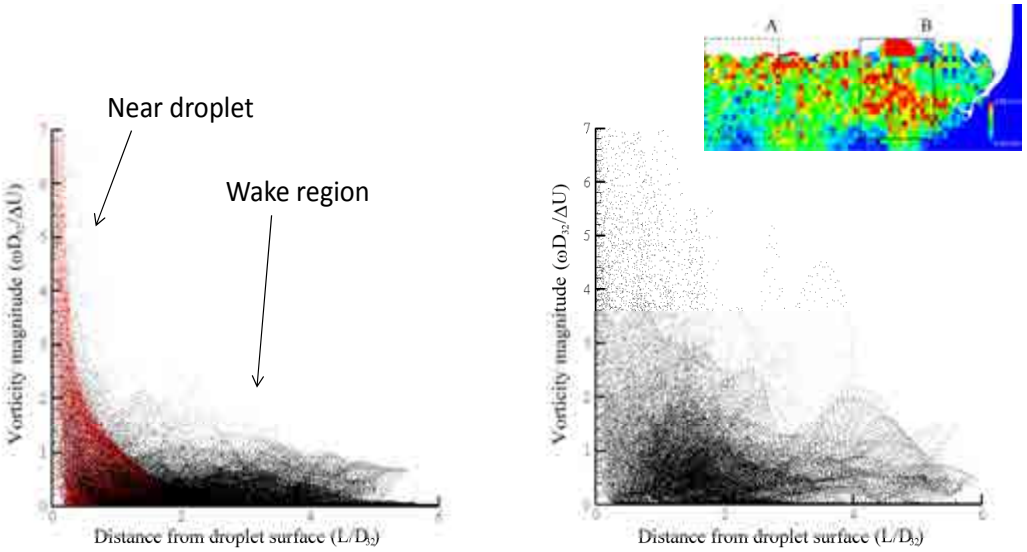
液滴周り渦度



領域A （低数密度） 領域B （高数密度）

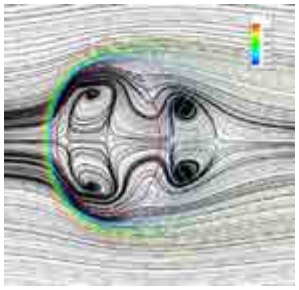
*Red scatter points are from single droplet simulation of the similar Re (~40) with evaporation and reactions.

- 領域Bのほうが、ウェイクの干渉が大きい
- 平均液滴間距離 : (A) l=7.9D_{32} and (B) l=3.3D_{32} $l \sim n^{1/3}$

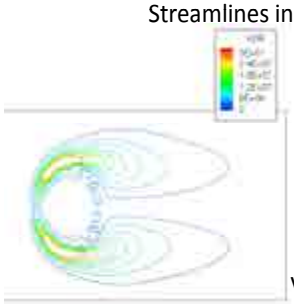
単液滴計算

- 「一様流」中に置かれた個々の液滴の蒸発

例 : Re=40, T_{air}=900K



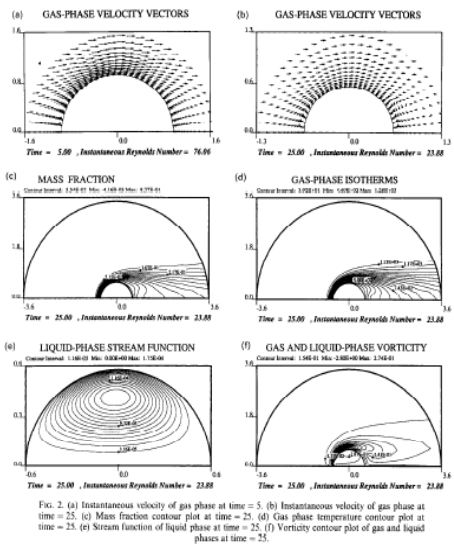
Streamlines in liquid C.G. frame



Vorticity magnitude

*この液滴は少しずつ変形しています

Cf.



Chiang, Raju, Sirignano (Int. J Heat Mass Transfer 1992)

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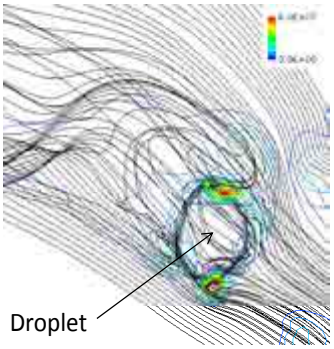
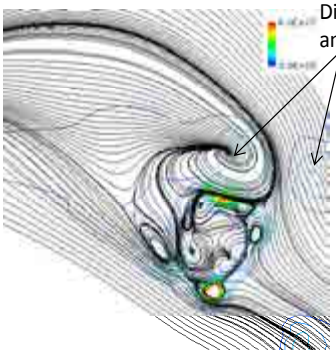
液滴数密度：低

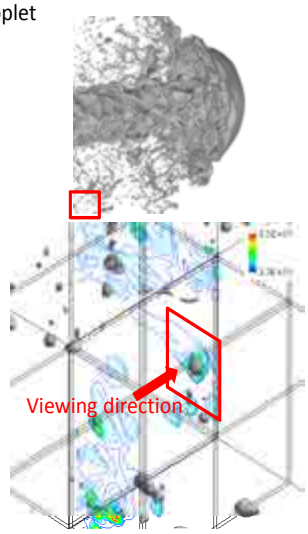


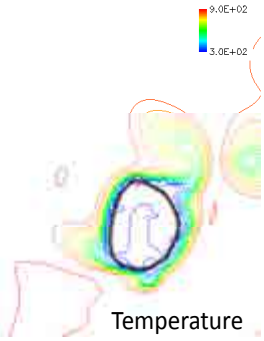
3D streamlines



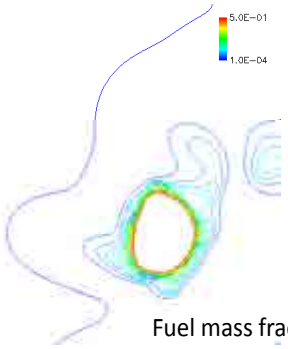
2D streamlines

Based on C.G. velocity of liquid. Color indicates vorticity.



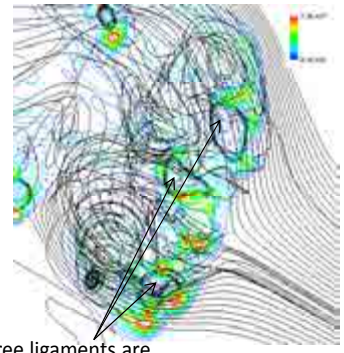


Temperature

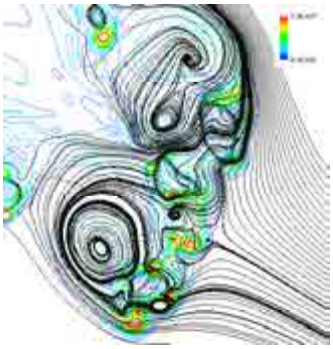


Fuel mass fraction

液滴数密度：高

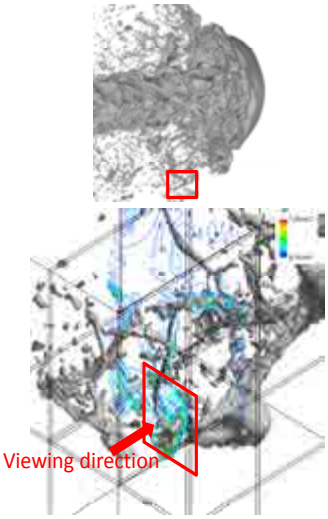


3D streamlines

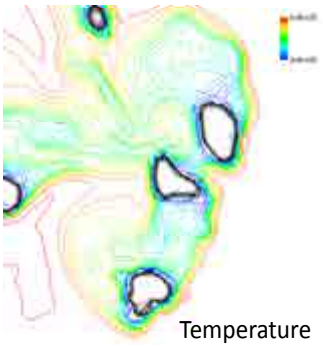


2D streamlines

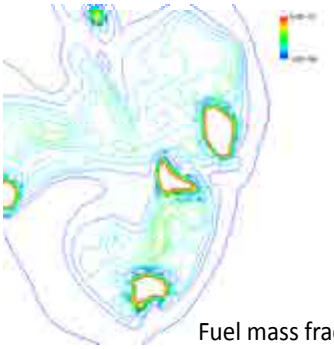
Based on C.G. velocity of liquid. Color indicates vorticity.



These are ligaments



Temperature



Fuel mass fraction

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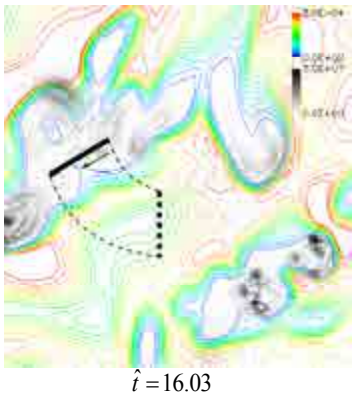
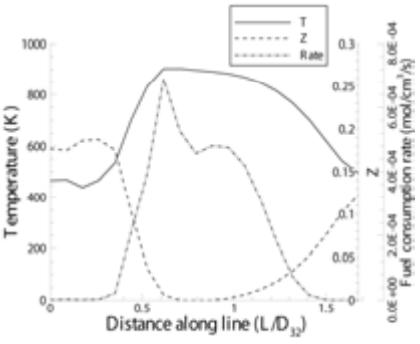
燃料蒸気クラスタの形成

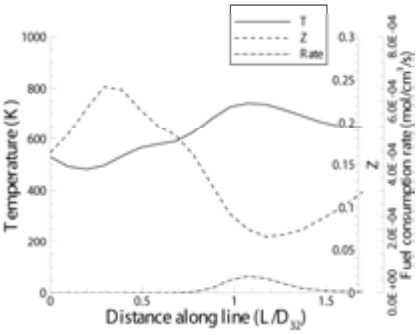
Color: reaction rate
Black-white: vorticity

$\hat{t}=15.71$



$\hat{t}=16.03$





Molecular diffusion τ_d

$\tau_d = L^2/D_{dif} = 5.4\text{e-}6\ \text{s}$

Or $\Delta\hat{t} = 5.4$

With
D_{dif}=3.4e-6m^2/s
$L=D_{32}$=4.3μm

Eddy turnover τ_e

$\tau_e = 4\pi/|\boldsymbol{\omega}| = 3.6\text{e-}7\ \text{s}$

Or $\Delta\hat{t} = 0.36$

With
$|\boldsymbol{\omega}| = 3.5\text{e}7\ \text{s}^{-1}$

Actual time difference

$\Delta\hat{t} = 0.32$

すでに結合しており、渦による近傍の混合促進が分かる

群燃焼数

数密度の高い領域Bでは、おおざっぱに

$$G = 2\pi n D_{32} R_c^2 = 5.7$$

With
R_c=0.25D_N
n=3.4e14 m^{-3}
D_{32}=4.3μm

External Group Combustion

- 相対速度による液滴周りの輸送
- 液滴間の干渉

液滴数密度が高いときの熱・物質輸送の修正モデルを現在構築中

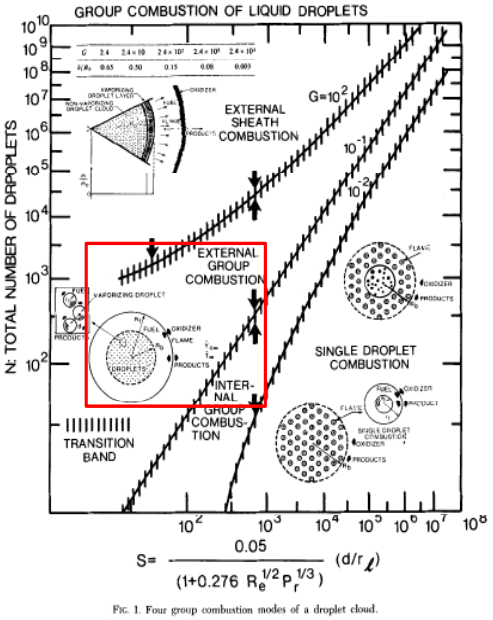


FIG. 1. Four group combustion modes of a droplet cloud.

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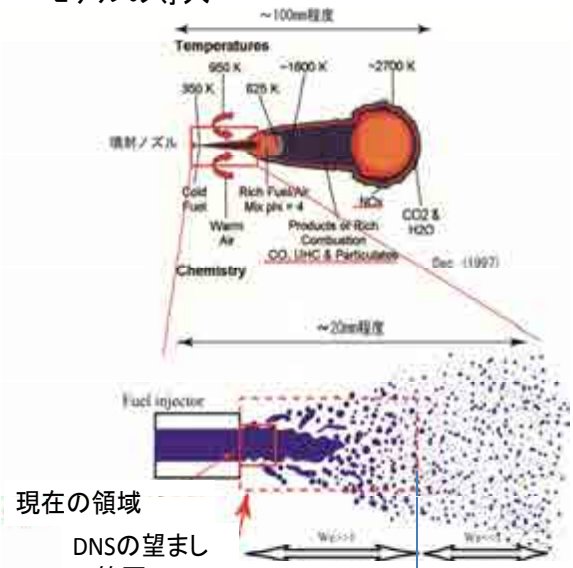
今後の展望：スケール拡張

•空間スケール
•少なくとも一次微粒化領域のカバー
＋ハイブリッド法（Euler-Euler, Euler-Lagrange）
•モデルの導入



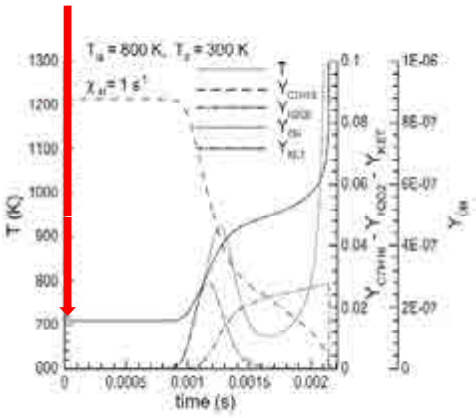
現在の領域

DNSの望ましい範囲

DNS (Euler-Euler)　LES (Euler-Lagrange)

•時間スケール
•着火遅れ時間程度までのカバー

現在の時間スケール



Viggiano (CNF 2010)

まとめ

– 噴射孔直下の液体燃料噴霧の挙動を詳細に見、そしてかなりの理解が進んだ
  • 実形状に由来する微粒化により液滴分布が決まり、その後の現象に影響する
  • 単液滴とみなせるところは従来モデルにさほど修正は必要ない
  • 液滴の密な領域は群形態に進んでいき、従来モデルは誤差が大きい可能性がある
    – 下流域でも気相の渦で液滴がクラスタリングするので要注意

– 今後の取り組み
  • モデリングのさらなる解析
  • 空間・時間スケールの拡張
  • 反応系等の高度化

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東京大学JAXA社会連携講座シンポジウム

Sep/27/2012

超臨界圧における極低温流体混合現象の高精度数値モデリング

寺島洋史（東大）
越　光男（東大）

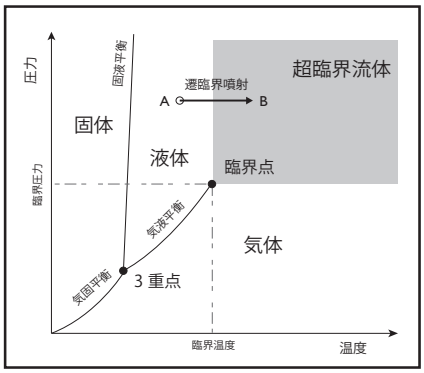
1

Backgrounds I

Pressure in rocket engine chamber

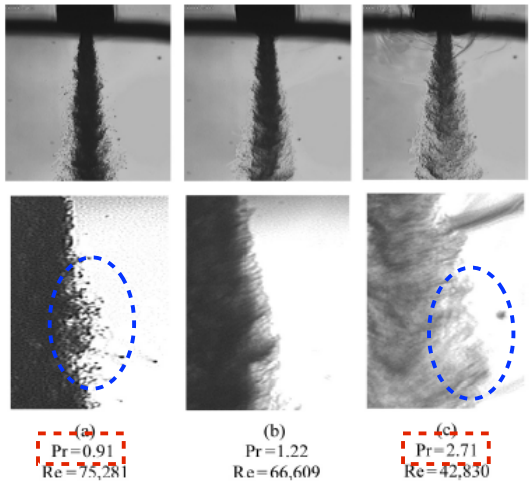
LE-7A engine

- 3~20 MPa: supercritical pressures



Mixing, followed by combustion

- Disappearance of surface tension and latent heat
- Stirring and diffusion process, rather than atomization: **Turbulent mixing**



Chehroudi et al. (2002)

2

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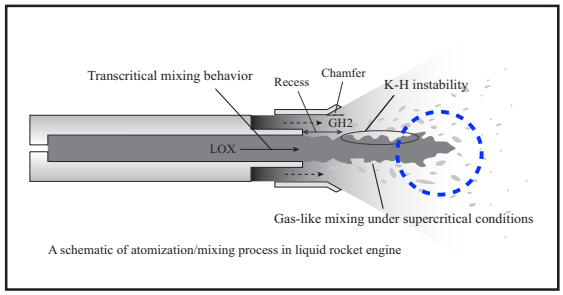
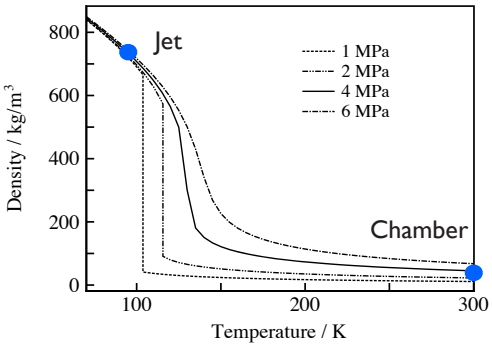
Backgrounds II

- Large difference of thermodynamic fluid properties: **cryogenic jet into supercritical fluids**



A schematic of atomization/mixing process in liquid rocket engine



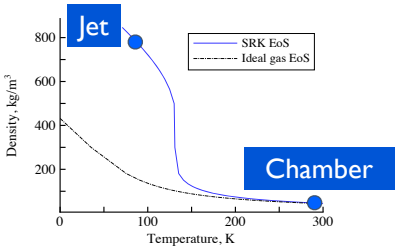
A diagram for nitrogen

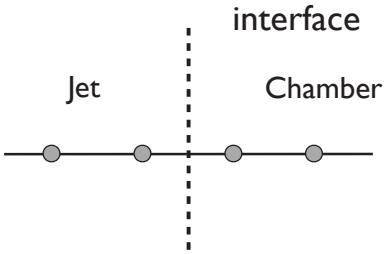
- **Real fluid effects**
- **Turbulent flows**
- **Large density contrast**

3

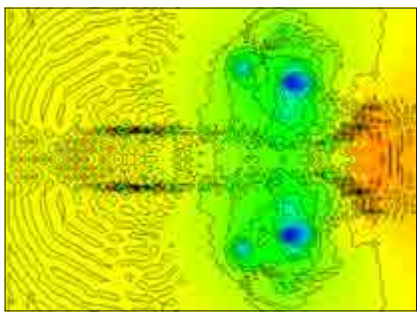
What the problem is

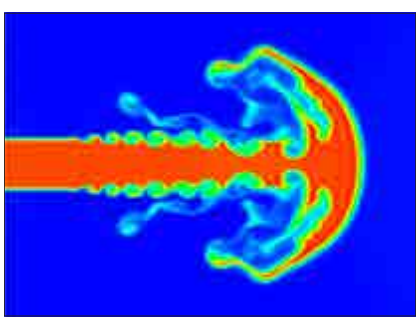
- **Turbulent flows** → High-order (central) schemes are preferred...,





- **Large contrast:** gas-liquid-like interface → Computational instability





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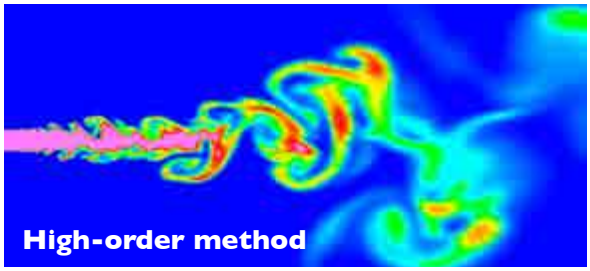
Superiority of high-order schemes

- To resolve a wide range of scales, acoustics, etc.,



5

Objectives

- Propose an approach for simulating supercritical cryogenic fluids, while using high-order central differencing schemes and general EoS

- Explore some distinctive characteristics of supercritical cryogenic jet mixings

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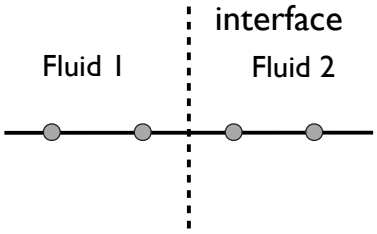
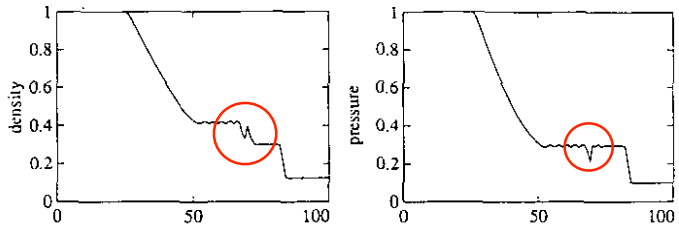
Present idea inspired by



I. Karni (JCP, 1994), Abgrall (JCP, 1996)

- maintaining velocity and pressure equilibriums at interface

- Spurious oscillations when using a conservative form in compressible multicomponent flows



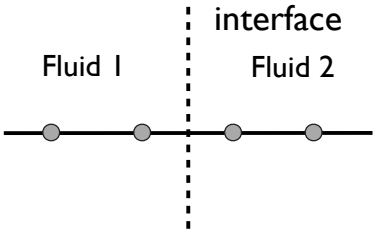
Karni (JCP, 1994)

Two-component shock tube problem (calorically perfect gas EoS)

Discretization of the governing equations

- The Euler equations in an 1-D form
- Central difference discretization plus Numerical diffusion term

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} D_j^c \left[\rho u - A_\rho\right]$$
$$(\rho u)_j^{n+1} = (\rho u)_j^n - \frac{\Delta t}{\Delta x} \left(D_j^c \left[\rho u u - A_{\rho u}\right] + D_j^c \left[p\right]\right)$$
$$E_j^{n+1} = E_j^n - \frac{\Delta t}{\Delta x} D_j^c \left[(E+p)u - A_E\right]$$



e.g.,

$D_j^c[f] = (f_{j+1} - f_{j-1})/2$: central differencing operator

$D_j^c\left[A.\right]$: numerical diffusion term

$$u_j^{n+1} = u_j^n = u$$

$$p_j^{n+1} = p_j^n = p$$

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Velocity equilibrium

Considering the mass and momentum equations,

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} u D_j^c \left[\rho - \frac{A_\rho}{u} \right]$$

$$(\rho u)_j^{n+1} = (\rho u)_j^n - \frac{\Delta t}{\Delta x} u u D_j^c \left[\rho - \frac{1}{u} \frac{A_{\rho u}}{u} \right]$$

→ $$A_{\rho u} = u A_\rho$$

- The velocity and pressure are uniform across an interface at a time step

- The velocity is unchanged at the next time step (**oscillation-free**)

$$u_j^{n+1} = u_j^n = u$$

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Pressure equilibrium

Considering the mass and energy equations,

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} u D_j^c \left[\rho - \frac{A_\rho}{u} \right]$$

$$(\rho e + \rho \frac{uu}{2})_j^{n+1} = (\rho e + \rho \frac{uu}{2})_j^n - \frac{\Delta t}{\Delta x} \frac{uu}{2} u D_j^c \left[\frac{2}{uu} \rho e + \rho - \frac{2}{uu} \frac{A_E}{u} \right]$$

- The velocity and pressure are uniform across an interface at a time step

→ $$A_E = A_{\rho e} + \frac{uu}{2} A_\rho$$

The energy equation is reduced to the internal energy equation:

→ $$(\rho e)_j^{n+1} = (\rho e)_j^n - \frac{\Delta t}{\Delta x} u D_j \left[\rho e - A_{\rho e} \right]$$

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Pressure equilibrium (*cont'd*)

with **a calorically perfect gas:** $p = (\gamma - 1)\rho e$

$$(\rho e)_j^{n+1} = (\rho e)_j^n - \frac{\Delta t}{\Delta x} u D_j \left[\rho e - A_{\rho e}\right]$$

$$\downarrow \quad A_{\rho e} = p A_\gamma$$

$$\left(\frac{1}{\gamma - 1}\right)_j^{n+1} = \left(\frac{1}{\gamma - 1}\right)_j^{n} - \frac{\Delta t}{\Delta x} u D_j^c \left[\frac{1}{\gamma - 1} - A_\gamma\right] \quad \& \quad A_E = \frac{uu}{2} A_\rho + p A_\gamma$$

- a well-known advection equation by Abgrall (JCP, 1996)

- The pressure is unchanged at the next time step (**oscillation-free**)

$$p_j^{n+1} = p_j^n = p$$

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Summary of numerical diffusion terms (fluxes)

a calorically perfect gas

$$\begin{pmatrix} A_\rho \\ A_{\rho u} \\ A_E \end{pmatrix} = \begin{pmatrix} 1 \\ u \\ \frac{uu}{2} \end{pmatrix} A_\rho + \begin{pmatrix} 0 \\ 0 \\ p \end{pmatrix} A_\gamma$$

- serving as an interface-capturing
- velocity equilibrium
- pressure equilibrium

$$\left(\frac{1}{\gamma - 1}\right)_j^{n+1} = \left(\frac{1}{\gamma - 1}\right)_j^{n} - \frac{\Delta t}{\Delta x} u D_j^c \left[\frac{1}{\gamma - 1} - A_\gamma\right]$$

- pressure equilibrium

• A_ρ and A_γ modeled by extending the LAD method (Cook: JCP 2004, Kawai: JCP 2008)

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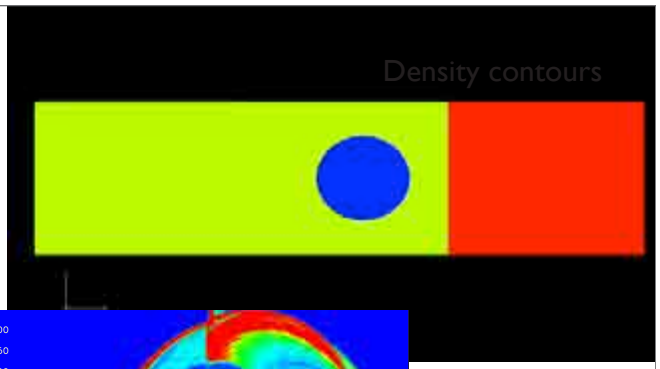
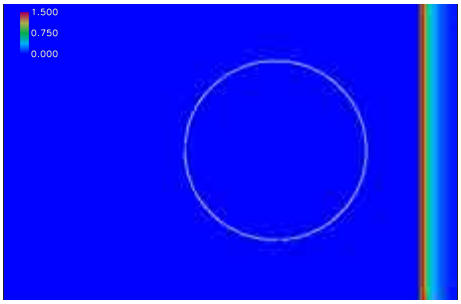
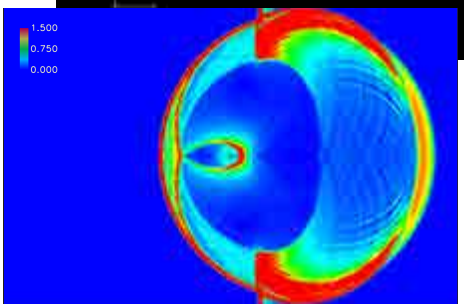
2-D shock-bubble interaction

- Experiment of Hass and Sturtevant (1987)
- 1300×361 with Δx=0.005

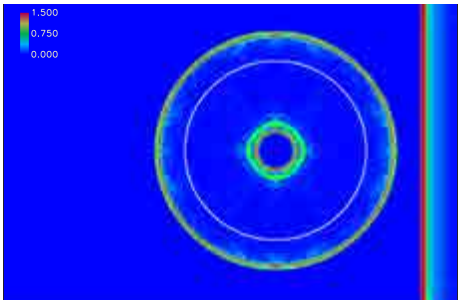


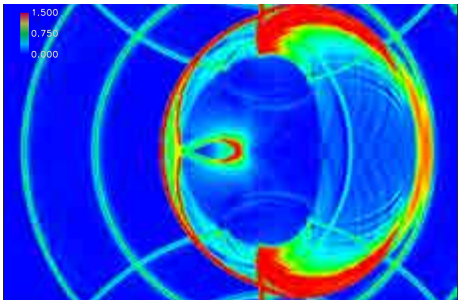
Present method Pressure gradient





FC method





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Extend to general EoS: pressure equilibrium

$$(\rho e)_j^{n+1} = (\rho e)_j^n - \frac{\Delta t}{\Delta x} u D_j \left[\rho e - A_{\rho e}\right]$$

the calorically perfect gas !!

$$\boxed{p = (\gamma - 1)\rho e} \longrightarrow \left(\frac{1}{\gamma - 1}\right)_j^{n+1} = \left(\frac{1}{\gamma - 1}\right)_j^{n} - \frac{\Delta t}{\Delta x} u D_j^c \left[\frac{1}{\gamma - 1} - A_\gamma\right]$$

Considering a Mie-Gruneisen-type or a van der Waals equations of state,

$$\boxed{p(\rho, e, Y_i) = F(\rho, Y_i)\rho e + G(\rho, Y_i)}$$

$$\longrightarrow \quad \boxed{\begin{aligned} (1/F)_i^{n+1} &= (1/F)_i^n - \frac{\Delta t}{\Delta x} u D_i \left[(1/F)\right] \\ (G/F)_i^{n+1} &= (G/F)_i^n - \frac{\Delta t}{\Delta x} u D_i \left[(G/F)\right] \end{aligned}}$$

K.M. Shyue, JCP., 2001

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- More complicated EOS

$$p = \frac{RT}{V - b_{srk}} - \frac{a_{srk}\alpha(T)}{V^2 + b_{srk}V}$$

: cubic EOS

$$p = \rho RT\left(1 + B(T)\rho + C(T)\rho^2 + \cdots\right)$$

: virial EOS

Look-up table-typed EOS

Attempting Abgrall's and Shyue's ideas seems to be difficult to general EOSs

15

Pressure evolution equation

- Karni (1996), Fedkiw (2001)
- Single-species case considered

$$p = f(\rho, e)$$

-- (c-1)

$$\frac{Dp}{Dt} = \left(\frac{\partial p}{\partial \rho}\right)_e \frac{D\rho}{Dt} + \left(\frac{\partial p}{\partial e}\right)_\rho \frac{De}{Dt}$$

-- (c-2): Pressure evolution equation

$$\begin{aligned} &\frac{\partial p}{\partial t} + \boldsymbol{u}\cdot\nabla p \\ &= \left[\left(\frac{\partial p}{\partial \rho}\right)_e + \frac{p}{\rho^2}\left(\frac{\partial p}{\partial e}\right)_\rho\right](-\rho\nabla\cdot\boldsymbol{u}) + \left(\frac{\partial p}{\partial e}\right)_\rho\left(\frac{1}{\rho}\nabla\cdot(\boldsymbol{\tau}\cdot\boldsymbol{u} - \boldsymbol{q})\right) \\ &= -\rho c^2\nabla\cdot\boldsymbol{u} + \frac{\alpha_p}{c_v\beta_T}\left(\frac{1}{\rho}\nabla\cdot(\boldsymbol{\tau}\cdot\boldsymbol{u} - \boldsymbol{q})\right) \end{aligned}$$

-- (c-3)

$$c = \left(\frac{\partial p}{\partial \rho}\right)_s = \left(\frac{\partial p}{\partial \rho}\right)_e + \frac{p}{\rho^2}\left(\frac{\partial p}{\partial e}\right)_\rho$$

$$c_v = \left(\frac{\partial e}{\partial T}\right)_V \qquad \alpha_p = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p \qquad \beta_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T$$

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The proposed governing equations set

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = \nabla \cdot (\varrho_\rho \nabla \rho),$$

- Interface-capturing

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u} + p\boldsymbol{\delta} - \boldsymbol{\tau}) = \nabla \cdot (\varrho_\rho (\boldsymbol{u} \otimes \boldsymbol{g}) \nabla \rho),$$

- Velocity equilibrium

$$\frac{\partial p}{\partial t} + \boldsymbol{u} \cdot \nabla p = -\rho c^2 \nabla \cdot \boldsymbol{u} + \frac{\alpha_p}{c_v \beta_T} \left(\frac{1}{\rho} \nabla \cdot (\boldsymbol{\tau} \cdot \boldsymbol{u} - \boldsymbol{q}) \right),$$

- Pressure equilibrium

$$p = \frac{RT}{V - b_{srk}} - \frac{a_{srk}\alpha(T)}{V^2 + b_{srk}V}$$

$$\varrho_\rho = C_\rho \frac{c}{\rho} \overline{\left| \sum_{l=1}^{n_d} \frac{\partial^r \rho}{\partial x_l^r} \Delta_l^{r+1} \right|}$$

Disadvantage: the energy is not conserved, resulting in incorrect shock strength or speed, while the mass and momentum are conserved

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Numerical methods

- Sixth-order compact difference scheme
- Eighth-order low-pass filtering (a free-parameter: 0.495)
- Third-order TVD Runge-Kutta scheme

- CFL = 0.4
- One-point jump at initial condition

- FC method: conventional fully conservative method

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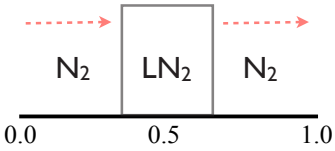
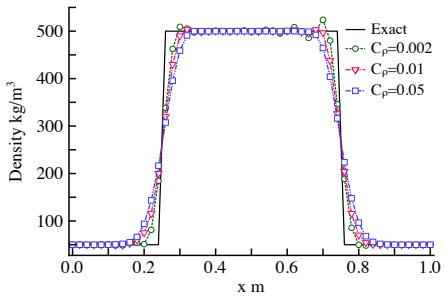
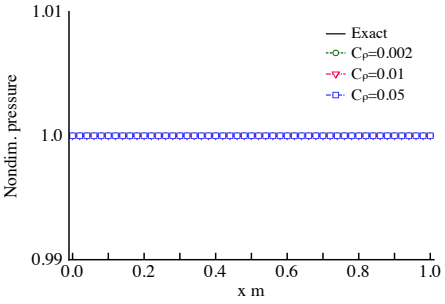
Advection of a contact discontinuity



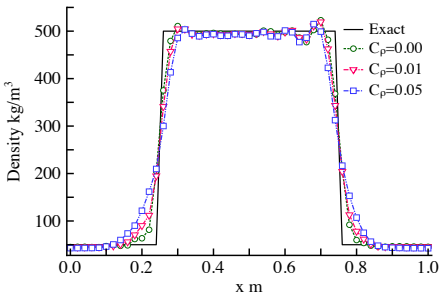
- 51 grid points with Δx=0.02
- Nitrogen single-species flow
- 5.0 MPa
- Density: 500/50, Temperature: 123/332

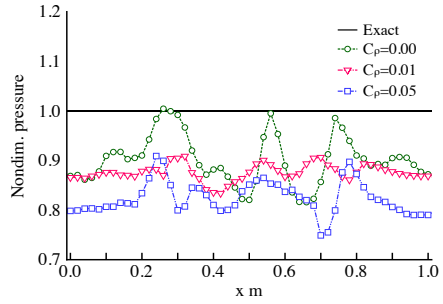
Present method





FC method





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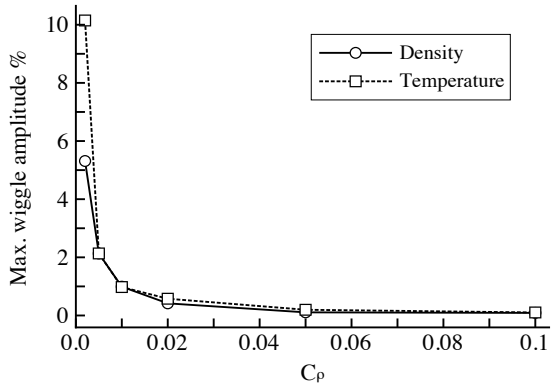
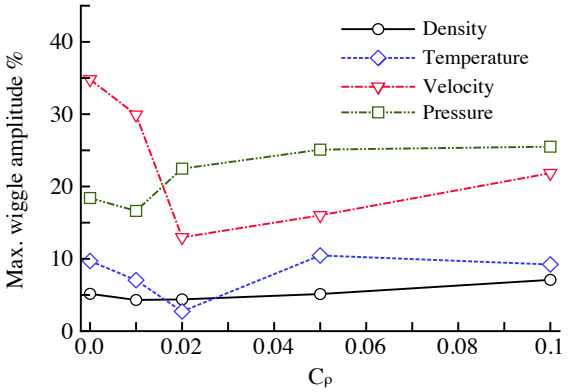
Unfavorable characteristics of a full conservation form

Present method



FC method



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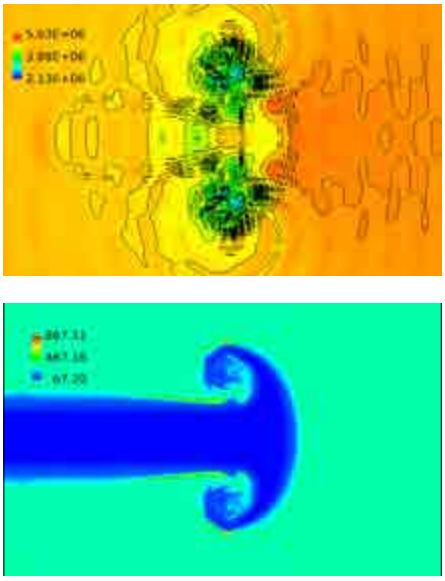
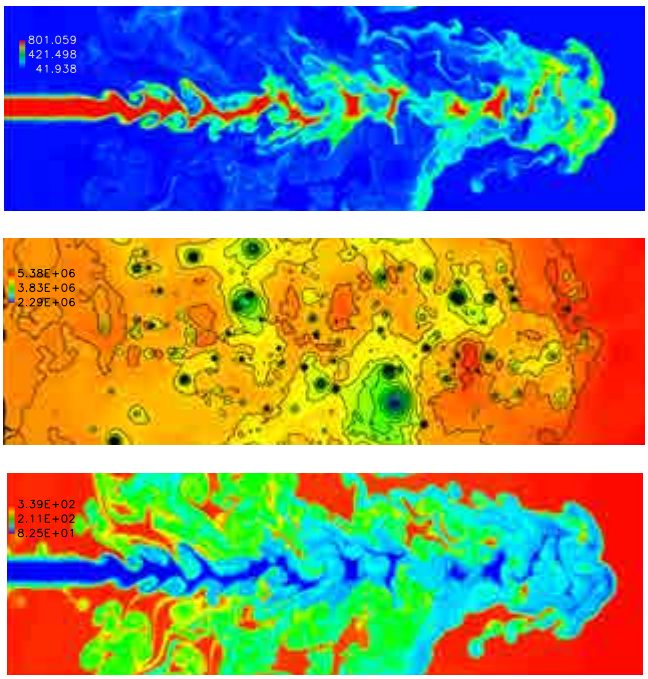
Performance of the proposed model

- Cryogenic nitrogen jet: Density: 800/50 kg/m^3, Temperature: 83/332 K, 5 MPa



Conventional (FC) method



Proposed method

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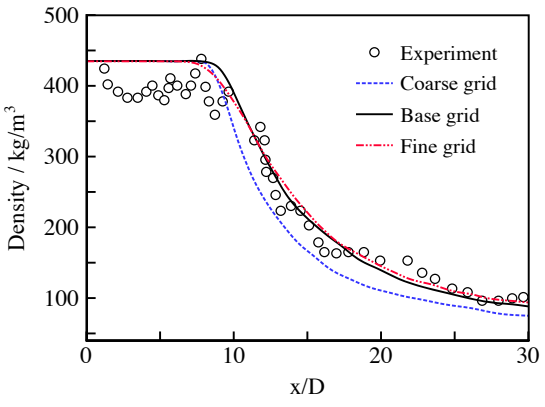
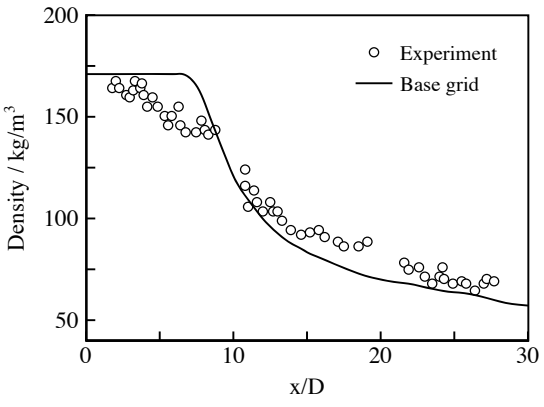
Validation of the proposed model

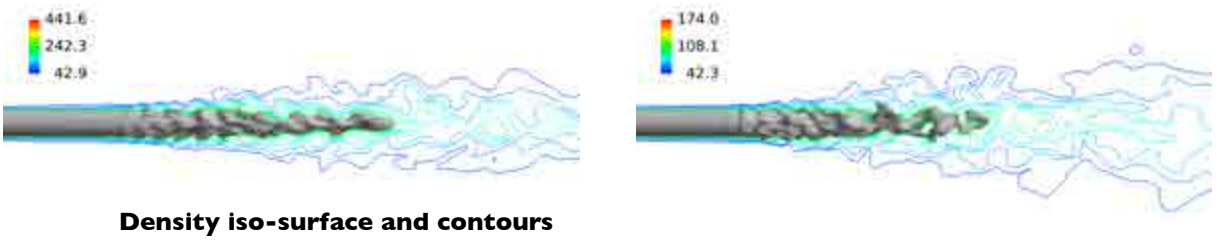
- Supercritical 3-D round jet in Mayer's experiment (Mayer et al., HMT 2003)

Case 3: T = 126 K, 4 MPa



Case 4: T = 137 K, 4 MPa





Density iso-surface and contours

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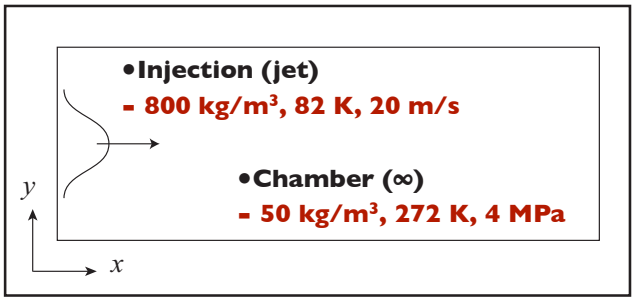
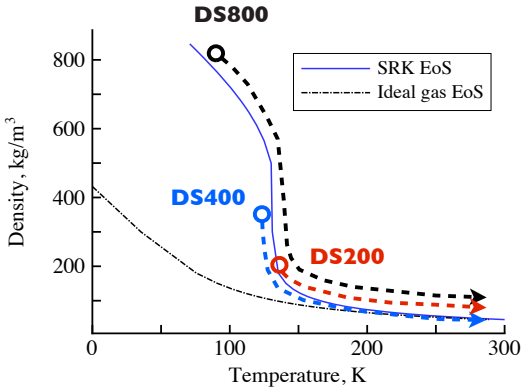
Conditions

$p_{cr} = 3.4$ MPa, $T_{cr} = 126.2$ K, $\rho_{cr} = 313.3$ kg/m^3

- Two-dimensional planar N_2 (single-specie) jet in supercritical pressure conditions
- 4 and 8 MPa





*Pseudo-critical temperature: 128 K at 4 MPa

Table 1. Conditions for 4 MPa case.

ρ_{jet} kg/m^3	u_{jet} m/s	T_{jet} K	Re$_{jet}$ $\times 10^5$	ρ_∞ kg/m^3	T_∞ K
800	20	82.1	1.2		
400	$20\sqrt{2}$	126.9	3.6	50.0	271.13
200	40	132.9	4.5		

*the same momentum used for jet

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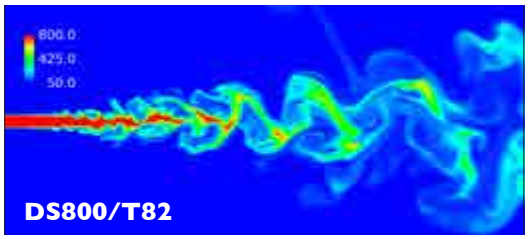
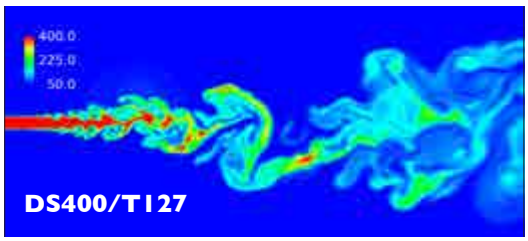
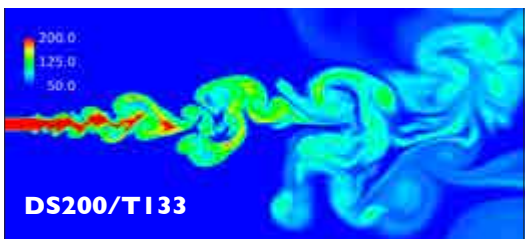
A unsteady jet mixing

T=100 K injection, 5 MPa







- Statistical data obtained over 10 ms

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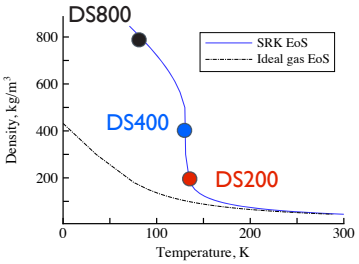
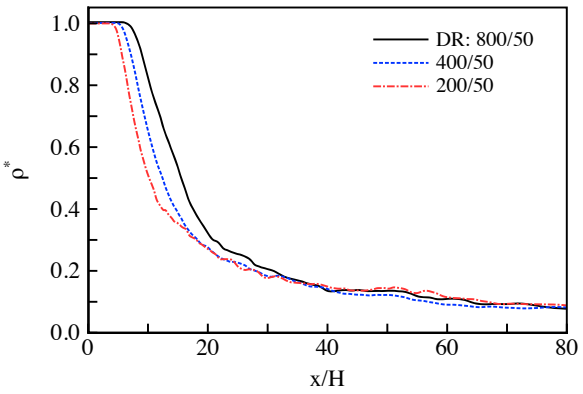
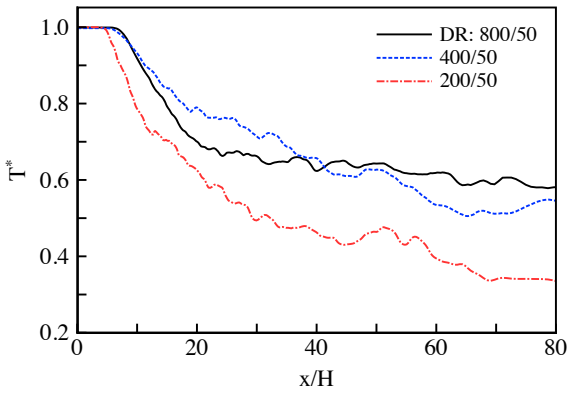
Results: mean properties on centerline

- 4 MPa







$$\rho^* = \frac{\rho - \rho_\infty}{\rho_{inj} - \rho_\infty}$$

$$T^* = \frac{T - T_\infty}{T_{inj} - T_\infty}$$

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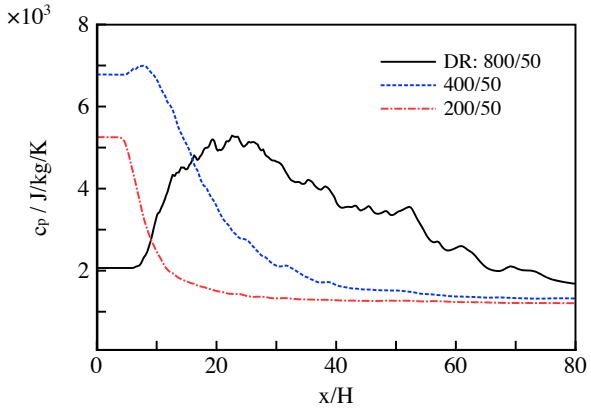
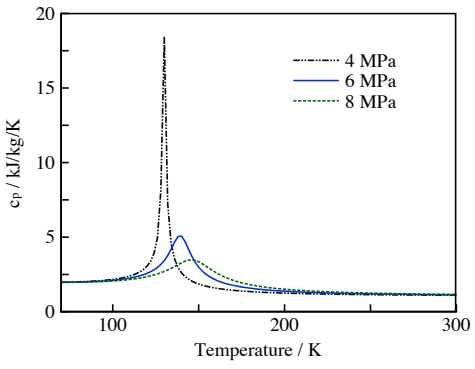
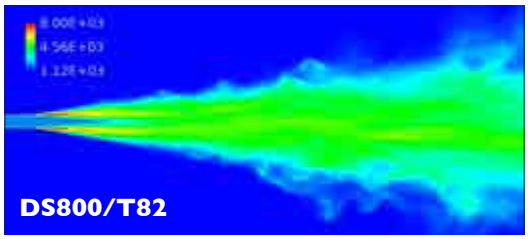
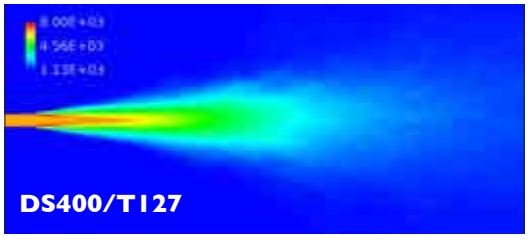
Why it happened: mean specific heat distributions









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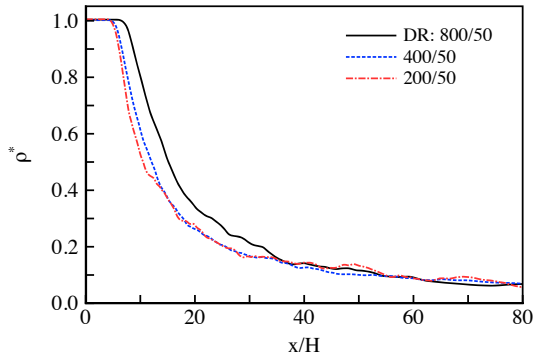
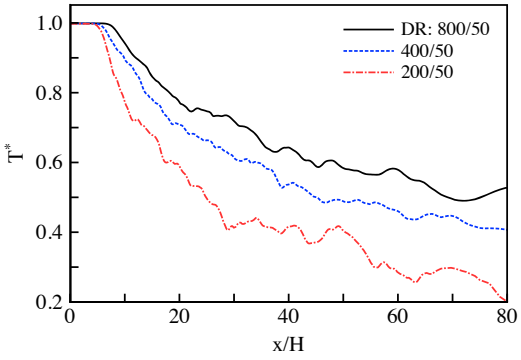
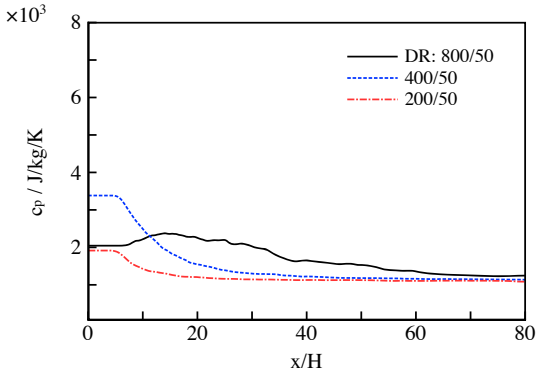
8 MPa case







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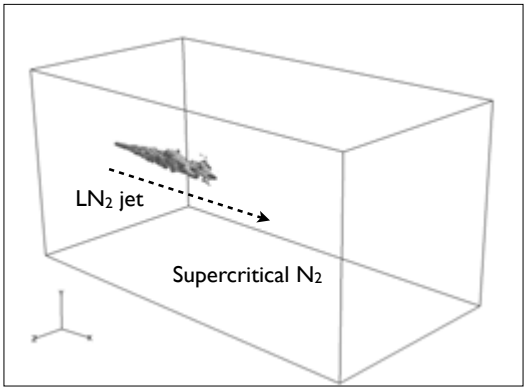
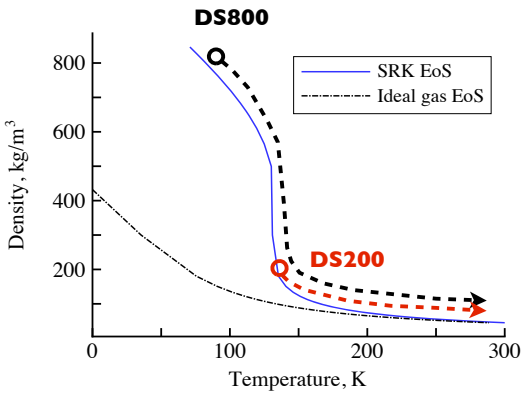
Demonstration on 3-D jet

$p_{cr} = 3.4$ MPa, $T_{cr} = 126.2$ K, $\rho_{cr} = 313.3$ kg/m^3

- Three-dimensional round N_2 (single-specie) jet in supercritical pressure conditions
- Injection geometry just changed: 2-D slit to 3-D circle, others are the same as the 2-D conditions
- Case1: 4 MPa, **82 K**, Case 2: 4 MPa, **133 K**





*Pseudo-critical temperature: 128 K at 4 MPa

- 398×293×293 grid points used

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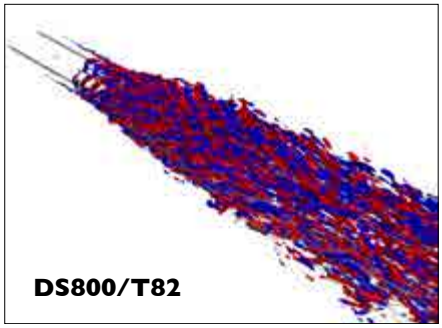
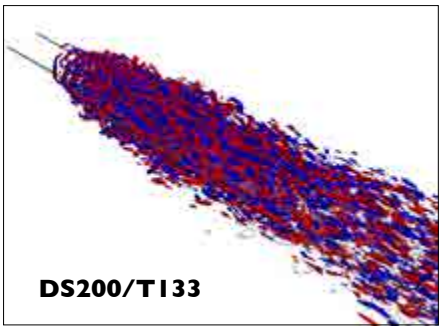
3-D Results

$p_{cr} = 3.4$ MPa, $T_{cr} = 126.2$ K, $\rho_{cr} = 313.3$ kg/m^3

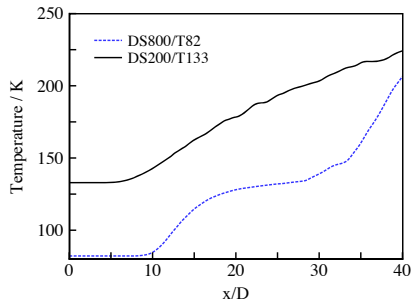
- There is no clear difference of vortical structures

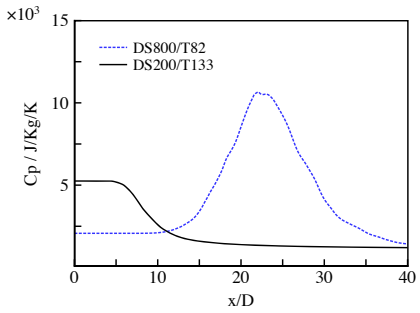




- Flattened temperature distribution appeared also in the 3-D round jet

*Pseudo-critical temperature: 128 K at 4 MPa





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Summary

- A strategy for simulating gas-liquid-like flows under supercritical pressures proposed

Satisfying the pressure and velocity equilibriums is a key to robust application of high-order schemes to severe thermodynamic fluid conditions

Terashima and Koshi, J. Computational Physics, 231(2012)

- A unique characteristic of supercritical jets successfully explored

The distinctive features of temperature caused by the interaction of multiple factors: a very low temperature injection, a variation of the specific heat, and mixing process

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液酸・液水高圧燃焼試験における燃焼不安定現象

宇宙航空研究開発機構
エンジン研究開発グループ

布目　佳央・田村　洋・冨田　健夫

平成24年9月27日

燃焼不安定性問題と噴射器設計

燃焼不安定性にかかわる問題はロケットエンジンの開発に大きな影響を及ぼす
- テスト-フェイル-フィックス型の開発
  →不具合発生時に、出戻りが発生し，開発期間・コストの大幅な増加
- バッフル・アコースティックキャビティの装着によるコスト・重量増など
  → その解決には多大な時間とコストが発生
- 燃焼不安定を精度良く予測するツールは未だ無し
- 現象の詳細・発生範囲も特定できていない

設計段階や研究フェーズでの現象把握・対処が重要！

- 要素試験による現象把握，リスク等の抽出
- 要素試験に裏打ちされた高度な解析手法（予測手法）の確立

経験依存の設計から、試験／解析データに裏打ちされた設計手法の確立へ

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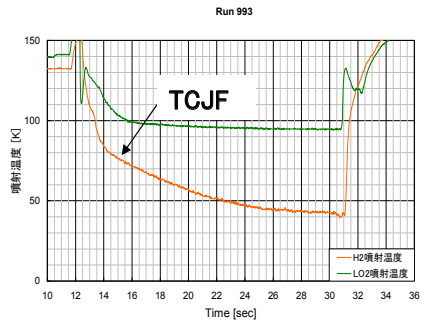
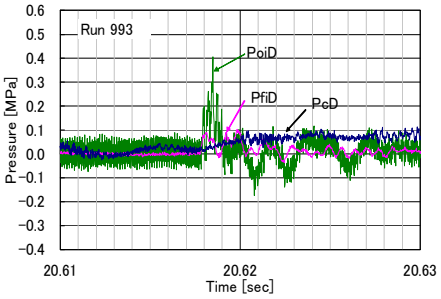
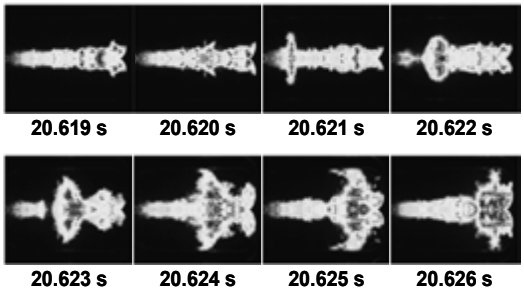
同軸型噴射器で見られた燃焼不安定事例（燃料噴射温度傾斜試験での燃焼の可視化）



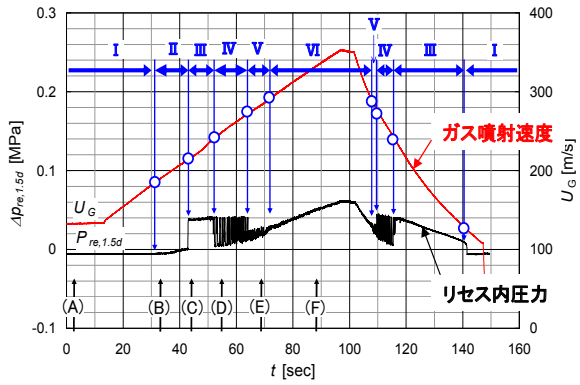


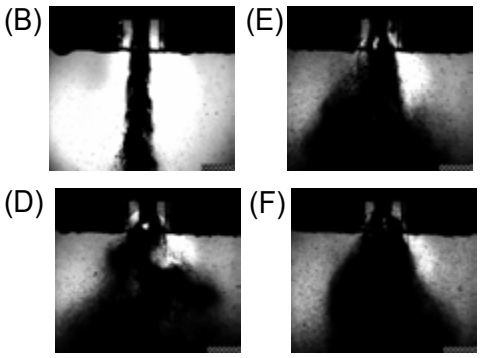
LOX/LH2, Pc= 6 MPa, O/F=6



・TCJFが約53 K以下となると、PoiDに圧力スパイクが発生し、その直後に噴射器出口で火炎がバースト的に発達するもととなる塊が噴射される現象が観察された.
→ TCJF低下による高周波振動の要因？
→ 圧力スパイクの発生原因は？
・歪み計測から、LOXポストも機械的に振動している事が判明.

同軸型噴射器で見られた噴流の自励振動（水・ガス窒素による同軸型噴射器の水噴霧試験）





- 同軸噴射器を模した矩形断面の噴射器による水・窒素の流し試験
- ガス流量を連続的に変化させるとき、リセス内の圧損がステップ状に上昇
- このときLOXポストは左右に大きく振動し，噴流が大きく蛇行して微粒化する現象が観察
- リセス内で微粒化が促進，外周のガス噴流の流路が閉塞されることが基で流体振動が発生.

LOX/LH2同軸型噴射器の燃焼試験でも，噴射圧が高周波で振動し、併せてLOXポストが振動すると考えられる現象が観察されており，ここでの観察結果と類似点が多い.

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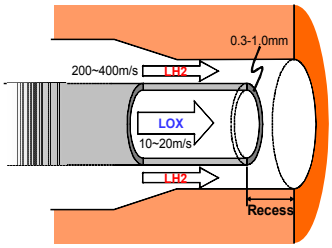
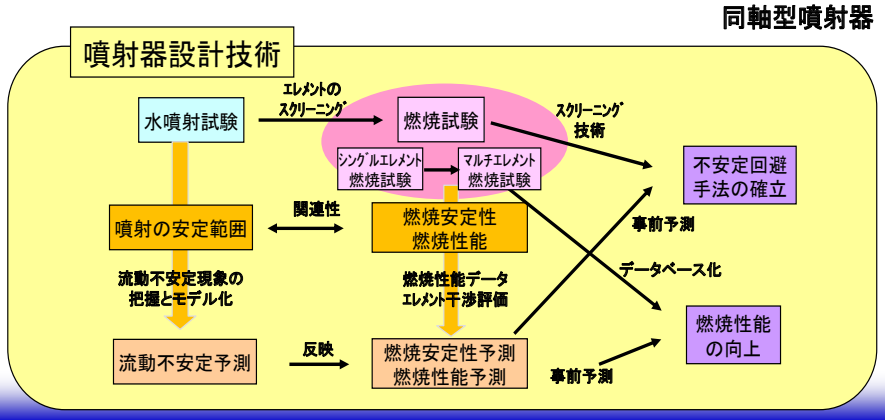
液体ロケットエンジンの噴射器設計

■噴射連成不安定
・ 作動条件により，同軸型噴射器内で噴流の流動不安定現象が生じ，燃焼現象と連成することで発生する燃焼不安定．
・ 発生メカニズムや噴射器形状・噴射条件との関連性は未だ不明．



同軸型噴射器



目的

複数の試験条件やエレメント形状での燃焼状況を把握し、液酸・液水ロケット噴射器の設計に必要な燃焼特性基礎データを取得する

- 7種類のエレメント形状の噴射器を対象に燃焼試験を実施
- 燃焼安定性に及ぼす水素噴射温度および噴射器形状の影響について評価
- 不安定燃焼が発生する条件の特定（閾値のマップ化 ）
- 数値シミュレーションの検証データの取得

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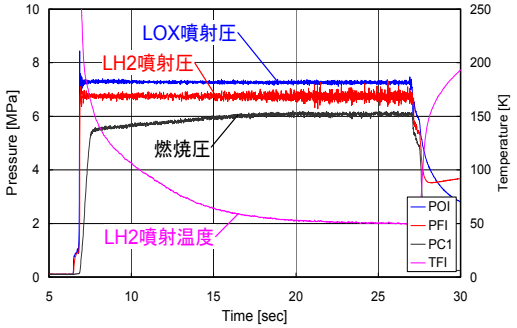
実験方法

◆ **試験条件範囲**

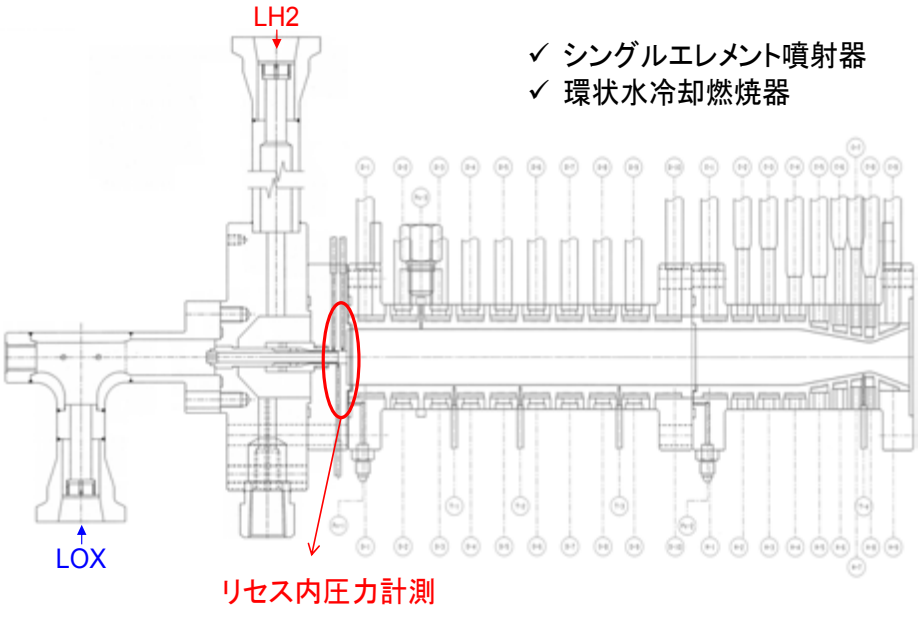
推進剤 ： LOX/LH2
燃焼圧 ：(6MPa), 7.5 MPa, 9 MPa
混合比 ：4 ～ 8
LH2噴射温度: 40 K ～150 K
(Rump test)
噴射速度比 ： 11 ～ 40
燃焼時間: 20～30秒



◆ **評価項目**

- リセス内の圧損特性 ：データ取得・流動不安定現象・ポスト振動等との関連性評価
- 燃焼の不安定現象 ： 発生範囲の特定，現象のモデル化，噴射器形状の影響

供試体概要



✓ シングルエレメント噴射器
✓ 環状水冷却燃焼器

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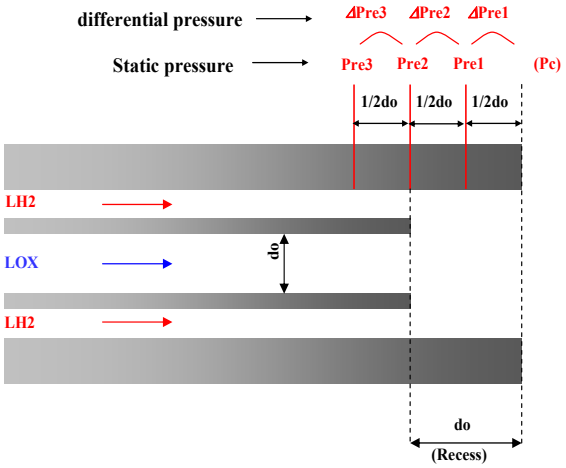
供試体概要（噴射器 1/2）

リセス圧力計測

シングルエレメント燃焼試験では，下図のような配置でリセス内圧力の計測を実施した



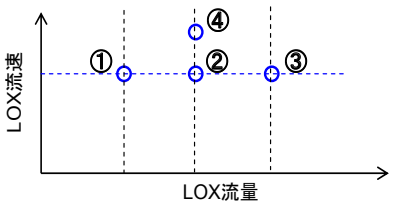
リセス内差圧の定義
ΔPre1 = Pre1 - Pc
ΔPre2 = Pre2 - Pre1
ΔPre3 = Pre3 - Pre2

供試体概要（噴射器 2/2）

供試噴射器	LOXポスト形状※	備考
Injector①	小口径／ストレート型	基準噴射器
Injector②	中口径／ストレート型	
Injector③	大口径／ストレート型	
Injector④	小口径／ストレート型	Injector①と同型，流量は②と同等

※リセス深さは全て1d_o，スワール無し．（d_o：LOXポスト内径）

ストレート型の各噴射器の形状は、右図のように，LOX流速がほぼ一定になるように設計．
（ただし，Injector④は除く）



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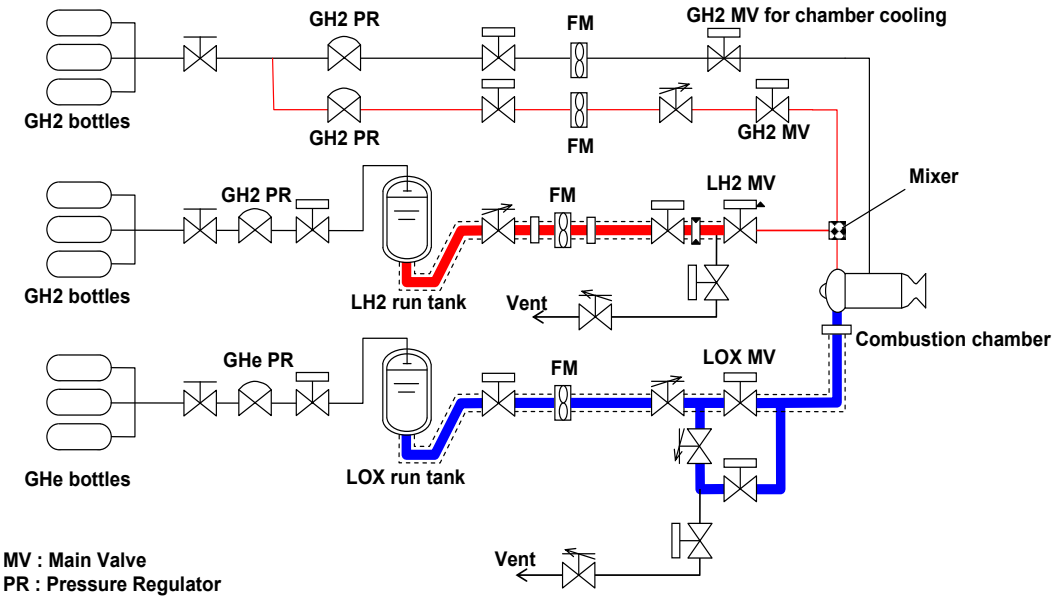
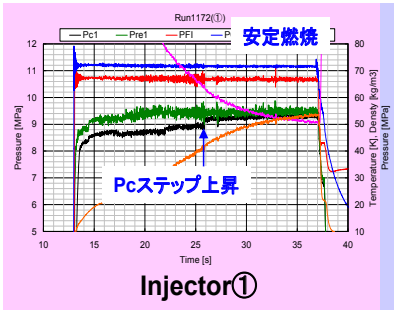
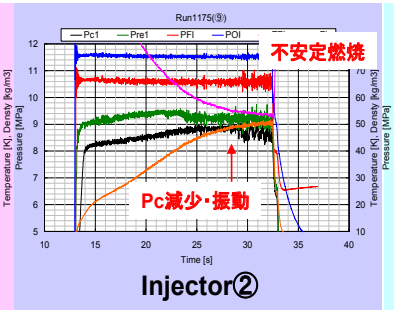
試験設備系統図
～角田宇宙センター液体水素ロケットエンジン要素試験設備～



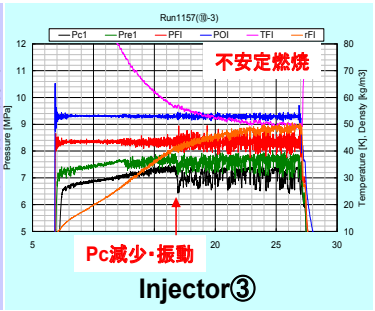
各噴射器の代表的な試験結果



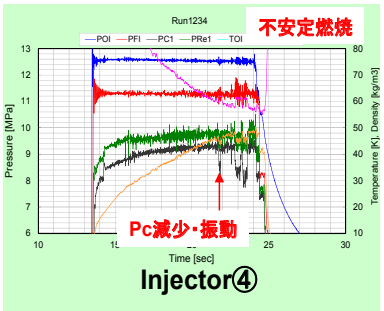
Injector①



Injector②



Injector③



Injector④

・ 大口径ほど，低噴射温度領域で，不安定燃焼に移行しやすい．
・ 小口径でも，流量増により，低噴射温度領域で大口径と同様の不安定燃焼に移行した．

小口径 → 大口径

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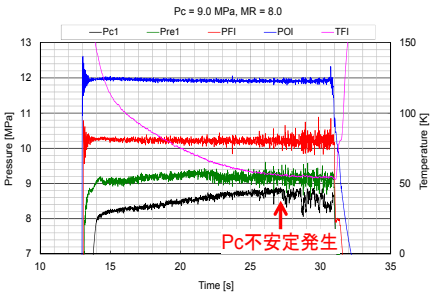
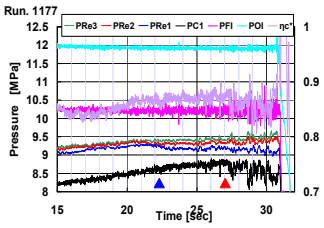
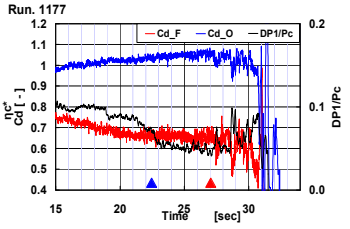
中孔径噴射器（②）の特徴（1/2）



圧力・LH2噴射温度の時間履歴

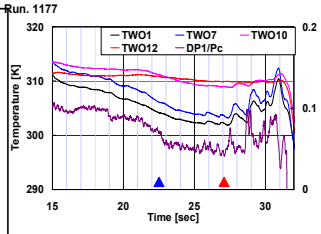


圧力・ηC*の時間履歴

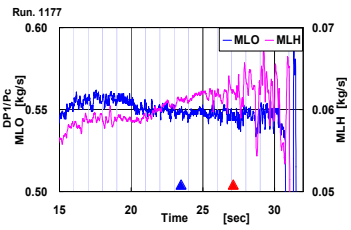


噴射器流出係数とΔPre1/Pcの時間履歴

- ✓ 燃焼中にΔPre1/Pcが減少（▲）
  - 各パラメータとの関連性が不明瞭
- ✓ 低LH2噴射温度域でPc不安定発生（▲）
  - Pc：減少，振動→ηC*：減少，振動（対応）
  - LH2噴射圧（PFI）：振動
  - ΔPre1/Pc：増加
  - 壁温度：増加→ ΔPre1/Pcと対応
  - 噴射器流出係数：減少→ ΔPre1/Pcと対応
  - 流量：脈動（やや減少）



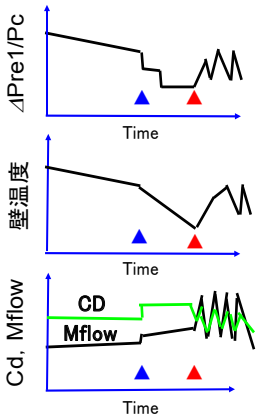
壁温度とΔPre1/Pcの時間履歴



流量の時間履歴

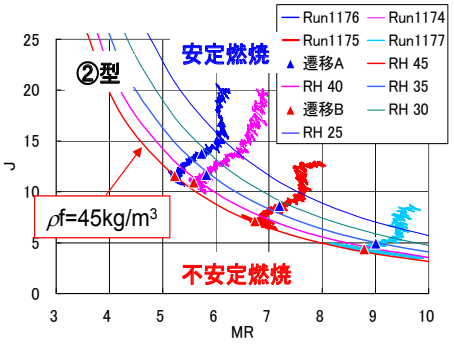
各パラメータの関連性から，リセス内にパルス振動を起こす現象が発生した可能性が高く、これによりhC*の減少，噴射器近くの熱負荷増大を招いたと考えられる．

中孔径噴射器（②）の特徴（2/2）



②型噴射器の模式図

②型噴射器の特徴は模式図に示す通り．
▲（B遷移点とする）が今回観察された燃焼不安定への遷移点と考えられる．下図は、J-MRマップ上にB遷移点をプロットしたものである．J-MRの関係式を以下のように導き，噴孔面積比，LOX噴射密度（ρ_o）を一定とするとρ_fをパラメータとした曲線が引け，B遷移点は概ねρ_f = 45 kg/m^{3}上に乗ることが分かる．
▲（A遷移点）は試験により傾向が一定せず，判定に多分な誤差を含むため，ここでの議論は避ける．



混合比と運動量比の関係

JとMRの関係式：$J = \dfrac{(\rho o/\rho f)}{MR^{\wedge}2 \times (Af/Ao)^{\wedge}2}$

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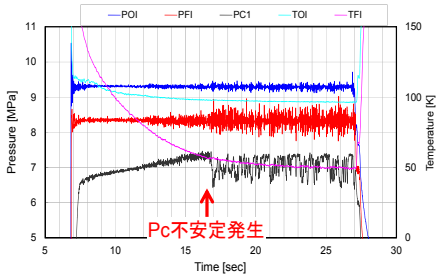
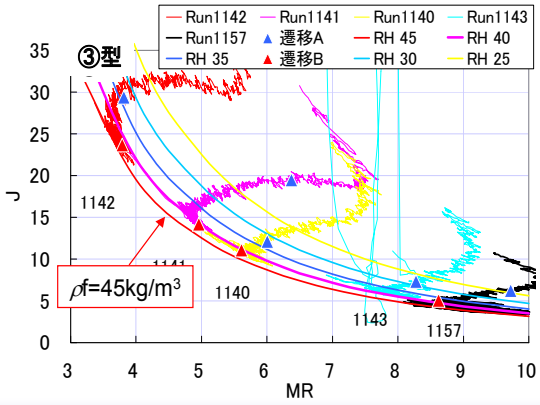
大孔径噴射器(③)の特徴



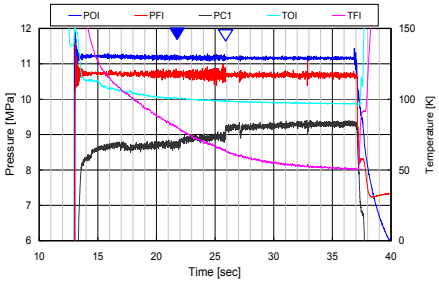
圧力・噴射温度の時間履歴

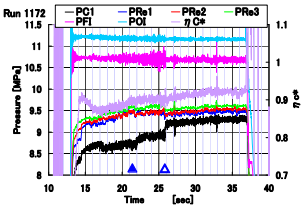
特徴は②型と同様

A遷移(▲)は、ρf≒30~35 kg/m3
B遷移(▲) は、ρf≒45kg/m3
▲は、ηc*ステップ減に対応

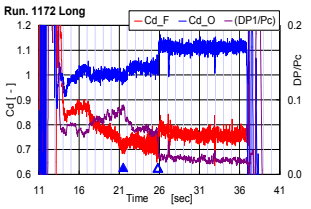


小孔径噴射器(①)の特徴(1/2)

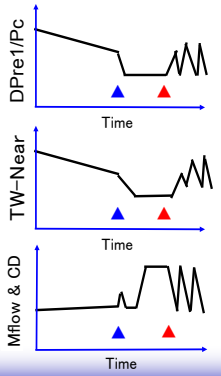




圧力・ηC*の時間履歴

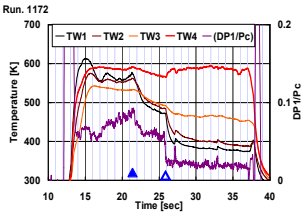


噴射器流出係数とΔPre1/Pcの時間履歴

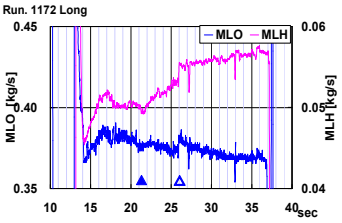


典型的な時間履歴
(模式図)

ΔPre1/Pc減は,
噴射面近くのTw減, Mflow増, Cd増.
ΔPre1/Pc増は,
噴射面近くのTw増, Mflow減, Cd減を招く.



壁温度とΔPre1/Pcの時間履歴



流量の時間履歴

低LH2噴射温度域で、燃焼不安定に遷移していない

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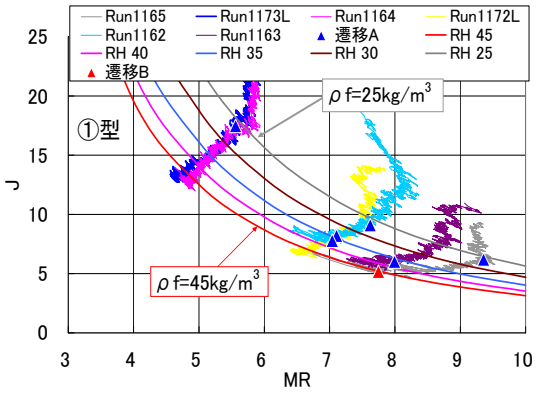
小孔径噴射器(①)の特徴(2/2)

⊿Pre1/Pc, Tw-near, Mflow & Cd の典型的な時間履歴の模式図を下に示した.

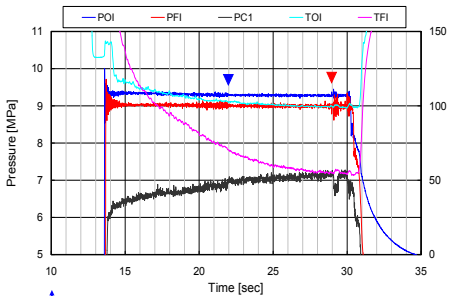
▲;⊿Pre1/Pcステップ減→A遷移

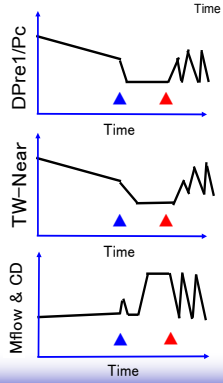
▲;⊿Pre1/Pcステップ増→B遷移

①型試験では, B遷移は最も高MRのRun1165でしか観察されなかった.



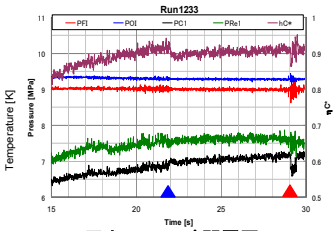
小孔径噴射器(④)の特徴



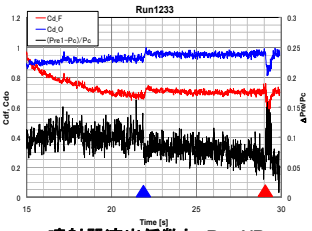


典型的な時間履歴
(模式図)

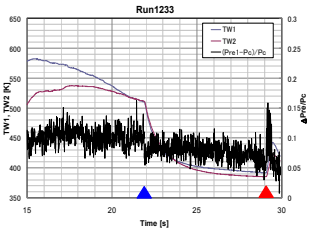
⊿Pre1/Pc減は, 噴射面近くのTw減, Mflow増, Cd増.
⊿Pre1/Pc増は, 噴射面近くのTw増, Mflow減, Cd減を招く.



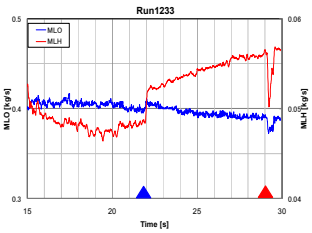
圧力・ηC*の時間履歴



噴射器流出係数と⊿Pre1/Pcの時間履歴



壁温度と⊿Pre1/Pcの時間履歴



流量の時間履歴

特徴は①型と同様だが、②型のような燃焼焼不安定遷移も発生

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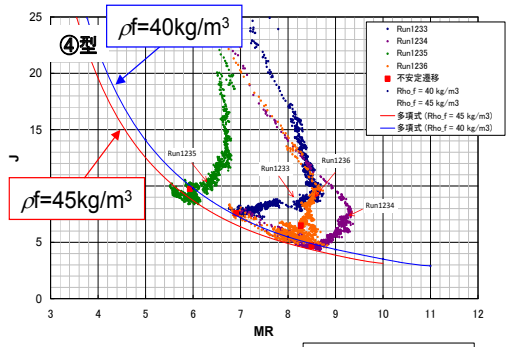
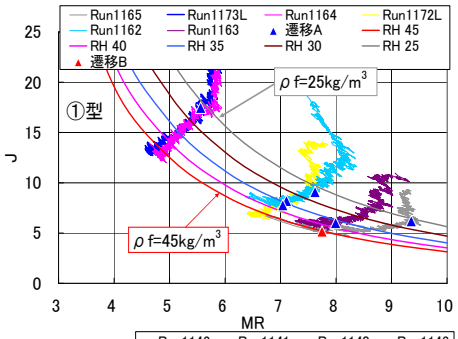
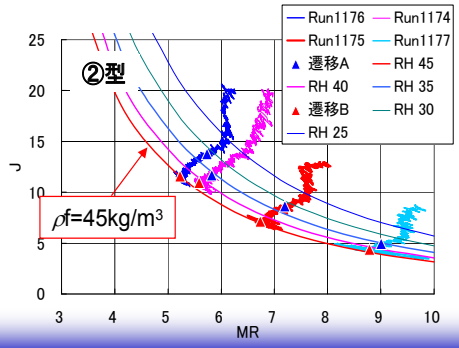
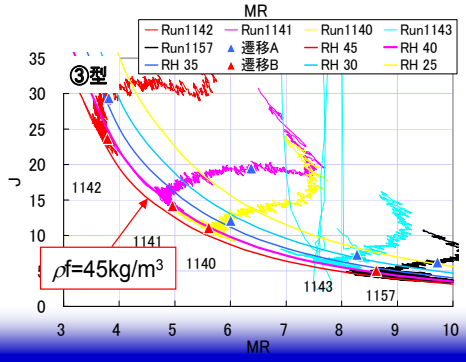
燃焼不安定限界のマップ化



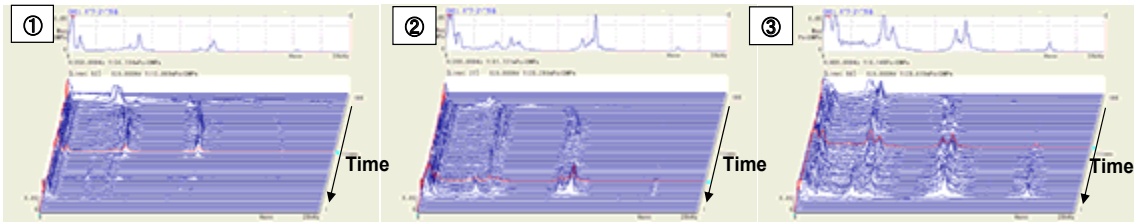


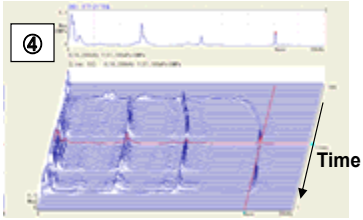




LOX噴射変動圧のFFT解析結果

高速系データ(LOX噴射変動圧)のFFT解析結果





・ どの噴射器にも1次～3次のLOXポストの音響固有値に相当する卓越した周波数が存在.
・ ①および④型では、燃焼中に発生するPcのステップ上昇とともにこれらの卓越周波数が消滅.
・ ②～④型では，低TFIにおけるPc変動およびPcステップ減少の発生により、1次～3次のLOXポスト音響固有に値相当するすべての周波数が卓越.

卓越周波数，リセス内圧損，噴射器近傍の燃焼室壁温度および噴射器流出係数の増減には強い関連性があり，噴射器内(リセス内)での燃焼形態の変化に対応しているものと考えられる.

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まとめ

・ 大口径ほど，低噴射温度領域で，不安定燃焼に移行しやすい．

・ 小口径でも，流量増により，低噴射温度領域で大口径と同様の不安定燃焼に移行した．
  ・ LOXポストの口径だけでは安定性は決まらない．つまり，大口径でも安定燃焼を実現できる形状・作動範囲がある？

・ 燃料不安定性とリセス内の圧損特性が強い関連性を示す
  ・ リセス圧計測により，今回観察された燃焼不安定は，リセス内での微粒化・混合・燃焼過程の変化によって引き起こされている可能性が高い．
  → 今後の現象モデルの構築とCFD等での検証が必要

・ 混合比と運動量比から燃焼不安定発生範囲をマップ化した。LH2噴射密度をパラメータとして整理をすることで、燃焼圧力に関係なく、発生範囲が整理できると考えられる。

・ LH2噴射器出口密度は40kg/m^{3}以下となる作動条件が望ましい。

謝辞

本研究を進めるにあたり，筑波宇宙センターエンジン研究開発グループの川島秀人氏，三菱重工業株式会社名古屋誘導推進システム製作所の渡邉真一郎氏をはじめ，多くの方々のご協力を賜りました．ここに感謝の意を表します．

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ロケットエンジンの化学反応機構

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東京大学工学系研究科　総合研究機構
JAXA社会連携講座

2012.9.27
「ロケットエンジンシミュレーションの最先端」シンポジウム

ロケットエンジンシシミュレーション＝CFD+化学反応

化学反応の取り扱い

1. Sheet model（=infinitely fast chemistry）
   特に乱流拡散燃焼:　混合速度<<反応速度
   EBU, EDCなど
2. Flamelet model
   火炎構造は混合分率によって一意的に決まる
   Flamelet table
3. **詳細反応機構**
   非定常現象（着火、消炎）
   保炎機構、振動燃焼

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概要

1. ロケットエンジン燃焼の詳細反応機構

1.1 水素の高圧燃焼反応 (LE-7,LE-X)

1.2 ヒドラジンの自己着火反応機構(衛星スラスター)

2. 詳細反応機構のCFDコードへの組み込み法に関する研究

2.1 詳細反応機構の簡略化法(RCCE法)

2.2 反応機構の高速積分法(MTS法)

目標:詳細反応機構に基づく
反応性流体シミュレーション技術の獲得

1.1 水素の高圧燃焼反応

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新しい高圧燃焼速度のデータ

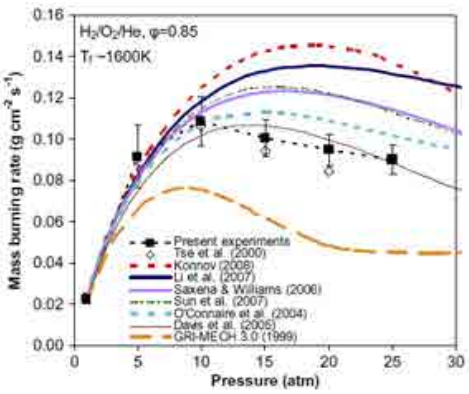
M.P.Burke, M.Chaos, F.L.Dryer, and Y.Ju, AIAA 2009-990
M.P.Burke, F。L.Dryer, and Y.Ju, AIAA 2010-776
M.P.Burke, M.Chaos, F.L.Dryer, and Y.Ju, Combust. Flame, 157 (2010) 618-631

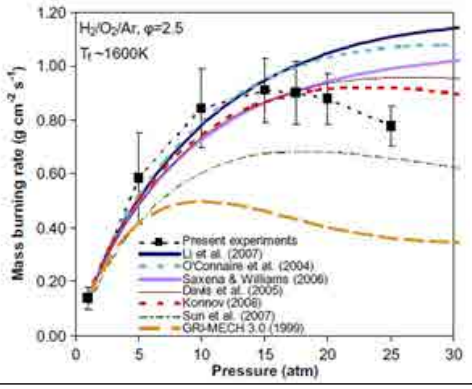
(a) 1 atm

(b) 15 atm

(c) 25 atm

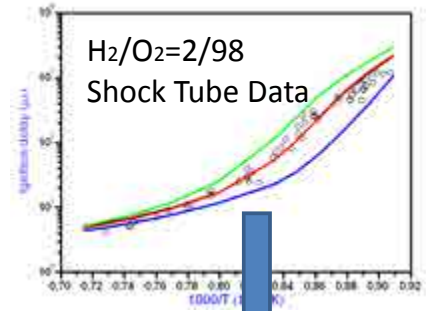
Fig. 2. Schlieren images of propagating flames at r_f = 2.5 cm for an $H_2/O_2/Ar$ mixture of equivalence ratio 2.5 and flame temperature of ~1600 K for various pressures.

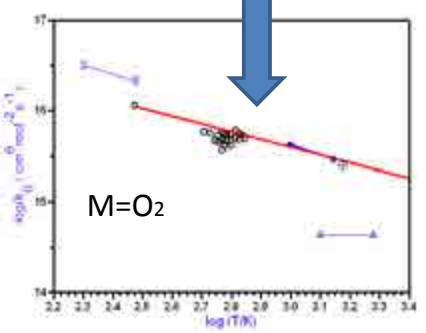




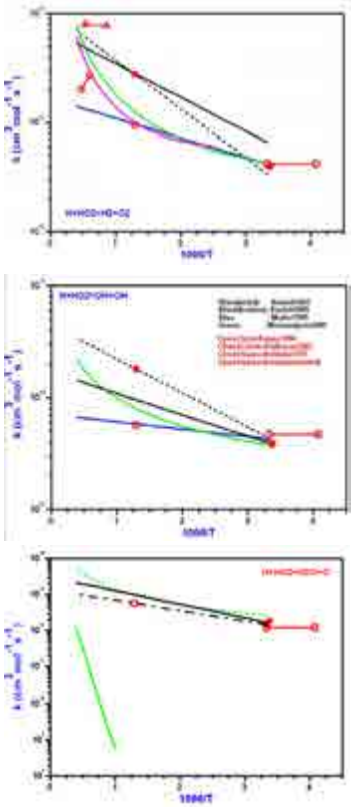
反応機構の再構築

H+O2+M=HO2+M：
Third Body efficiencies

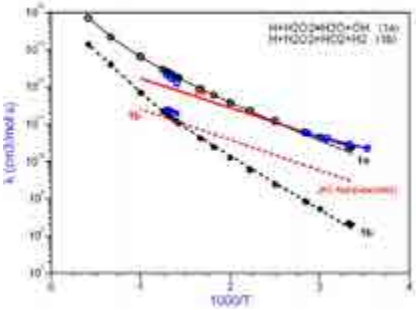




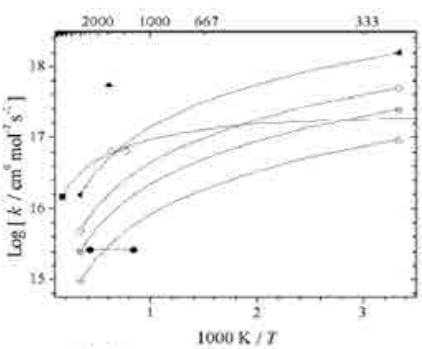
H+HO2 channels



H+H2O2 Reactions



H+OH+M=H2O+M



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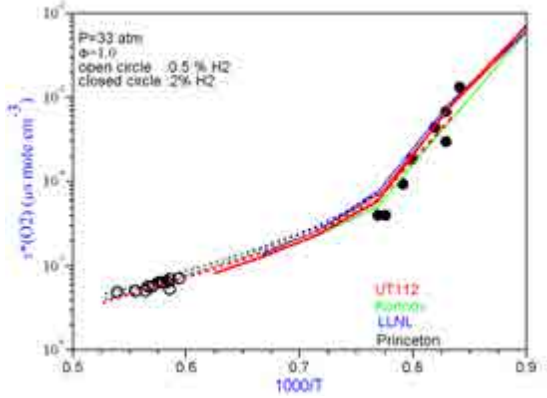
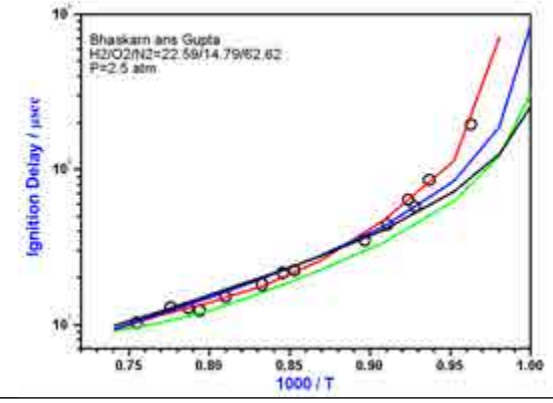
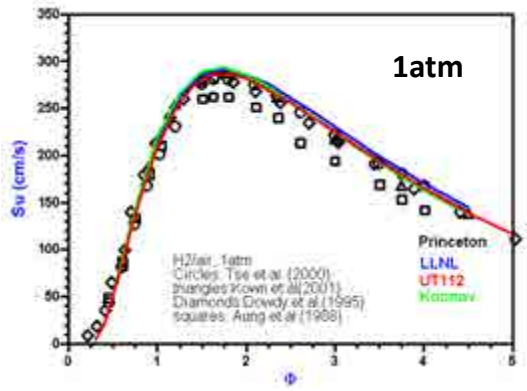
Validation

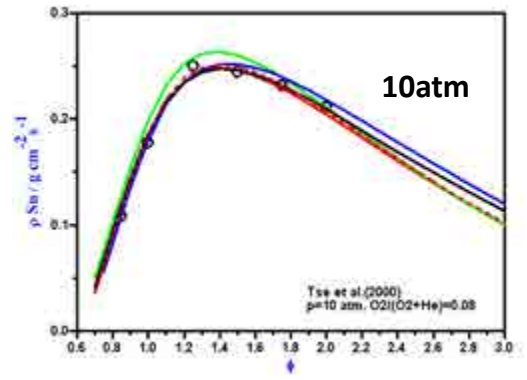
Ignition Delay



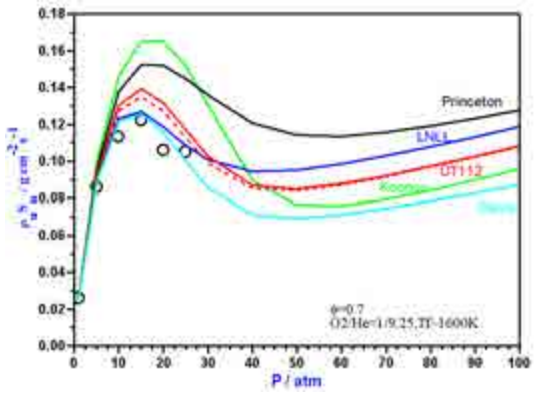


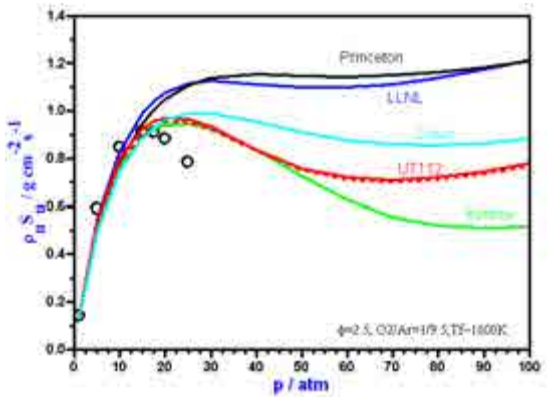
Burning Velocity



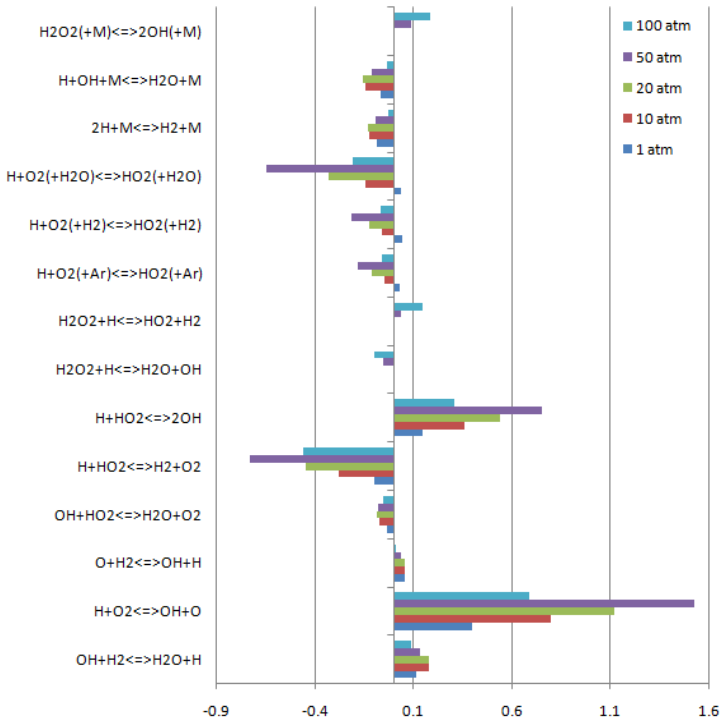


燃焼速度の圧力依存





Sensitivity Analysis
ϕ=2.5, H_2/O_2/Ar



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水素の高圧燃焼：まとめ

水素の詳細反応機構に含まれるすべての素反応の速度定数を再検討し、新規反応機構を提案した。

（主要な改良点）

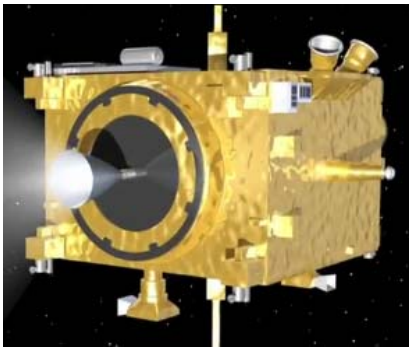
- $H+O_2+M$の第三体効果（$M=H_2O,O_2,H_2$)
- $H+HO_2$、$H+H_2O_2$の反応速度定数

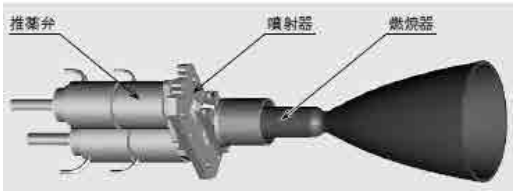
既往の機構に対して

燃焼速度の圧力依存性が改善された。

燃料過多の反応機構に関してはさらなる検討が必要。

1.2 ヒドラジンの自己着火反応機構





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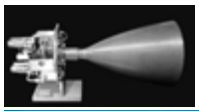
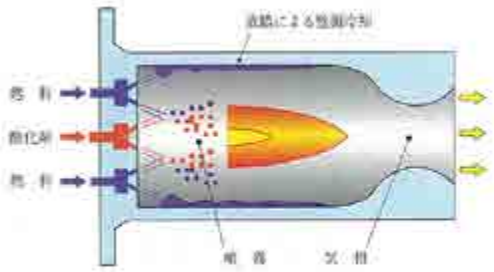
研究の背景



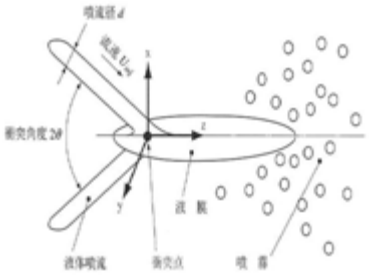
宇宙機の軌道・姿勢制御のためのロケットエンジン（スラスター）

（あかつき：JAXAホームページより）

（コウノトリ：JAXA　ホームページより）



第1図　二液スラスタ
Fig. 1　Bi-propellant thruster



第2図　衝突噴流式ノズル
Fig. 2　Schematic of impinging jets

松野ら：
石川島播磨技報
44(2004)

既往の研究のまとめと問題点

$N_2H_4(liq)$ → 液相反応（イオン反応？） → 着火せず
$RN_3(Solid)$の生成？

$N_2O_4(liq)$ → 液相反応（イオン反応？）

液相反応（イオン反応？） → 蒸発
$N_2H_4(g)+NO_2(g)$ → 気相反応 → 着火爆発

疑問点？

1. 液相反応の機構と生成物（RN_3はなぜできるか）
2. 沸点以下のN_2H_4がなぜ瞬時に蒸発できるのか
   （化学反応による発熱？　または　共沸？）
3. $N_2H_4(g)+NO_2(g)$はなぜ着火源なしに着火するのか

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N_2H_4/NO_2の気相反応機構の構築.

Available Information

1. A N_2H_4 thermal decomposition mechanism:

Konnov A.A., Ruyck, J.D., "Kinetic modeling of the decomposition and flames of hydrazine", Comb. Flame 124:1060126 (2001).

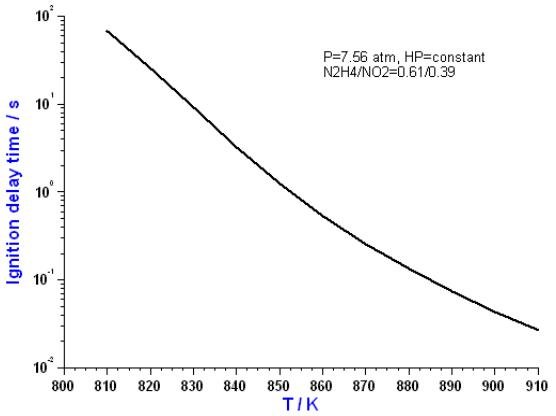
2. A review on N/H/O elementary reactions:

Dean, A.M., Bozzelli, J.W., "Combustion chemistry of nitrogen", in Gas Phase Combustion Chemistry, ed. By Gardiner, W.C.Jr., Springer-Verlag (2000).

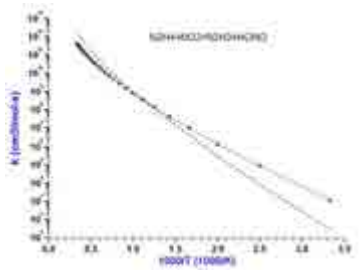
A Base Mechanism: 34 species with 239 reactions

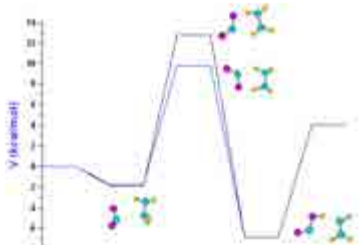
(Ohminami et al., AIAA-2009-5044)

これまでの情報のみから
作った反応機構では
800K以下では自着火しない！
=> Missing Reactions
$NO_2+N_2H_4$

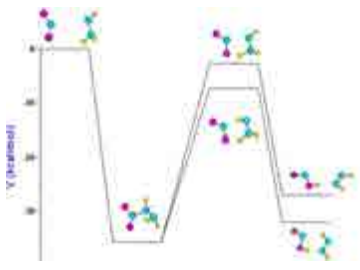


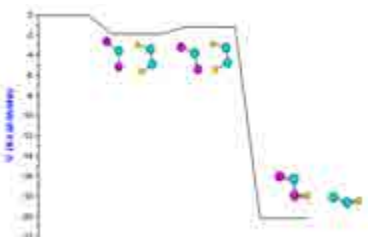
NO_2とN_2H_4は直接反応するか？

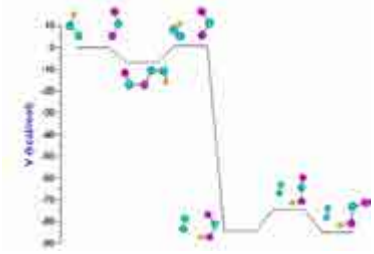


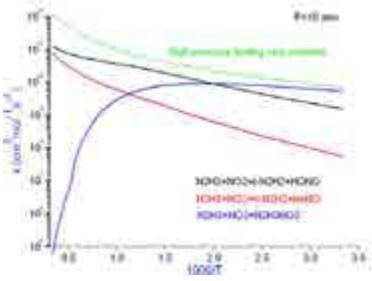


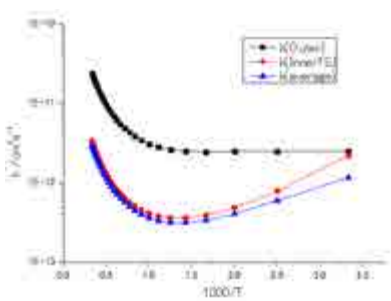
$N_2H_4+NO_2 = N_2H_3+HONO$
$N_2H_3+NO_2 = N_2H_2+HONO$
$N_2H_2+NO_2 = N_2H+HONO$
$N_2H+NO_2 = N_2+HONO$
N_2生成による熱発生
=>反応の加速=>熱爆発

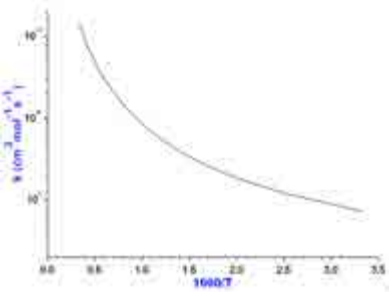












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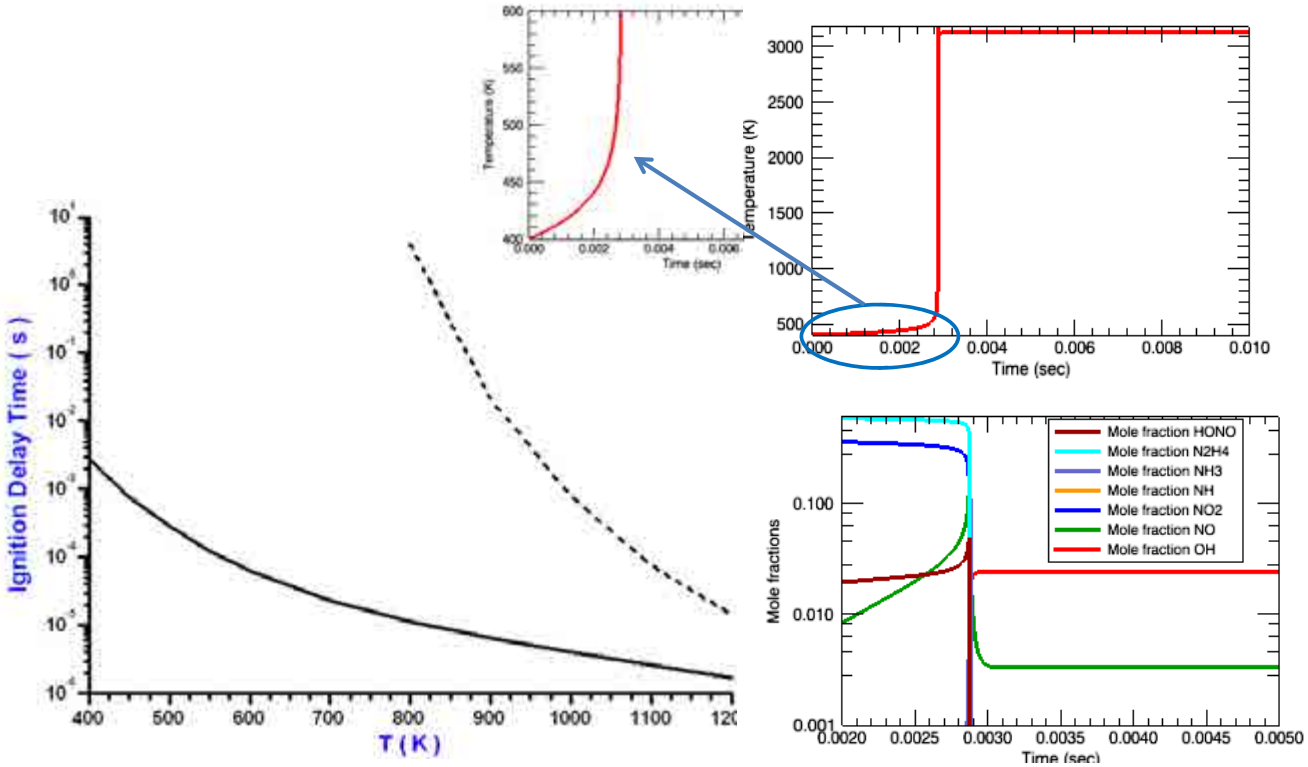
NO_2+N_2H_mを含む反応機構によるシミュレーション



HP=constant,P=7.54 atm,
N_2H_4/NO_2=0.61/0.39

実験値との比較

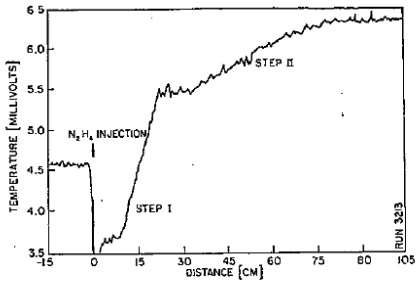
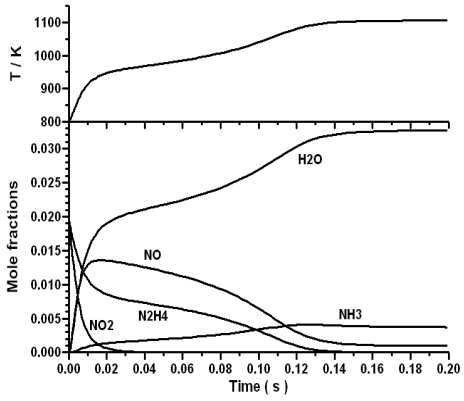


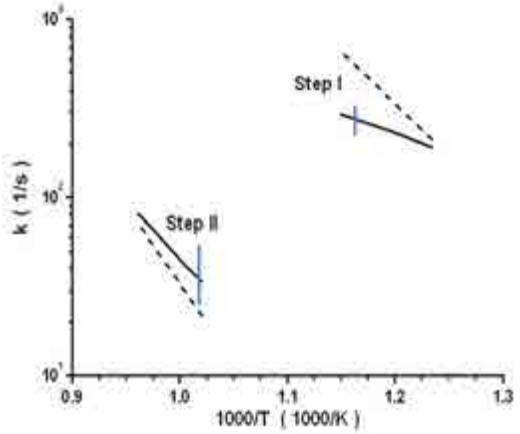
FIG. 2. Flow-reactor-temperature profile for the reaction of hydrazine and nitrogen dioxide, showing a two-step behavior.

R. F. Sawyer and I. Glassman,
Proc. Inst. Combust., pp.861-869 (1967)
A flow tube experiment,
NO_2/N_2 flow (T=810-1000K)
Liq. N_2H_4 injection

Step I: $N_2H_4+NO_2 \rightarrow 0.5N_2H_4+H_2O+NO+0.5N_2$ (fast)
Step II: $0.5N_2H_4+NO \rightarrow H_2O+N_2$. (slow)



T_0=800 K, P_0=1 atm, p(N_2H_4)=p(NO_2) =15 Torr



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ヒドラジンの反応：まとめ

ヒドラジンとNO_2の詳細反応機構を構築した。

$N_2H_4+NO_2$とその後続反応
量子化学計算＋支配方程式解析により
反応経路を明らかにして速度定数を算出した。

低温でのヒドラジン/NO_2混合気の自己着火反応機構が明らかになった。

NO_2によるN_2H_nからの逐次的な水素引き抜きによるN_2生成
N_2生成による発熱と反応の加速=>熱爆発

ヒドラジンのNO_2による燃焼反応は2段階で起こる。

Step I: $N_2H_4+NO_2 \rightarrow 0.5N_2H_4+H_2O+NO+0.5N_2$ (fast)
Step II: $0.5N_2H_4+NO \rightarrow H_2O+N_2.$ (slow)

2. 詳細反応機構のCFDコードへの組み込み法に関する研究

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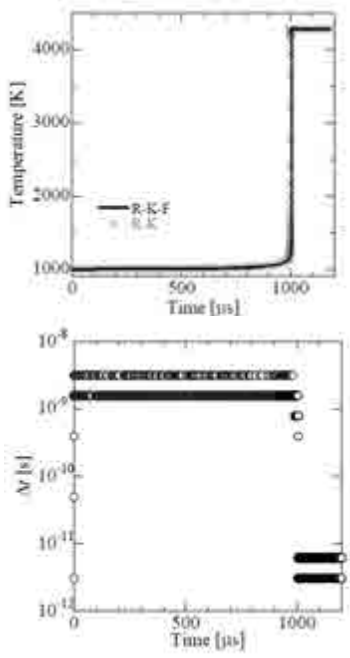
詳細反応機構をCFDコードに組み込む場合の問題点

1）化学反応式硬直性（stiffness）による時間刻み幅の制限，
2）化学種移流方程式数の増加，
3）多成分輸送係数の計算時間の増加



H_2/O_2=2/1, T_0=1000K, P_0=150 atm

Huge Number of Species and Reactions

```
species
h h2 o o2 oh h2o n2 co hco co2 ch3 ch4 ho2 h2o2 ch2o ch3o c2h6
c2h4 c2h5 ch2 ch c2h c2h2 c2h3 ch3oh ch2oh ch2co hcco c2h5oh
pc2h4oh sc2h4oh ch3co ch2cho ch3cho c3h4-a c3h4-p c3h6 c4h6 nc3h7
ic3h7 c3h8 ic4h7 ic4h8 c4h7 c4h8-2 c4h8-1 sc4h9 pc4h9 tc4h9 ic4h9
ic4h10 c4h10 ch3coch3 ch3coch2 c2h5cho c2h5co c5h9 c5h10-1 c5h10-2
ic5h12 ac5h11 bc5h11 cc5h11 dc5h11 ac5h10 bc5h10 cc5h10 ic5h9
nc5h12 c5h11-1 c5h11-2 c5h11-3 neoc5h12 neoc5h11 c2h5o ch3o2
c2h5o2 ch3o2h c2h5o2h c2h3o1-2 ch3co2 c2h4o1-2 c2h4o2h o2c2h4oh
ch3co3 ch3co3h c2h3co c2h3cho c3h5o c3h6ooh1-2 c3h6ooh1-3 c3h6ooh2-1
c3h6ooh1-2o2 c3h6ooh1-3o2 c3h6ooh2-1o2 nc3h7o ic3h7o nc3h7o2h
ic3h7o2h nc3h7o2 ic3h7o2 c3h6o1-3 ic4h8o ic4h8oh ic2c4h8oh ic4h7o
c4h7o c4h8oh-1 c4h8oh-2 o2c4h8oh-1 o2c4h8oh-2 c4h8ooh1-2o2 c4h8ooh1-3o2
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c4h8o1-3 c4h8o1-4 c4h8o2-3 cc4h8o pc4h9o sc4h9o ic4h9o tc4h9o
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cc5h11o2 dc5h11o2 ac5h11o
bc5h11o cc5h11o dc5h11o a
bc5h10ooh-a bc5h10ooh-c b
dc5h10ooh-a dc5h10ooh-b d
ac5h10ooh-co2 ac5h10ooh-d
cc5h10ooh-ao2 cc5h10ooh-b
dc5h10ooh-co2 a-ac5h10o a
b-dc5h10o c-dc5h10o c5h11
c5h11o2h-2 c5h11o2h-3 c5h
```

CFDへの組み込み <= 反応機構の簡略化

Reduction とLumping

DRG: Directed Relation Graph
T.Lu, C.K.Law, Proc. Combust. Inst., 30 (2005) 1333

PCA: Principal Component Analysis
S.Vajda, P.Valko, T.Turnyi, Int. J. Chem. Kinet., 17(1985) 55

CSP: Computaional Singular Perturbation
S.H.Lam, D.A.Goussls, Int. J. Chem. Kinet., 26(1994) 461

ILDM: Intrinsic Low-Dimensional Manifolds
U.Maas, S.B.Pope, Combust. Flame, 88 (1992) 239

RCCE：Rate-Controlled Constrained Equilibrium
J.C.Keck, D.Gillespie, Combust. Flame, 17,237(1971)

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2.1 RCCE法の開発と問題点

RCCE （Rate-Controlled Constraint-Equilibrium）

Jones and Rigopoulos, Combust. Theory Modelling, 11, 755 (2007)

Gibbs Free energy and chemical potential

$$g = \sum_{j=1}^{N} \mu_j n_j \quad (1)$$ N:number of chemical species、 n_j :mol/g

$$\mu_j = \mu_j^o + RT \ln p_j / p^0 = \overline{\mu_j^0} + RT \ln n_j / n \quad (2)$$ p^0 :1bar

$$\overline{\mu_j^0} = \mu_j^0 + RT \ln p / p^0 = H_j^0 - TS_j^0 + RT \ln p / p^0 \quad (3)$$

$$n = \sum_j n_j \quad (4)$$

Constraints

$$b_i = \sum_{j=1}^{N} a_{ij} n_j \quad (i = 1,....,M_e) \quad (5)$$ **M_e=number of elements**

$$d_k = \sum_{j=1}^{N} c_{kj} n_j \quad (k = 1,.....,M_c) \quad (6)$$ **M_c=number of constraints**

Lagrangean : L $\quad L = g + \sum_i \overline{\lambda_i} b_i + \sum_k \overline{\beta_k} d_k$

$$\frac{\partial L}{\partial n_j} = 0 \Rightarrow n_j = n \exp\left(-\frac{\overline{\mu_j^0}}{RT}\right) \exp\left(\sum_i \lambda_i a_{ij}\right) \exp\left(\sum_k \beta_k c_{kj}\right) \quad (7)$$

$$\lambda_i = -\overline{\lambda_i} / RT, \quad \beta_k = -\overline{\beta_k} / RT$$

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For H,p=constant conditions

Thermodynamic constraints

$$h = \sum_j H_j n_j \quad (8)$$

$$p = n\rho RT \quad (9)$$

Kinetic constraints

$$d(d_k)/dt = \sum_j c_{kj}(dn_j/dt) = \sum_j c_{kj} W_j \quad (10)$$

$W_j \Leftarrow$ From detailed chemical kinetic nechanism

Index 1 Solution: Solve the algebric Eqs.(5),(6),(8),(9) and differential eq. (10).

Index 0 Solution: (constraint potentials) formulation
Differential equations for $M_e + M_c + 2$ variables

$$\rho, T, \lambda_i\ (i = 1,....,M_e), \beta_k\ (k = 1,....,M_c)$$

From eq.(7)

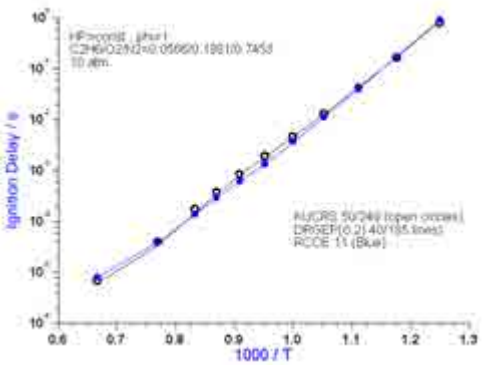
$$\frac{\partial n_j}{\partial \lambda_i} = a_{ij} n_j \quad \frac{\partial n_j}{\partial \beta_k} = c_{kj} n_j \quad \frac{\partial n_j}{\partial T} = \frac{1}{T}\left(\frac{H_j^0}{RT} - 1\right) n_j \quad \frac{\partial n_j}{\partial \rho} = -\frac{n_j}{\rho} \quad (11)$$

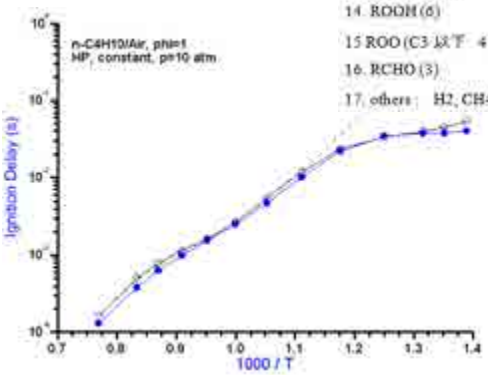
Solver of DAE used in the present study: DASPK

RCCE（H,P=一定）の例：C_2H_6と$n\text{-}C_4H_{10}$

1	Fuel	C2H6			
2	Oxidant	O2			
3		H			
4		O	OH		
5	Products	H2O	O2		
6	RCO	CO			
7	RCOO	HO2	CH3OO	C2H5OO	
8	ROOH	H2O2	CH3OOH	C2H5OOH	
9	RCHO	CH2O	CH3CHO		
10		H2	CH4	C2H4	C2H2
11	M				

1. BASE 束縛条件
（H2-O2 系、6 つ）
O2、H2+CO2、CO、H, OH+O, M
2. RH （燃料）
3. R （C4H9 の異性体 4 種類）
4. ROO （C4H9 2 種類）
5. QOOH（C4H8OOH 6 種）
6. QOOH （C3 以下 3 種）
7. HOOQOO (HOOC4H8OO 6 種)
8. ketOOH (3)
9. ketRO (3)
10. AldOOH (5)
11. Alken (4)
12. Allyl (2)
13. CycEther (7)
14. ROOH (6)
15. ROO (C3 以下 4 種類)
16. RCHO (3)
17. others : H2, CH4, C2H6, C2H2, CH2CHO





DRGEP （黒）実線(88/338) 点線（69/291)
RCCE （青）36束縛条件

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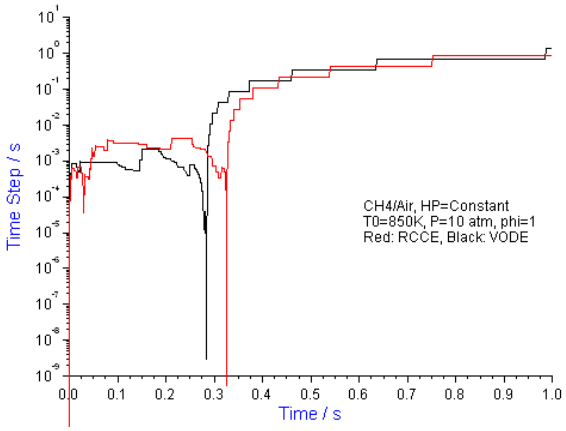
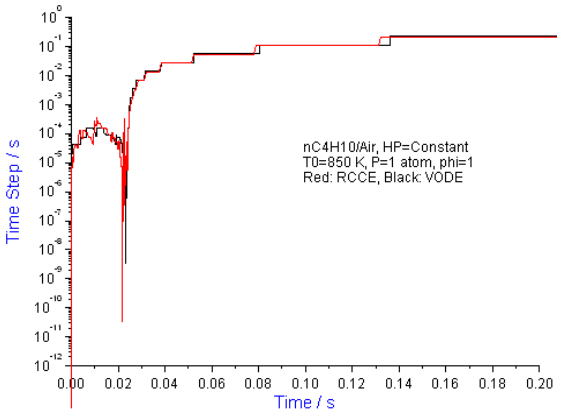
RCCE法で高速化されるか？

H,P=Const. の場合の計算時間 （秒）
(T_0=850 K, P=10 atm, ϕ=1）

	CH_4/Air	C_2H_4/Air	nC_4H_{10}/Air	nC_7H_{16}/Air
Species/Reactions	66/337	48/249	111/426	373/1071
VODE	0.85	0.73	2.02	9.19
RCCE (# of constraints)	0.61 (9)	0.45 (11)	3.37 (36)	8.97 (26)





CFDへのRCCE法の組み込み

＜1次元オイラー方程式の場合＞

$$\frac{\partial \mathbf{Q}}{\partial t}+\frac{\partial \mathbf{E}}{\partial x}=\mathbf{S} \qquad \mathbf{Q}=\begin{bmatrix}\rho\\ \rho u\\ e\\ \rho Y_k\end{bmatrix},\quad \mathbf{E}=\begin{bmatrix}\rho u\\ \rho u^2+p\\ (e+p)u\\ \rho u Y_k\end{bmatrix},\quad \mathbf{S}=\begin{bmatrix}0\\ 0\\ 0\\ \dot{\omega}_k\end{bmatrix}$$

k=1,…,N
N: speciesの数

2nd order Strang-type Fractional Step method

$$Q^{n+1}=L_{PDE}^{\frac{1}{2}\Delta t}L_{ODE}^{\Delta t}L_{PDE}^{\frac{1}{2}\Delta t}Q^{n}$$

$$L_{PDE}^{\frac{1}{2}\Delta t}:\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial x}=0$$ ⇐ 流体計算

$$L_{ODE}^{\Delta t}:\frac{dQ}{dt}=S$$ ⇐ 反応計算 ⇐ ρ、eが一定のRCCE法

流体計算における化学種の保存式 （N組）をどうするか？

$$\frac{\partial \rho Y_k}{\partial t}+\frac{\partial \rho u Y_k}{\partial t}=0,\quad k=1....N$$

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束縛条件に対する保存式

束縛条件 $b_l = \sum_{k=1}^{N} a_{lk} n_k , \quad l = 1,.....,M$

M:束縛条件の数 (M<<N)

化学種の保存式

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u Y_k}{\partial x} = 0, \quad k = 1....N$$

$Y_k = W_k n_k$ なので

$$\frac{\partial \rho n_k}{\partial t} + \frac{\partial \rho u n_k}{\partial x} = 0$$

a_{lk} を掛けてkについての和をとると

$$\frac{\partial \rho b_l}{\partial t} + \frac{\partial \rho u b_l}{\partial x} = 0 , \quad l = 1,.....,M$$

N組の保存式の代わりにM(<<N)組の式を解けばよい。

RCCE法：まとめ

RCCE法を適用することにより

1．化学反応方程式
　化学種の微分方程式（数百～数千）
　　=>束縛条件の微分方程式（数十）

2．移流方程式
　化学種の移流（数百～数千）
　　=>束縛条件の移流（数十）

未解決の問題

RCCE法のDAEがよりStiffになってしまう場合がある
　=> MTS（時間積分）＋RCCE（移流）

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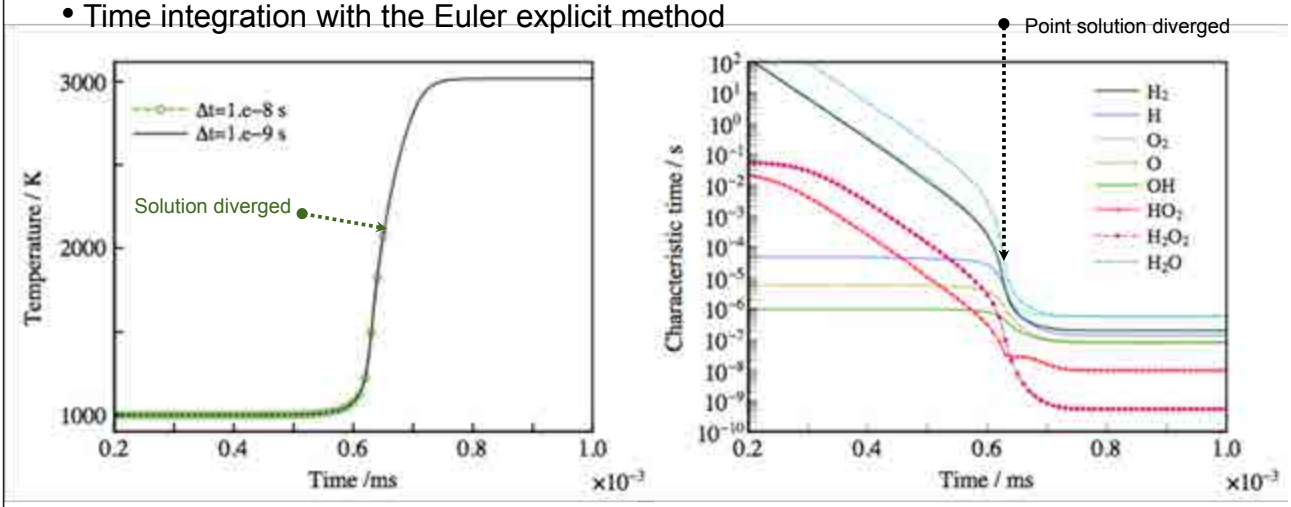
2．2 反応方程式の高速積分法
MTS（Multi TimeScale）法

素反応の特性時間

$$\frac{dY_k}{dt} = \omega_k \frac{W_k}{\rho}$$

$$\frac{dT}{dt} = -\frac{\sum h_k \omega_k W_k}{\rho c_p}$$

- H2/O2 = 2.0/1.0, T=1000 K, p = 0.1 atm
- 11 species, 34 reactions
- The characteristic time evaluated with CHEMKIN-II library: $\tau_k = \frac{X_k}{D_k}$ $\omega_k = C_k - D_k$
  - Time integration with the Euler explicit method



- The computation with Δt=1.e^{-8} s failed

- The characteristic time could be comparable to the time step size required

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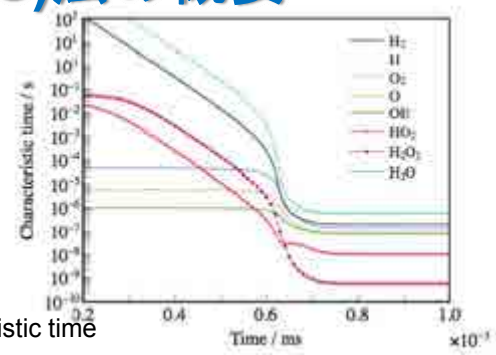
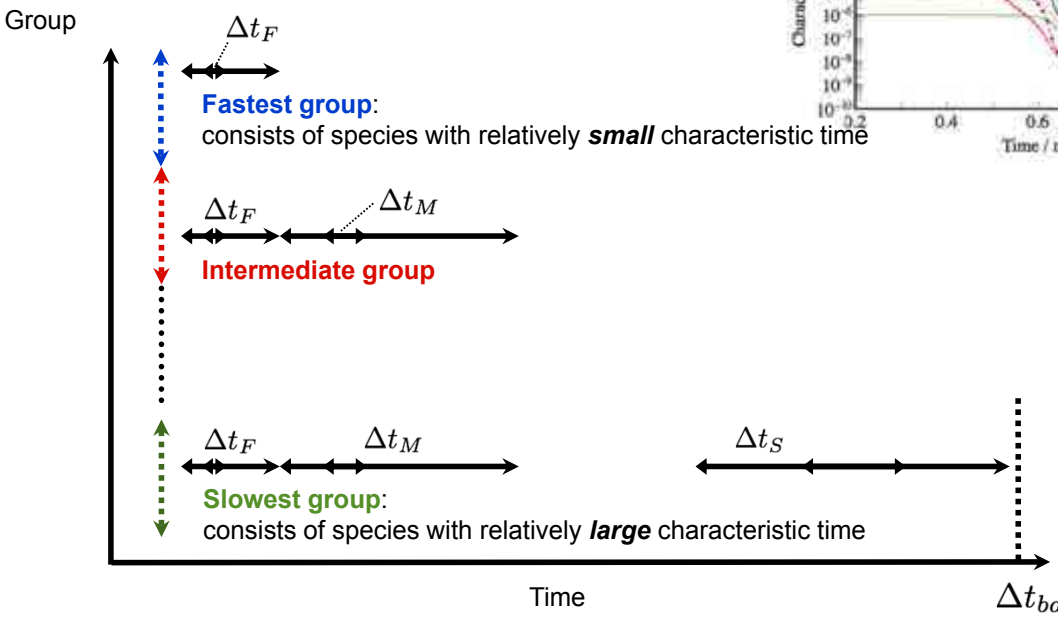
Multi-timescale (MTS)法の概要

Ref.: X. Gou, W. Sun, Z. Chen, and Y. Ju,
Combustion and Flame, 2010



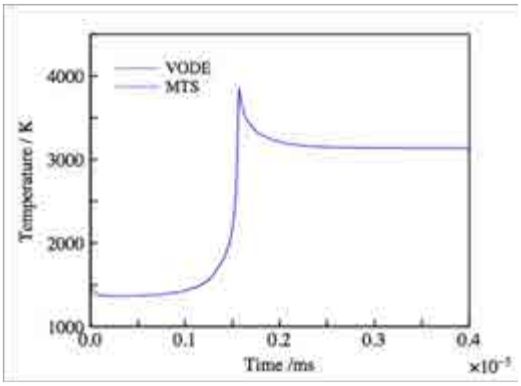


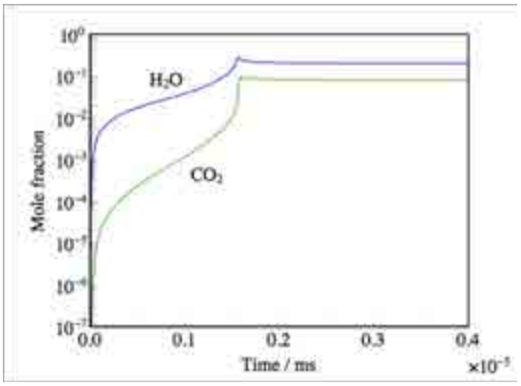
: may correspond to CFD

- *An assumption: Fast groups are expected to converge quickly*

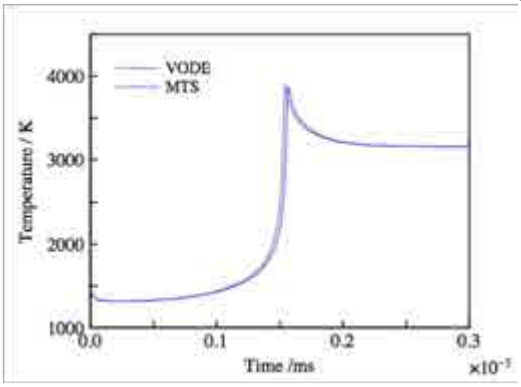
MTS と VODE(陰解法)の比較

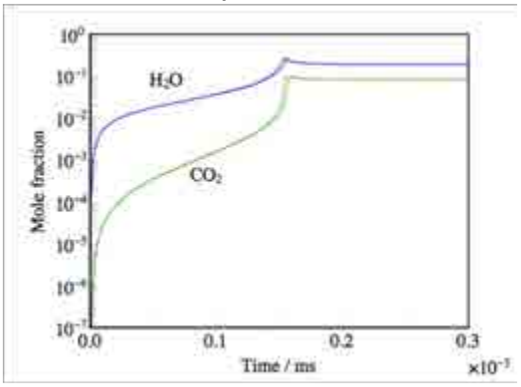
- nC4H10/O2 = 2.0/13.0, T=1500 K, p = 0.1 atm, 146 species, 554 reactions)





- nC7H16/O2 = 1.0/11.0, T=1500 K, p = 0.1 atm, 373 species, 1071 reactions)





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MTSとVODEの計算時間の比較

- Computations on iMac, quad core, Intel Core i7

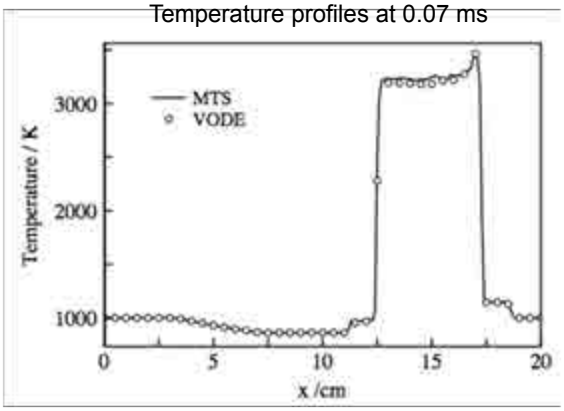
/O2	species #	Initial temperature	Initial pressure	CPU time / s		Saving / %
				VODE	MTS	
H2	11	1000	0.1	9.53	7.99	**16.1**
CH4	68	1800	0.1	231.3	40.26	**82.6**
C4H10	146	1500	0.1	537.7	53.67	**90.0**
C7H16	373	1500	0.1	2424.0	100.03	**95.8**

- Saving = (VODE-MTS)/VODE
- Note: elapsed times are different among each case; CPU time not proportional to species #
- Note: VODE without initialization parameter provides much faster CPU time

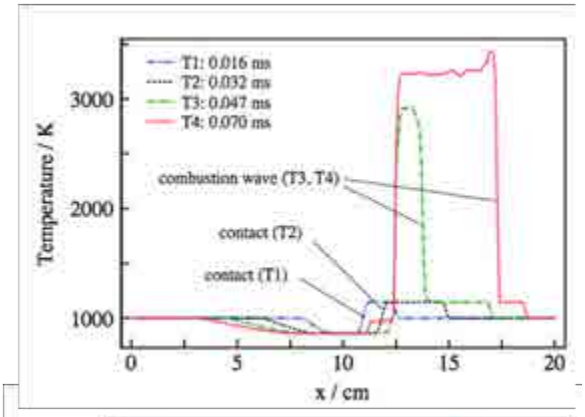
MTS法のCFDへの組み込みの例：衝撃波問題

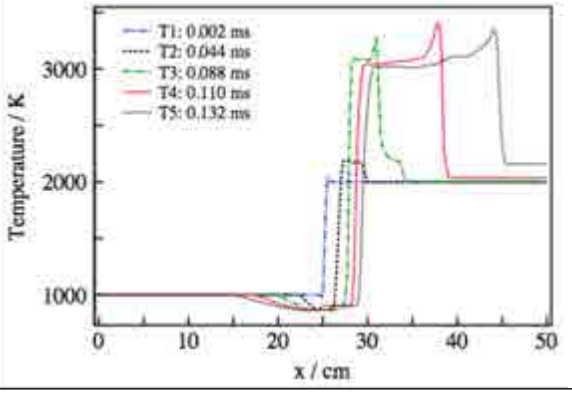
- Stoichiometric H2/O2 mixture at 1000 K
- 11 species, 34 reactions
- p_left/p_right=1.0/0.3

Temperature profiles at 0.07 ms



Time histories of temperature profiles with MTS





- Stoichiometric CH4/Air mixture
- 68 species, 334 reactions by KUCRS
- p_left/p_right=1.0/0.3,
  T_left/T_right=1000/2000

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MTS法：まとめ

- MTS法による反応方程式の高速解法を開発
  - 広範な条件で安定・高速・高精度であることを実証
  - 化学種の数が多くなるとVODEより大幅に高速
- MTS法のCFDへの組み込みの実証
  - MTS法は陽解法であるため特に有利

今後の課題

- 可変時間刻みによるさらなる高速化
- 移流・拡散を解くための化学種のReduction
  - <=RCCE/MTS法の開発

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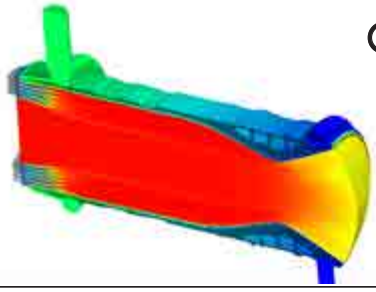
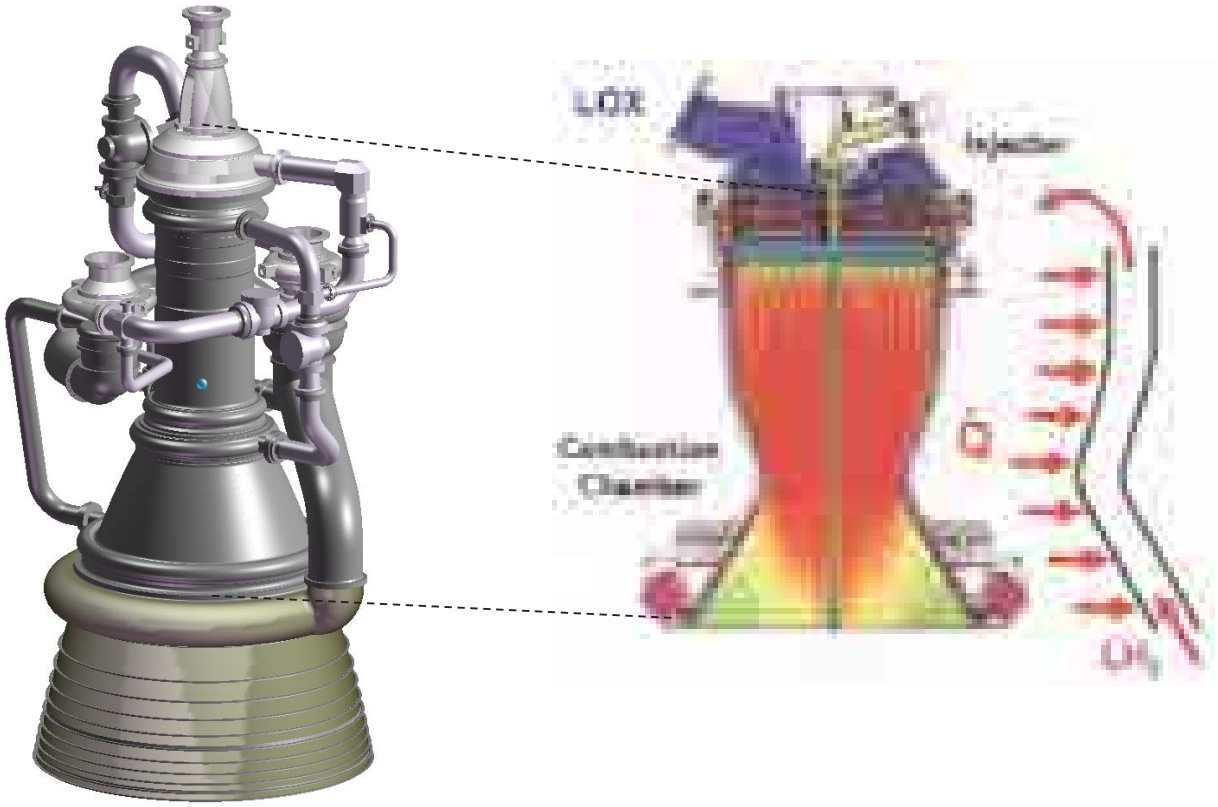
液体ロケットフルスケール燃焼器 再生冷却性能予測手法の提案

宇宙航空研究開発機構
情報・計算工学センター

○大門　優、根岸　秀世、山西　伸宏



背景　ロケットエンジン燃焼器



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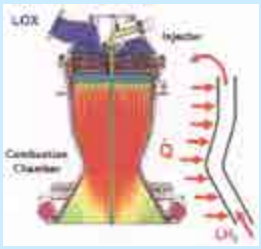
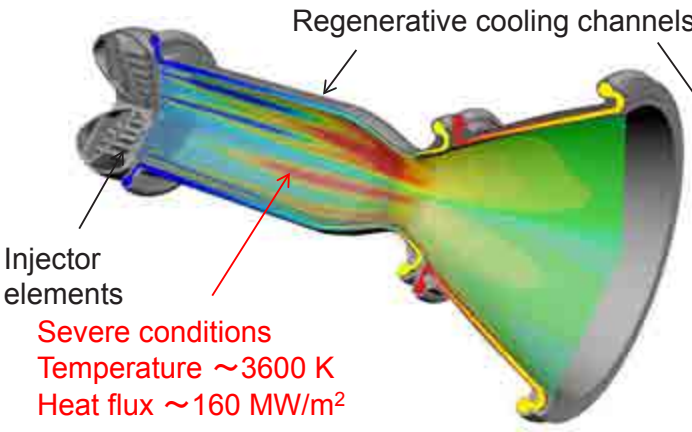
背景 再生冷却技術

再生冷却の役割

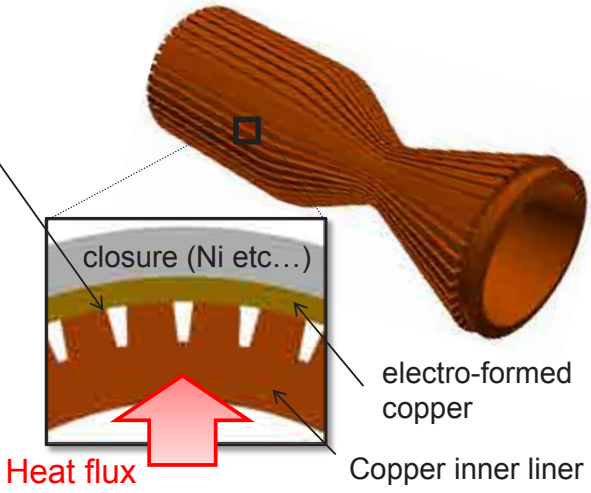
- 小さな圧力損失を保ちながら壁面を冷却する
- ターボポンプを回すためのエネルギーを得る
  （エキスパンダーブリードサイクル）



Prog. in Astronautics and Aeronautics, Vol. 200, AIAA, 2004.



再生冷却燃焼器概念図

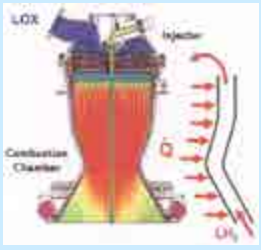


燃焼器構造部分概念図

背景 再生冷却性能予測に対してCFDの適用

再生冷却の役割

- 小さな圧力損失を保ちながら壁面を冷却する
- ターボポンプを回すためのエネルギーを得る
  （エキスパンダーブリードサイクル）

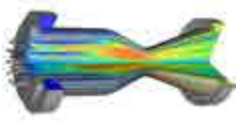


Prog. in Astronautics and Aeronautics, Vol. 200, AIAA, 2004.

エンジン開発における再生冷却への要望:

- 壁面を効率的に冷却し、効率的にエネルギーを得る
- ✓ 燃焼器内部の物理現象を理解する必要がある:
  燃焼ガス、冷却材流れ、熱伝導特性
- ✓ 再生冷却性能を予測する:
  - 燃焼ガス側、冷却材側の壁面熱流束
  - 壁面温度
  - 冷却材流れの圧力損失と昇温量

CFDを利用して再生冷却性能予測をしたい



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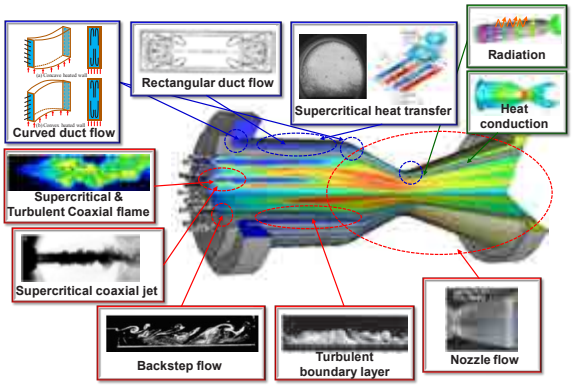
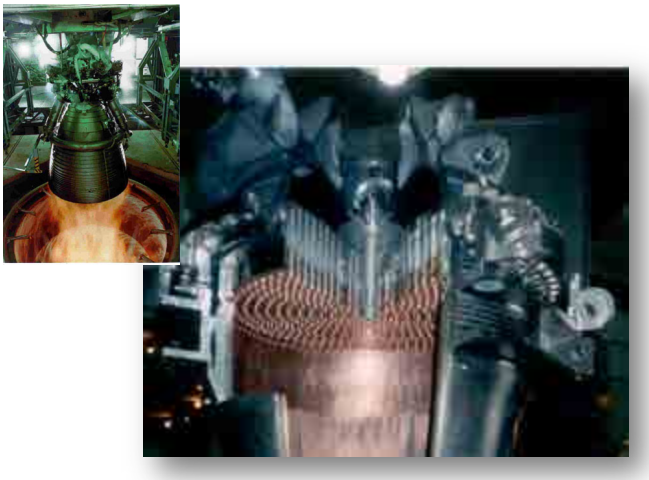
背景　フルスケール再生冷却性能予測解析の課題

【燃焼器側壁面熱流束予測の課題】

- 物理モデル
  - 各物理モデルの精度
  - 物理モデルの集合
  - 計算時間とのトレードオフ



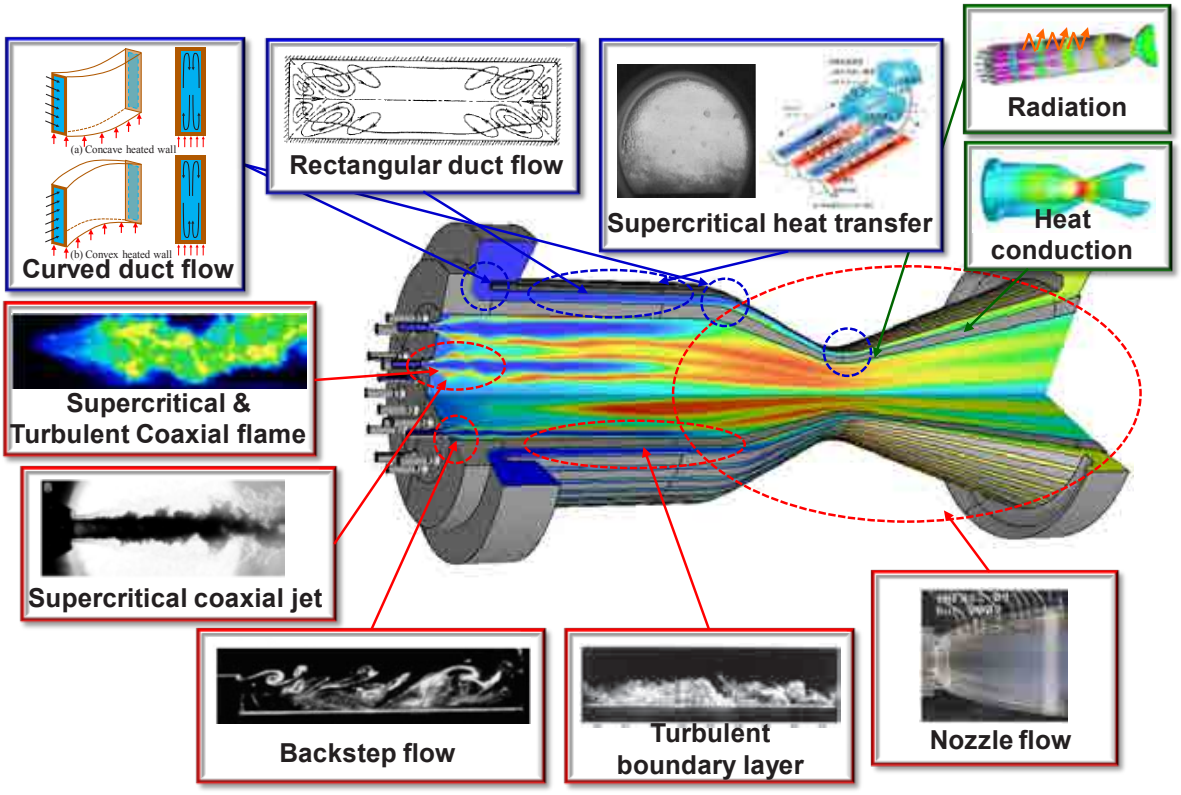
- インジェクターの数
  - 計算負荷低減



計算時間との戦い

5

物理現象の集合　⇒　物理モデルの集合



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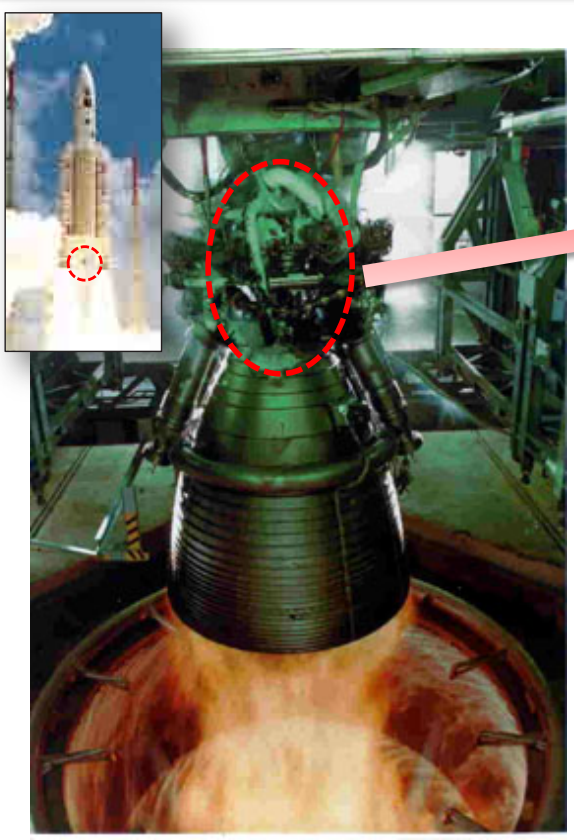
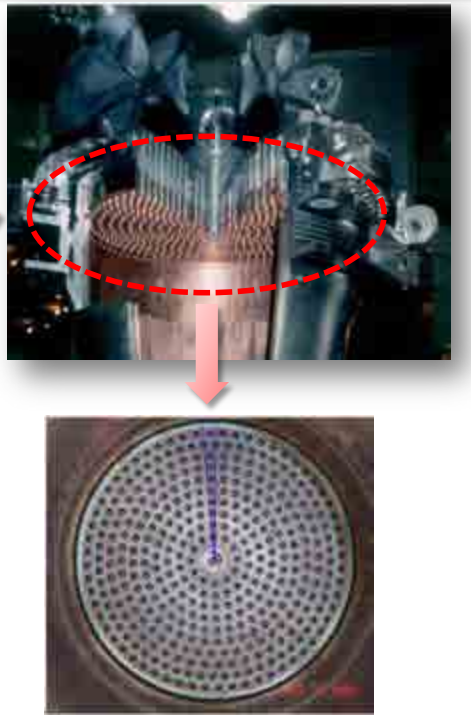
フルスケールを実現するための壁：ｲﾝｼﾞｪｸﾀの数



Vulcain II; the booster stage engine of ARIAN V



フルスケール燃焼器は数百本のｲﾝｼﾞｪｸﾀを持つ
⇒解析負荷が高い（全周12年、一部4.5ヵ月）
⇒ **計算の効率化、簡略化手法が必須**

7

目標および本公演内容

【目標】

- フルスケール燃焼器の再生冷却性能を**数週間**で評価する手法を開発する。
  - 評価項目：**液面熱流束**、壁面温度、冷却材流れ圧力損失昇温量

【キー技術】

- 複数の物理モデルの精度評価
  - 計算負荷とのトレードオフ ⇨ JAXA社会連携講座
- インジェクター簡略化手法

【講演内容】

- 燃焼ガス側壁面熱流束検証方法
- 燃焼ガス側壁面熱流束検証結果
- 効率的なﾓﾃﾞﾘﾝｸﾞの検証およびﾌﾙｽｹｰﾙ燃焼器への適用結果

8

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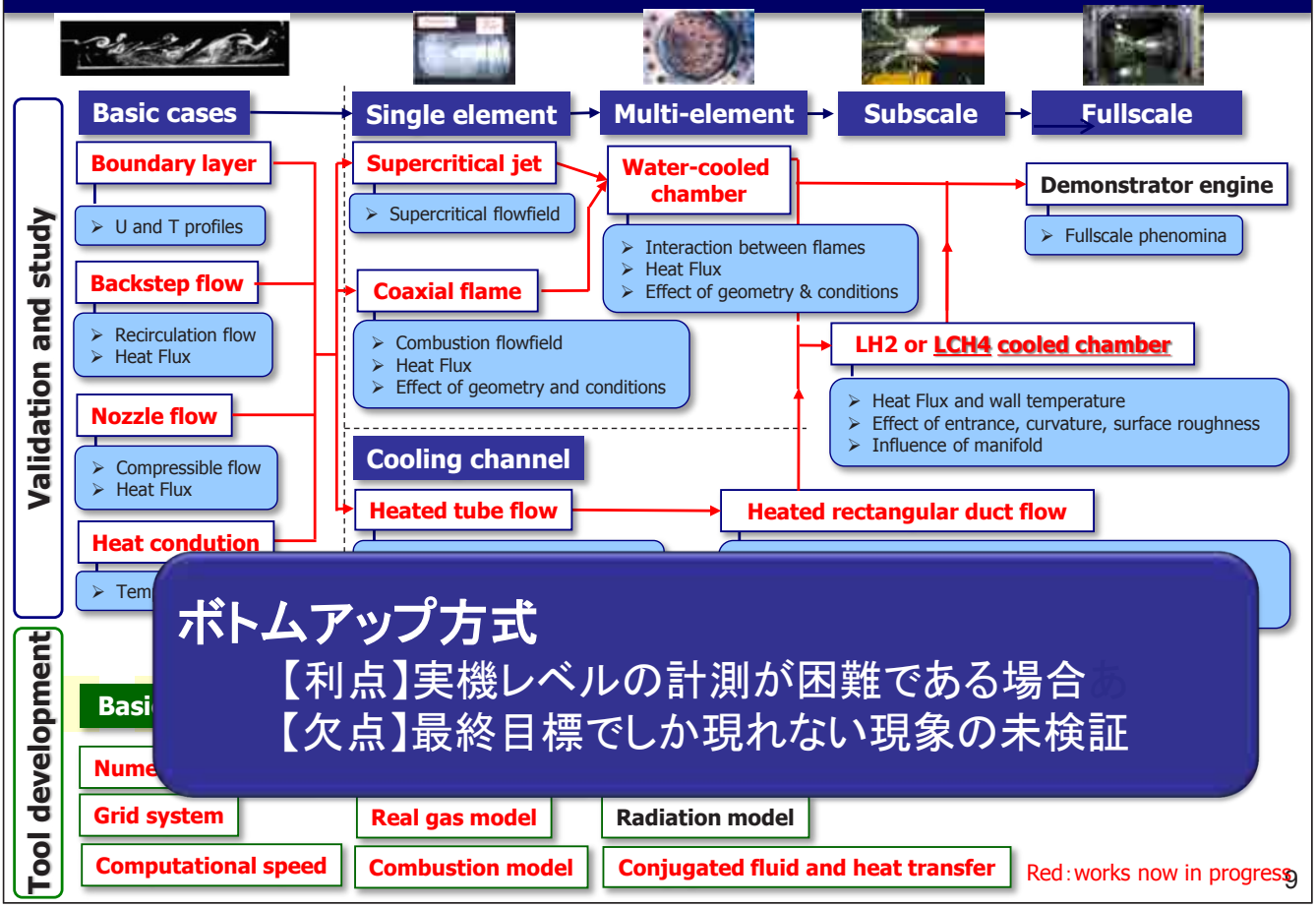
検証作業（ボトムアップ方式）



解析手法

- **Solver:** CRUNCH CFD developed by CRAFT Tech.
- **Governing eq.:** 3D compressible RANS
- **Convective terms:** 2nd order upwind
- **Viscous terms:** Central differencing
- **Turbulence model:** Low-Re-type k-ε model *Papp, JPP, 2011*
- **Combustion model:** Laminar finite rate (8species and 21 reactions) *Shimizu and Koshi, JPP, 2011*
- **Equation of state:** Soave-Redlich-Kwong EoS
- **Transport properties:** Ely and Hanley model

連携講座発の反応モデル

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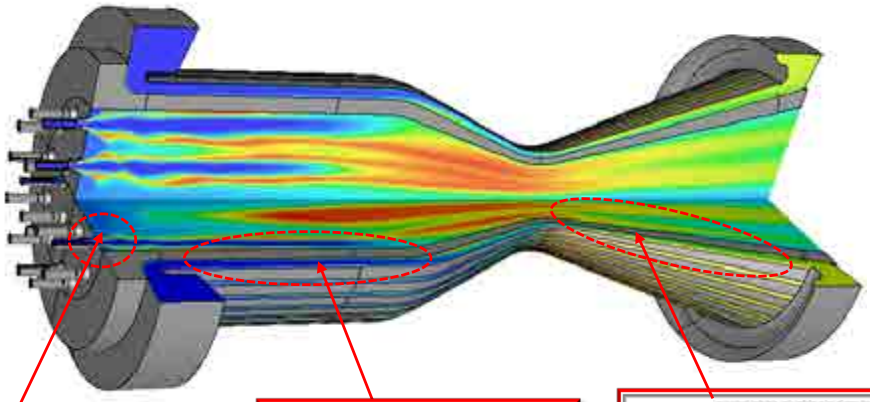
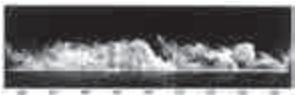
壁面漸近挙動モデルの検証



Recirculation flow on Heated Expansion Tube



Turbulent Boundary Layer on Heated Flat Plate

Turbulent Boundary Layer with Pressure Gradient

壁面熱流束に着目し壁面漸近挙動モデルの評価を実施

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壁面漸近挙動モデルの検証

Validation and study

Basic cases → Single element → Multi-element → Subscale → Fullscale

- Boundary layer
  - U and T profiles
- Backstep flow
  - Recirculation flow
  - Heat Flux
- Nozzle flow
  - Compressible flow
  - Heat Flux
- Heat condution
  - Temperature profile

- Supercritical jet
  - Supercritical flowfield
- Coaxial flame
  - Combustion flowfield
  - Heat Flux
  - Effect of geometry and conditions
- Cooling channel
- Heated tube flow
  - Supercritical heat transfer
  - Heat Flux and wall temperature

- Water-cooled chamber
  - Interaction between flames
  - Heat Flux
  - Effect of geometry & conditions
- LH2 or LCH4 cooled chamber
  - Heat Flux and wall temperature
  - Effect of entrance, curvature, surface roughness
  - Influence of manifold
- Heated rectangular duct flow
  - Effect of entrance, curvature, surface roughness
  - Heat Flux and wall temperature
  - Difference between heated tube and rectangular duct

- Demonstrator engine
  - Fullscale phenomina

Tool development

Feedback

Basic features
- Numerical scheme
- Grid system
- Computational speed

Key physical model
- Turbulence model
- Real gas model
- Combustion model
- Heat condution
- Radiation model
- Conjugated fluid and heat transfer

Red：works now in progress

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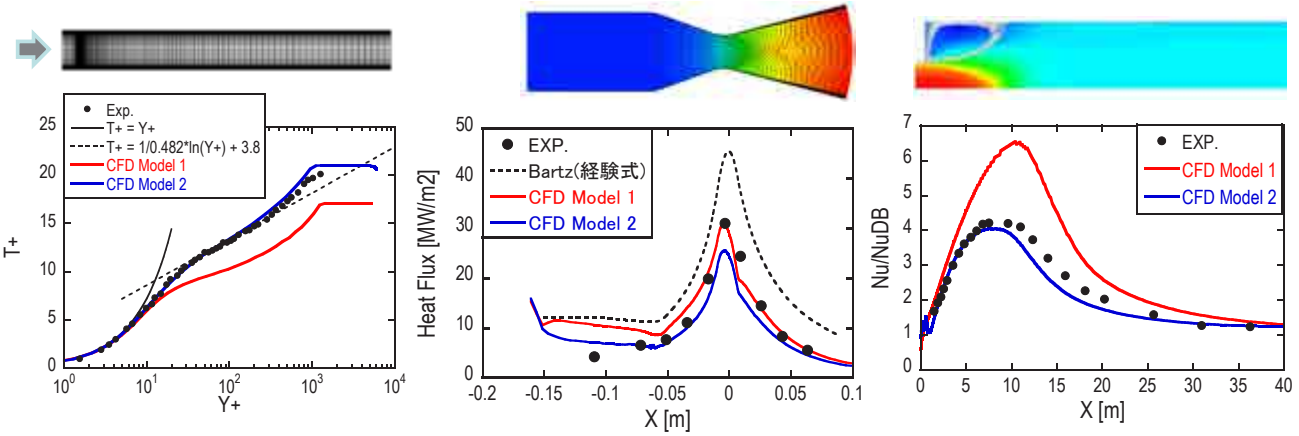
壁面漸近挙動モデルの検証

加熱平板　　ノズル　　加熱拡大管



Near-Wall Model	加熱平板	ノズル	加熱拡大管
Model 1 (Low-Re)	Fair	Good	Bad
Model 2 (Two-layer)	Good	Fair	Good

- 流れ場の特徴によって，適切な壁面漸近挙動が異なる。

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壁面漸近挙動ﾓﾃﾞﾙ　GH2/GO2ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験

Validation and study

- Basic cases
  - Boundary layer
    - U and T profiles
  - Backstep flow
    - Recirculation flow
    - Heat Flux
  - Nozzle flow
    - Compressible flow
    - Heat Flux
  - Heat condution
    - Temperature profile
- Single element
  - Supercritical jet
    - Supercritical flowfield
  - Coaxial flame
    - Combustion flowfield
    - Heat Flux
    - Effect of geometry and conditions
  - Cooling channel
  - Heated tube flow
    - Supercritical heat transfer
    - Heat Flux and wall temperature
- Multi-element
  - Water-cooled chamber
    - Interaction between flames
    - Heat Flux
    - Effect of geometry & conditions
- Subscale
  - LH2 or LCH4 cooled chamber
    - Heat Flux and wall temperature
    - Effect of entrance, curvature, surface roughness
    - Influence of manifold
  - Heated rectangular duct flow
    - Effect of entrance, curvature, surface roughness
    - Heat Flux and wall temperature
    - Difference between heated tube and rectangular duct
- Fullscale
  - Demonstrator engine
    - Fullscale phenomina

Feedback

Tool development

- Basic features
  - Numerical scheme
  - Grid system
  - Computational speed
- Key physical model
  - Turbulence model
  - Real gas model
  - Combustion model
  - Heat condution
  - Radiation model
  - Conjugated fluid and heat transfer

Red：works now in progress

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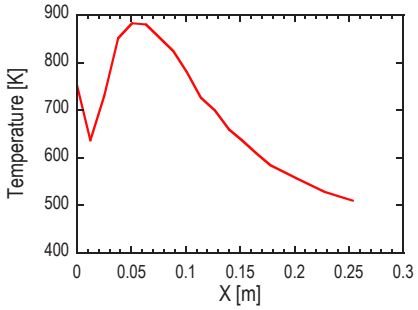
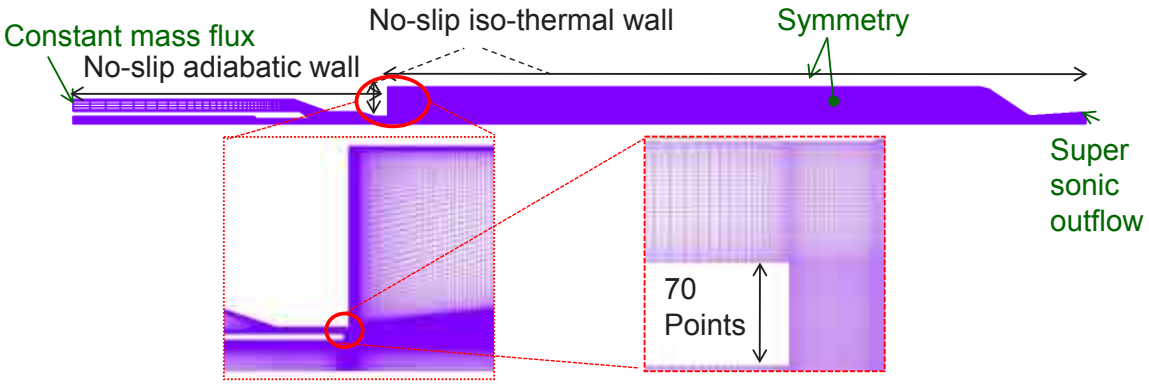
壁面漸近挙動ﾓﾃﾞﾙ GH2/GO2ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験

- 対象: GH2/GO2 ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験
- 条件;
  - 燃焼圧力 = 5.2MPa
  - 燃料温度 = 800 [K]
  - 酸化剤温度 = 711 [K]
  - 燃料流量 = 3.31 × 10-2 [kg/s]
  - 酸化剤流用 = 9.04 × 10-2 [kg/s]
  - 壁面温度 = 空間分布あり固定 (右図参照)
- 格子
  - 322000 点
  - 最少格子幅 = 0.3 μm (Y+ < 1 in all zone)

Marshall et al. (Penn. State Univ.), AIAA-2005-3572, 2005.





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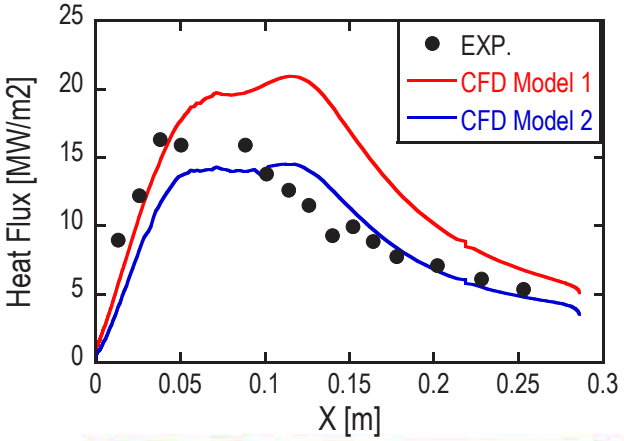
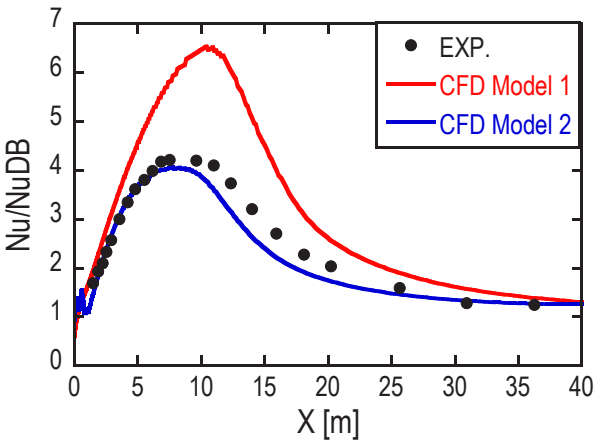
壁面漸近挙動ﾓﾃﾞﾙ GH2/GO2ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験

Single Element Injector



Temp. with Stream line

Expansion Tube



Vel. with Stream line

- ｼﾝｸﾞﾙｴﾚﾒﾝﾄ熱流束分布はModel 2 の方が，Model1よりも良い結果を示している.
  - 拡大管と同じ傾向を持つ.
- ｼﾝｸﾞﾙｴﾚﾒﾝﾄでは再循環領域における熱流束レベルを適切に評価できる壁面漸近挙動モデルを使う必要がある.

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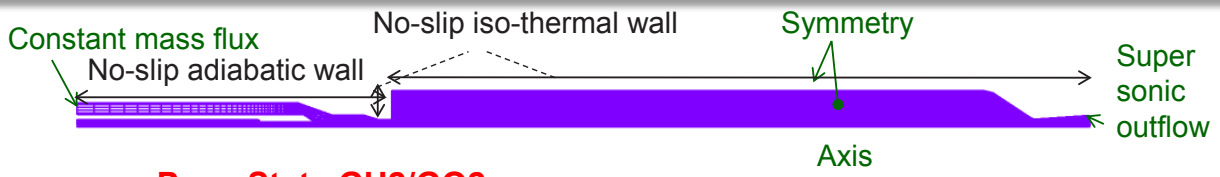
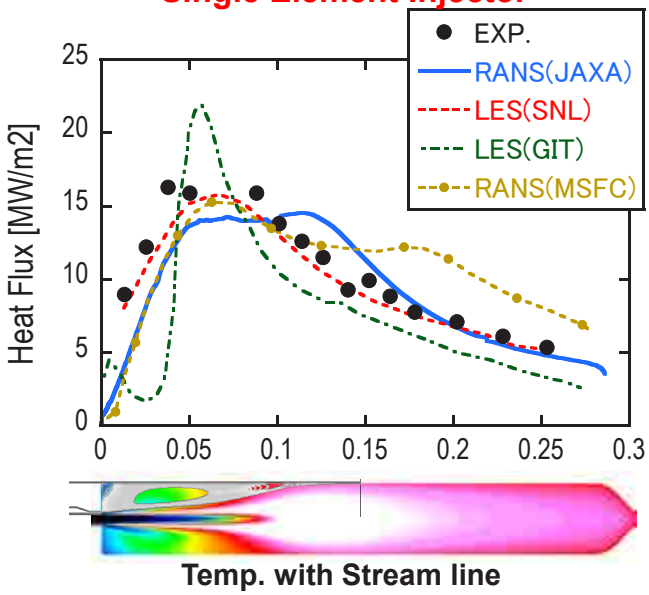
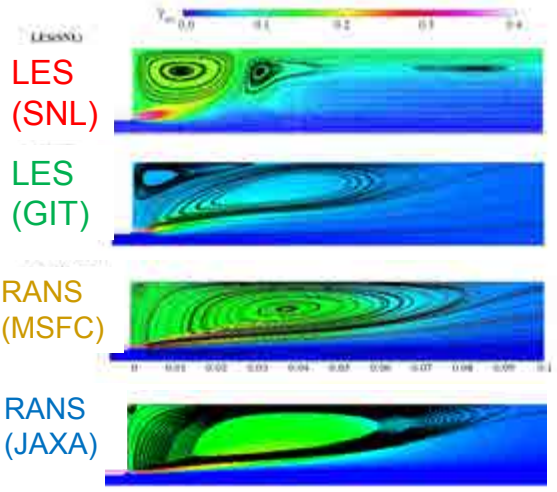
米国の結果との比較　GH2/GO2ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験



Penn State GH2/GO2 Single Element Injector



Temp. with Stream line



- RANS解析にしては妥当だが、
  - フルスケール燃焼器では循環小さい
    ⇒**よりフルスケールに近いｻﾌﾞｽｹｰﾙ燃焼器での検証が必要**

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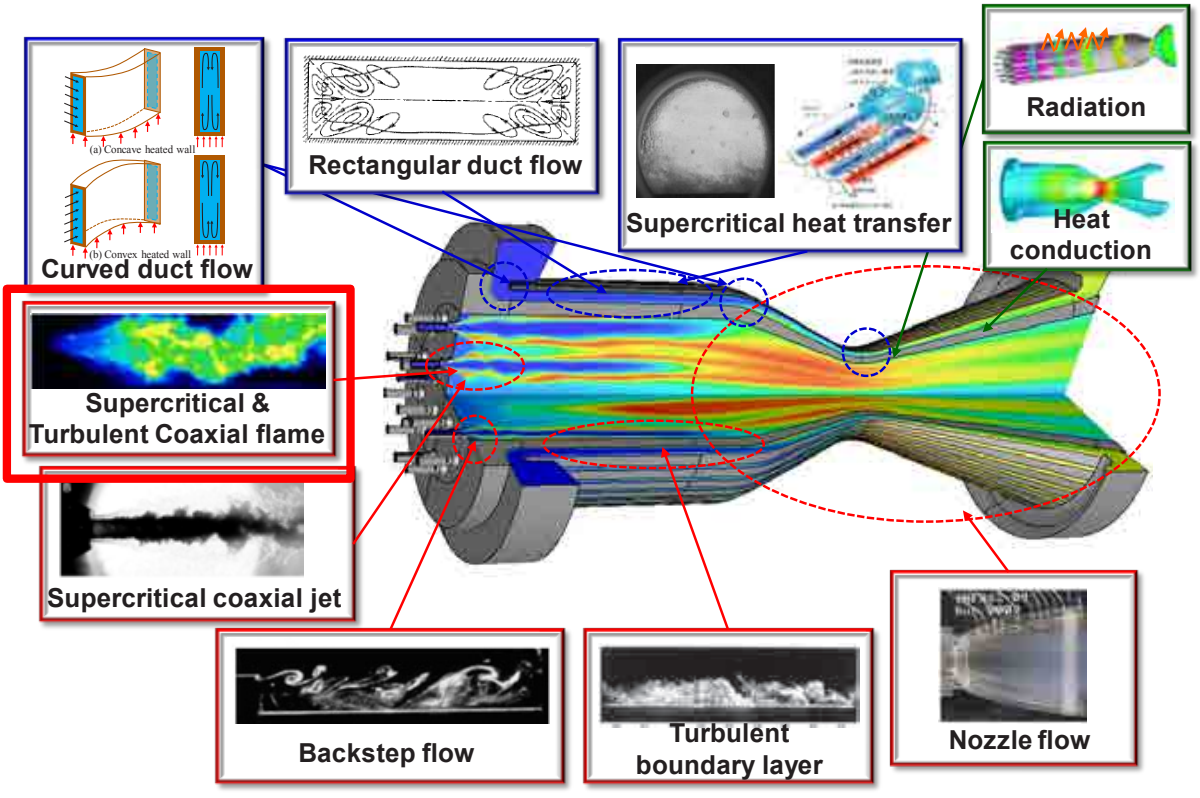
燃焼モデル　GH2/GO2ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験



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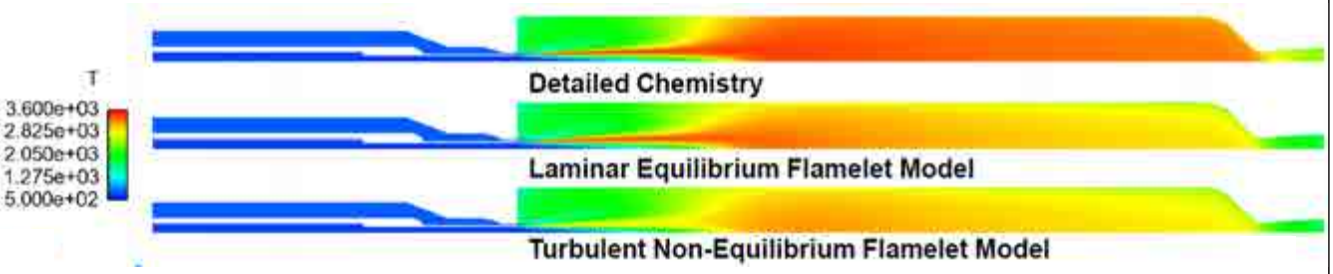
燃焼モデル GH2/GO2ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験



- Flameletモデルを導入し計算負荷の低減を狙った。
  - 【利点】
    - 方程式の数が詳細反応と比較して少ない。
      5+2+8本から5+2+2本に低減⇒計算速度約2倍
    - 副次的ではあるが解析が安定する。
  - 【欠点】
    - 熱損失、圧力変化を伴う系に適用するには改良が必要

- Laminar finite rateモデル（＋詳細反応モデル）との比較。
  - 燃焼器下流にて詳細反応モデルよりも燃焼温度が低い。
  - 壁面近傍、ノズル内部での温度変化に差異が生じている。

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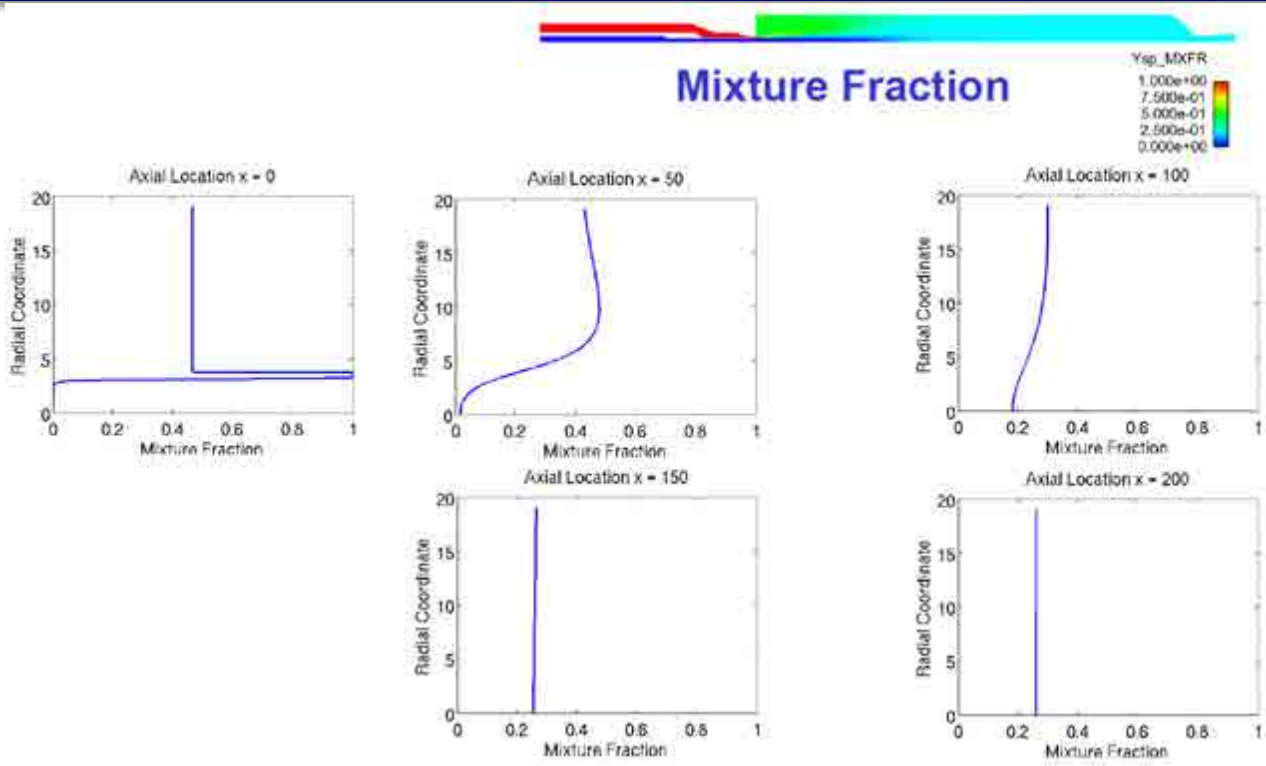
燃焼モデル GH2/GO2ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験



- Laminar finite rateモデル（＋詳細反応モデル）との比較。
  - X=150mm以降では混合分率が一定となり反応進行が止まる。

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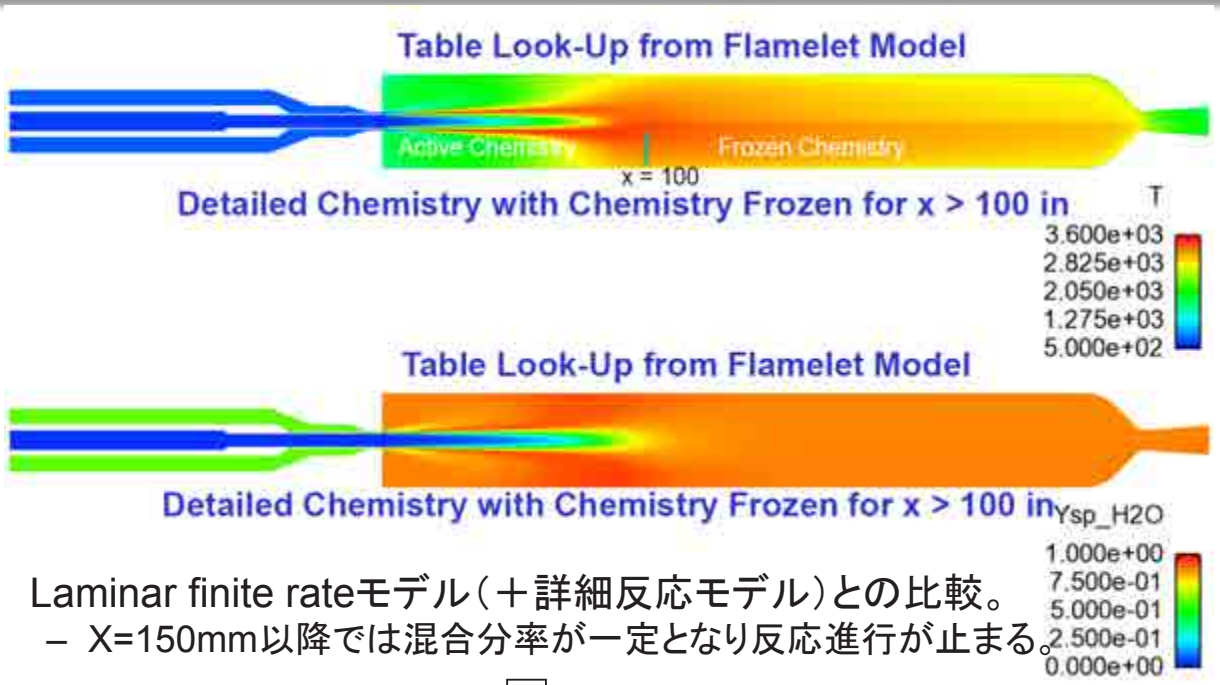
燃焼モデル　GH2/GO2ｼﾝｸﾞﾙｴﾚﾒﾝﾄ燃焼試験



- Laminar finite rateモデル（＋詳細反応モデル）との比較。
  - X=150mm以降では混合分率が一定となり反応進行が止まる。

⇩

  - 詳細反応モデルにてx=100mm以降で反応を強制的に凍結すると、Flameletモデルで観察された温度降下を再現できる。
    ⇒**【Flameletモデルの欠点】混合が起こらないと反応進行が止まる。**

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燃焼モデル　Flameletモデルの活用

- Flameletモデルを導入し計算負荷の低減を狙った。
  - 【利点】
    - 方程式の数が詳細反応と比較して少ない。
      5+2+8本から5+2+2本に低減⇒計算速度約2倍
    - 副次的ではあるが解析が安定する。
  - 【欠点】
    - 熱損失、圧力変化を伴う系に適用するには改良が必要
    - 混合が起こらないと反応進行が止まる。

⇩

初期解を効率的に作成するためにFlameletモデルを利用し、最終解では詳細反応モデルを使用
⇒ **解析にかかる総時間が約1/3に低減**

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サブスケール燃焼器による検証と簡略化手法検討

Validation and study

Basic cases → Single element → Multi-element → Subscale → Fullscale

- Boundary layer
  - U and T profiles
- Backstep flow
  - Recirculation flow
  - Heat Flux
- Nozzle flow
  - Compressible flow
  - Heat Flux
- Heat condution
  - Temperature profile

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  - Supercritical flowfield
- Coaxial flame
  - Combustion flowfield
  - Heat Flux
  - Effect of geometry and conditions
- Cooling channel
- Heated tube flow
  - Supercritical heat transfer
  - Heat Flux and wall temperature

- Water-cooled chamber
  - Interaction between flames
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- LH2 or LCH4 cooled chamber
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  - Difference between heated tube and rectangular duct

- Demonstrator engine
  - Fullscale phenomina

Tool development

Feedback

Basic features
- Numerical scheme
- Grid system
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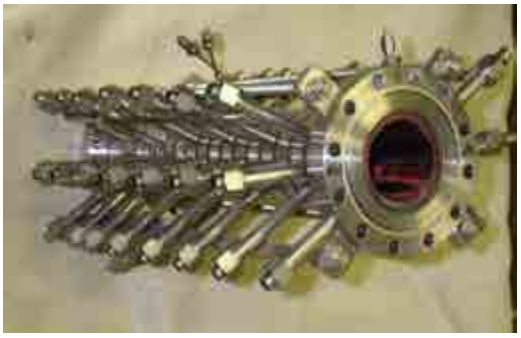
Key physical model
- Turbulence model
- Real gas model
- Combustion model
- Heat condution
- Radiation model
- Conjugated fluid and heat transfer

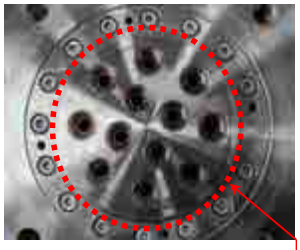
Red : works now in progress

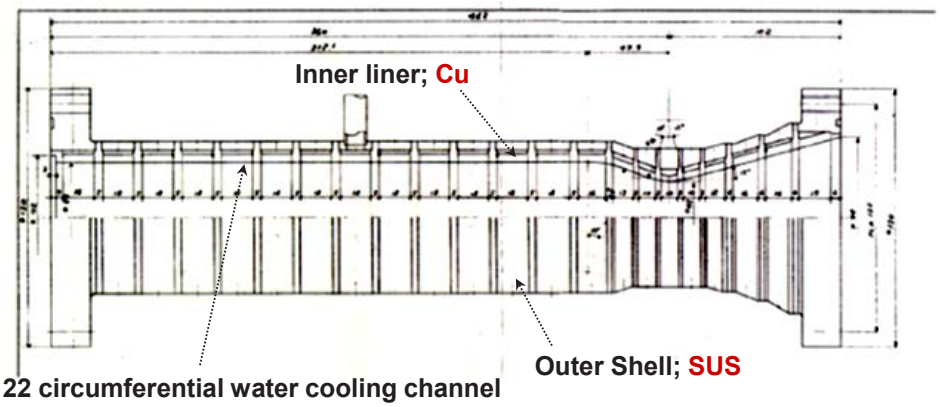
23

サブスケール燃焼器による検証と簡略化手法検討

- 燃焼圧力: 5.0 MPa
- 混合比: 6.5
- 噴射速度比: 50
- 噴射温度: 99 K for GH2
  97 K for LOX







12 co-axial injector elements

Throat Diameter = 42 mm
Face plate to Throat = 360 mm

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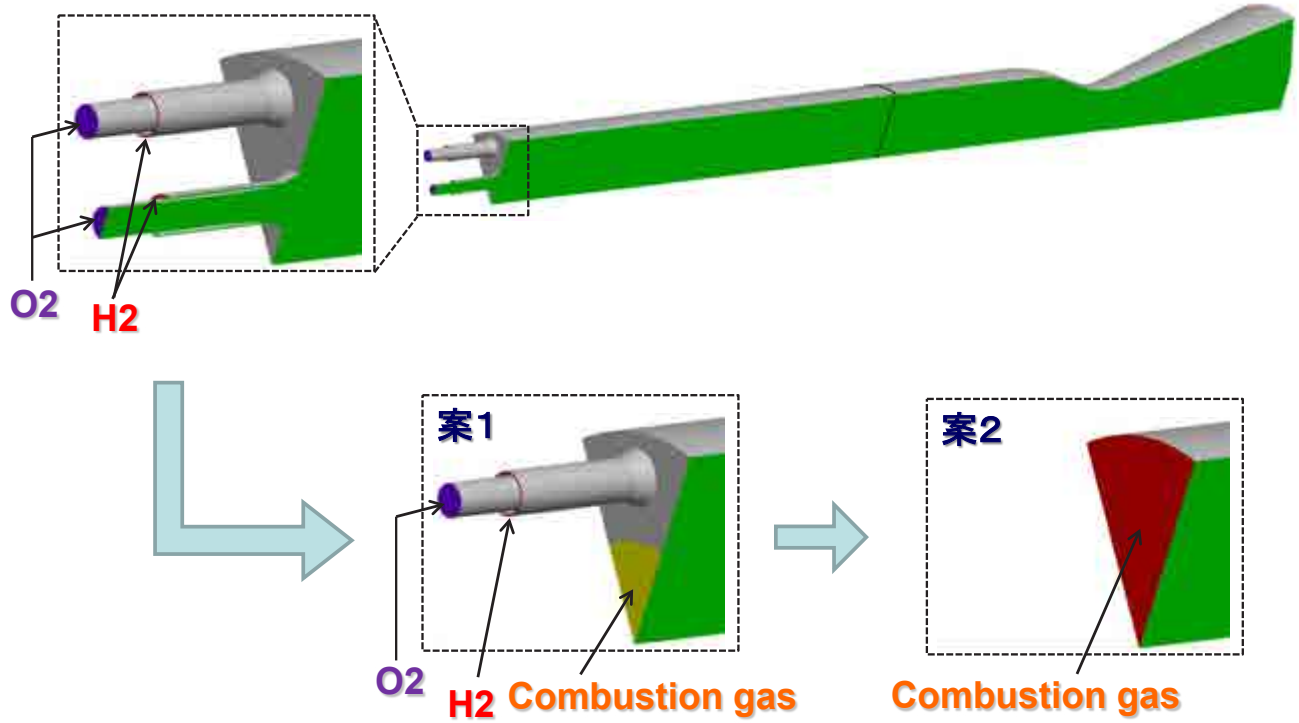
サブスケール燃焼器による検証と簡略化手法検討

- **案1**：壁面熱流束に大きな影響を有する最外周エレメントのみ考慮
- **案2**：エレメントを完全無視



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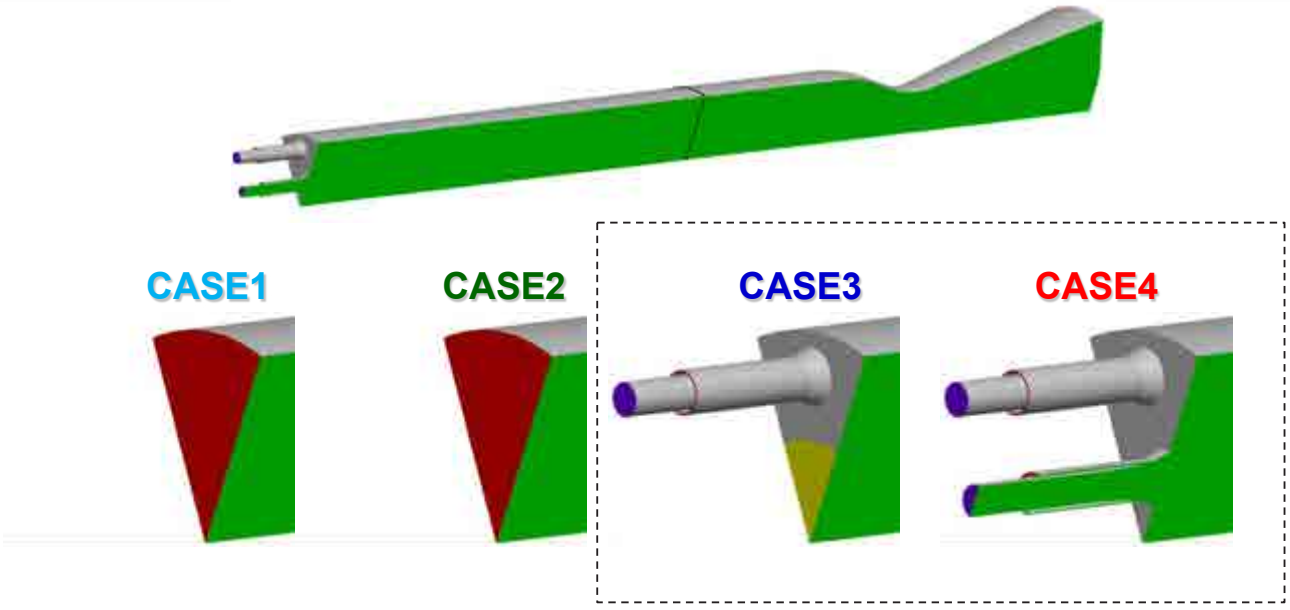
サブスケール燃焼器による検証と簡略化手法検討



CASE1: 全面燃焼ガス噴射、化学反応無
CASE2: 全面燃焼ガス噴射、化学反応有
CASE3: 最外周エレメント考慮、内側は燃焼ガスで模擬、化学反応有
CASE4: 実形状、化学反応有

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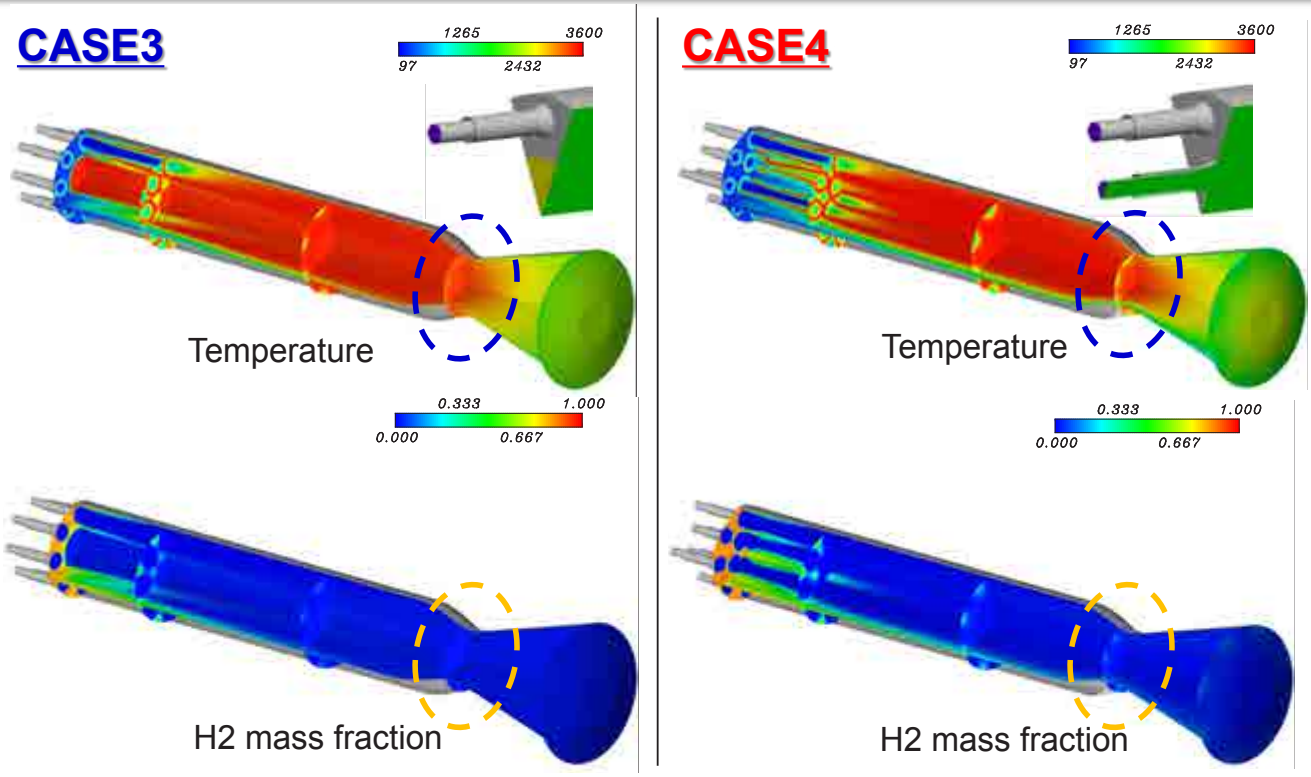
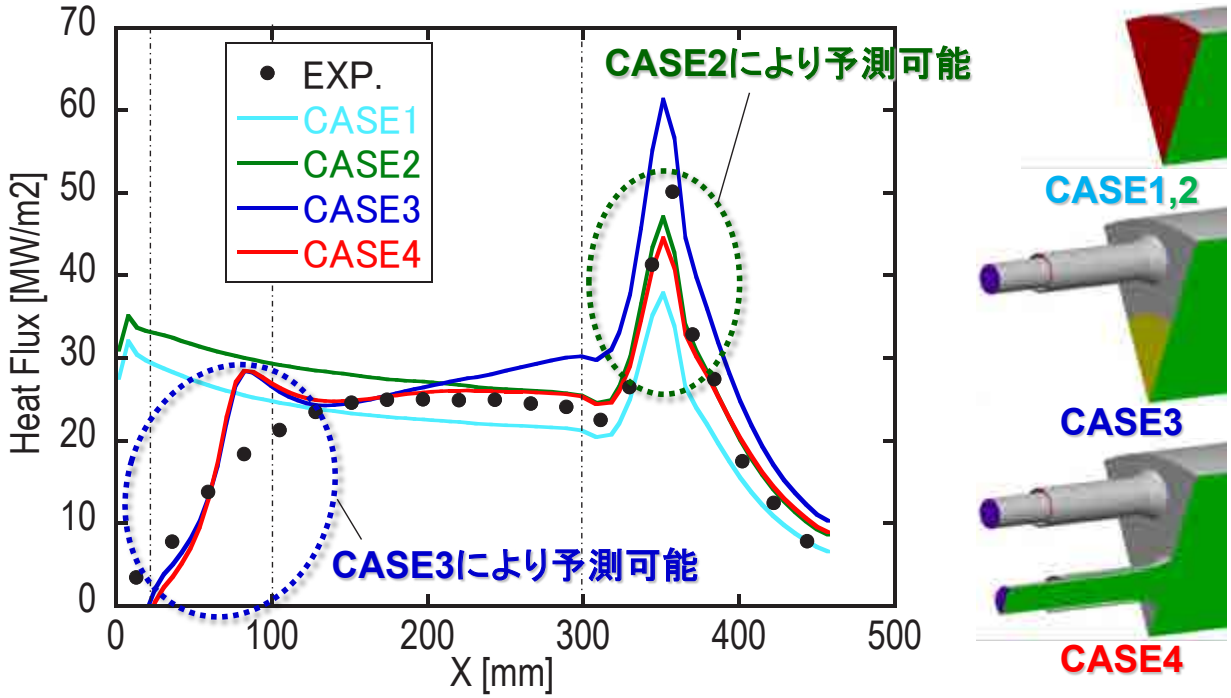
サブスケール燃焼器による検証と簡略化手法検討



- 内側エレメント無視でも全体的な傾向は模擬できている
- 壁面近傍の未燃水素濃度に差異あり ⇒ 壁面熱流束分布に影響する可能性あり

サブスケール燃焼器による検証と簡略化手法検討



- **Case 1 vs 2:** 化学反応の考慮は必須
  ⇒ 温度境界層及びノズル温度低下による化学種組成が重要
- **Case 3 vs 4:** 内側エレメント無視による平行部下流での過大評価
  ⇒ 壁面近傍を流れる未燃水素量の予測が重要

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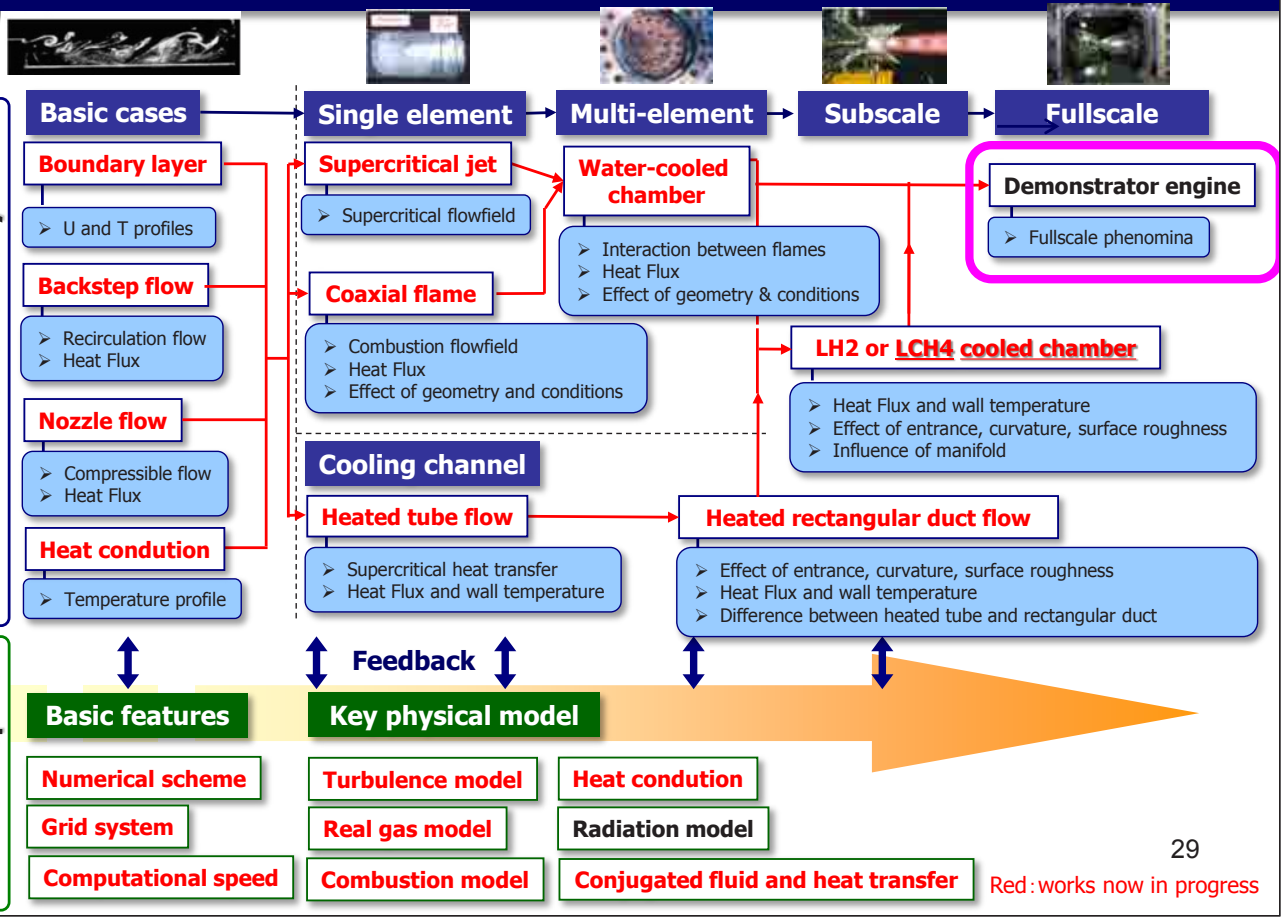
フルスケール燃焼器　簡略化手法の適用



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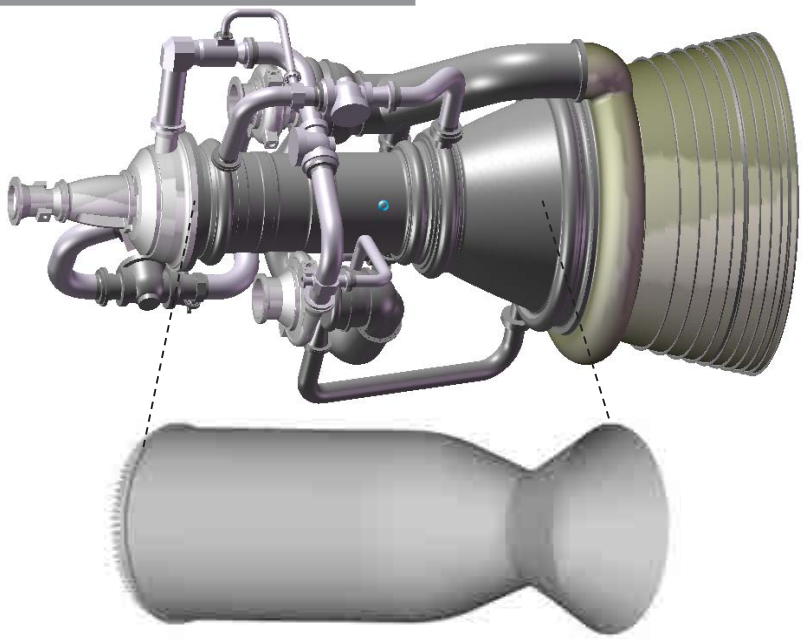
Red：works now in progress

フルスケール燃焼器　簡略化手法の適用

◆ フルスケール燃焼器　(LE-X)

- 燃焼圧力: 12 MPa
- 混合比: 6程度



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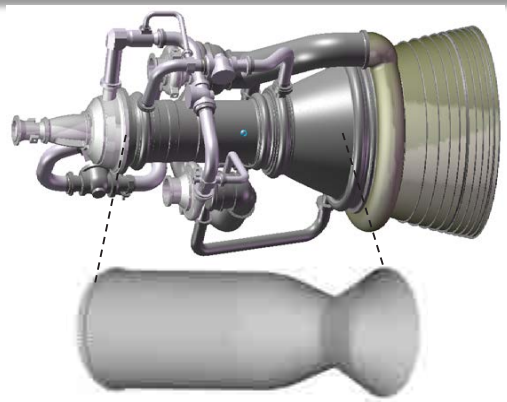
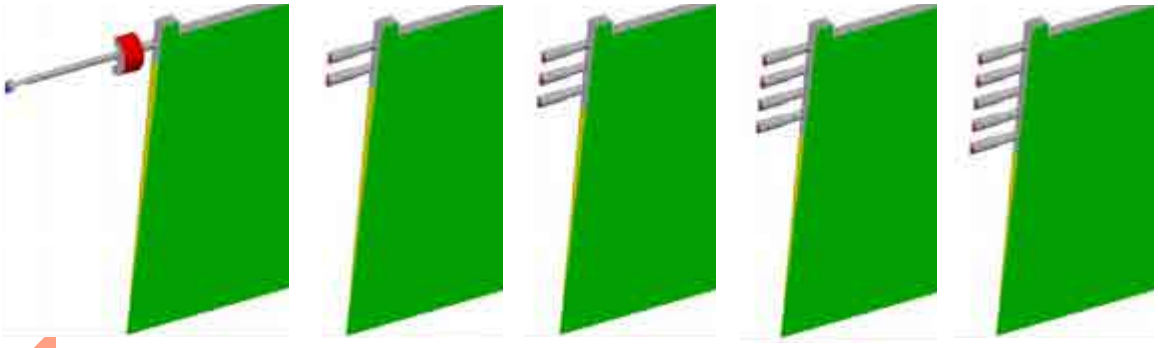
フルスケール燃焼器 簡略化手法の適用





Lower Computational Cost

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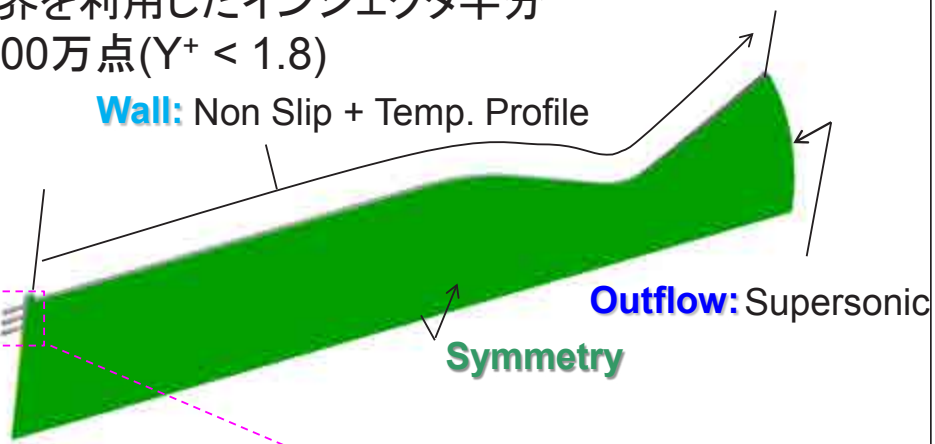
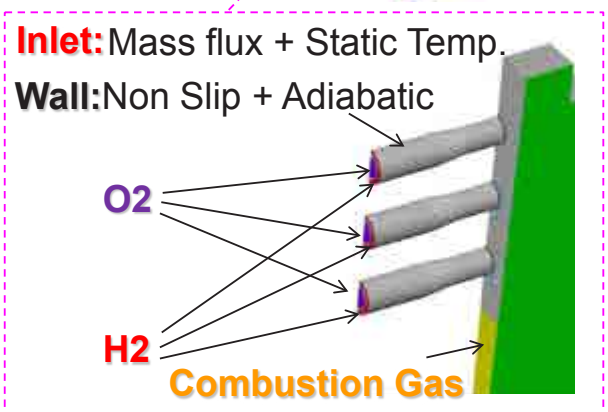
最外周のエレメント列数を1－5列と変化させて熱流束に対する列数の影響を調査

フルスケール燃焼器 簡略化手法の適用

- **解析領域**：対象境界を利用したインジェクタ半分
- **総格子点数**：約1000万点($Y^+ < 1.8$)





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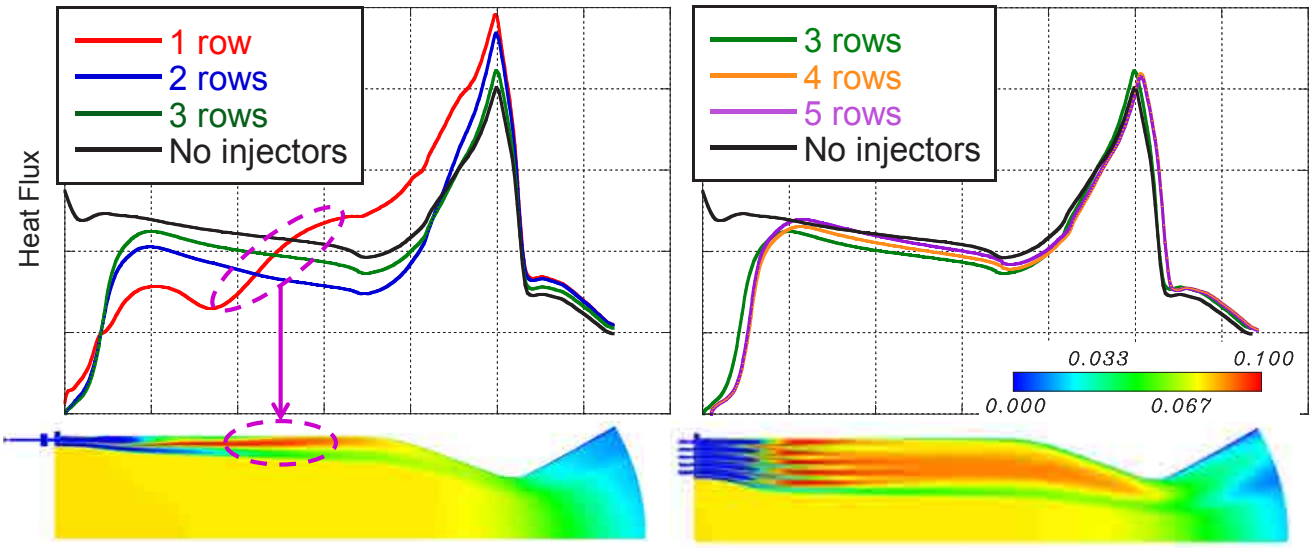
フルスケール燃焼器　簡略化手法の適用



OH mass fraction distributions

- 外側インジェクタ5列を考慮することで解析結果は収束する。
- 収束解のノズル部分はインジェクタを考慮しない2次元軸対象解析結果に近づく.
  - ノズル部の2次元軸対象解析結果の信頼性はｻﾌﾞｽｹｰﾙで確認済み
    ⇒ フルスケール燃焼器熱流束予測には**5列の解析結果を選択**

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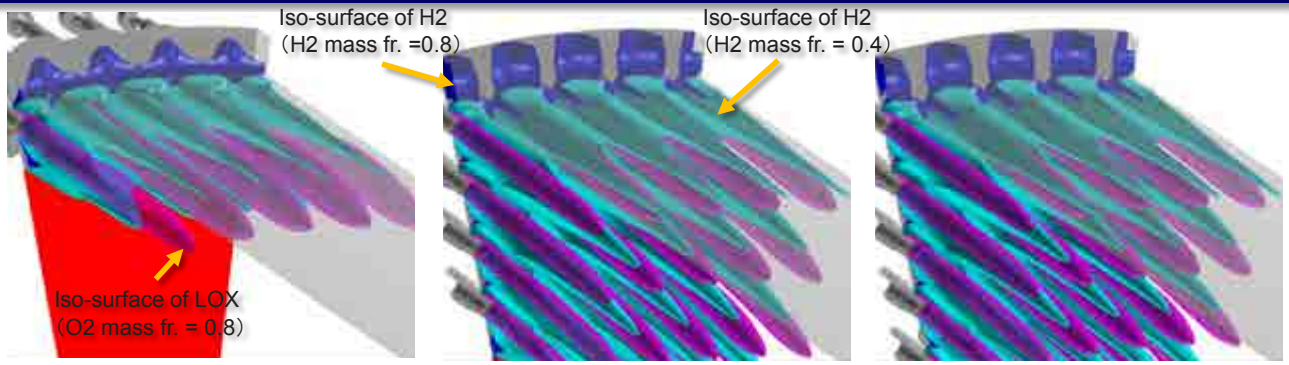
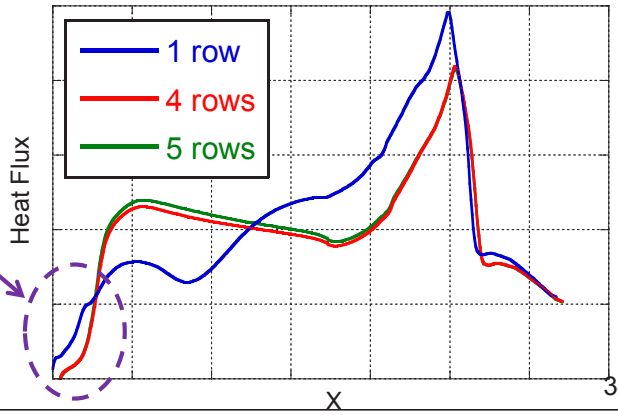
フルスケール燃焼器　簡略化手法の適用



1 row　　4 rows　　5 rows

➢ 壁面近傍に存在する未燃の水素量は1列の方が、4-5列と比較して少ない

➢ 未燃水素量が少ないと壁面近傍の温度が高くなり熱流束が高くなる



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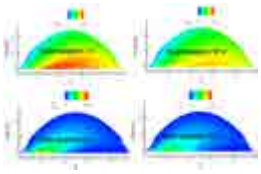
効率的なモデリングによる解析時間の短縮

オリジナル	コード効率化（コードチューニング）	Flamelet導入（初期解作成）	形状簡略化（燃焼ガスコア導入）
4.5か月	9週間	3週間	1週間

1/2　1/3　1/3

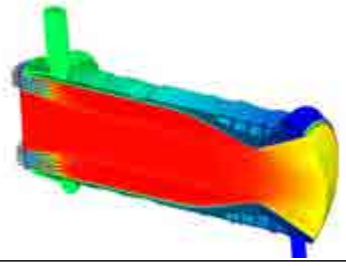


【目標】

- フルスケール燃焼器の再生冷却性能を数週間で評価する手法を開発する。

⇒ **目標ほぼ達成**

（冷却側とのカップリングを実施中
AIAA JPC 2013にて発表予定）



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まとめ

- 「フルスケール燃焼器の再生冷却性能を数週間で評価する」という目標に向かい、物理モデル評価、検証解析、簡略化手法の燃焼ガス側壁面熱流束への影響検討を行った。
  - 物理モデル評価
    - 壁面漸近挙動モデル
    - 燃焼モデル
  - 検証解析
    - 基礎非燃焼流れ
    - シングル、マルチインジェクタ燃焼試験
  - 簡略化手法
    - 内側インジェクタの簡略化
  - フルスケール燃焼器への適用 ⇒ 成功

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残った課題と今後の目標

- 亜臨界圧燃焼

  ⇒微粒化モデル、噴霧燃焼技術の導入（井上先生発表）

- 非定常現象理解

  ⇒次の発表へ（JAXA松山氏）

  ⇒RCCEなどさらなる計算負荷軽減手法の実装（越先生発表）

  ⇒高次精度解析の燃焼場への実装（寺島先生発表）

連携講座の知見のさらなる活用と実装（実現）

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ロケットエンジン燃焼に関する LES 燃焼解析

東京大学 JAXA 社会連携講座シンポジウム

2012年9月27日, 東京大学 浅野キャンパス
武田先端知ビル5階 武田ホール

松山 新吾
宇宙航空研究開発機構　研究開発本部

はじめに

- 近年の著しい計算機能力の向上により, 詳細な乱流燃焼シミュレーションが可能になってきている
  - DNS : 数十億点規模, LES : 数億点規模
- ロケット燃焼についても, 同様に DNS / LES が行われ始めている
- 今後, ロケット燃焼器の開発において, 特に LES が重要なツールになるものと期待
  - 燃焼振動や不安定現象など, 非定常性が支配的な問題
- 本講演では, JAXA 研究開発本部（ARD）においてこれまで実施した, 液体ロケット燃焼器に関する燃焼シミュレーションの事例を紹介する
  1. 超臨界圧 LO_X/GH_2 同軸噴流火炎のLES
  2. ロケット燃焼器内部における高周波燃焼振動のLES

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1. 超臨界圧 LO_X/GH_2 同軸軸噴流火炎のLES

背景

- LE-7A エンジンの燃焼室圧力は約120気圧，超臨界圧力環境下で燃焼が生じる（$P_{c,O2}$=50気圧）
- 極低温状態（約100K）で噴射された液体酸化剤（LO_x）を伴う燃焼
- ロケット燃焼シミュレーションの研究を開始した当初，JAXA/ARDには超臨界圧・極低温物性を扱うことが出来る燃焼コードが存在しなかったため，超臨界圧燃焼コードを開発する必要があった
- 超臨界圧燃焼コードを開発し，LE-7A を想定した LO_X/GH_2 火炎のシミュレーションを実現することを目標とした

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研究の目的

- Flamelet モデルを用いた LES により, 超臨界圧力における LO_X/GH_2 同軸噴流火炎の燃焼シミュレーションを実現
- 燃焼試験データとの比較により, flamelet LES コードの予測精度を検証
  - DLR P8 燃焼器, 60気圧燃焼試験
  - Shadow graph
  - OH*, H_2O 自発光イメージ
  - 大規模渦構造の長さスケール

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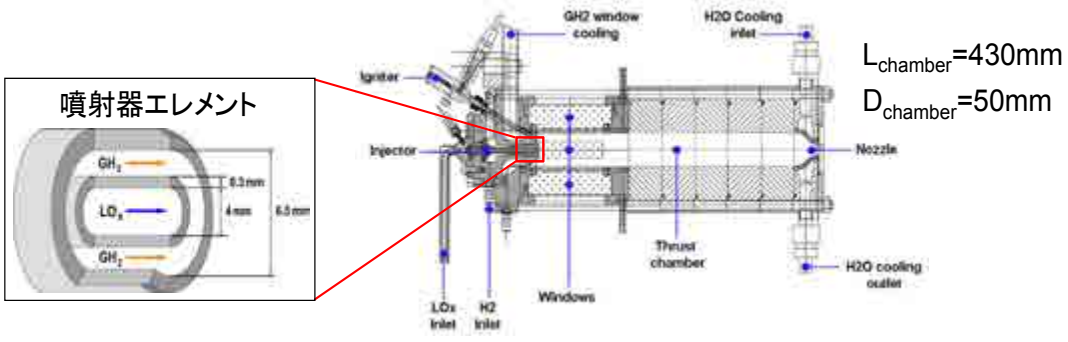
解析の対象（DLR P8燃焼器, 60気圧燃焼試験）

• 6MPa case of LO_X/GH_2 combustion experiment by the P8 combustor at the DLR (Ivancic and Mayer, *J of Propulsion and Power*, 18, 2002, 247-253.)



燃料・酸化剤・パージガス 噴射条件

	LO_X	GH_2	GH_2 purge
Velocity [m/sec]	25	310	300
Temperature [K]	127	125	293
Density [kg/m^3]	925	11.4	4.81
Reynolds no. [-]	1.15×10^6	2.86×10^6	6.63×10^5
$P_{chamber}$ [MPa]	6.0（$P_{c,O2}$=5.04MPa を超える）		

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数値計算手法

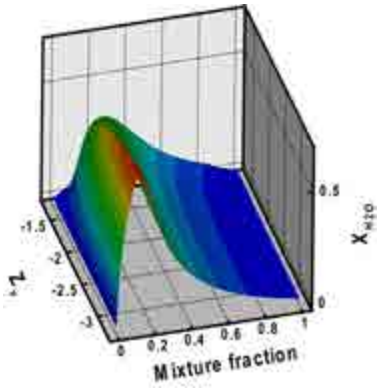
- 支配方程式
  - 三次元 filtered Navier-Stokes 方程式（ρ, ρu, ρv, ρw, E, $\rho\zeta$）
  - 超臨界圧力環境を仮定，液体酸素（LO_X）は気相的に取り扱う
- SGSモデル: 標準 Smagorinsky モデル（C_s=0.2）
- 乱流シュミット数：Sc_t =0.4, 乱流プラントル数：Pr_t =0.7
- 高圧・極低温状態における実在気体効果を考慮
  - 状態方程式: Soave-Redlich-Kwong 状態方程式（SRK EoS）
  - 熱力学状態量（C_p, H, S）: Departure function による評価
  - 輸送係数（μ, κ）: Chung et al. method
  - 輸送係数（D_{ij}）: Chapman-Enskog theory + SRK EoS
- 対流流束: AUSM$^+$-up スキーム（三次精度 MUSCL）
- 時間積分: 二段 Runge-Kutta 法
- 並列化：領域分割（MPI） + OpenMP, 288CPUs on JSS (Fujitsu FX1)

6

乱流燃焼モデル

- Laminar flamelet モデル
- Flamelet テーブルを参照することにより乱流燃焼をモデル化
- 混合分率 ζ, スカラー散逸速度 χ, 混合分率のSGS変動 ζ_v の 3変数
- CHEMKIN OPPDIF コードにより flamelet テーブルを構築
- Li らによる 8化学種 (H_2, O_2, OH, H_2O, H, O, HO_2, H_2O_2), 19反応モデル
- presumed β-shaped PDF により混合分率の SGS 変動を考慮
- $\zeta_v = C\Delta^2|\nabla\zeta|^2$, C=0.13

Example of flamelet library
(Mole fraction of H_2O)



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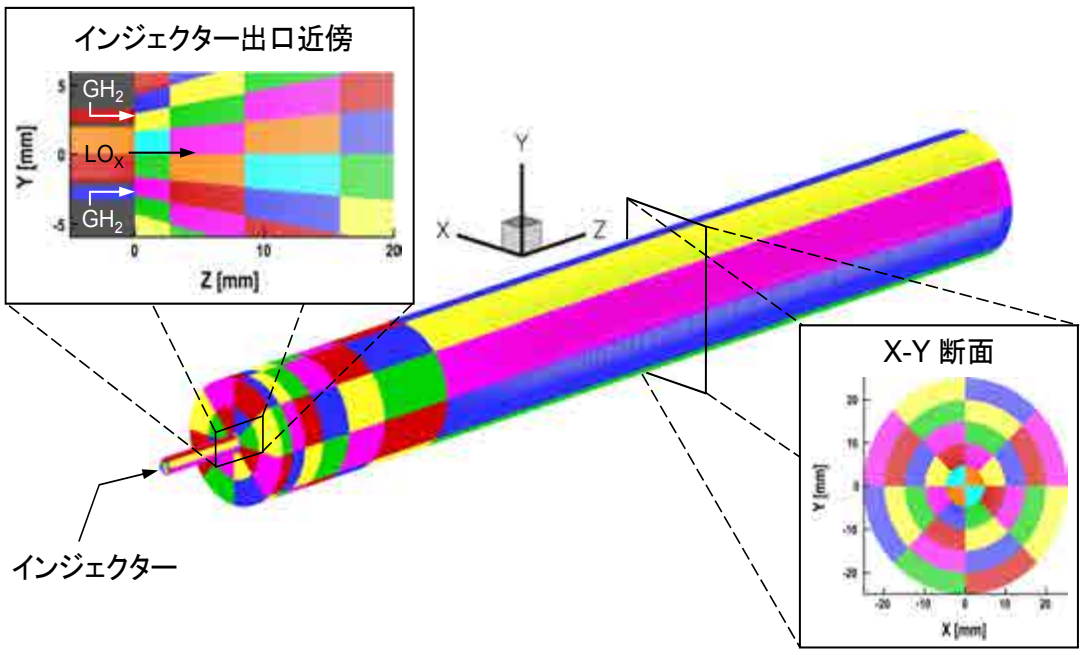
計算格子の例



- 総格子点数: 6100万セル（1056×160×320 + 1056×80×80）
- 最少格子幅:（軸方向）50μm,（半径方向）20μm,（周方向）40μm

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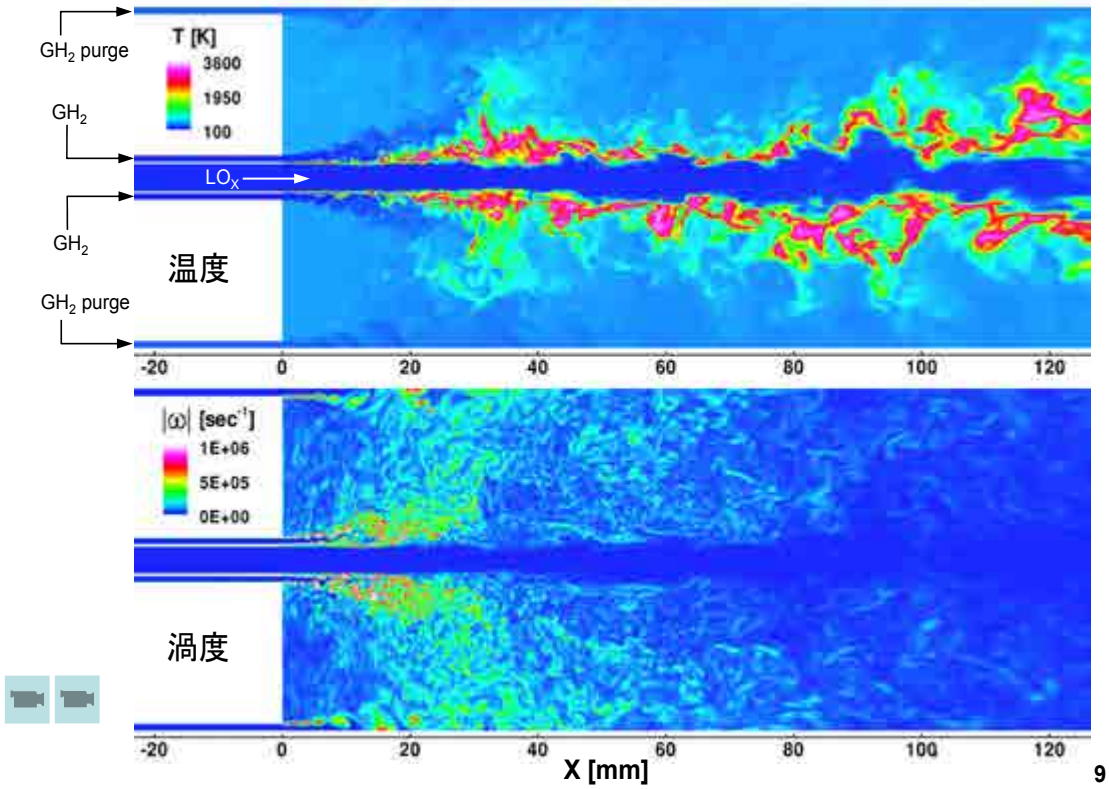
計算結果：瞬時流れ場



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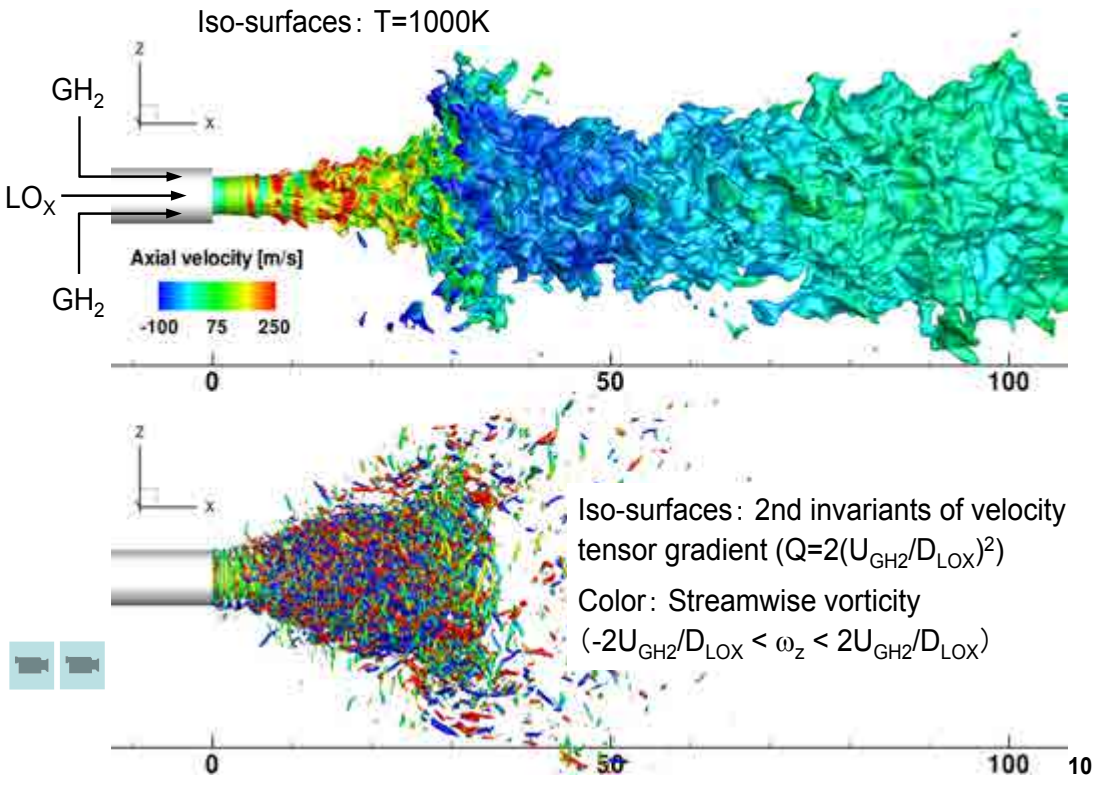
計算結果：流れ場の三次元構造



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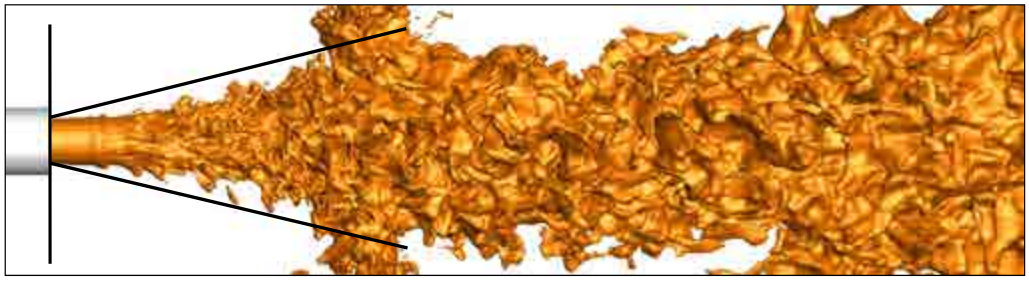
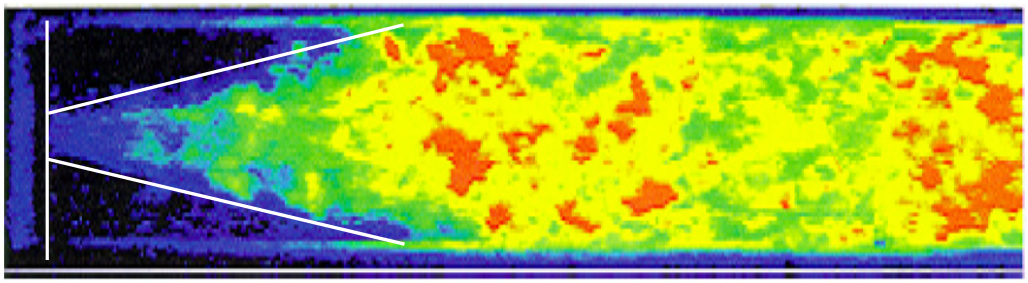
実験データとの比較：火炎形状

Present LES (X_{H2O}=0.1)



H_2O emission image (instantaneous image, 100mm × 25mm)



* B. Ivancic et al., AIAA Paper 99-2211.

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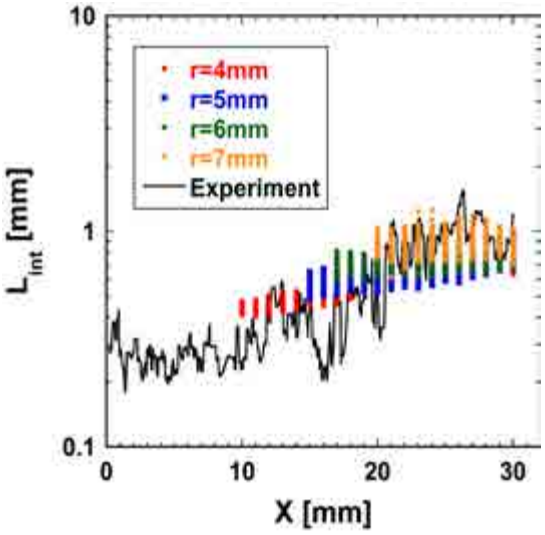
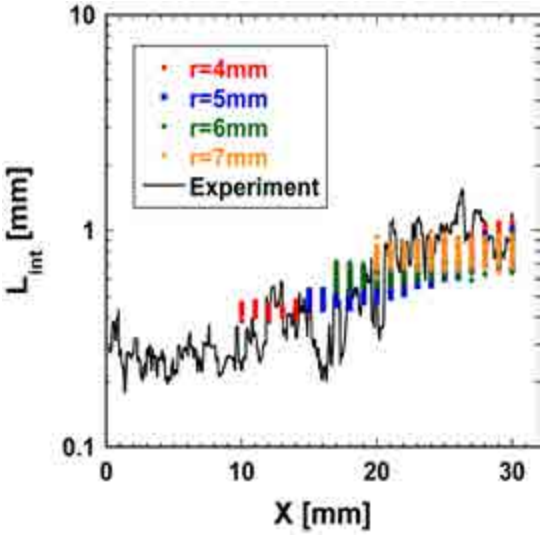
実験データとの比較：長さスケール

Integral length scale L_{int} by U_r'



Integral length scale L_{int} by U_θ'



✓ LESと実験データは良い一致を示す
✓ 半径方向と周方向の速度変動はほぼ同じ長さスケールを持つ

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まとめ：LO_X/GH_2 同軸噴流火炎のLES

- Flamelet モデルを用いた LES により, 超臨界圧力における LO_X/GH_2 同軸噴流火炎の燃焼シミュレーションを実現
  - DLR P8 燃焼器, 60気圧燃焼試験
- 実験データとの良い一致
  - Shadowgraph: 密度分布
  - H_2O 自発光イメージ: 火炎形状
  - 大規模渦構造の長さスケール: 乱流構造

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2. ロケット燃焼器内部における高周波燃焼振動のLES

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研究の背景

- ロケットエンジンの開発では，燃焼振動・燃焼不安定が常に大きな問題
- 高周波燃焼振動（数kHz）の発生は燃焼器の破損・焼損につながる
- 設計が進んだ段階で燃焼振動が発生した場合，設計変更・エンジン改修に時間とコストが費やされるため，設計の初期段階で発生の有無を評価することが重要
- 燃焼シミュレーションの中で燃焼振動を発生させることができれば，燃焼器内部のあらゆる情報を調べることが可能
- レイリーインデックス，$\int_V \left\{ \frac{(\gamma_0 - 1)p'q'}{\gamma_0 p_0} \right\} dV$
  - 圧力変動と発熱率変動とのカップリングの指標，燃焼振動の増幅項に相当
- 燃焼シミュレーションの結果を利用して，燃焼器内部のレイリーインデックスや，開口部からの流出による減衰などを評価，圧力変動の増減との関係を明らかにする

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研究の目的

- ロケット燃焼器を模擬した燃焼シミュレーションを実施, 高周波燃焼振動を発生させることを試みる
  - – H_2/O_2 インジェクター, 大気圧燃焼試験
  - – インジェクター偏心配置による火炎・圧力変動相互作用の促進
  - – 加振による強い横方向モードの発生
- 燃焼シミュレーションの結果を利用してレイリーインデックスなどを評価, 火炎と圧力変動の相互作用メカニズムを理解する

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解析対象

- 大気圧燃焼試験（JAXA/ARD ジェットエンジン技術センターにおいて実施）
- H_2/O_2 同軸型インジェクターを偏心配置, 燃焼室出口を開放
- 火炎がインジェクターリム部から離脱するような条件において, 1Tモードの圧力変動（±3kPa）が発生

燃焼器の概要

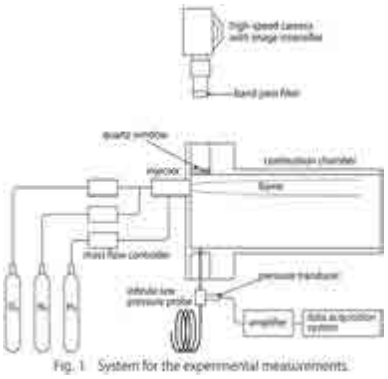
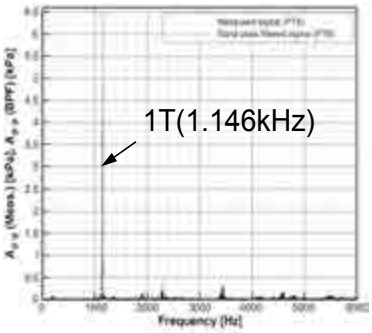
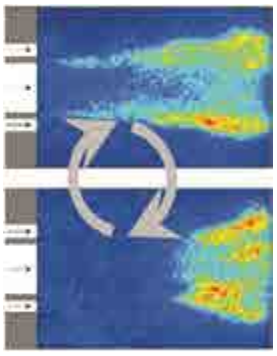


Fig. 1 System for the experimental measurements.

圧力変動のFFTスペクトル



OH自発光画像



* T. Shimizu et al., *AIAA Journal* 49(10), pp.2272-2281, 2011.

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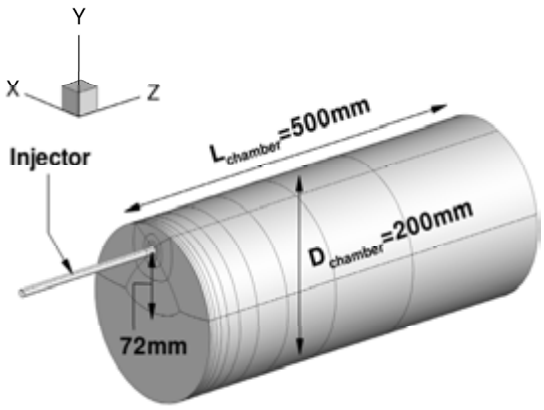
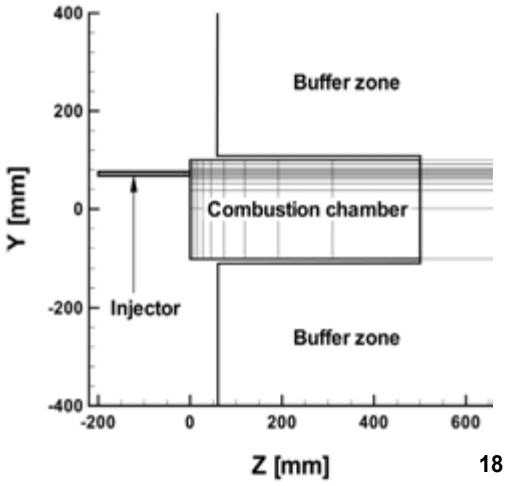
解析条件など

- 円筒形燃焼器($L_{chamber}$=500mm, $D_{chamber}$=200mm)
- インジェクター流入部において H_2/O_2 噴射流量・温度を固定
- 燃焼室出口は開放し, 巨大なバッファー領域を接続
- バッファー領域の外部境界を大気圧(0.1MPa)に固定
- 格子点数 = 800万点, 最小格子幅 = 100μm

燃焼室およびインジェクター



バッファー領域



18

数値計算手法

- 支配方程式: 三次元 filtered Navier-Stokes 方程式
- SGSモデル: 使用しない
- 詳細反応モデル:
  - 7化学種(H_2, O_2, OH, H_2O, H, O, HO_2)
  - 13反応モデル(based on Li et al., *Int.J.Chem.Kinet.* 36, pp.1-10.)
- 熱力学的諸量: NASA Glenn データベース
- 輸送係数: CHEMKIN データベース
- 対流流束: AUSM$^+$-up スキーム(五次精度 WENO)
- 時間積分: 三段 三次 Runge-Kutta 法
- 並列化: 領域分割(MPI) + OpenMP, 289CPU

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噴射条件

- 火炎がリムに付着するケース（付着火炎）
  - 燃料：100% H_2, 酸化剤：100% O_2
  - U_{H2}=190m/sec, U_{O2}=100m/sec, O/F=5.11
  - 燃焼試験では圧力変動が発生せず
- 火炎がリムから離脱するケース（離脱火炎, JEDI 堀 暖 氏による解析）
  - 燃料：100% H_2, 酸化剤：53% O_2 + 47% N_2（モル比）
  - U_{H2}=108m/sec, U_{O2}=168m/sec, O/F=8
  - 燃焼試験では 1T モードの圧力変動が発生

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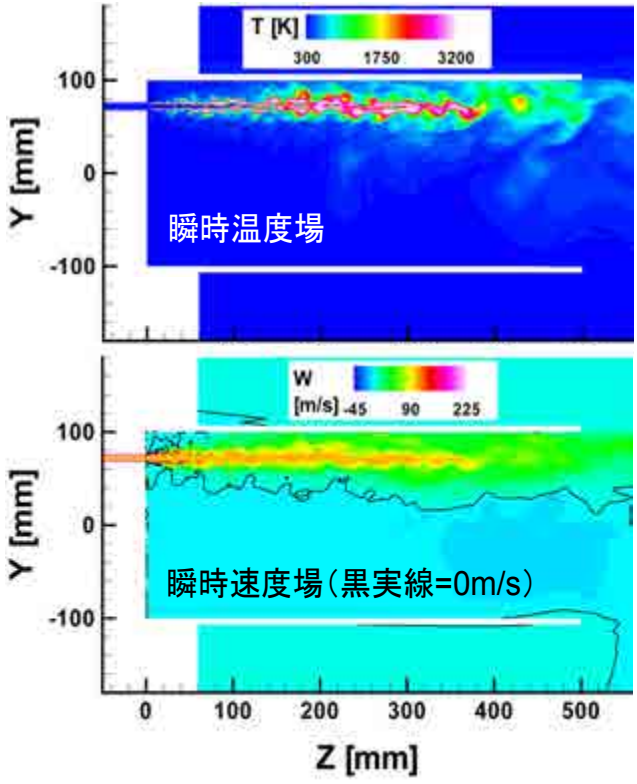
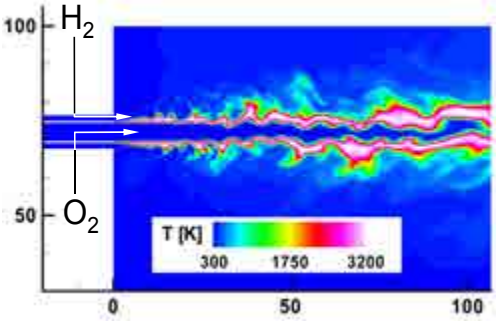
付着火炎：燃焼場の概要



インジェクター近傍



- 約50msecの解析を実施, 燃焼室内部の流れ場は定常的な状態
- 火炎はインジェクターのリム部に付着し, 拡散火炎を形成
- 燃焼室下半分の領域はほぼ速度が 0 でよどんだ状態

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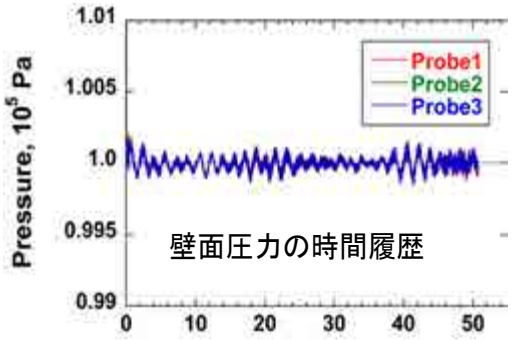
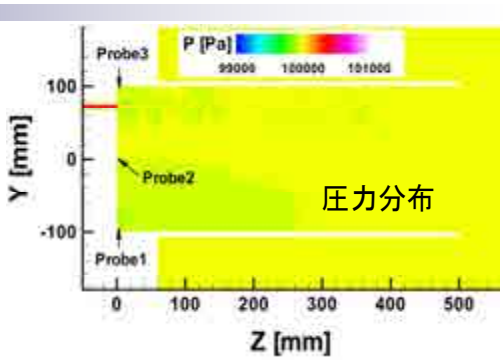
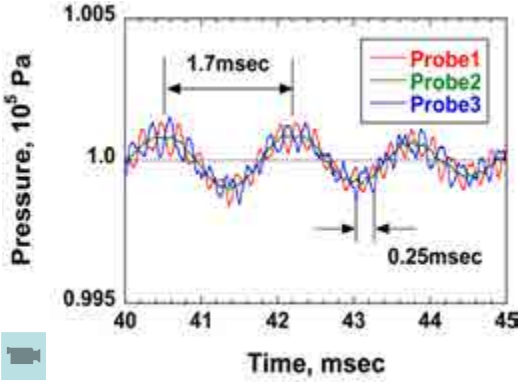
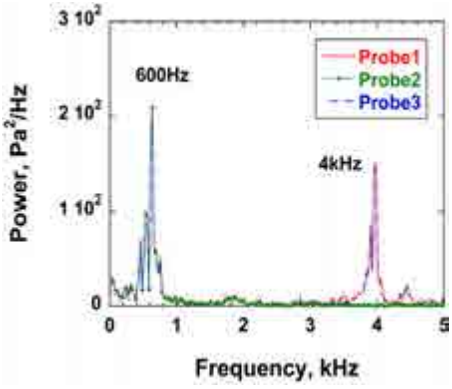
付着火炎：燃焼室内部の圧力場





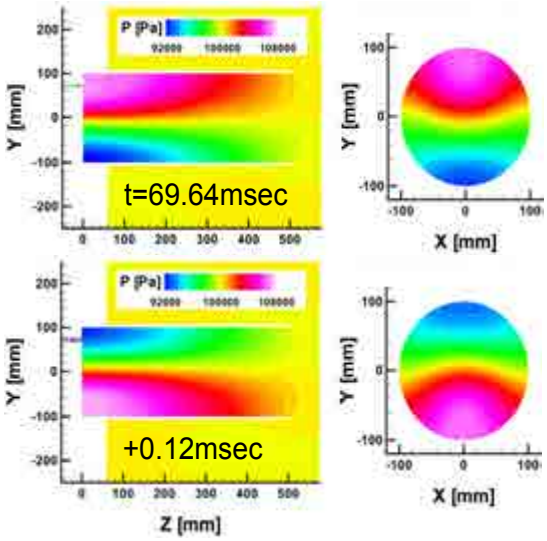


圧力変動のFFTスペクトル

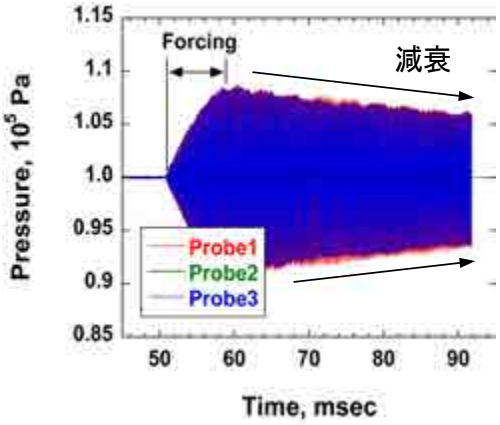


22

付着火炎：加振による横方向モードの発生



壁面圧力の時間履歴



- 燃焼室壁面（Y<0mm）に沿って人工的なエネルギー生成項を付加し，加振を実施
- 加振によって，強い横モードの圧力変動（±8%）が発生
- 1T モードの圧力変動に相当，0.12msec（4kHzの半周期）で圧力分布が反転
- 加振を停止後，変動レベルは維持できずに減衰

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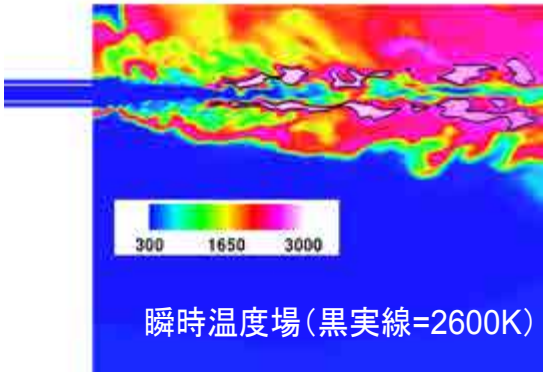
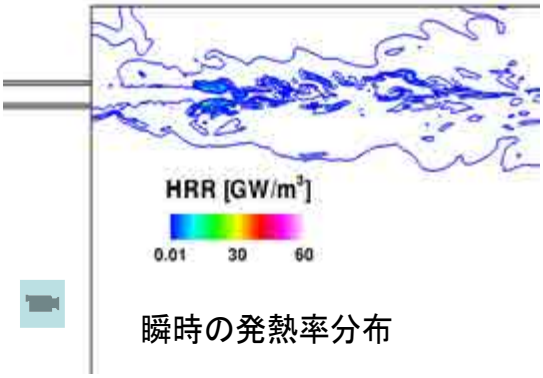
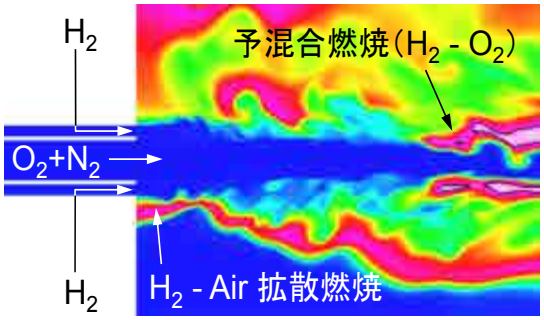
離脱火炎：燃焼場の概要





瞬時の発熱率分布

インジェクター近傍



- 水素噴流の外側に拡散燃焼，リムから離脱した火炎は予混合燃焼
- 予混合燃焼による高い発熱率と大きな空間変動
- H_2 - Air 燃焼, T_{max}=2400K
- H_2 - O_2 燃焼, T_{max}=3000K

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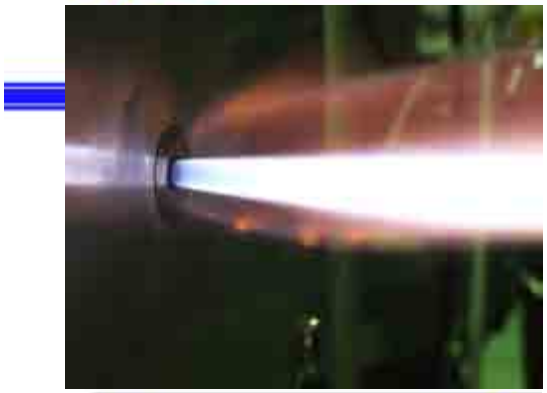
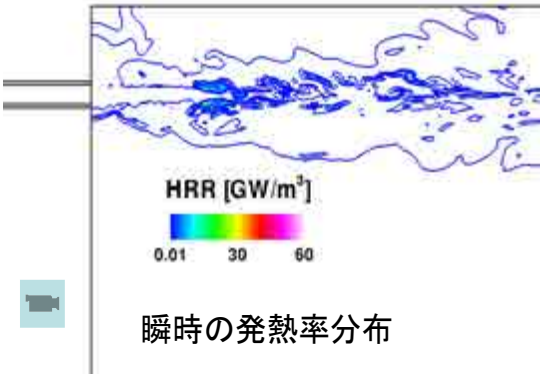
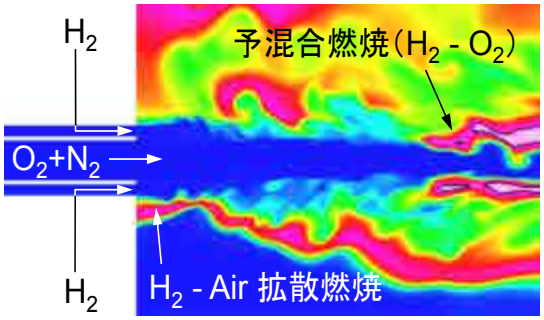
離脱火炎：燃焼場の概要





瞬時の発熱率分布

インジェクター近傍



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- 予混合燃焼による高い発熱率と大きな空間変動
- H_2 - Air 燃焼, T_{max}=2400K
- H_2 - O_2 燃焼, T_{max}=3000K

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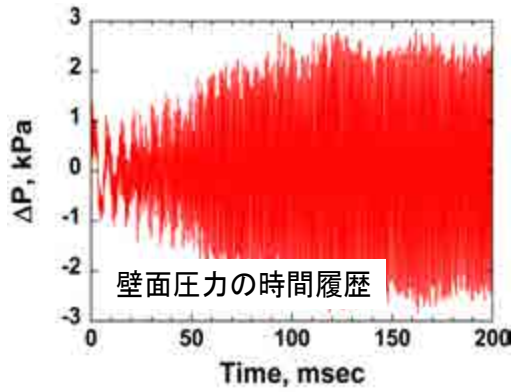
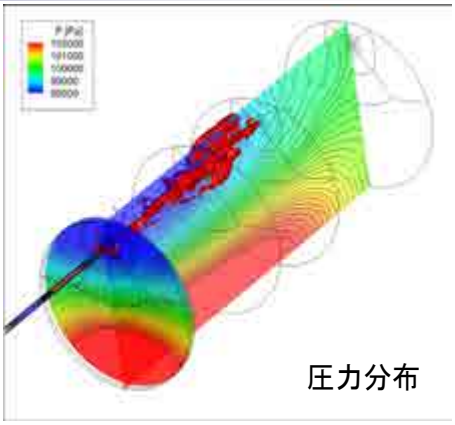
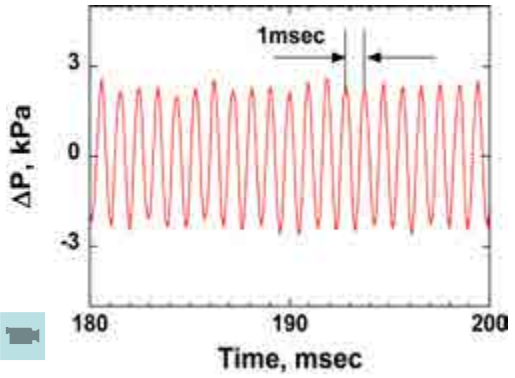
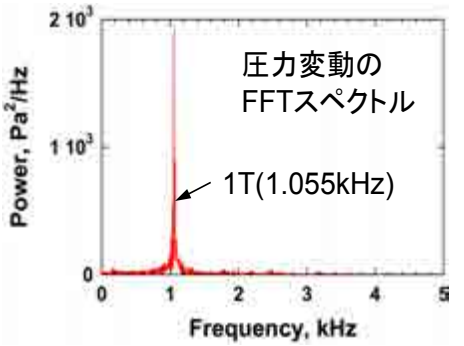
離脱火炎：燃焼室内部の圧力場









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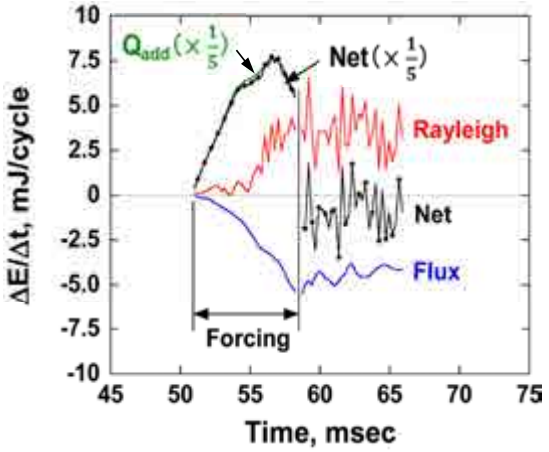
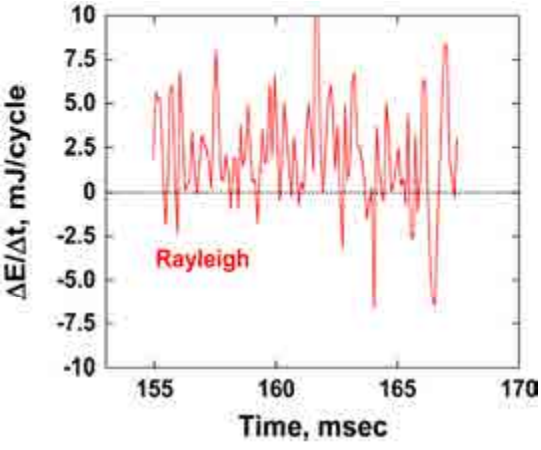
音響エネルギー収支の解析

付着火炎の場合



離脱火炎の場合



- 付着火炎の場合，
  - 音響エネルギー増加のほとんどは加振で付加したエネルギー（Q_{add}）による
  - 加振を実施しないと Rayleigh 項（ $\int_T\int_V \frac{\gamma_0-1}{\gamma_0 p_0} p'q' dV dt$ ）は非常に小さく，振動が自励的に発達する見込みは低い
  - 加振停止後，燃焼室出口からの流出（Flux, $-\int_T\int_S p'\mathbf{u}'\cdot\mathbf{n}\, dS dt$ ）が大，圧力変動は減衰

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まとめ:高周波燃焼振動のLES

- ロケット燃焼器を模擬して燃焼シミュレーションを実施, 高周波燃焼振動を発生させることを試みた
- 噴射条件の違いにより, 異なる2つの燃焼形態（付着火炎と離脱火炎）
- 付着火炎の場合,
  - 拡散燃焼, 大きな圧力変動は発生しない
  - 加振により強い横方向モードを発生, 加振停止後, 圧力変動は減衰
  - Rayleigh 項が小さく, 圧力変動が自励的に発達する見込みは少ない
- 離脱火炎の場合,
  - 拡散燃焼（H_2 - Air）と予混合燃焼（H_2 - O_2）が混在
  - 1T モード（1kHz）に対応する圧力変動が自励的に発生
  - 予混合燃焼による発熱変動が比較的大きな Rayleigh 項を発生させる要因と思われる

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課題, 将来の展望

- 超臨界圧 LO_X/GH_2 同軸噴流火炎のLES
  - 超臨界圧力における LO_X/GH_2 火炎のシミュレーションを実現
  - 入手可能な燃焼試験データと良い一致, ただし, 限定的な比較であるため, 継続的なコードの検証が必要
  - 検証用データの不足, 高圧環境下での検証用データを取得するため, 計測技術の向上が必要
  - 解析コストの問題, 現状では1ケースに1ヶ月, 次期スパコンが導入されると3日で1ケースの解析が期待できる
- 高周波燃焼振動のLES
  - LES 燃焼解析により燃焼振動をとらえることは可能, ただし, 適切な乱流モデル・燃焼モデルの選択が重要
  - 付着火炎（拡散火炎）に対しても, 自励的に振動が発達する条件を模索
  - 燃焼シミュレーションデータの解析から, 圧力変動の増幅・減衰メカニズムを把握できるものと期待

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東京大学JAXA社会連携講座シンポジウム(2012/09/27 東京)

宇宙輸送機の推進薬挙動予測に関する研究

東京大学 航空宇宙工学専攻　姫野 武洋
JAXA/JEDI　谷 直樹
JAXA/ISAS　野中 聡
JAXA/輸送本部　杵淵 紀世志

UT JET PROPULSION LABORATORY

液体ロケットに関係する自由表面流

自由表面流

とても身近ではあるが、
形を説明したり予測するのはとても難しい。

東京大学とJAXAは協力して、
航空宇宙推進機関内部の
自由表面流の熱流動を予測できる知見と技術の
獲得に努めている。

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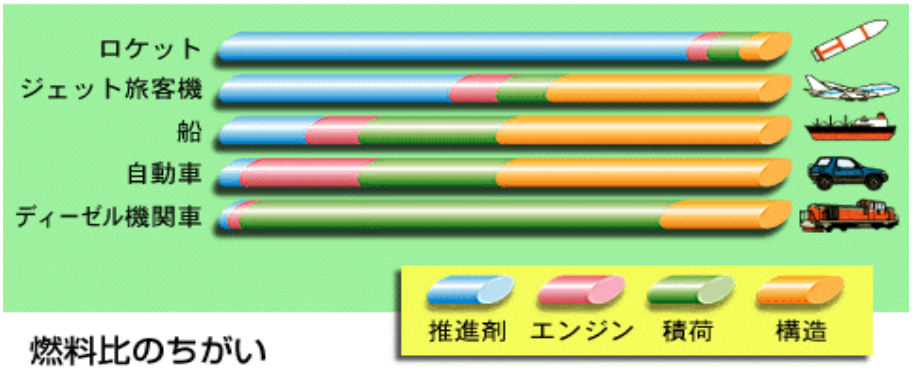
ロケットが搭載している推進剤

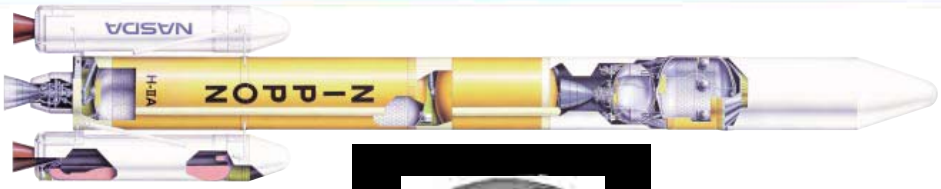


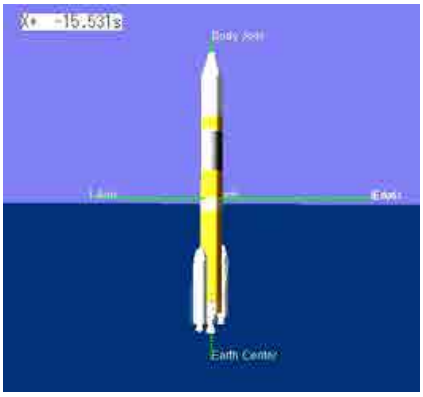
燃料比のちがい

缶ビール 4.6%

卵 11%

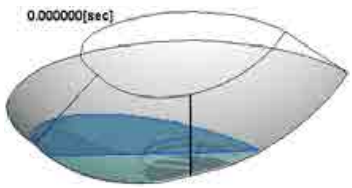
液体ロケットに関係する自由表面流
(1/5) 推進薬タンクでのスロッシング





宇宙輸送機の
姿勢変化と推力変動に伴って
内部加速度は時間的に変化する。

スロッシングは
重心移動に伴う
推力ミスアライメント
を伴うため、
航法誘導上有害
意図せぬ
熱伝達促進を伴うため、
タンク圧制御上有害



(Himeno and Watanabe 2004)

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重力支配の流れ と 界面張力支配の流れ
流体管理

・・・ **着眼点**

宇宙開発利用の進展に伴い、宇宙輸送システムの推進機関や軌道上構造物の熱管理機器など、地上とは異なる加速度環境で液体を利用する場面が増えつつある。

これらの流体機器を構成する液体貯蔵容器や蒸発・凝縮器の内部は、気液両相の共存系となるが、推力や姿勢変動を伴う宇宙機内部の動的加速度環境や、比重差による液体駆動を期待できない軌道上の低重力環境では、液体を望ましい位置に保持し、思い通りに搬送するという、流体管理 (fluid management) が非常に難しくなる。

今後、軌道上で運用される流体機器の信頼性を向上させ、同時に開発コストと運用リスクを低減するためには、その設計・計画段階から作動流体の挙動を適切に予測する技術が求められる。特に、貯蔵容器や流路内部の自由表面流を考える場合、液体の重心移動などの動力学特性に注目するだけでなく、伝熱や相変化までも考慮し、共存する気体との熱交換に起因する熱流動特性を把握することが重要である。

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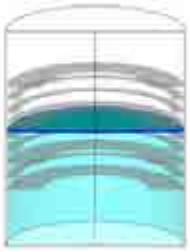
東京大学

JAXA

UT-JAXA Collaboration

液体挙動予測
圧力変化予測
沸騰現象予測



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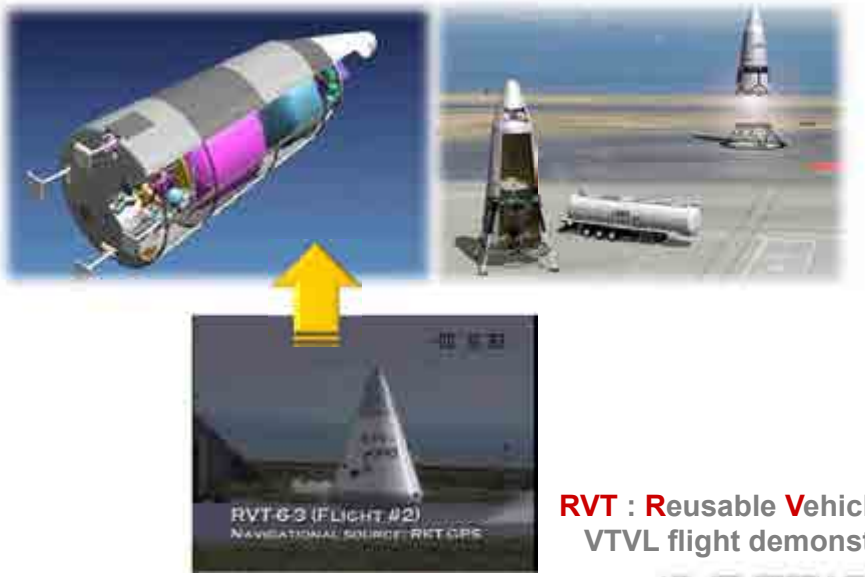
Sloshing Prediction in a Model Tank with Baffles

RSR : Sub-orbital Reusable Sounding Rocket

As the evolutional program of RVT,
JAXA/ISAS worked out
the conceptual design of reusable launch vehicle for sounding missions.



RVT : Reusable Vehicle Testing
VTVL flight demonstrator

Sloshing Prediction in a Model Tank with Baffles

RSR : Sub-orbital Reusable Sounding Rocket

As the evolutional program of RVT,
JAXA/ISAS worked out
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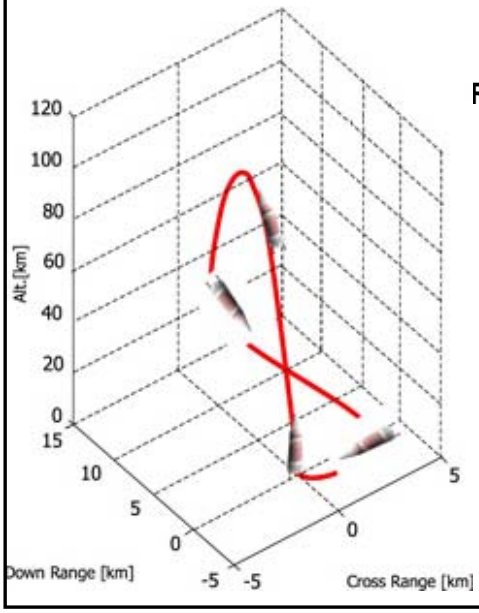

Reusable sub-orbital rocket vehicle was designed
for upper-air observation around 120 km height,

for microgravity experiments
during its weightless flight for 180 sec and

as a test bed to clarify
the actual costs and reliability
of the reusable launch systems.

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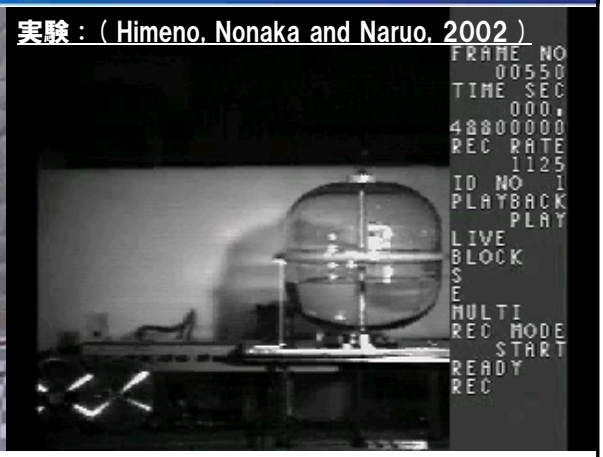
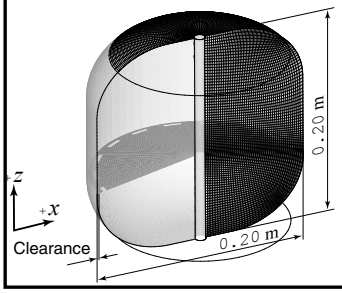
液体推進薬のタンクスロッシング
実験と数値解析によるアプローチ

計算：（ Himeno, 2003 ）

実験：（ Himeno, Nonaka and Naruo, 2002 ）

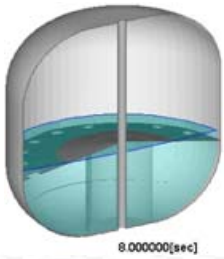




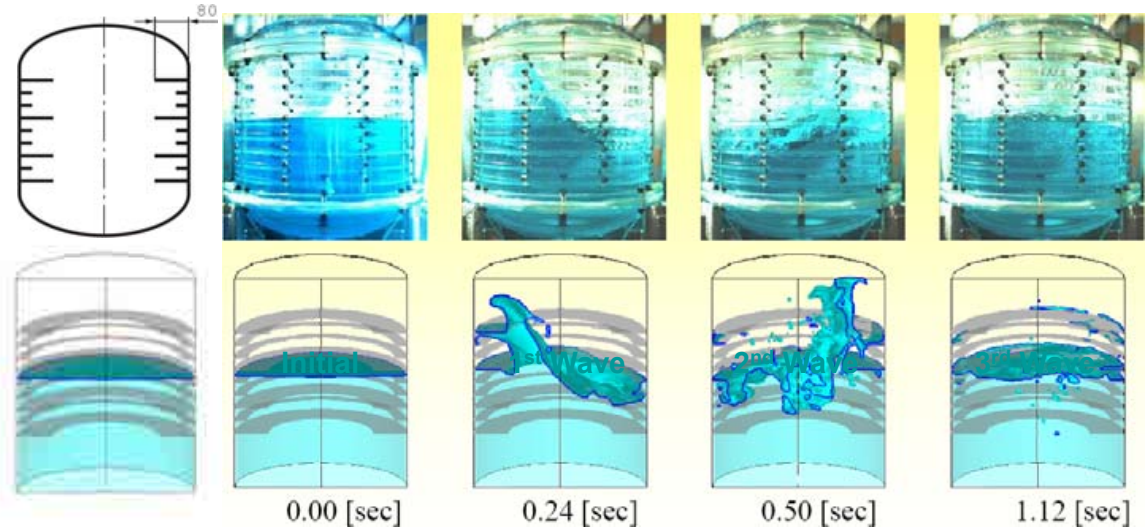
Ref. AIAA 2005-3931 (Himeno)

- 相似流れについて
  実験と計算の相関を確認
- 実機飛行条件を計算で予測

CIP-LSM (東大コード) で計算



液体推進薬のタンクスロッシング
実験と数値解析によるアプローチ



Ref. AIAA 2007-5557 (Himeno & Watanabe)
AIAA Liquid Propulsion Best Paper Award, 2008

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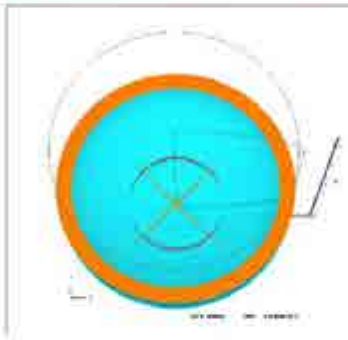
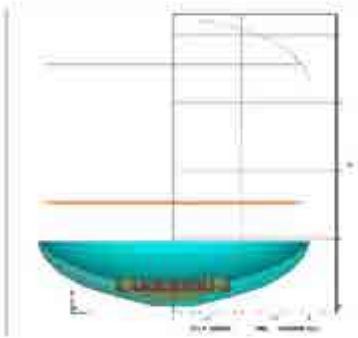
液体推進薬のタンクスロッシング
実機運用事前検討への適用





Sloshing caused by slight disturbance in lateral direction under low-g condition during coasting flight of upper stage.

Numerical code : **CIP-LSM**
Hybrid PLIC-VOF and level-set
developed in University of Tokyo

東大コードをJAXAおよびメーカーに供与
H-IIA上段高度化ミッションの成立性検討・
バッフル配置最適化検討に使用

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CIP-LSM

流体解法 : Thermo CIP-CUP (TCUP)
界面捕獲 : MARS + LSM
相変化 :

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CIP-LSM

流体解法 ： Thermo CIP-CUP (TCUP)

界面捕獲 ： MARS + LSM

相変化 ：

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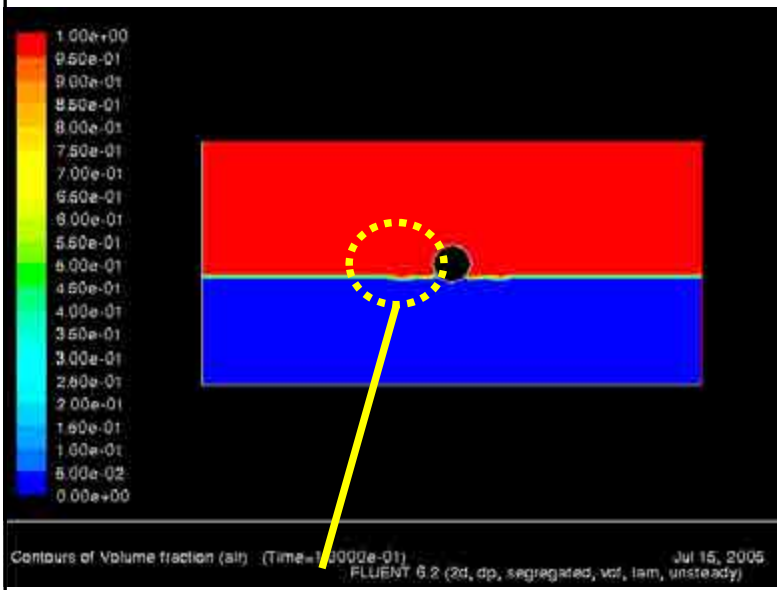
界面捕獲 : Original-VOF

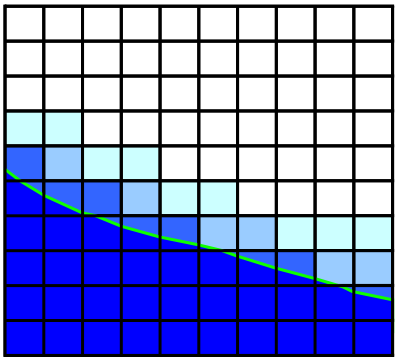
VOF関数の数値的散逸



VOFの数値的散逸

気液の非物理的かつ不可逆な混合

セル内部の
液体の偏在が
考慮されていない。



界面勾配を考慮すべき

→ PLIC-VOF

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界面捕獲：MARS + LSM

(Himeno, 2003)

Distance Function

Distance function ϕ

From the distribution of ϕ

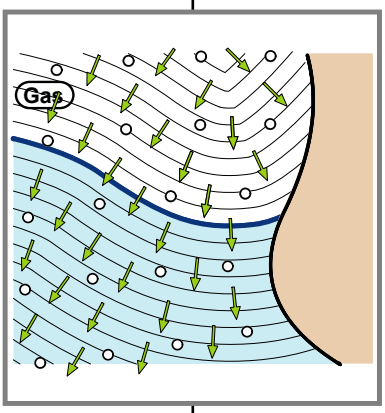
Normal Vector

$$\vec{n}_S = \frac{\nabla\phi}{|\nabla\phi|}$$

Curvature

$$\kappa = \nabla\cdot\vec{n}_S = \nabla\cdot\left(\frac{\nabla\phi}{|\nabla\phi|}\right)$$

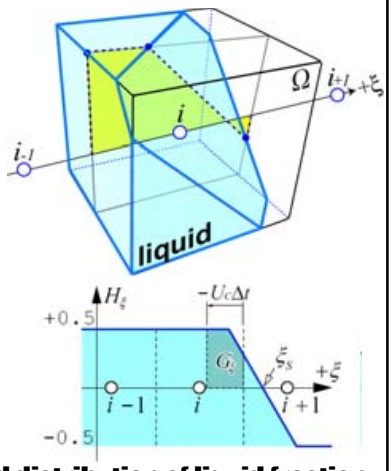
are precisely computed



Surface tension is computed by CSF model

MARS

VOF distribution



Interpolated distribution of liquid fraction

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界面捕獲：MARS + LSM

(Himeno, 2003)

Distance Function

Distance function ϕ
overset
around moving interface

From the distribution of ϕ

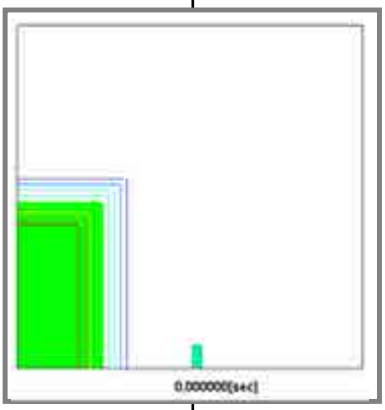
Normal Vector

$$\vec{n}_S = \frac{\nabla\phi}{|\nabla\phi|}$$

Curvature

$$\kappa = \nabla\cdot\vec{n}_S = \nabla\cdot\left(\frac{\nabla\phi}{|\nabla\phi|}\right)$$

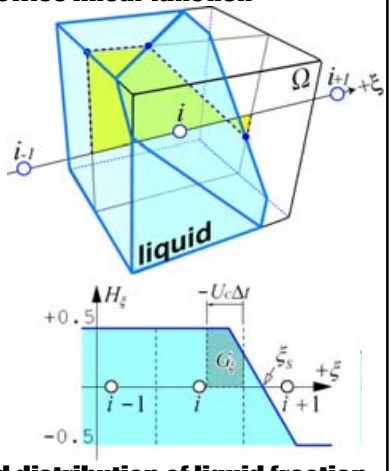
are precisely computed



Surface tension is computed by CSF model

MARS

VOF distribution
re-constructed with
piecewise linear function



Interpolated distribution of liquid fraction

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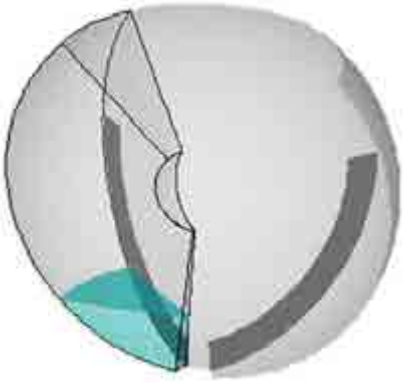
Simulation for Surface Tension Devices

Future Works on Satellite Tanks



数値計算 (姫野)

落下塔実験 (IHI・今井ら)

We are now conducting the simulation
to design surface tension devices for satellite tanks.

東京大学

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液体挙動予測
圧力変化予測
沸騰現象予測

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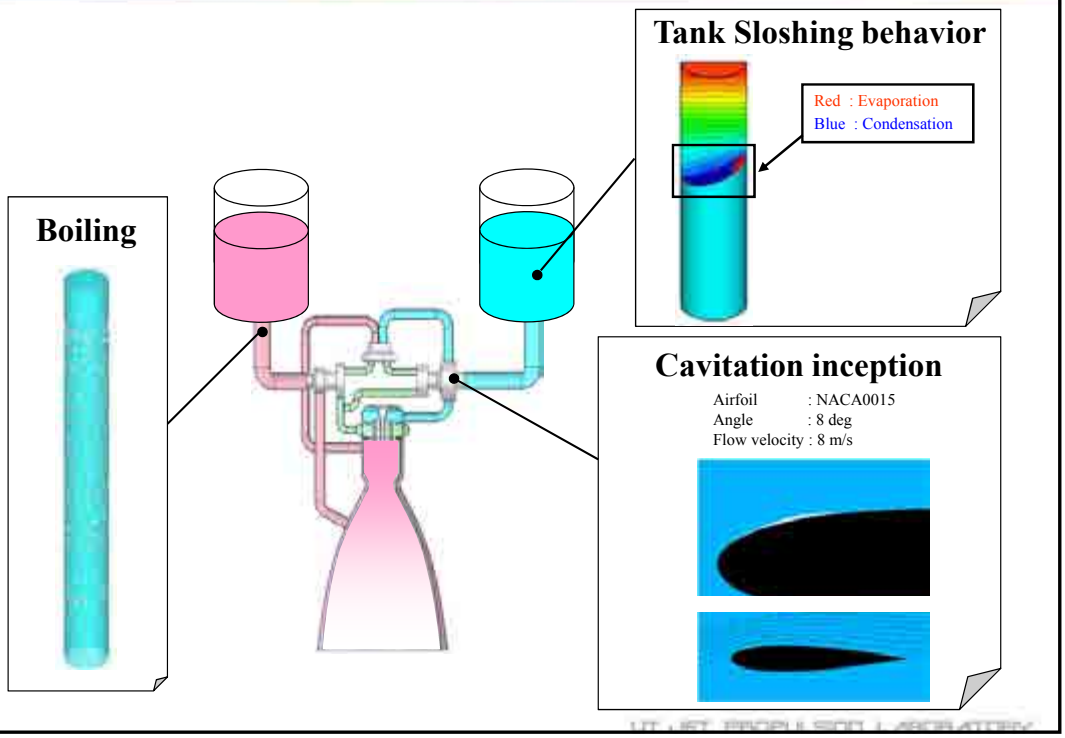
液体ロケットに関係する自由表面流
相変化を伴う熱流体管理・予測



液体ロケットに関係する自由表面流
微小重力・長秒時飛行の実現

ロングコースト、エンジン再々着火を実現するための上段推進系の技術開発

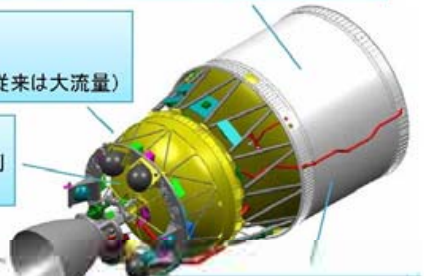
ベント水素ガスによる推薬静定(リテンション)
- ✓従来はヒドラジンガスジェット推力のGによりタンク底部に推薬を静定
- ✓高度化ではロングコースト中、LH2蒸発ガス噴射の推力を活用(ガスジェット推薬の節約)

LOX予冷量の削減
- ✓機外へ投棄する予冷用推薬量の削減
- ✓長時間コースト中の小流量予冷の適用(従来は大流量)

低液位でのエンジン着火
- ✓再々着火時の低液位でのスロッシング抑制(ターボポンプガス吸込みリスクの低減)

エンジン再々着火およびスロットリング
- ✓加圧制御・液温制御

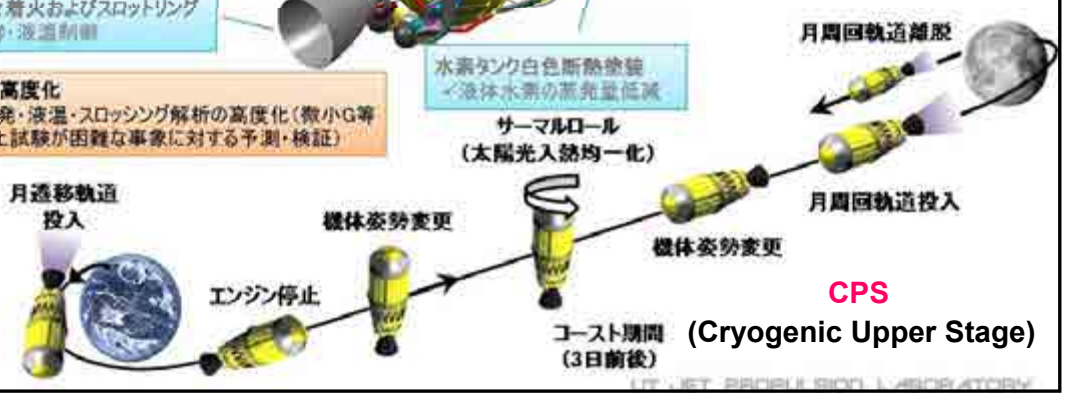
解析技術の高度化
- ✓予冷・蒸発・液温・スロッシング解析の高度化(微小G等により地上試験が困難な事象に対する予測・検証)



水素タンク白色断熱塗装
✓液体水素の蒸発量低減

高度化H-IIA

無効推進薬の最小化
低重力下での液体捕獲
がカギ



CPS
(Cryogenic Upper Stage)

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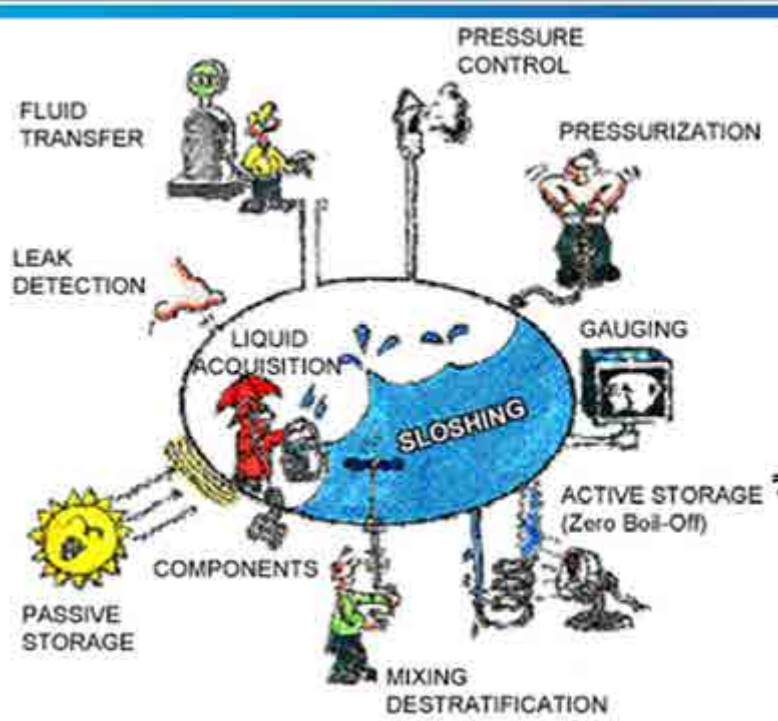
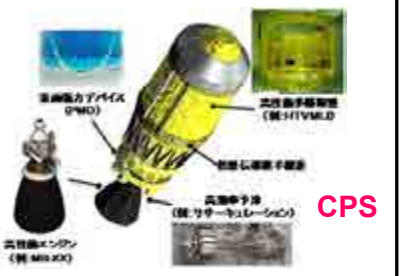
液体ロケットに関係する自由表面流
将来宇宙輸送インフラのための課題



AIAA-2005-1148 (David J. Chato)



Re-fuel on orbit

液体ロケットに関係する自由表面流
将来宇宙輸送インフラのための課題

上段推進系(推薬マネジメント) 技術ロードマップ

宇宙輸送ミッション マイルストン	H-IIA高度化	次期基幹ロケット(H-X) CPS Blk 1	CPS Blk 2
目的地	静止軌道	静止軌道・月周辺	小惑星・火星
ミッション時間	～5時間	～1週間	～1年
蒸発量抑制	白色断熱塗装 タンク熱流体解析(簡易モデル)	MLI断熱(展開機構等開発) タンク熱流体解析(詳細モデル) 軌道上入熱解析	極低温冷凍機 ベントガスシールド
微小G下での液体推薬制御	ベントリテンション プルーム希薄流解析 スロッシング解析	PMD(ベーン/メッシュ) 表面張力支配流解析	推薬コンディショニング
エンジン予冷	トリクル予冷 アイドル予冷 予冷解析(簡易モデル)	ブリード予冷効率化 予冷解析(詳細モデル)	リサーキュレーション
タンク与圧エンジン高機能化	極低温He与圧 エンジンスロットリング	高Ispアイドル燃焼	タップオフ与圧 アイドル/スロットル立上げ

JAXA 杵淵 (2012[宇科連発表予定])

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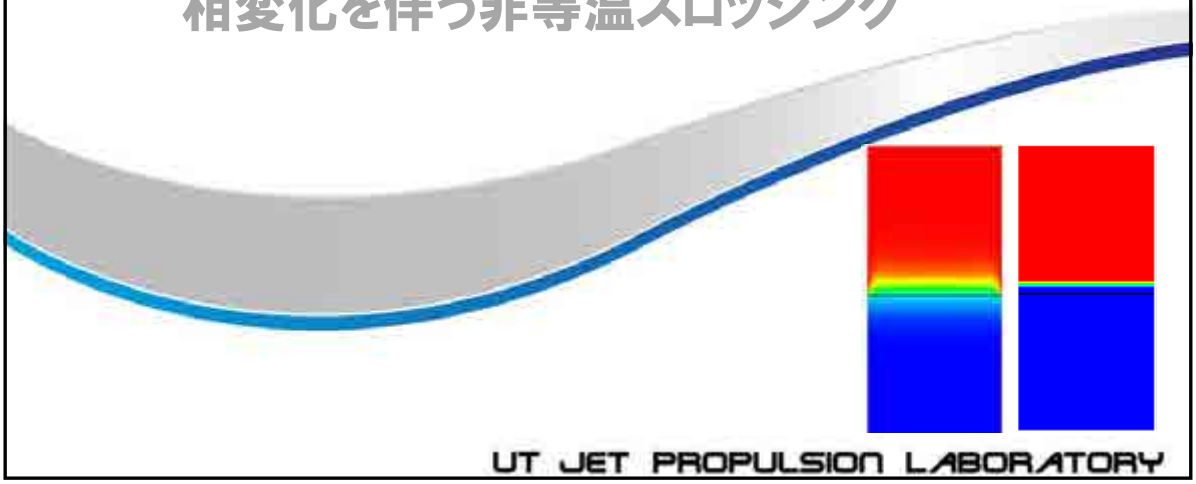
相変化を伴わない非等温スロッシング
相変化を伴う非等温スロッシング



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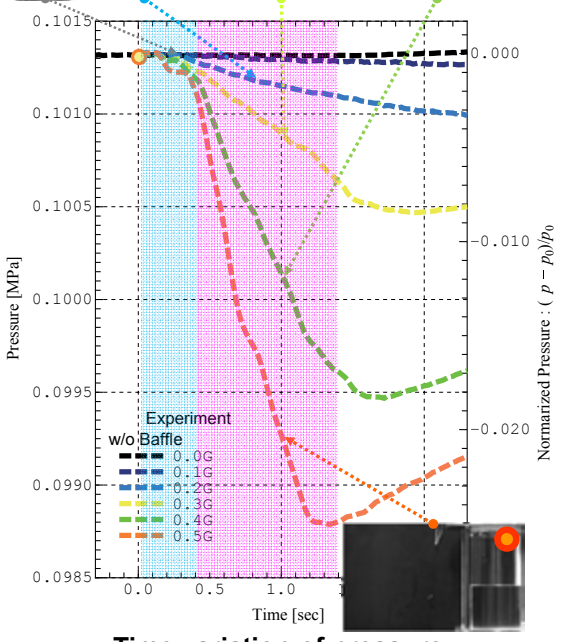
液体推進薬のタンクスロッシング
非等温スロッシングに伴う気液間伝熱促進と圧力変化



Time variation of pressure

模型実験：温度差 ΔT =15 K
供試液体：シリコンオイル(低温)/空気(高温)
相変化なし

Table 2 : Heat transfer from gaseous phase

Test ID	a	ΔP_{01}	ΔQ_{01}
Case 0	0.00 G	+/−	+/−
Case 1	0.10 G	-32 Pa	0.09 J
Case 2	0.20 G	-173 Pa	0.49 J
Case 3	0.30 G	-429 Pa	1.22 J
Case 4	0.40 G	-1185 Pa	3.38 J
Case 5	0.50 G	-2054 Pa	5.85 J

静定させた場合と比べ、
スロッシングを伴う場合、桁違いのΔp

砕波と飛沫の発生は、
更に伝熱を促進し大きな Δp を与える

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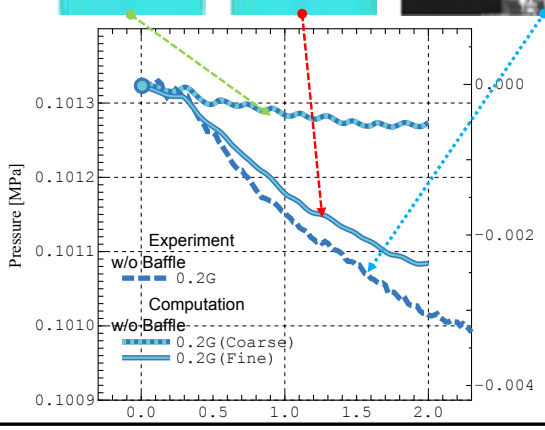
液体推進薬のタンクスロッシング
非等温スロッシングに伴う気液間伝熱促進と圧力変化



砕波を伴わない場合は、
ある程度 細かな格子 を用いると、
圧力変化 Δp を良く再現できる。

(液体の動きだけなら粗い格子でもOK)

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相変化を伴わない非等温スロッシング
相変化を伴う非等温スロッシング

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液体推進薬のタンクスロッシング
極低温スロッシングに伴う気液間相変化促進と圧力変化

LN_2 および LH_2 を用いた実験を実施
@ 能代多目的実験場(2011)

クライオスタットをローラースライダに載せ、
電動加振機で揺さぶる

液体推進薬のタンクスロッシング
極低温スロッシングに伴う気液間相変化促進と圧力変化

異種加圧 (LN_2/GHe)

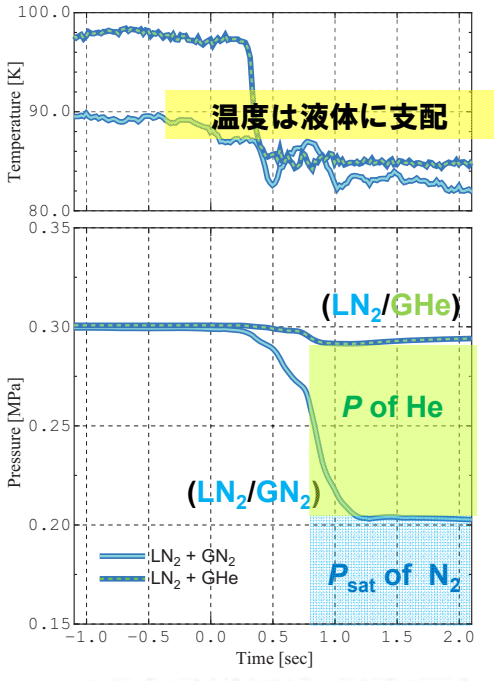
見た目は
シリコンオイルの場合
(不揮発性=相変化なし)
と変わらない

同種加圧 (LN_2/GN_2)

霧の発生 !!

同時に、タンク圧が
0.7 秒間に 0.1 MPa 急降下

温度は10%低下なのに
圧力は30%以上低下
凝縮が発生した



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CIP-LSM

流体解法 ： Thermo CIP-CUP (TCUP)
界面捕獲 ： MARS + LSM
相変化 ：

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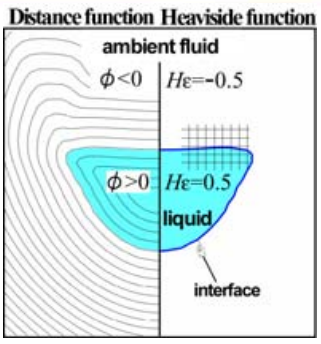
相変化：CIP-LSM の特長
：高精度な界面捕獲の発展性：相変化モデルとの親和性

CIP-LSM (CIP based Level Set method and MARS)

MARS(PLIC-VOF)で移流

level-set 関数を用い
液体の形状を把握

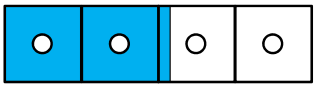
VOFを基に
level-set 関数を再生成

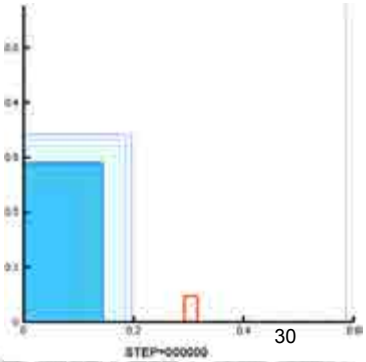


利点
- 移流時の液体の体積保存性が良い
  ⇒ 相変化による界面移動か
  数値的な散逸なのか差別化する上で重要

- 界面に数値的（人工的）な厚みがない
  ⇒ 物性値や密度の不連続をシャープに取り扱える

※ １つ分のセル間で気液が切り替わる





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相変化：支配方程式の記述 → 潜熱項の離散化モデル
：高精度な界面捕獲の発展性

潜熱項

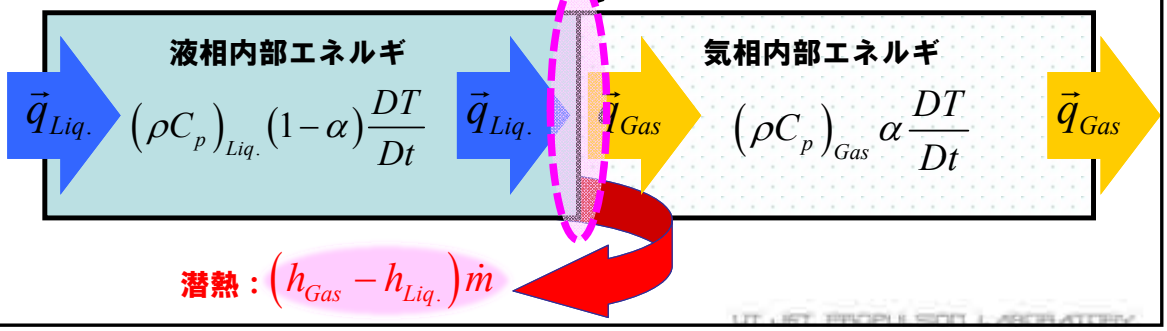
界面でのみ $\delta_S = 1$ となる

・エネルギ式 (顕熱の式)

$$\rho C_p \frac{DT}{Dt} = -\nabla \cdot \vec{q} + \dot{Q} - \left(h_{Gas} - h_{Liq.}\right)\dot{m}\delta_S$$

界面を挟んで成立する
顕熱と潜熱のジャンプ条件

$$\vec{q}_{Gas} - \vec{q}_{Liq} = \dot{m}\left(h_{Gas} - h_{Liq.}\right)\vec{n}$$



潜熱：$\left(h_{Gas} - h_{Liq.}\right)\dot{m}$

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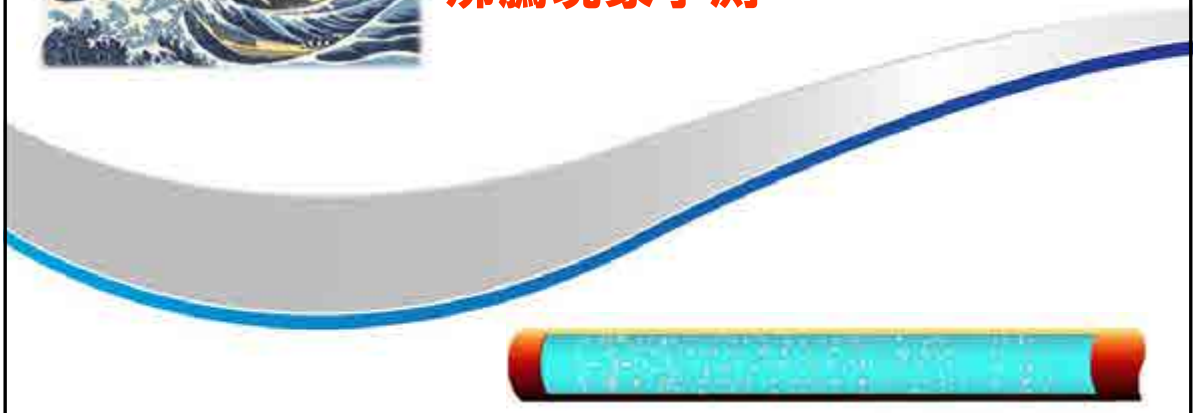
液体挙動予測
圧力変化予測
沸騰現象予測



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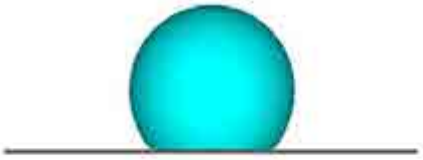
液体推進薬の配管内対流沸騰熱伝達予測へ向けて
相変化モデルの構築と自由表面流直接解析

検証 ：沸騰離脱気泡 (CIP-LSM+相変化+界面張力+多次元+重力) 梅村 (2012)

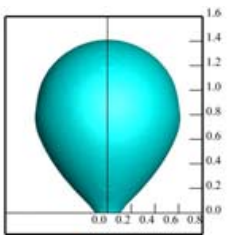


梅村・姫野 (2011)

Bubble Shape Prior to Departure

Exp.(Vijay K. Dhir : 2001)

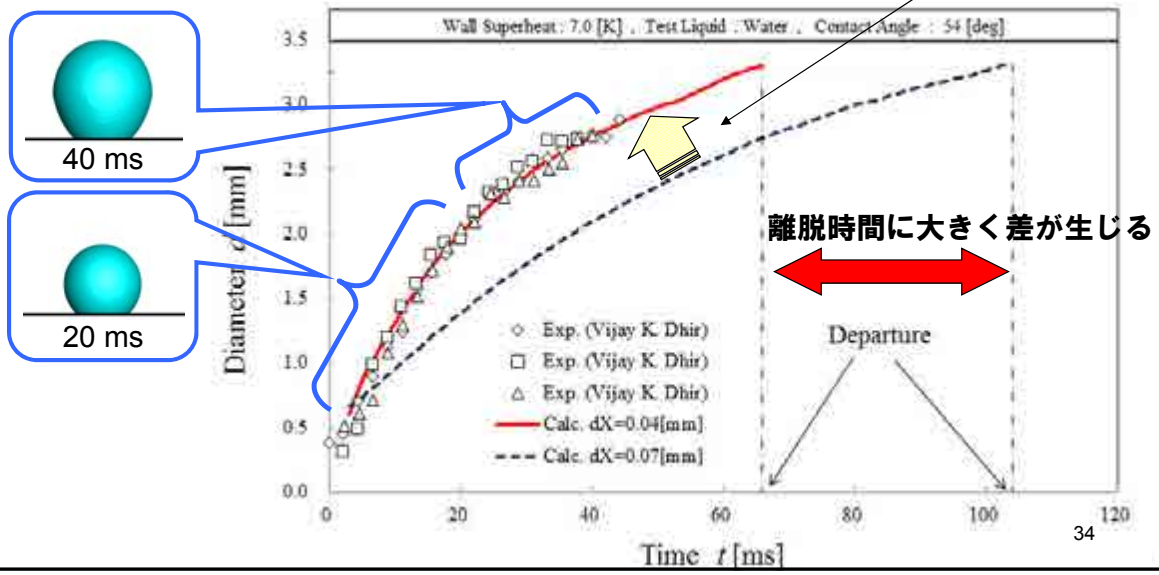
Calc.



液体推進薬の配管内対流沸騰熱伝達予測へ向けて
相変化モデルの構築と自由表面流直接解析

検証 ：沸騰離脱気泡 (CIP-LSM+相変化+界面張力+多次元+重力) 梅村 (2012)

ステファン問題と同様に格子の幅を小さくするに従い実験結果に漸近する
浮力によって気泡が上昇を開始すると成長速度が遅くなる



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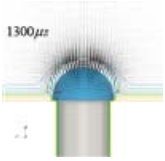
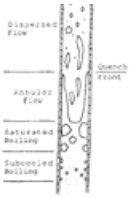
液体推進薬の配管内沸騰熱伝達
沸騰気泡成長モデルの構築による大スケール解析

沸騰現象解明を目的とした解析



解析対象のスケール ： 数μm～数mm

トリクル予冷を考える際に必要な解析



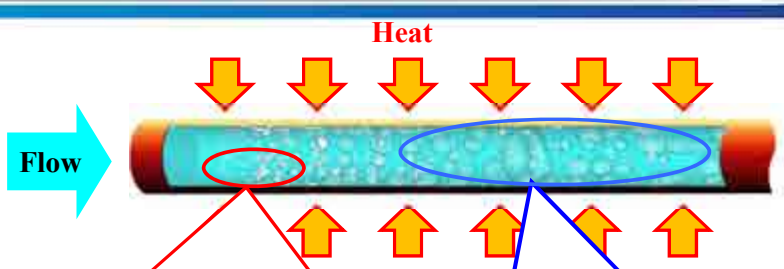
蒸発や表面張力が支配的であり
泡が合体しながら流れていく様子

解析対象のスケール ： 数cm～数m

計算領域が数cmオーダーの沸騰流解析に適する相変化モデル構築が必要

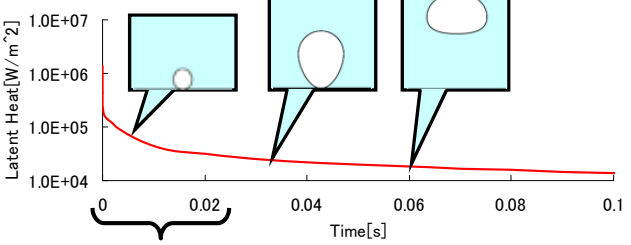
微小重力環境における少質量流量での沸騰流解析手法の構築を目指す

液体推進薬の配管内沸騰熱伝達
沸騰気泡成長モデルの構築による大スケール解析



単位面積当たりの蒸発量

多 ← → 少



高格子解像度が必要

泡の動き・合体調査のため
計算領域を広く取りたい

壁面上の気泡生成・
気泡成長をモデル化
することで計算負荷を
軽減させる！！

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液体推進薬の配管内沸騰熱伝達
沸騰気泡成長モデルの構築による大スケール解析

流体　　水
最小格子幅　0.4 mm

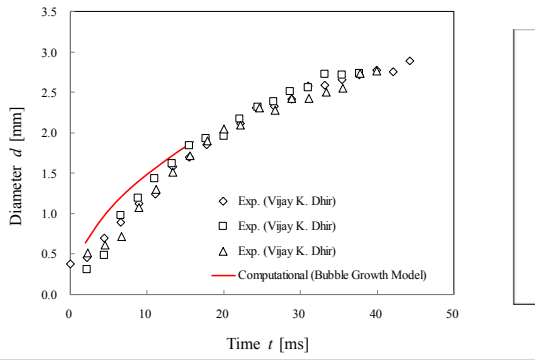
キャビティサイズ　0.03 mm
接触角　54.0 deg
壁面過熱度　7.0 ℃

格子幅10倍

実験と良い一致を見せた
気泡離脱の解析

最小格子幅
0.04 mm

気泡発生・成長モデル



CIP-LSM
+
気泡発生・成長モデル

UT JET PROPULSION LABORATORY

東京大学

まとめ

UT JET PROPULSION LABORATORY

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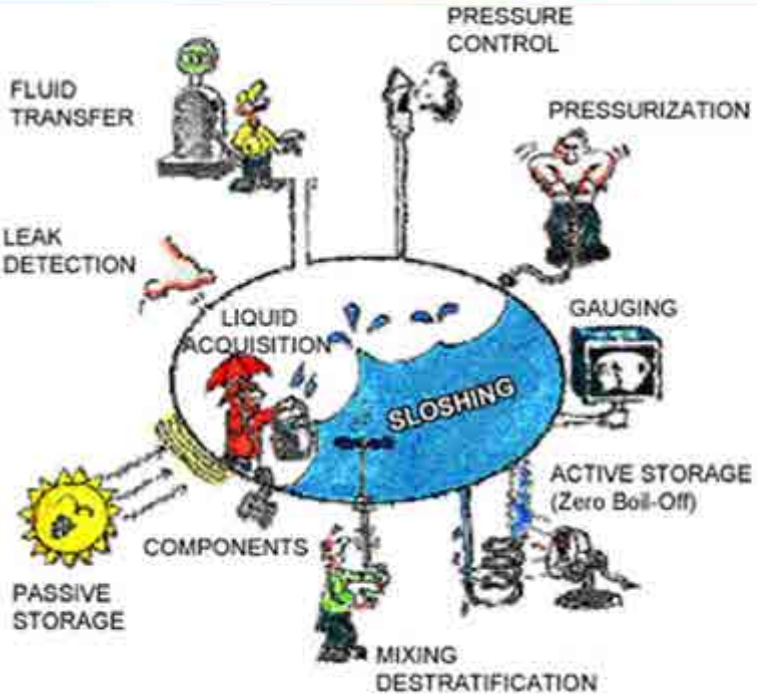
液体ロケットに関係する自由表面流 将来宇宙輸送インフラのための課題



AIAA-2005-1148 (David J. Chato)

RLV

Re-fuel on orbit

まとめ

界面追跡にMARSを採用し、形状捕捉にLSMを援用した自由表面流解析手法として、界面厚みを排除したCIP-LSMを提案した。

界面を挟む熱流束のジャンプ条件を基づきスタッガード位置に集中した相変化モデルを考案した。

三次元物体適合格子を用いて、様々な加速度環境に置かれた自由表面流を、相変化と表面張力を考慮して模擬できる可能性を示した。

微粒化など格子スケールと同等の現象を適切に模擬できるか、さらに微小スケールの現象をどのようにモデル化できるかが今後の課題。

ベンチマークとしての実験データはますます重要。
過去の開発で蓄積された試験のトレース = 温故知新、
クライテリア理解の深化と再構築 = 世代間継承
が重要。次期社会連携講座での活動。

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JAXA社会連携講座シンポジウム(9/26, 9/27)@東京大学 武田ホール

IHI

二液スラスタに関する基礎試験および数値解析

株式会社 IHI
熱流体研究部 高和*, 松野

東京大学
井上助教, 姫野准教授, 渡辺教授

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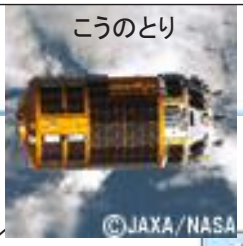
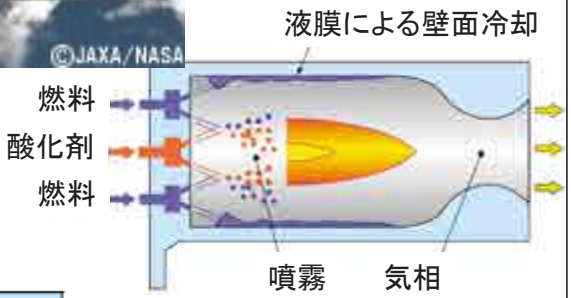
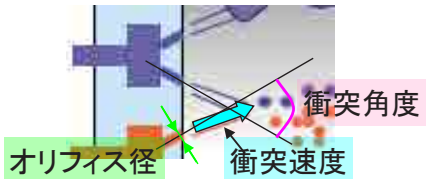
研究ビジョン

IHI

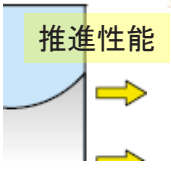
- 対象製品
  - 人工衛星・宇宙探査機の姿勢制御用スラスタ／ロケットエンジン燃料噴射ノズル
  - IHIエアロスペースで開発中のHTV用スラスタ
- 研究背景
  - 設計パラメータと推進性能との現象論的関係性が完全には解明されていない







関係性: ？



  - 計測が困難
    - 噴霧が高密度
    - 燃料(ヒドラジン)が毒性，NTOとの組み合わせで　自発着火

数値解析的なアプローチであれば計測の困難さを解消⇒現象解明が可能

ビジョン

人工衛星・宇宙探査機の姿勢制御用スラスタ／ロケットエンジンの燃料噴射ノズルの解析評価手法の開発

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研究ロードマップ

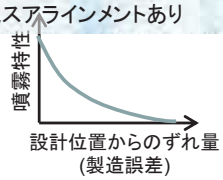
IHI

H26年度IAに技術移管！

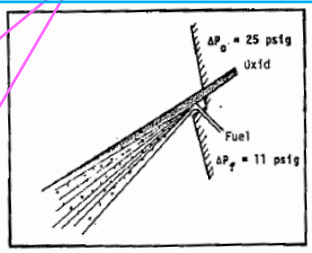
出資元	H23年度 上期	H23年度 下期	H24年度 上期	H24年度 下期	H25年度 上期	H25年度 下期	H26年度 上期	H26年度 下期
	CIP-LSM法の社内への導入		各現象の試験による再現(データ取得)		LNGエンジンへの適用検討・性能評価		燃焼まで解析!	
		検証解析（同種衝突、IHIﾃﾞｰﾀ）			検証試験（異種ﾍﾟﾈﾄﾚｰｼｮﾝ）			
			検証試験（同種ﾍﾟﾈﾄﾚｰｼｮ	検証試験（ﾐｽｱﾗｲﾒﾝﾄ）				
			スラスタ性能の簡易予測手法確立		微粒化状態からスラスタ性能評価手法確立			
基盤研			2相3種流解析のためのソルバ改修				キャビテーションなどの影響評価	
			並列化対応		異種液体衝突解析対応のソルバ			
					気相乱流考慮	液相蒸発考慮	化学反応考慮	

H24

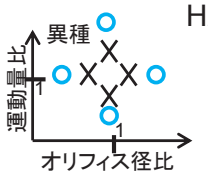
ミスアラインメント時の噴霧特性の定性的評価・傾向知見の獲得

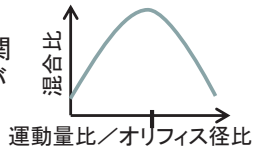


H25



運動量比とオリフィス径比の関係でペネトレーションの発生が判断できる，また液体の混合比を判断できるなど





アウトプットイメージ

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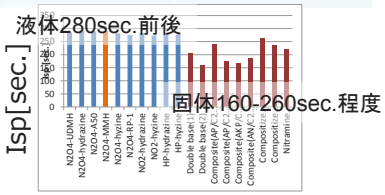
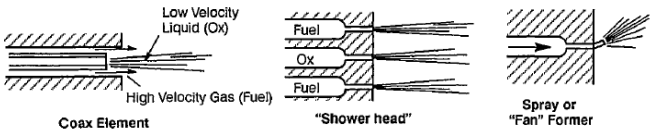
背景

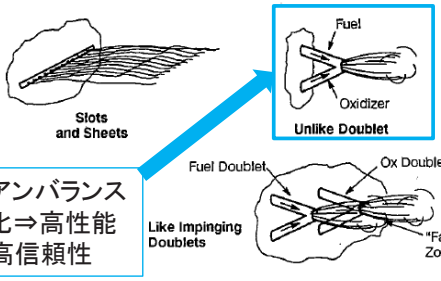
IHI

- 推進器: 人工衛星の軌道変更・姿勢制御
- 液体推進器: 自己着火性を用いた二液式が安定かつ高性能
- 噴射器タイプ(Impinging type)
  - 適切な混合比，急速な微粒化，速やかかつ安定的な燃焼

	長所	短所
液体	点火系が必要なし 推力調整が容易	構造が複雑 取り扱いが困難
固体	構造が簡単 取り扱いが容易	点火系が必要 推力調整が困難







○比較的噴射条件をそろえられる
○良い混合
×微細な孔の数が多くなる
×酸化剤リッチになり易い
×安定性に問題

×噴射条件アンバランス
○良い微粒化⇒高性能
○安定的⇒高信頼性

D. K. Huzel, D. H. Huang, Modern Engineering for Design of Liquid-Propellant Rocket Engines, Progress in Astronautics and Aeronautics, Vol. 147

二液式Unlike Doubletタイプに焦点を当てる

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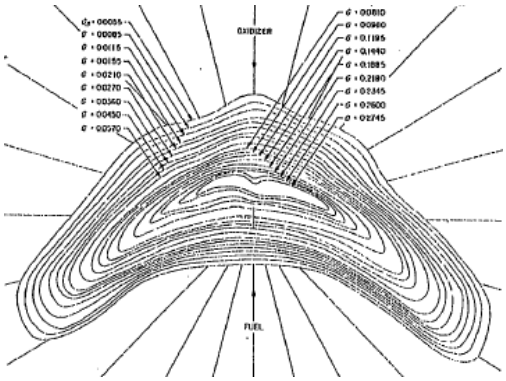
過去の研究①

J. H. Rupe, An Experimental Correlation of the Nonreactive Properties of Injection Schemes and Combustion Effects in a Liquid-Propellant Rocket Engine Part I. The Application of Nonreactive Spray Properties to Rocket Motor Injector Design, NASA Technical Report, No. 32-255

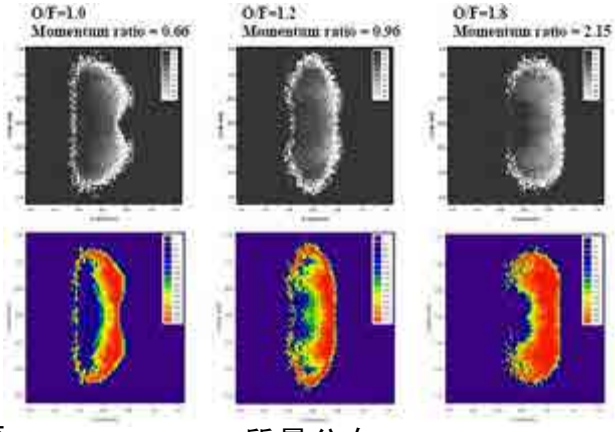
- いくつかの噴射器形状・噴射条件で非燃焼異種衝突試験
- 下流位置での質量Flux分布
- スラスタ設計の指針を構築
- 可視化はないため，現象として不明な点がある



Fuel: 径2.5mm, 41.6m/s
Oxi.: 径4.5mm, 26.2m/s　44°，15.2cm下流

T. Yuan, C. Chen, B. Huang, A PLIF Observation of the Impingements of NTO/MMH Simulants for a 5-lbf Rocket

- 非燃焼，異種，同径(0.3mm)，運動量比(1.0～2.2)，衝突角60°
- PLIF法を用いた質量分布および混合比
- 高混合比を実現する条件などを明らかにしている
- 同径かつ液相の可視化はなし



質量分布

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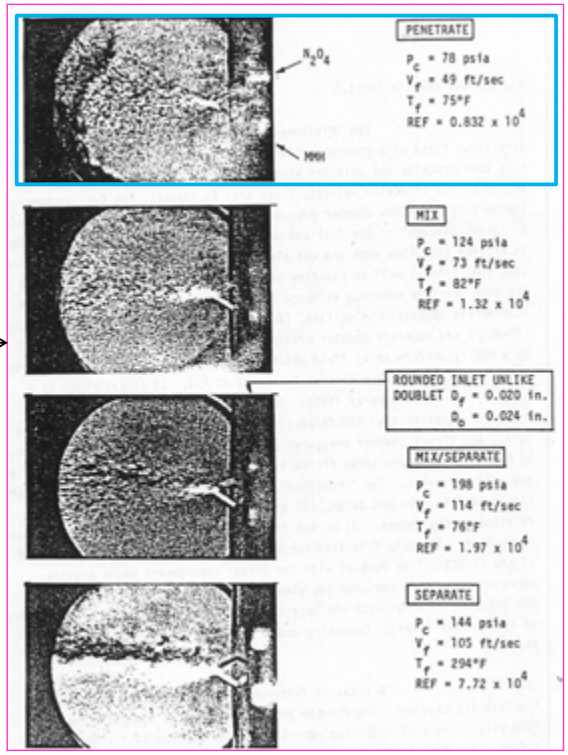
過去の研究②

B. R. Lowver, High Performance N2O4/AMINE Elements “BLOWAPART”, NASA CR-160273

項目	単位	値，種類
液体		N2O4/MMH，N2O4/A-50，N2O4/N2H4
チャンバ圧力	kPa	400 – 7,000
燃料温度	℃	12.7 – 148.9
燃料噴射速度	m/s	9.1 – 61.0
衝突角度2θ	℃	32，60，90

- 非燃焼
- 可視化
- 衝突条件により変化する衝突後の二液の状態を4種類に種別化
- その一つにペネトレーション現象を確認
- 以降においてペネトレーション現象について調査された例は少ない



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目的

- 噴流衝突実験において径比および運動量比を大きく変化させ微粒化現象の変化を調査する
  - ペネトレーション現象を含めた包括的な条件
- 実験と対応する条件下の数値解析を実施し解析的再現性を評価する
  - 自由界面法(CIP-LSM法)を用いた解析

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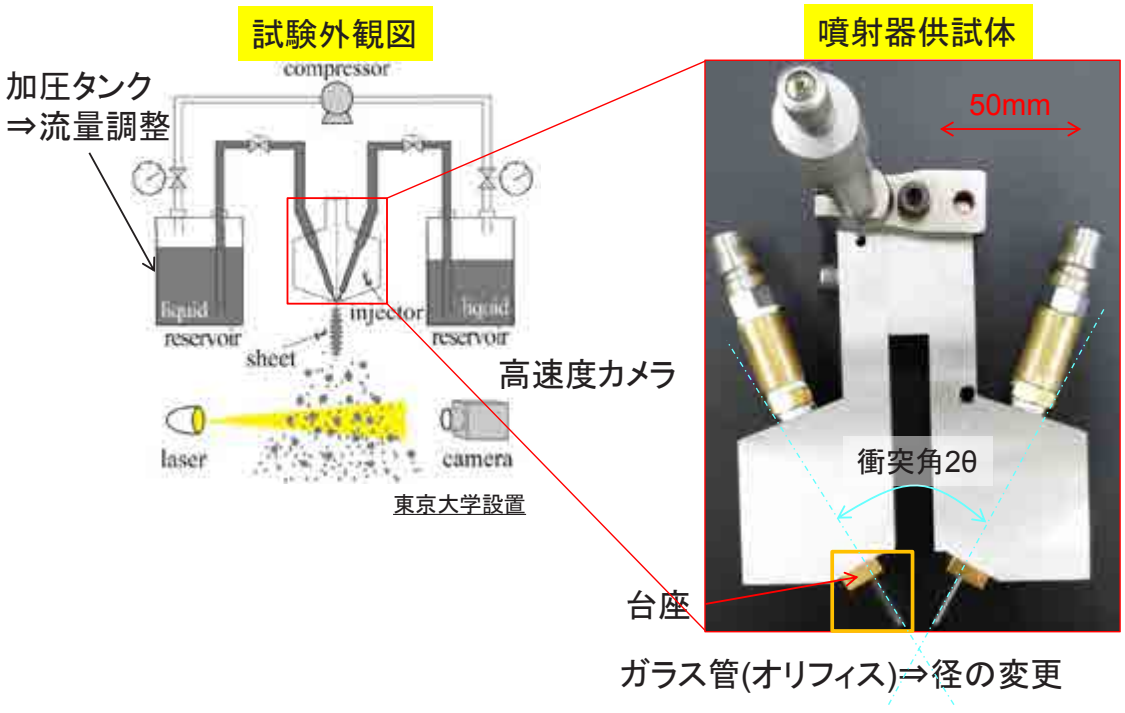
噴流衝突試験方法



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計測項目

IHI

	項目	計測技術		目的	本発表
定性的	可視化	ハイスピードカメラ	Photron FASTCAM APX-RS	衝突点近傍および微粒化の様子を撮影する	○
	断面液相通過領域可視化	レーザー	DANTEC DYNAMICS DualPower 135-15	下流方向断面における水が通過した領域の可視化	×
	混合状態	蛍光剤の使用	Rhodamine B	2液の混合状態を把握する	×
	質量Flux	パタネータ法	自作	下流方向任意の面で通過する質量Flux分布を計測	×
定量的	粒径・速度	画像処理		微粒化効率にどのような影響があるか調査する	×

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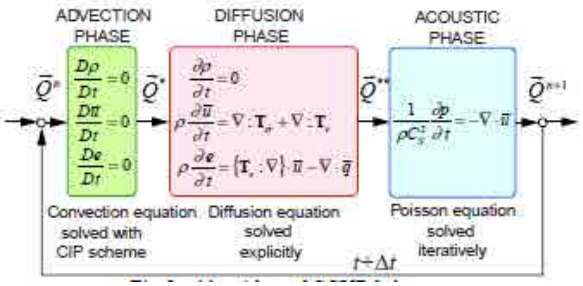
衝突微粒化解析方法

IHI

姫野 武洋, 根岸 秀世, 野中 聡, 井上 智博, 渡辺 紀徳, 鵜沢 聖治,「様々な加速度環境における自由表面流の数値解析(CIP法, MARS法, Level-set法を協調した解法の改良, 日本機械学会論文集B編, Vol. 76, No. 765, pp. 778-788, 2010

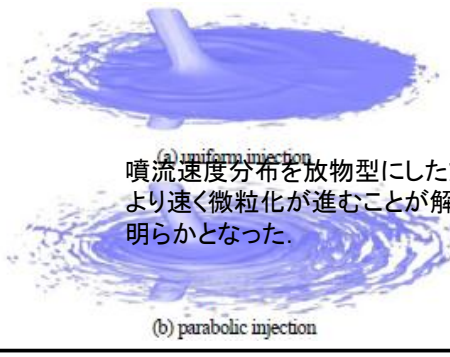
- CIP-LSM法(姫野ら)
  - 移流項: CIP法
  - 界面追跡法: Level-set法 + MARS法
  - 表面張力計算法: CSF法



- 過去の解析例
  - 噴流の速度分布の違いによる衝突後の微粒化傾向の変化をCIP-LSM法により調査(井上ら)
- 衝突微粒化の適用性はあるが, 今回は径比や運動量比の幅広い条件での適用性を検証

スラスタ設計における非設計点への対応力

井上 智博, 渡辺 紀徳, 姫野 武洋,「燃料噴射弁近傍における液膜挙動と微粒化特性の数値解析」, 第23回数値流体力学シンポジウム, 2009



噴流速度分布を放物型にした方がより速く微粒化が進むことが解析的に明らかとなった.

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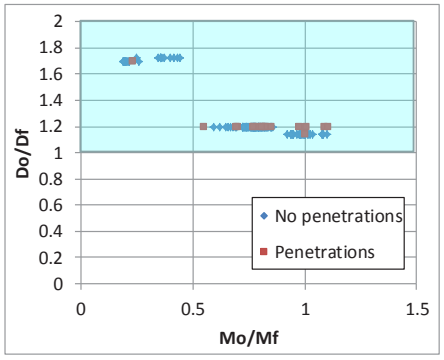
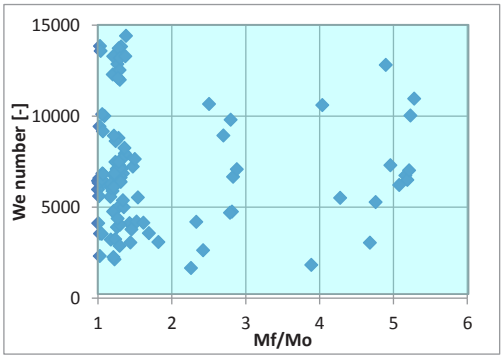
噴射条件

NASAデータの試験条件





運動量比=(相手噴流の運動量)／(基準噴流の運動量)

本研究の試験条件

径	運動量	衝突角度	We数	Re数
1mm	0.009 ～ 0.07 [kg/s m/s]	40°	200 ～ 13,000	6,000 ～ 45,000
1.2mm		50°		
1.6mm		60°		
2.0mm				

本発表における条件

- 比の大きい領域を実施した
- 今後他の条件においても実施する

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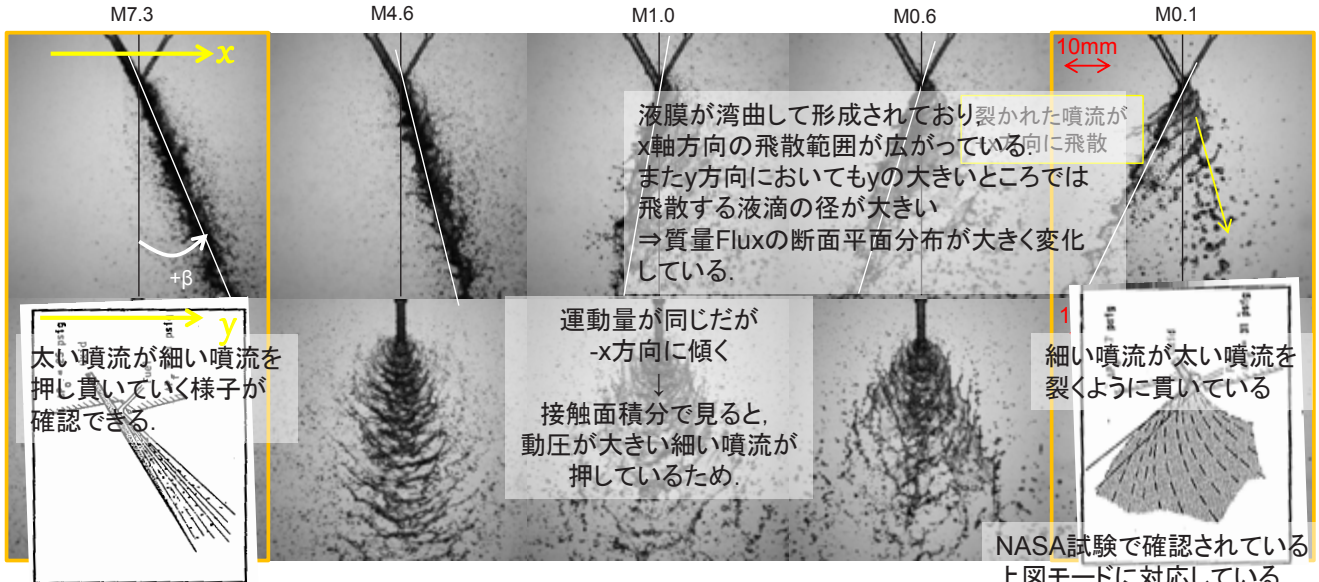
可視化結果(1mm径規準, 径比2.0)

太い噴流の運動量が高い ⟷ 細い噴流の運動量が高い



$$\tan\beta = \frac{\dot{w}_1 v_1 \sin\theta_1 - \dot{w}_2 v_2 \sin\theta_2}{\dot{w}_1 v_1 \cos\theta_1 + \dot{w}_2 v_2 \cos\theta_2}$$

		基準	#1	#2	#3	#4	#5	#6
運動量比	–		7.33	4.55	1.37	0.97	0.58	0.12
流速	m/s	17.6	22.3	17.6	9.66	8.12	6.26	2.87
We数	–	3674	13457	8364	2520	1783	1058	223
衝突後角度β	°		18.9	13.6	−5.1	−10.4	−17.0	−26.9

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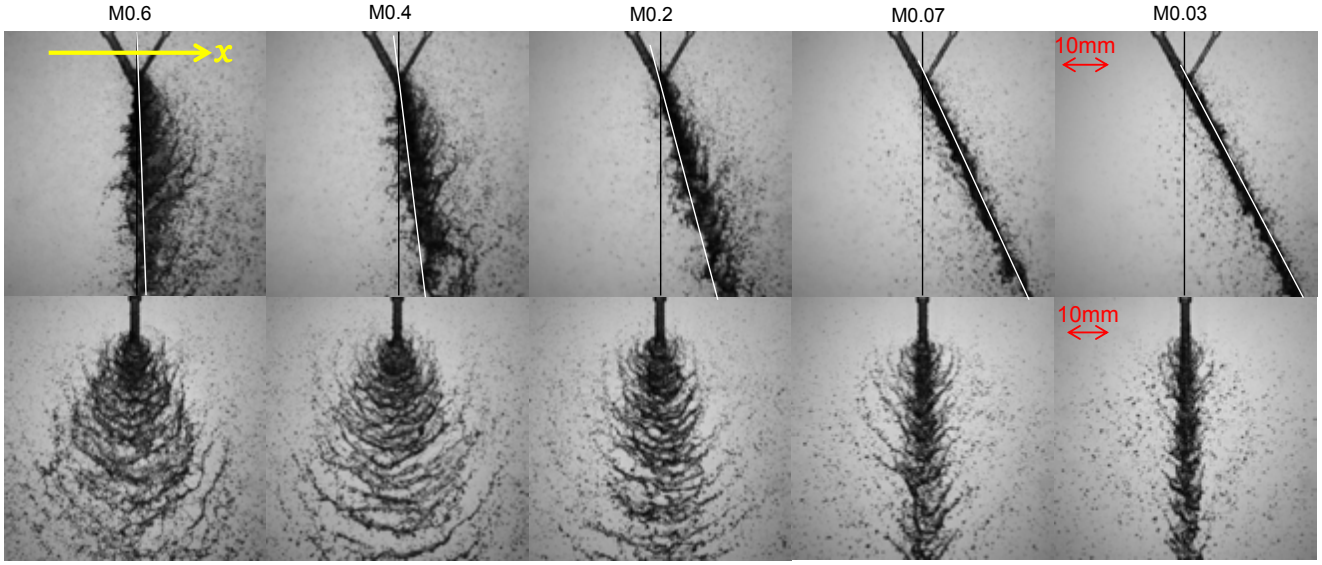
可視化結果(2mm径規準，径比0.5)

IHI

細い噴流の運動量が高い ←――――――――――→ 太い噴流の運動量が高い



太い噴流が運動量で勝っているため
+x方向に傾き，大きくなるにつれて
正面(下段)での液膜の形成が
小さくなる.

		基準	#1	#2	#3	#4	#5	
径	mm	2	0.5（径比2:1）					
運動量比	–		0.57	0.4	0.23	0.07	0.03	
流速	m/s	17.6	26.5	22.4	16.9	9.1	5.89	
We数	–	8364	9478	6771	3871	1121	469	
衝突後角度β	°		1.2	6.6	14.6	24.9	27.8	

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解析結果(1mm径規準, 径比2.0)

()内数字は運動量比

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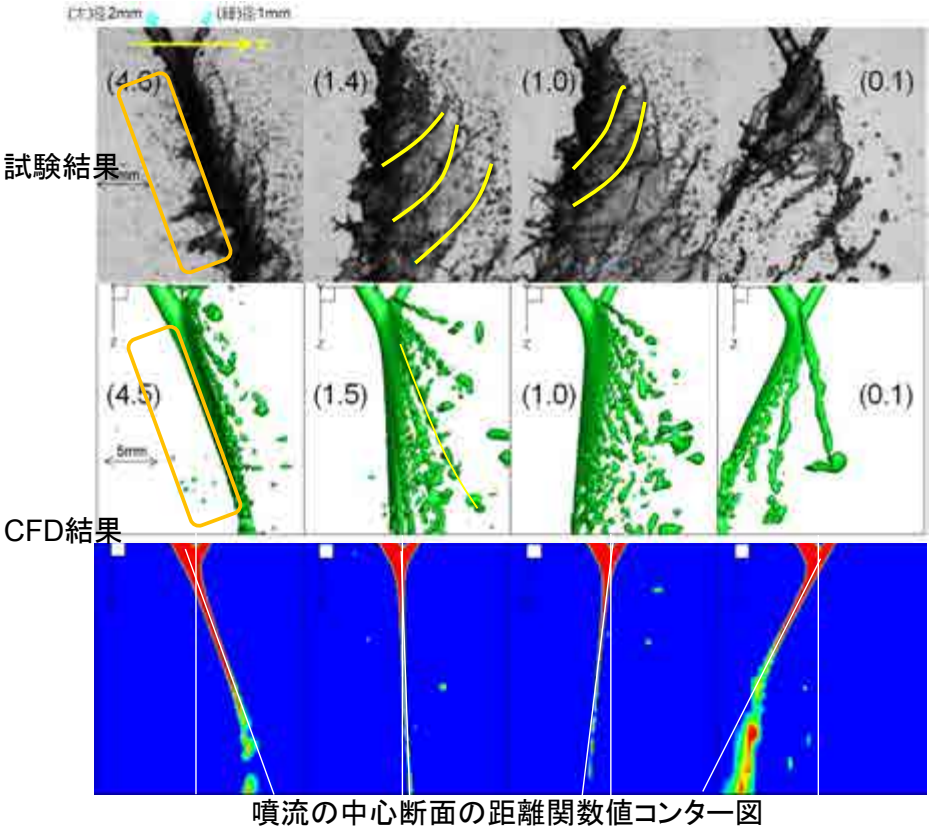

噴流の中心断面の距離関数値コンター図

- 衝突後の傾きなどの傾向は再現できていると考えられる.
- しわの方向や液滴の飛散状況がやや異なる

⇒メッシュ粗密の適性がないためと考えられる

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メッシュ依存性(1mm径規準, 径比2.0, 運動量比4.5)

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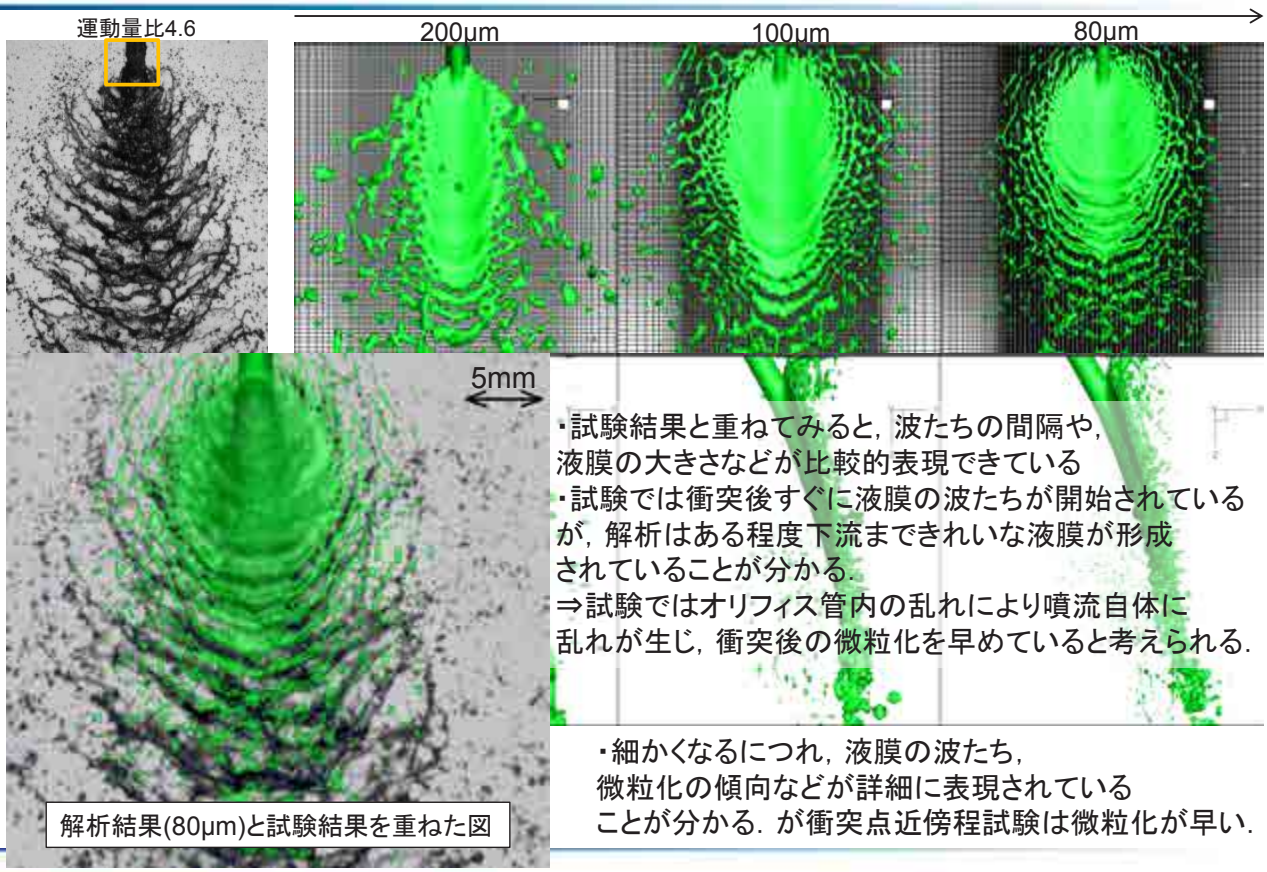

解析結果(80μm)と試験結果を重ねた図

・試験結果と重ねてみると，波たちの間隔や，液膜の大きさなどが比較的表現できている
・試験では衝突後すぐに液膜の波たちが開始されているが，解析はある程度下流まできれいな液膜が形成されていることが分かる．
⇒試験ではオリフィス管内の乱れにより噴流自体に乱れが生じ，衝突後の微粒化を早めていると考えられる．

・細かくなるにつれ，液膜の波たち，微粒化の傾向などが詳細に表現されていることが分かる．が衝突点近傍程試験は微粒化が早い．

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メッシュ依存性(1mm径規準, 径比2.0, 運動量比1.5)

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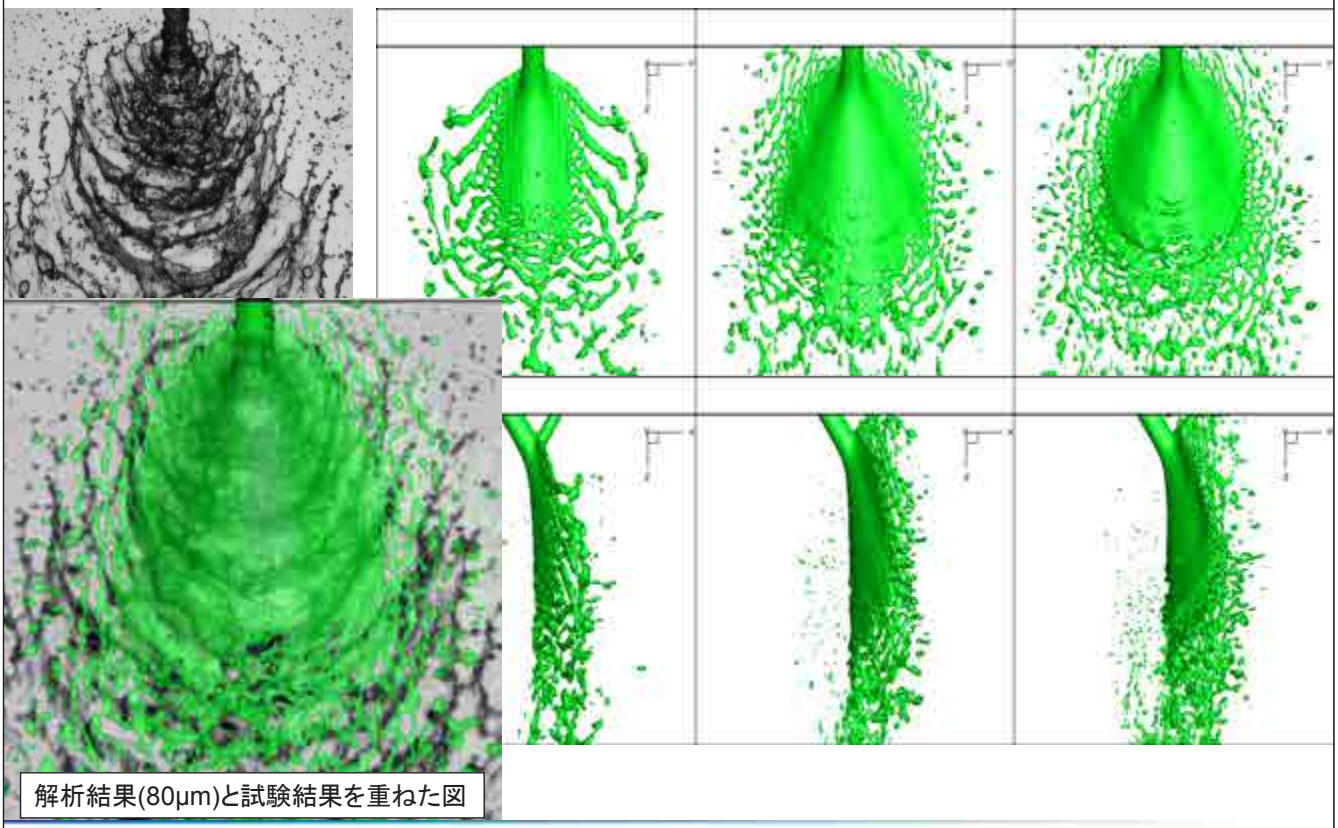

解析結果(80μm)と試験結果を重ねた図

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解析結果と試験結果の比較(1mm径規準, 径比2.0, 運動量比1.5)

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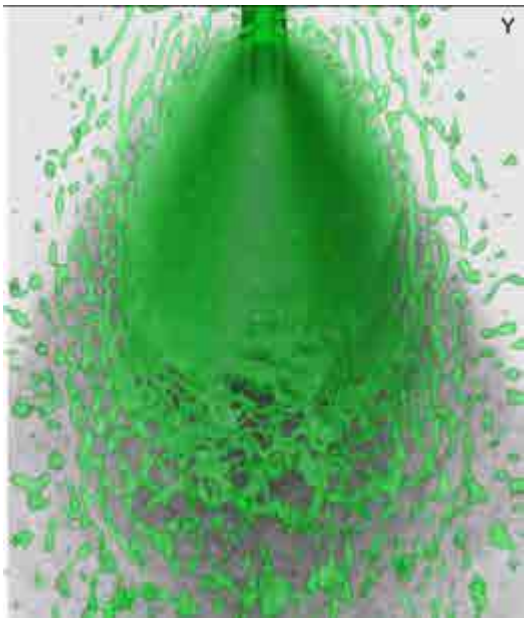
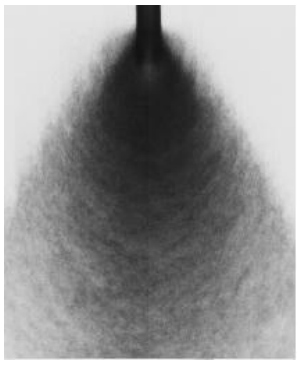
- 連続撮影画像を平均化した画像と解析結果を比較
  - 数値解析は噴流に乱れがなく，定常的な液膜の形成のため，瞬時結果で比較する





液膜の縁が概ね
解析の液膜部分を捕えている
と考えられる.

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まとめ

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- 径比2で運動量を広く変化させる二液噴流衝突実験を実施し，以下のような結果を得た
  - 太い噴流の運動量と細い噴流の運動量のぶつかり合いで最終的な角度が決まる
    - 径比による接触面積の違いのため，接触部分の動圧の大きさによって角度は決まる
    - 概ね理論式で算出できる角度となることが分かった
  - 運動量を振っていく中で，液膜の形成に起因して液滴が飛散する領域が変化し，質量の断面平面分布が大きく変わる傾向であることが，本結果からもわかる
  - ペネトレーション現象は径の大小に関わらず運動量比の大きな差で発生することが分かり，貫き方は径と運動量の大小関係により変化する
- 実験と対応する条件下の数値解析をCIP-LSM法を用いて実施した
  - 衝突後の傾き角度に関しては概ね再現性がある
  - 細かくすると液膜の状態などが詳細に表現され，試験結果にも一致する傾向が見られた
- 本連携講座の研究成果を応用することで実機設計評価のめどが得られた

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Advances in Rocket Engine Modeling and Simulation, and its Future

NQ-45498

液体ロケットエンジン設計への流体解析技術の適用

宇宙航空研究開発機構

三菱重工業(株)
航空宇宙事業本部
液体ロケットエンジン設計課

平成24年9月27日

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目次

NQ-45498

1. ロケットエンジン燃焼器内部の流れ
2. エンジン開発におけるCFDの役割
3. 解析モデル構築の取組み
   3.1 ミキサー流れ解析
   3.2 燃焼反応流れ解析
4. LE-X燃焼器単体試験へのCFD適用事例
5. まとめ

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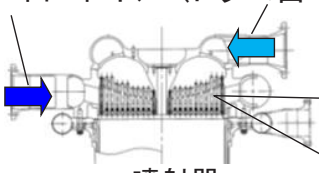
1. ロケットエンジン燃焼器内部の流れ

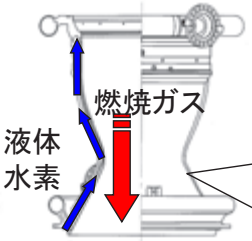
NQ-45498 三菱重工

水素
毎秒530L
（ドラム缶2本半）

酸素
毎秒180L
（ドラム缶1本）



噴射器



燃焼室

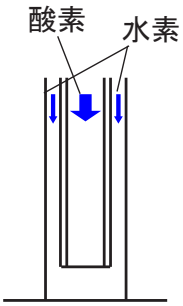
2.1m

①打上げ能力

- 重量低
- 燃焼効率高

⇩

- **高温高圧で燃焼**
- **エレメントから同軸噴射**
  - コンパクトな燃焼室
  - 燃焼効率（98%以上）



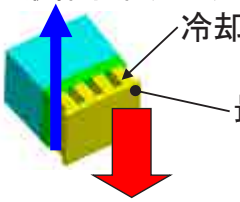
②構造強度

- 高温
- 高圧

⇨ **冷却溝構造**

- 薄肉化で冷却性能を向上
- 高圧の厳しい作動条件

液体水素（30K）



燃焼ガス（3500K以上）

熱流束（~80MW/m2）

H-2Aロケット1段エンジン（LE-7A）

重量	推力	燃焼圧
1.8 ton	110 ton	12.0MPa

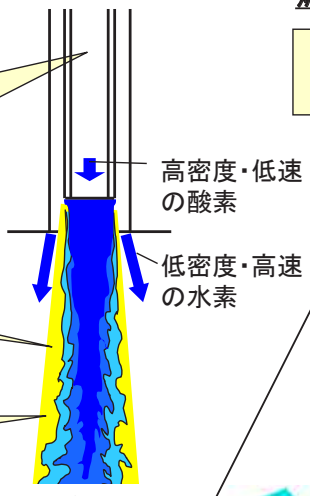
2

1. ロケットエンジン燃焼器内部の流れ

NQ-45498 三菱重工

水素、酸素の同軸火炎

上流の流量分布により
エレメント間で
燃焼の分布が発生



水素、酸素の速度せん
断層で乱流拡散燃焼

エレメント間の
火炎干渉

⇩

- 燃焼効率
- 燃焼安定性
- 壁に伝わる熱量

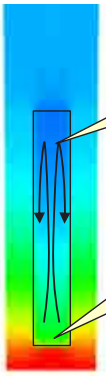
燃焼反応流れ

- 膨張、加速による組成変化
- 高速のため非平衡

⇨ 推力

	温度 [K]	圧力 [MPa]
平行部	3600	12
スロート	3300	7.1
ノズル出口	1400	0.04

冷却剤流れ



2次流れによる温度、流速分布

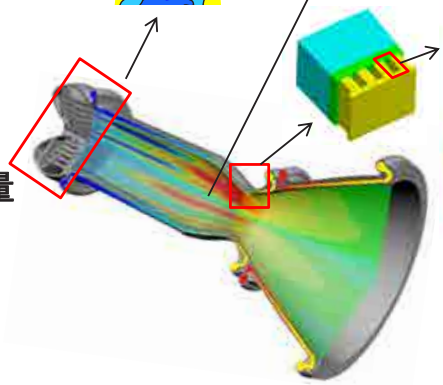
壁温との大きな温度差
⇒境界層での温度勾配大

⇩

- 冷却剤圧損
  （エンジン作動点）
- 壁温（燃焼室寿命）

⇧ 伝熱

温度分布



3

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1. ロケットエンジン燃焼器内部の流れ

NQ-45498 三菱重工

水素、酸素の同軸火炎

上流の流量分布により
エレメント間で
燃焼の分布が発生

燃焼反応流れ

・膨張、加速による組成変化
・高速のため非平衡

⇨ 推力

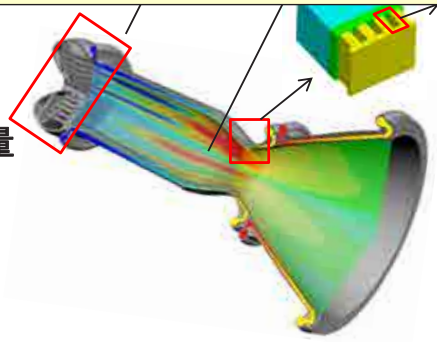
	温度 [K]	圧力 [MPa]
平行部	3600	12
スロート	3300	7.1

高密度・低速
の酸素

予測が難しい複雑な現象

・経験則（実験式）適用の範囲は限定⇒試験で確認
・CFD解析が精度向上に有効

・燃焼効率
・燃焼安定性
・壁に伝わる熱量



伝熱

温度分布

・冷却剤圧損
（エンジン作動点）
・壁温（燃焼室寿命）

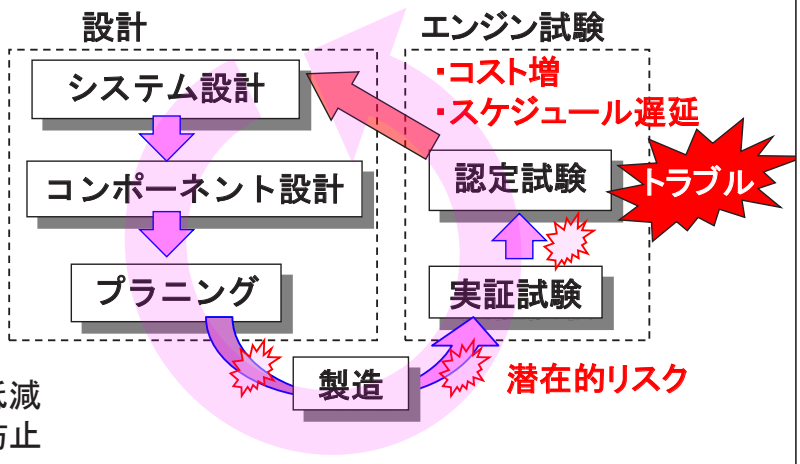
4

2. エンジン開発におけるCFDの役割

NQ-45498 三菱重工

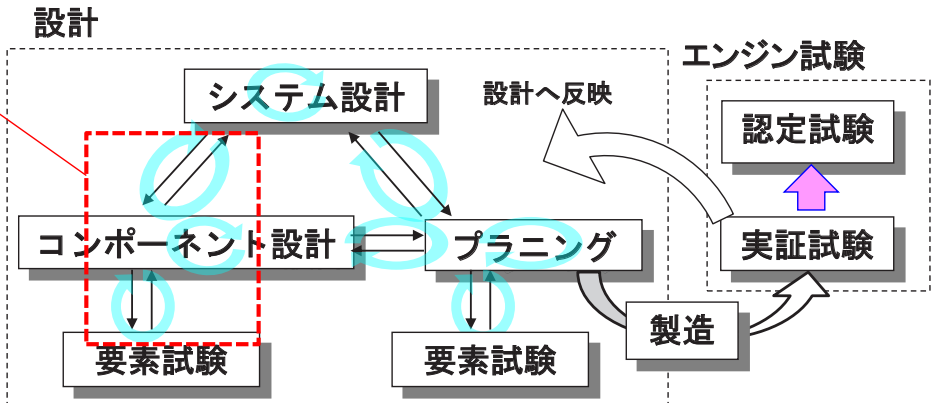
これまでのエンジン開発

試験で確認
⇒トラブル発生の場合、
コスト・スケジュールへの影響大



これからのエンジン開発

高精度解析により事前にリスクを低減
⇒試験での大きなトラブル発生を防止



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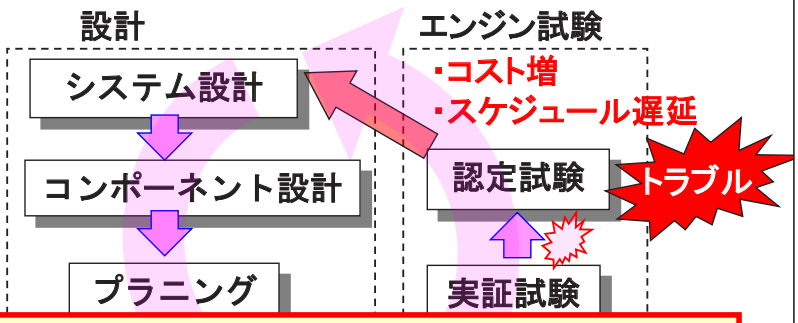
2. エンジン開発におけるCFDの役割

NQ-45498 三菱重工

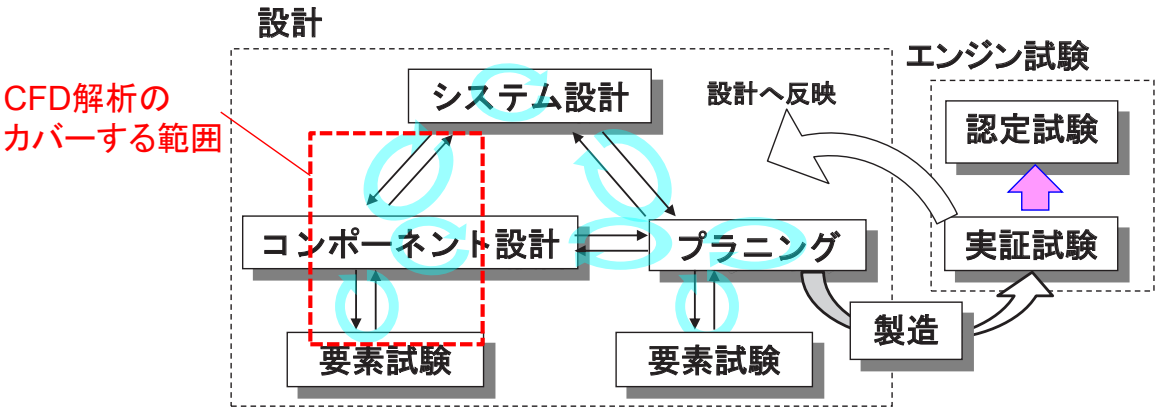
これまでのエンジン開発

試験で確認

⇒トラブル発生の場合、
コスト・スケジュールへの影響大



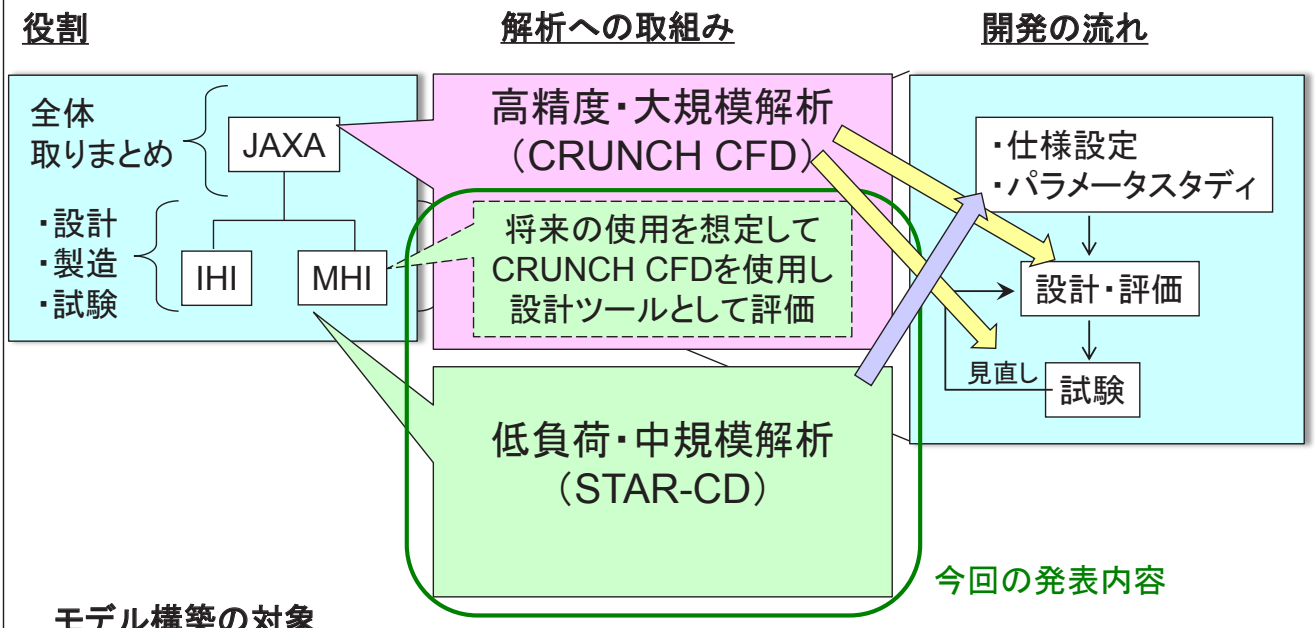
JAXA、MHIで高精度CFDモデル開発に取組み、研究開発中の新エンジンLE-Xへ適用



6

3. 解析モデル構築の取組み

NQ-45498 三菱重工



今回の発表内容

モデル構築の対象

- 噴射器上流
  - 酸素ドーム流れ
  - ミキサー流れ
- 燃焼反応流れ
- 冷却剤流れ

**評価を通して
適用するツール、モデルを決定する。**

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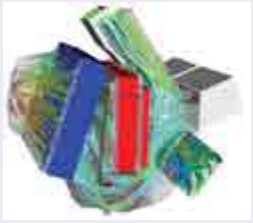
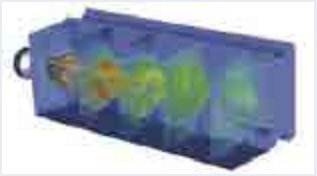
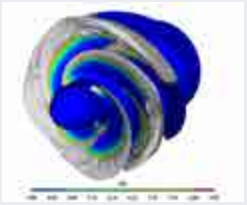
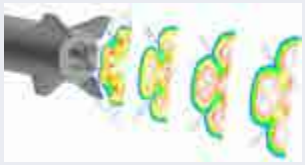
3. 解析モデル構築の取組み

NQ-45498 三菱重工

	STAR-CD	CRUNCH CFD
特徴	①圧力ベースソルバー	①密度ベースソルバー
	②低マッハ数、非圧縮流れに強い	②高マッハ数、圧縮性流れに強い
	③ユーザインタフェース機能が充実	③ユーザインターフェース機能を整備中
適用	④ユーザサブルーチンで対応	④ソースコードレベルで対応
	⑤MHI計算サーバを使用（~24CPU）	⑤JAXAスパコンを使用（~1000CPU）
解析事例	F1空力 熱交換器内部流  工業用ガスバーナー 	キャビテーション  噴流の干渉 超音速噴流 

※解析事例は各ソルバーのマニュアルより抜粋

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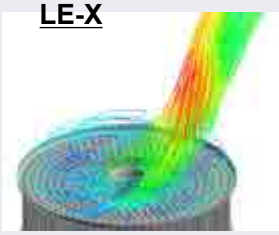
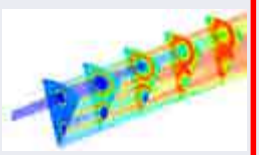
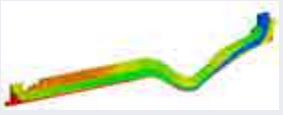
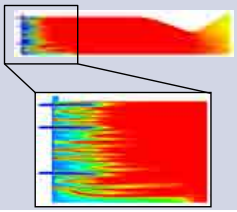
3. 解析モデル構築の取組み

NQ-45498 三菱重工

スケジュール

	酸素ドーム流れ	ミキサー流れ	燃焼反応流れ	冷却剤流れ
2010	サブスケール試験	現行エンジン	今回の発表内容	
2011	LE-X 	LE-X	サブスケール試験 	サブスケール試験 
2012			LE-X 	LE-X

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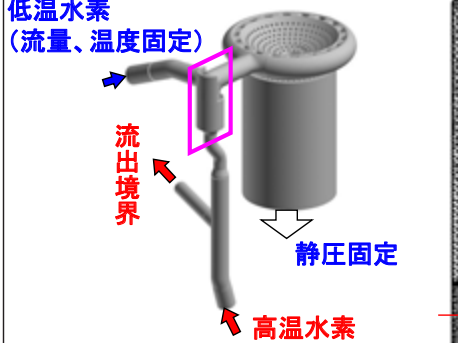
3.1 ミキサー流れ解析

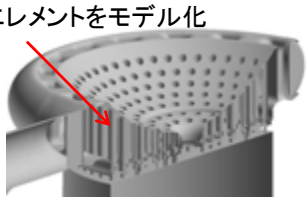
NQ-45498 三菱重工

解析モデル(現行エンジン)

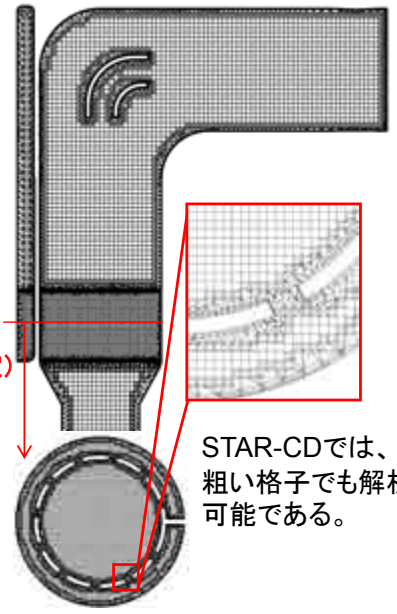


噴射器部(断面図)

全エレメントをモデル化

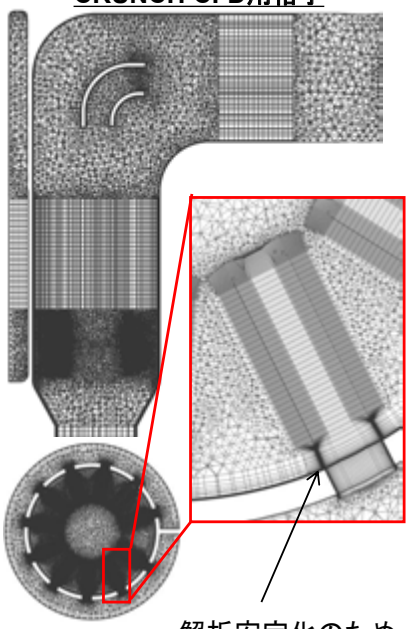


STAR-CD用格子



STAR-CDでは、粗い格子でも解析可能である。

CRUNCH CFD用格子



解析安定化のため温度勾配の大きい部分に格子を寄せている。

解析ソルバー	物性モデル	壁面モデル	乱流モデル	格子点数	解析時間
CRUNCH-CFD	実在流体	壁関数	標準k-ε	1700万点	140hr (400CPU)
STAR-CD	理想流体	壁関数	標準k-ε	700万点	70hr(8CPU)

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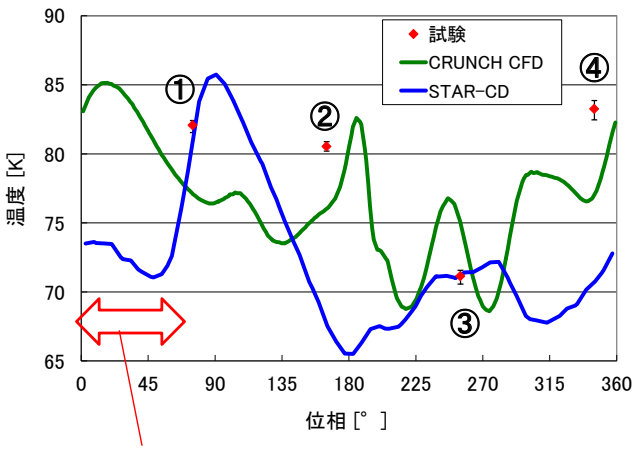
3.1 ミキサー流れ解析

NQ-45498 三菱重工

ミキサー下流の温度分布

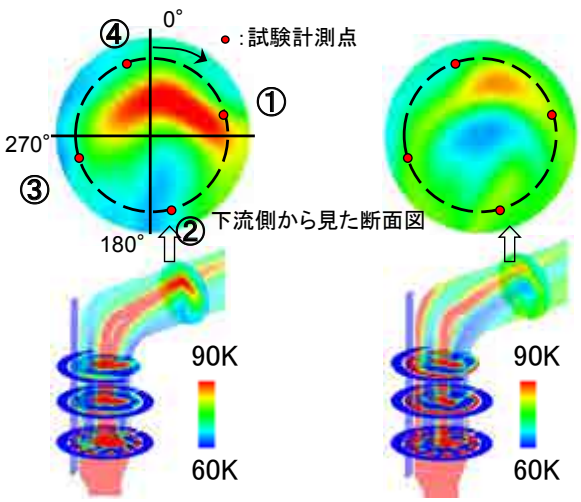
【試験との比較】
試験では③付近で温度が低い。
⇒CRUNCH CFDでは大まかに傾向を捉えられている。

【解析間の比較】
・CRUNCH CFDの方が④～①付近で温度が高い。
⇒高温領域が壁面に近い影響



CRUNCH CFDの方が温度が高い

STAR-CD **CRUNCH CFD**



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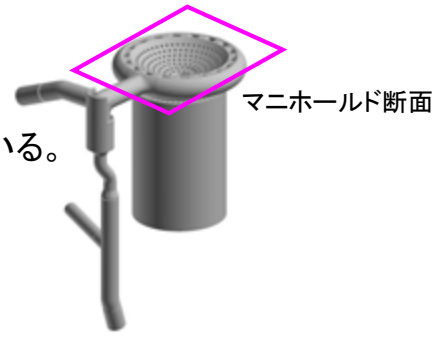
3.1 ミキサー流れ解析

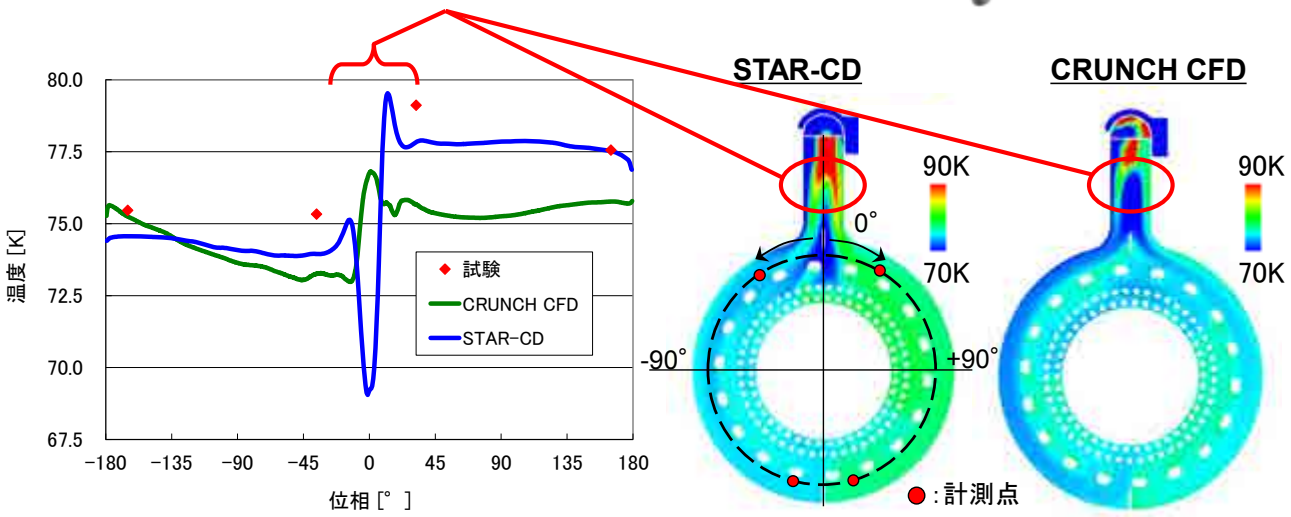
NQ-45498 三菱重工

噴射器マニホールド内の温度分布

【試験との比較】
右側の温度＞左側の温度
⇒STAR-CD、CRUNCH CFDともに傾向を捉えられている。

【解析間の比較】
入部付近（0度位相）で分布の傾向が異なる。
⇒上流配管内の分布の差が影響





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3.1 ミキサー流れ解析

NQ-45498 三菱重工

現行エンジンは計測点が限定
⇒流れ場の検証が十分ではない。

【LE-X燃焼器単体試験】
・2013年実施予定
・計測点を増やし、詳細に精度を検証

LE-X対象の解析

CRUNCH CFD

STAR-CD

高温部の位置が異なる。

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3.2 燃焼反応流れ解析

NQ-45498 三菱重工

サブスケール燃焼試験(水冷却)を対象

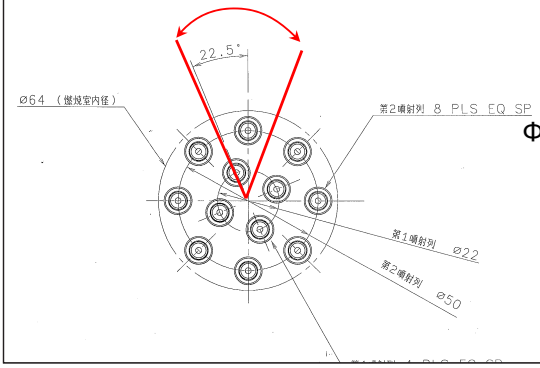
・噴射面で静圧(燃焼圧)を計測
・環状に流れる冷却水の温度上昇から熱流束を算出
・燃焼室内面の壁温は冷却水側で構築した実験式から算出

燃焼条件

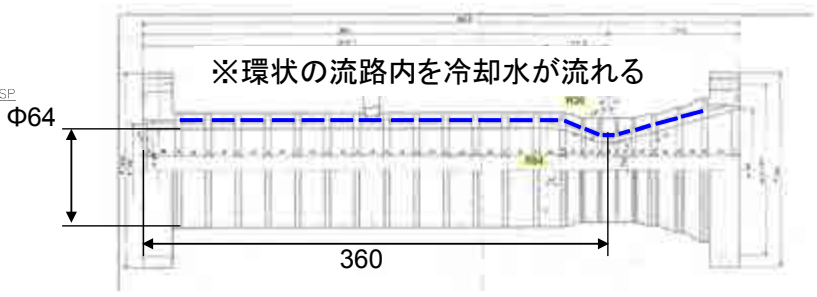
燃焼圧 [MPa]	5.01
混合比	6.49

エレメント配置

※周方向の対称性から
45度分をモデル化



燃焼室概形状



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3.2 燃焼反応流れ解析

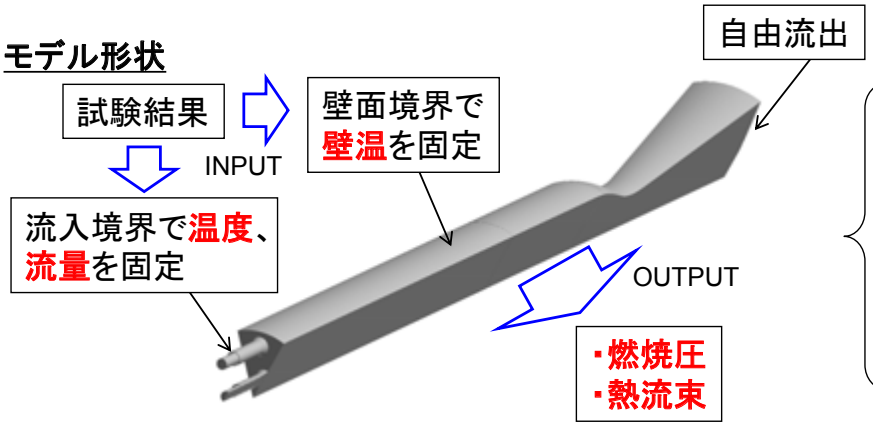
NQ-45498 三菱重工

【燃焼効率】
流量、スロート面積を試験と合わせて燃焼圧を試験と比較
【熱流束】
軸方向分布を試験と比較

$$\eta_{C^*} = \frac{C^*}{C^*_{theory}}$$

$$C^* = \frac{P_c A_t}{\dot{m}}$$

モデル形状



η_{C^*} :燃焼効率
C^*_{theory} :理論特性排気速度
C^* :特性排気速度
P_c :燃焼圧
A_t :スロート面積
$\dot{m}$:流量

解析ソルバー	物性モデル	乱流モデル	壁面モデル	反応モデル	格子点数	解析時間
CRUNCH-CFD	実在流体	標準k-ε	Near Wall Model	詳細反応	770万点	170hr (400CPU)
STAR-CD	理想流体	標準k-ε	壁関数	詳細反応	90万点	140hr (8CPU)

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3.2 燃焼反応流れ解析

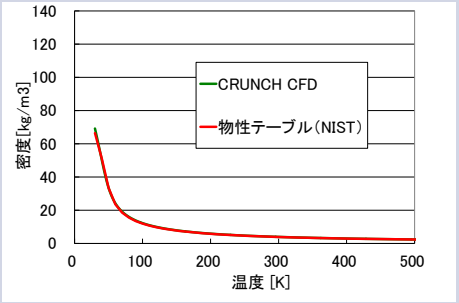
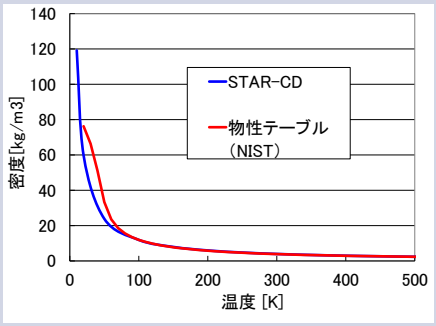
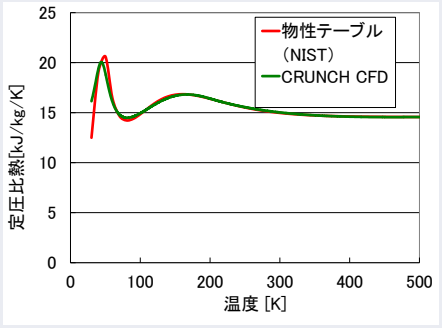
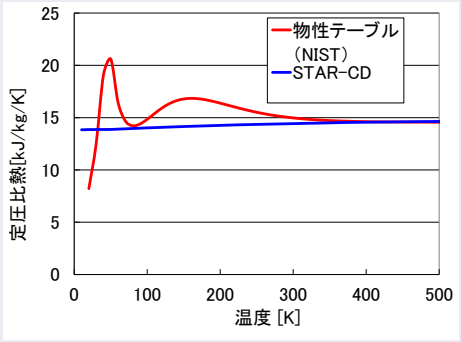
NQ-45498 三菱重工

理想流体の物性設定

流入温度を調整して密度（運動量）を試験と合わせている。

流入温度

	H2温度 [K]	O2温度 [K]
CRUNCH	100.1	98.1
STAR	100.7	17.3

	CRUNCH CFD	STAR-CD
密度		
定圧比熱		

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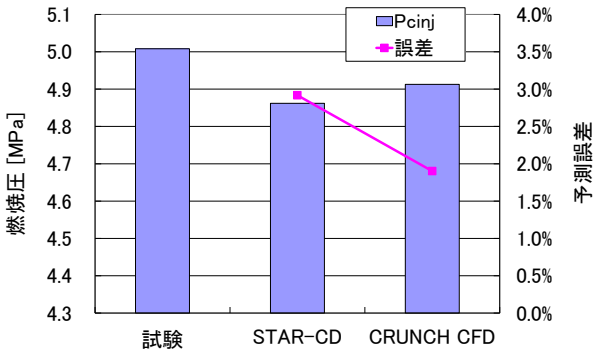
3.2 燃焼反応流れ解析

NQ-45498 三菱重工

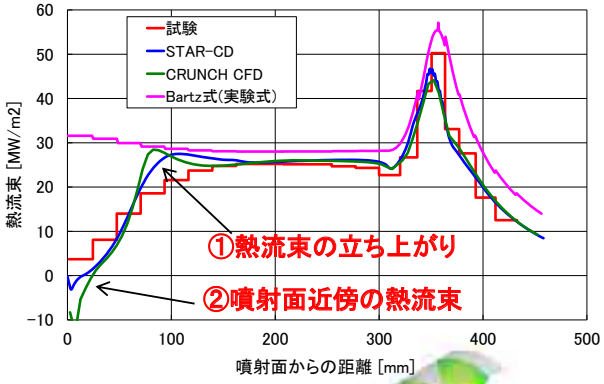
燃焼圧

・試験結果をほぼ再現
・CRUNCH CFDの方が試験に近い。



熱流束

・平行部、スロート部の傾向を捉えられている。
・CRUNCH CFDとSTAR-CDは同程度である。
・噴射面近傍に精度向上の余地あり。



CRUNCH CFD
0K 3500K

STAR-CD
0K 3500K

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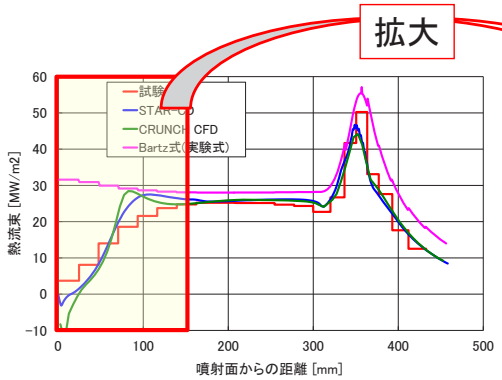
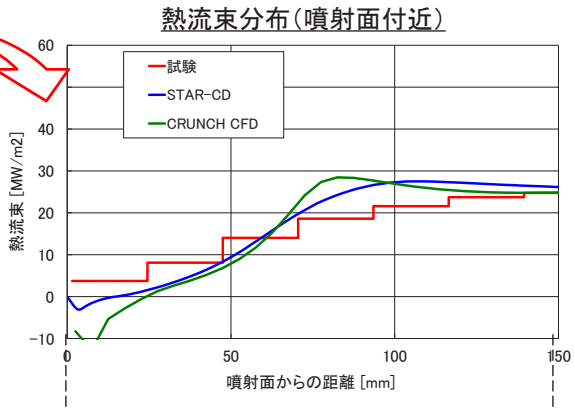
3.2 燃焼反応流れ解析

NQ-45498 三菱重工

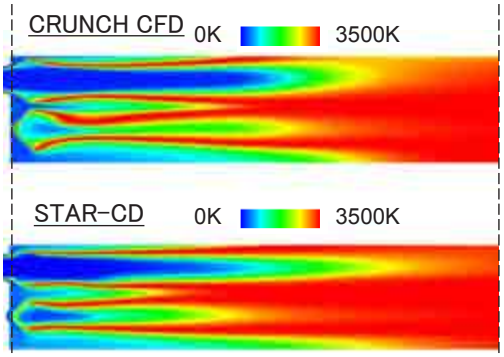
①熱流束の立ち上がり





・解析では同軸上の火炎が壁面に近づくのに伴い、熱流束が上昇する。

・試験では解析よりも緩やかに上昇
⇒火炎の形状が精度よく捉えられていない可能性



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3.2 燃焼反応流れ解析

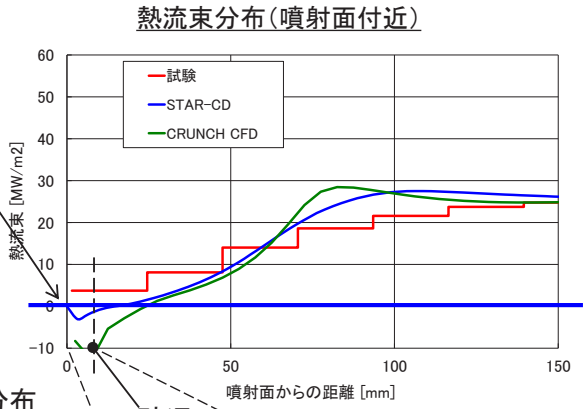
NQ-45498 三菱重工

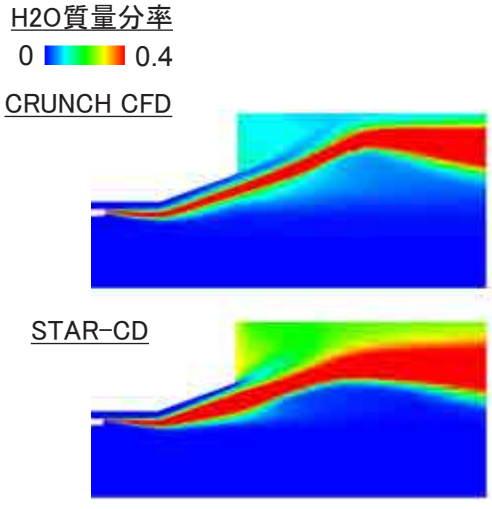
②噴射面近傍の熱流束

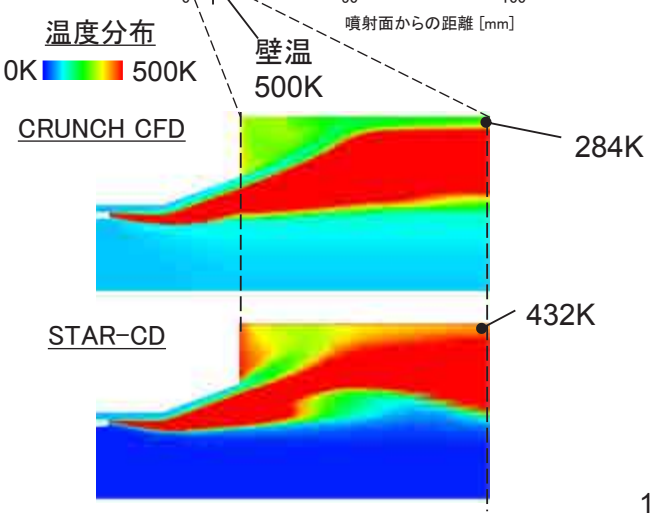
・流体温度＜壁面温度となり熱流束が負

・CRUNCH CFDの方がSTAR-CDよりも燃焼ガスの拡散が小さく、壁面付近の温度が低い。

・循環構造と火炎の干渉が実現象と異なる可能性







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4. LE-X燃焼器単体試験へのCFD適用事例

NQ-45498 三菱重工

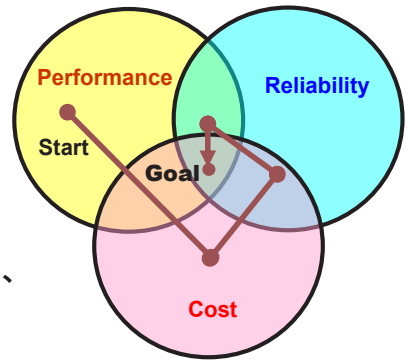
LE-Xエンジン

・次期基幹ロケット用の
1段エンジンとして研究開発中

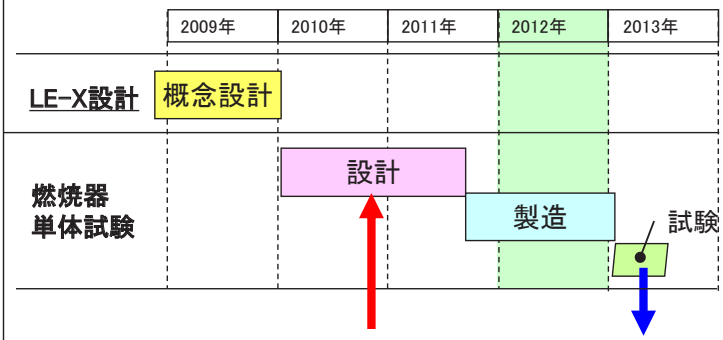
・信頼性、コスト、性能の
バランスの取れたエンジン

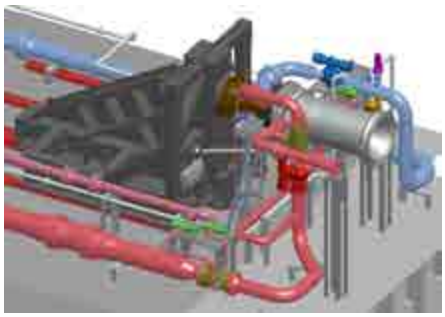
・高精度解析を設計初期から適用し、
信頼性を定量的に評価

・実機大燃焼器の燃焼試験準備中



LE-Xエンジン





燃焼器単体試験のレイアウト

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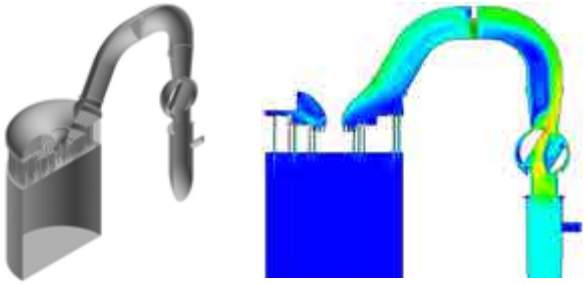
4. LE-X燃焼器単体試験へのCFD適用事例

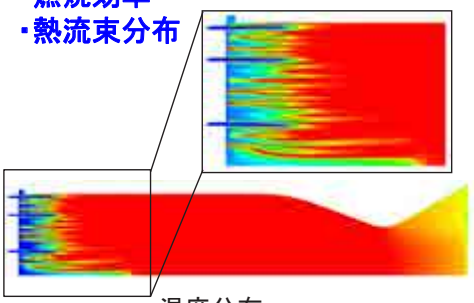
NQ-45498 三菱重工

酸素側の流量分布

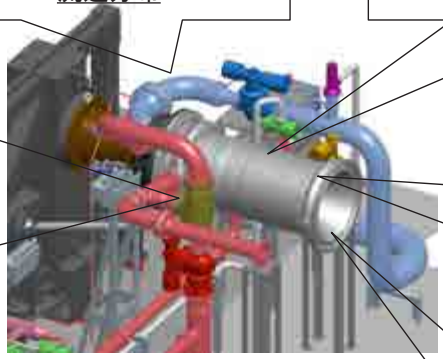


解析モデル（断面図）　流速分布

・燃焼効率
・熱流束分布



温度分布



水素側の流量分布

温度分布

・冷却剤圧損
・壁温分布

冷却剤流量分布

静圧分布

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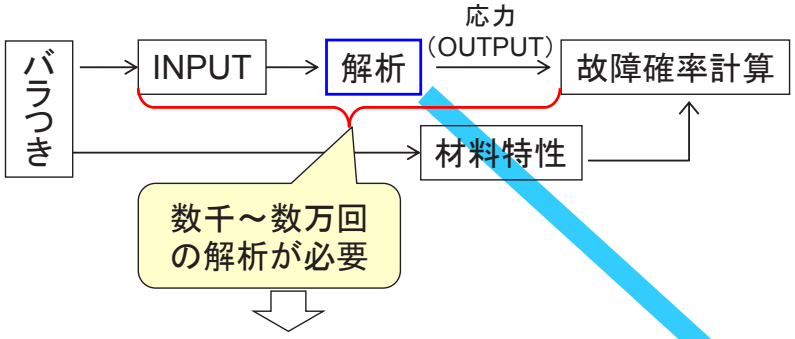
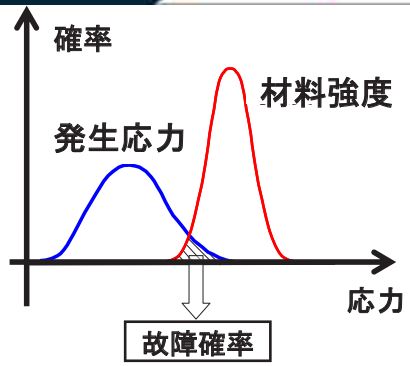
4. LE-X燃焼器単体試験へのCFD適用事例

NQ-45498 三菱重工

信頼性の定量評価（故障確率算出）

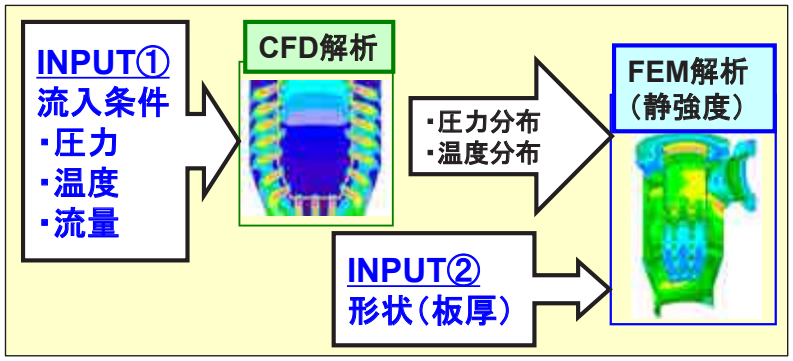




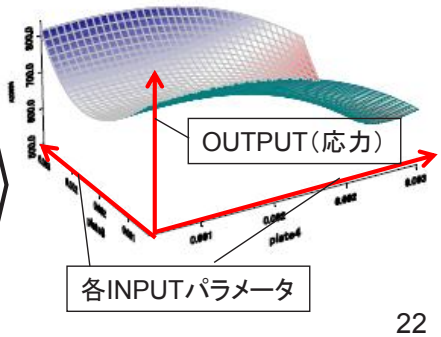
数十回（多数回）の解析によりINPUTとOUTPUTの関係を近似式化する。（応答曲面）

中規模の解析モデルが必要

ミキサーの評価例



応答曲面



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5. まとめ

NQ-45498 三菱重工

・JAXA、MHIで燃焼器の高精度CFD解析モデルの構築に取り組んでいる。
　JAXA⇒設計の検証に適用する高精度の大規模モデル
　MHI　⇒設計に適用する中精度、中規模モデル

・要素試験、エンジン燃焼試験を対象に精度を検証し、
　エンジン開発における各解析モデルの適用方針が定まりつつある。

・特に燃焼CFD解析では、噴射面近傍の熱流束の予測精度に
　向上の余地があり、引き続き精度検証とモデル改良に取組む。

・構築した解析モデルは研究開発中のLE-Xエンジン設計に
　順次適用されている。

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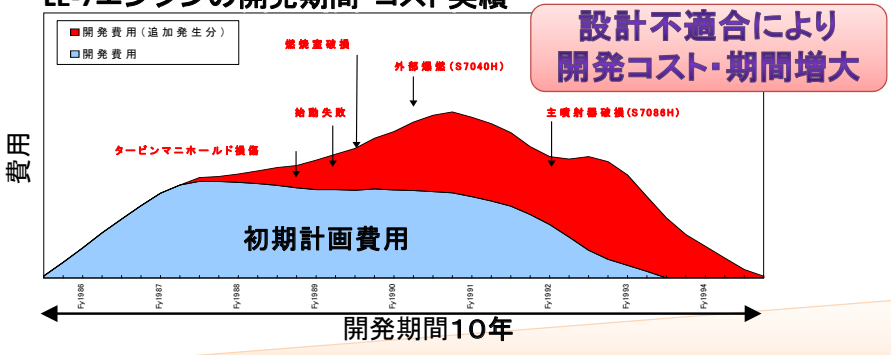
東京大学JAXA社会連携講座シンポジウム　2012年9月27日

ロケットエンジンシミュレーションにおける今後の展望

JAXA/JEDI
山西伸宏
根岸秀世，谷洋海

従来のロケットエンジン開発プロセス

LE-7エンジンの開発期間・コスト実績



設計不適合により
開発コスト・期間増大

JAXA/JEDI(情報・計算工学センター)の目標
シミュレーション技術を始めとする情報化技術で
ロケットエンジン開発にイノベーションを起こす

2

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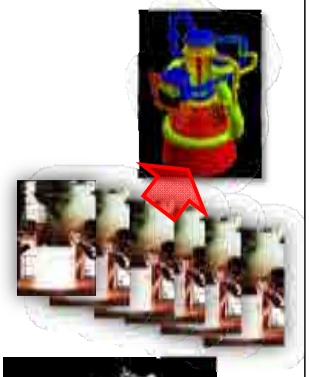
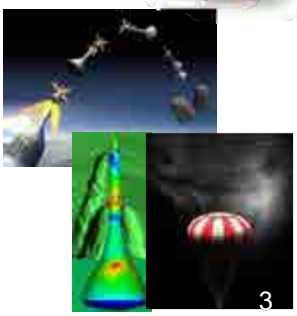
JAXAシミュレーションの最終目標

シミュレーションによる設計技術を導入した新たな開発プロセスで、将来の宇宙航空ミッションの低コスト/短期間化・高性能/高信頼化を実現する世界へ



【設計評価におけるコスト低減の実現】

- 設計初期段階でシミュレーションにより潜在的な不具合因子を洗い出すことで、開発後期での事故を未然に防止し、不具合対策によるコスト・期間を削減する
- 膨大な回数の試験が必要な設計評価(例えば有人輸送ミッションに不可欠なロケットエンジン設計信頼度)にシミュレーションを活用することで、試験回数を減らし、コスト・期間を大幅に削減する



【広範囲な設計探査の効率化の実現】

- 試験では網羅できないほど広範囲に機体やエンジンの作動状況を予測することで、信頼性や安全性の正確な評価に貢献する
- 膨大な数のコンポーネントからなる全体システムを各コンポーネントごとに切り分けて作動状況を予測することで、複雑な全体システムの信頼性や安全性の評価の効率化を図る
- 人間の経験則の延長では導けない新しい設計値を効率的に探索することで、最適な設計解を提案する

3

最終目標達成に向けた具体策

4

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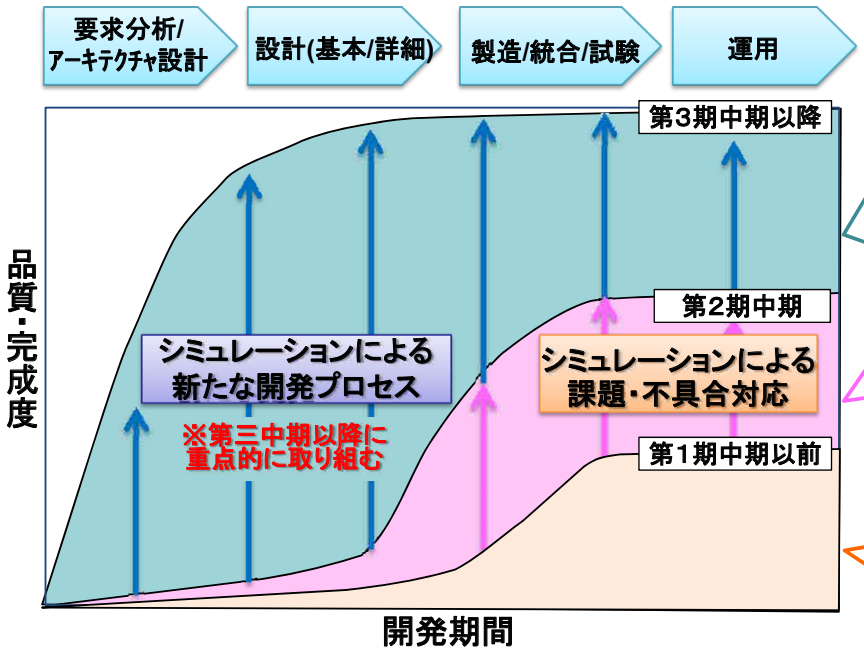
新たな開発プロセスの実現に向けたステップアップ

第１期中期ではシミュレーションによって、主に課題・不具合対応に貢献してきた。第２期中期ではこれらに加えて、漸く開発後期における設計手法の一つとして活用し始めている。第３期中期以降では、情報化技術を用いて開発初期段階からコスト/期間、安全性/信頼性、運用性の最適解を検討できる開発プロセスの中で、フロントローディングなシミュレーションを実施し、ミッションの低コスト化、短期間化、高信頼化を実現する。



第３期中期
開発初期段階からシミュレーションによる革新的設計手法を活用し、低コスト化、短期間化、高信頼化を実現

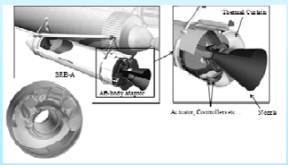
第２期中期
運用フェーズにおいて不具合対応に貢献するとともに、**開発後期において**設計手法の一つとして最適化や性能確認のためにシミュレーションを活用。また、宇宙輸送分野以外にも展開

第１期中期以前
運用フェーズにおいてシミュレーションによりミッションの不具合対応に貢献

5

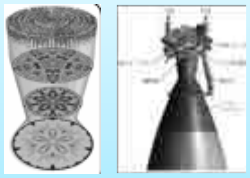
第１期・第２期におけるステップアップ

【第１期中期】 運用フェーズにて課題・不具合対応に貢献


H-IIA/F6の事故原因究明

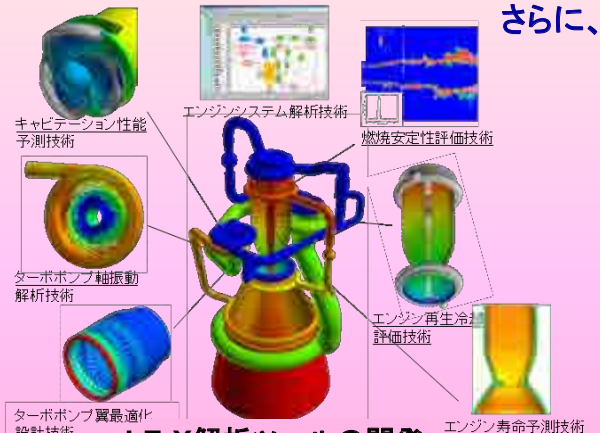
LE-7Aの改良開発

LE-5Bの改良開発

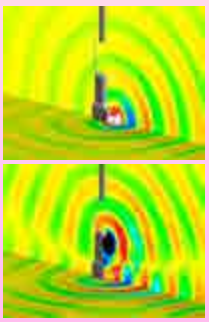

LNGエンジン燃焼器の開発

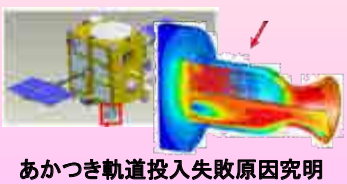
シミュレーション基盤技術の高度化、他分野への展開

【第２期中期】 開発後期及び運用フェーズにおける課題・不具合対応に貢献
さらに、宇宙輸送分野以外への展開開始



LE-X解析ツールの開発


打ち上げ時音響解析
イプシロンロケット設計支援


あかつき軌道投入失敗原因究明

ASTRO-H熱環境・内圧予測

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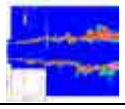
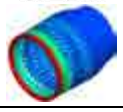
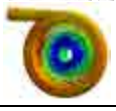
第2期までのツール開発達成状況

LE-Xプロジェクト支援として実施した波及成果

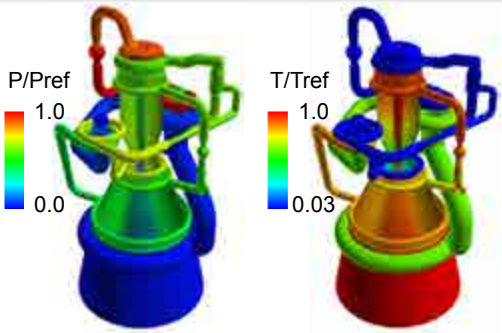
システム解析技術 → 燃焼器系解析技術 → 供給器系解析技術

	エンジンシステム解析	燃焼安定性評価	再生冷却性能評価	燃焼室寿命予測	ターボポンプ翼最適設計	キャビテーション性能予測	ターボポンプ軸振動解析	エンジン全系解析技術
設計解析技術								
第2期の目標	開発初期段階でシステム成立性を予測可能なツールの開発	実機燃焼器における燃焼振動発生予測及び発生までの余裕を評価するツール開発	開発初期段階で燃焼器の再生冷却性能を予測可能なツールの開発	開発初期段階で燃焼器の寿命を予測可能なツールの開発	最適化技術を適用した高性能翼設計支援ツールの開発	開発初期段階にてキャビテーション不安定現象を予測するツールの開発	開発初期段階にて実液中のターボポンプ軸振動を予測可能なツールの開発	開発した7つの解析技術を統合しエンジンシステム全体のハザード評価を実現する
目標達成	**達成** ・開発したツールでLE-X複数燃焼器化検討に適用 ・概念検討の標準ツールとして普及	**達成** ・開発したツールをLNGエンジン設計に適用 ・開発したツールをLE-X設計に適用	**達成** ・開発したツールをMHIへ技術導入 ・世界初のエンジン燃焼器熱-流体強連成解析を実現	**達成** ・開発したツールでLE-5Bの損傷メカニズムを解明 ・相互検証でメーカ解析技術を高度化	**達成** ・世界初の多段/非定常解析での翼最適化を実現 ・開発したツールをLE-X/FTP設計に適用	**達成** ・世界最高レベルの性能予測ツールを実現 ・旋回キャビメカニズムを解明(世界初)	**達成** ・世界的にも希少な軸振動解析手法を構築 ・LE-Xの軸振動過大リスクを評価	**達成** ・世界初のエンジン全系高精度シミュレーションを実現 ・LE-Xのハザード事象評価に活用
輸送ミッション本部での評価	・これまでにない汎用的なエンジン概念検討ツールを構築し、輸送本部に展開されたことは評価する ・今後は非定常性能予測を実現するツール開発に期待する	・燃焼安定性はLE-9開発での最大リスクの1つであり、その定量的リスク評価が可能となるレベルまで本手法は**引続き改良**されたい	・再生冷却性能はLE-9開発での最大リスクの1つであり、その定量的リスク評価が可能となるレベルまで本手法は**引続き改良**されたい	・従来ツールではできない現象を再現し、LE-X等の設計・研究計画に反映した。 ・定量的リスク評価が可能となるレベルまで本手法は**引続き改良**されたい	・LE-X/FTPタービンの定性的な方針を得るという点で有効であった ・今後は定量的な効率予測にも期待する	・LE-Xのインデューサ設計にJEDIの成果が反映された ・より確度の高い定量的リスク評価のために**引続き改良**されたい	・今中期の目標は達成見込みであるが**引続き改良**を希望 今後はメカシール、流体軸受、Squeeze-filmダンパなど動特性評価や多領域最適化での貢献に期待	・設計に使用するレベルには達していないが将来的なポテンシャルを示した。今後は精度向上及び非定常への対応と設計への適用に向けた**改良に期待**したい
次期中期計画への展開	・**開発の第1フェーズは終了**する ・次の開発フェーズへの移行判断のため輸送本部を中心にツールの有効性を評価した上で、随時改良開発に対応	・**開発の第1フェーズは終了**する ・次の開発フェーズとして輸送本部が目指す定量的リスク評価を実現するために**改良開発を継続**	・**開発の第1フェーズは終了**する ・次の開発フェーズとして輸送本部が目指す定量的リスク評価を実現するために**改良開発を継続**	・**開発の第1フェーズは終了**する ・次の開発フェーズとして輸送本部が目指す定量的リスク評価を実現するために**改良開発を継続**	・**開発の第1フェーズは終了**する ・次の開発フェーズへの移行判断のため輸送本部を中心にツールの有効性を評価した上で、随時改良開発に対応。	・**開発の第1フェーズは終了**する ・次の開発フェーズへの移行判断のため輸送本部を中心にツールの有効性を評価した上で、随時改良開発に対応。	・**開発の第1フェーズは終了**する ・次の開発フェーズへの移行判断のため輸送本部を中心にツールの有効性を評価した上で、随時改良開発に対応。	輸送本部が期待する実設計への適用と最終的にはシミュレーションによるエンジンQTの実現を目指し**改良開発を継続**

第2期で得られた世界的成果例

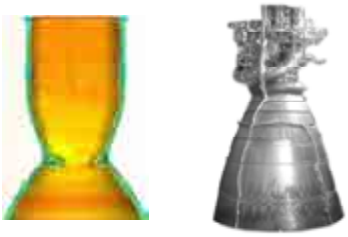
ロケットエンジンEnd-to-Endシミュレーション

ロケットエンジン設計解析ツールを組み合わせ、従来実施が困難とされたエンジン全系の高精度シミュレーションを実現し、性能評価に貢献。さらに、システム全体のハザード評価に適用。



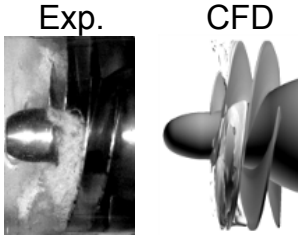
燃焼室スロート縮小の解明

改良型LE-5Bエンジンのエンジン試験で発生した燃焼室スロート縮小を対象に、非定常な熱・流体・構造連成解析を実現し、スロート縮小を解明。エンジン設計現場における設計解析技術の高度化へ貢献。



キャビテーション性能評価

キャビテーション不安定への流量の影響及びそのメカニズムについてターボ機械分野のトップジャーナルに掲載。さらに、CNESインデューサ共同研究に適用し、定量的予測精度は世界最高レベルであることを確認。



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第2期で得られたLessons Learned(1/3)

■ ツール開発

- ﾌﾟﾛｼﾞｪｸﾄ支援に適用した際に機能不十分が発覚し緊急で機能追加が必要となった
  ➔【教訓】実際のプロジェクト支援解析を想定したツール開発計画を策定する
- 世の中に物理モデルが存在しないものは結局最後まで検討できなかった
  ➔【教訓】重要物理モデルは早期に選定し、存在しなければ東大社会連携講座や共同研究を活用して新たに構築する

■ ツール検証

- CFD検証専用の試験データがなく物理モデルまで踏み込む検証ができなかった
  ➔【教訓】共同研究等を活用しCFD検証データ取得も含めてツール開発計画を検討する
- 試験データが存在するものでも質の低いものが多く、検証に苦労した
  ➔【教訓】試験の概念検討に参加し、少しでも検証に有用な試験となるよう調整する
- 試験では可視化情報が乏しく、現象を十分に理解することができないままツール開発を余儀なくされた（特に燃焼器系解析技術）
  ➔【教訓】試験ではなるべく可視化情報も取得するよう調整する

9

第2期で得られたLessons Learned(2/3)

■ 計算機環境

- JSS特別利用枠を申請しても必要十分な計算資源を利用することは困難であり、計算規模や内容に制約を受けた
  ➔【教訓1】計画当初から計算規模は十分に考えておく
  【教訓2】JAXA外の計算機の利用も検討する
- 特殊なｱｰｷﾃｸﾁｬの計算機(JSS)向けに解析ツールの最適化をする必要があり、多くの追加費用と時間が必要となった
  ➔【教訓】基盤となる計算機は極力標準的なものにする

■ 前/後処理

- 大規模や大量解析では格子作成、可視化など前/後処理作業に多くの時間が必要だった
  ➔【教訓】解析ツールだけでなくその前/後処理も含めて効率的な仕組みを考える
- 計算規模が大きくなるに伴い計算機環境の制約で前/後処理ができないことが発生した
  ➔【教訓】計算機環境は先の状況を見据えて十分な性能のものを調達しておく

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第2期で得られたLessons Learned(3/3)

■ メーカへの技術移転

- ツール開発をしながら技術移転を進めたため適用実績のない解析対象などでは不具合が発生した
  ➔【教訓】技術移転は適用実績のあるものから始める
- 限られた時間内でJEDIと同じ解析スキルまで習得させるために当初予想以上の技術指導や支援を要し、JEDI側の開発・検証作業を遅延させることがあった
  ➔【教訓】メーカ社員がJEDIに一定期間出向して中・長期的にスキル習得を図るなど人材交流の仕組みも利用する
- メーカ既存解析ツールの代替技術とするには解析精度、計算コストに対する厳しい要求があり、JEDI側の当初認識と相違があった
  ➔【教訓】ツール開発初期から目標精度に対する共通認識をメーカと作る

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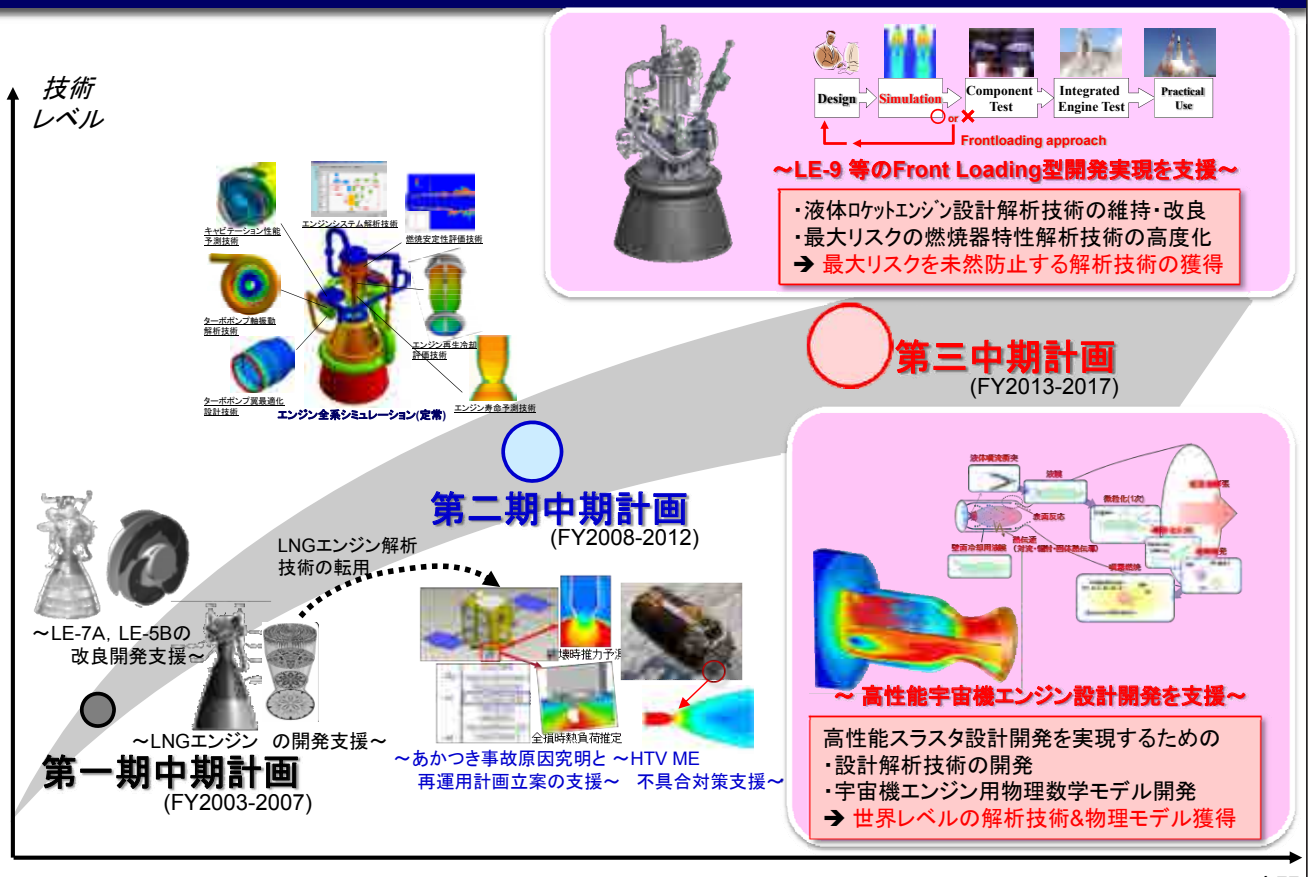
ロケットエンジン設計解析技術の変遷と次期中期ビジョン



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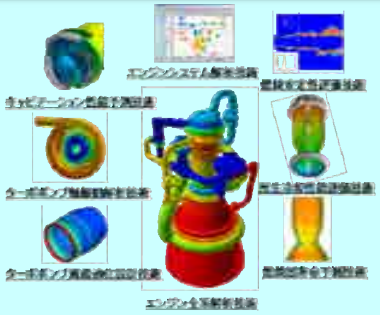
第3期のロケットエンジン解析技術の高度化

～開発した解析技術を新たな開発プロセスに活用～



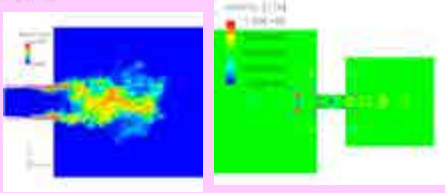
1. 液体ロケットエンジン設計解析技術の維持・改良・適用

- 第二中期計画で構築した各種ツール・ノウハウの維持
- プロジェクトからの要望に応じた改良開発(必要に応じて随時)
- ロケットエンジンモデリング委員会の運営により、現社会連携講座で獲得された知見の維持・継承

～新たな開発プロセス実現に向けたさらなる技術開発～

2. 燃焼安定性評価技術

- 今中期に構築した各分析ツールを適用・高度化し、融合することで、燃焼安定性の定量的リスク評価を実現。
  - 燃焼解析：ｻﾌﾞｽｹｰﾙ以上の実燃焼器解析実現と高度化
  - 音響解析：音響デバイス・噴射器等の評価の高度化・最適化
  - 安定性評価手法：上記2つを融合したリスク評価の実現



燃焼安定性評価解析ツール

3. 燃焼器性能・寿命評価技術

- 再生冷却及び寿命予測技術の更なる高度化を図る
  (起動・停止過渡状態などの非定格作動状態も含む)
  - 燃焼器寿命予測の高精度化
    ➔【打ち手】再生冷却解析ツール、全系システム解析との連成実現
  - 非定格作動状態(スロットリング、起動・停止過渡時)の予測実現
    ➔【打ち手】亜臨界圧燃焼＆伝熱解析技術の構築

燃焼性能・寿命評価解析ツール

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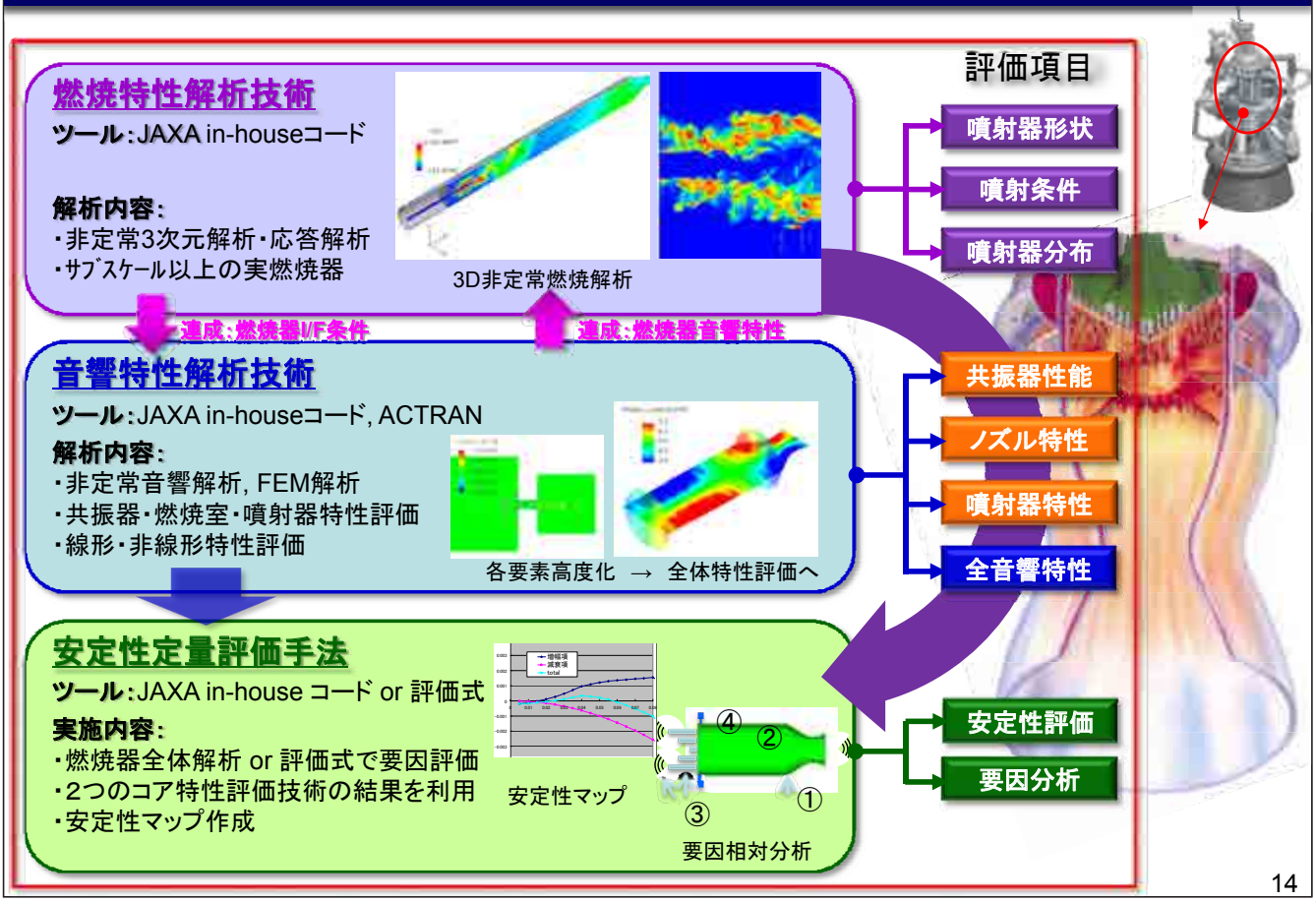
燃焼安定性評価技術; 目指す解析ツールのイメージ



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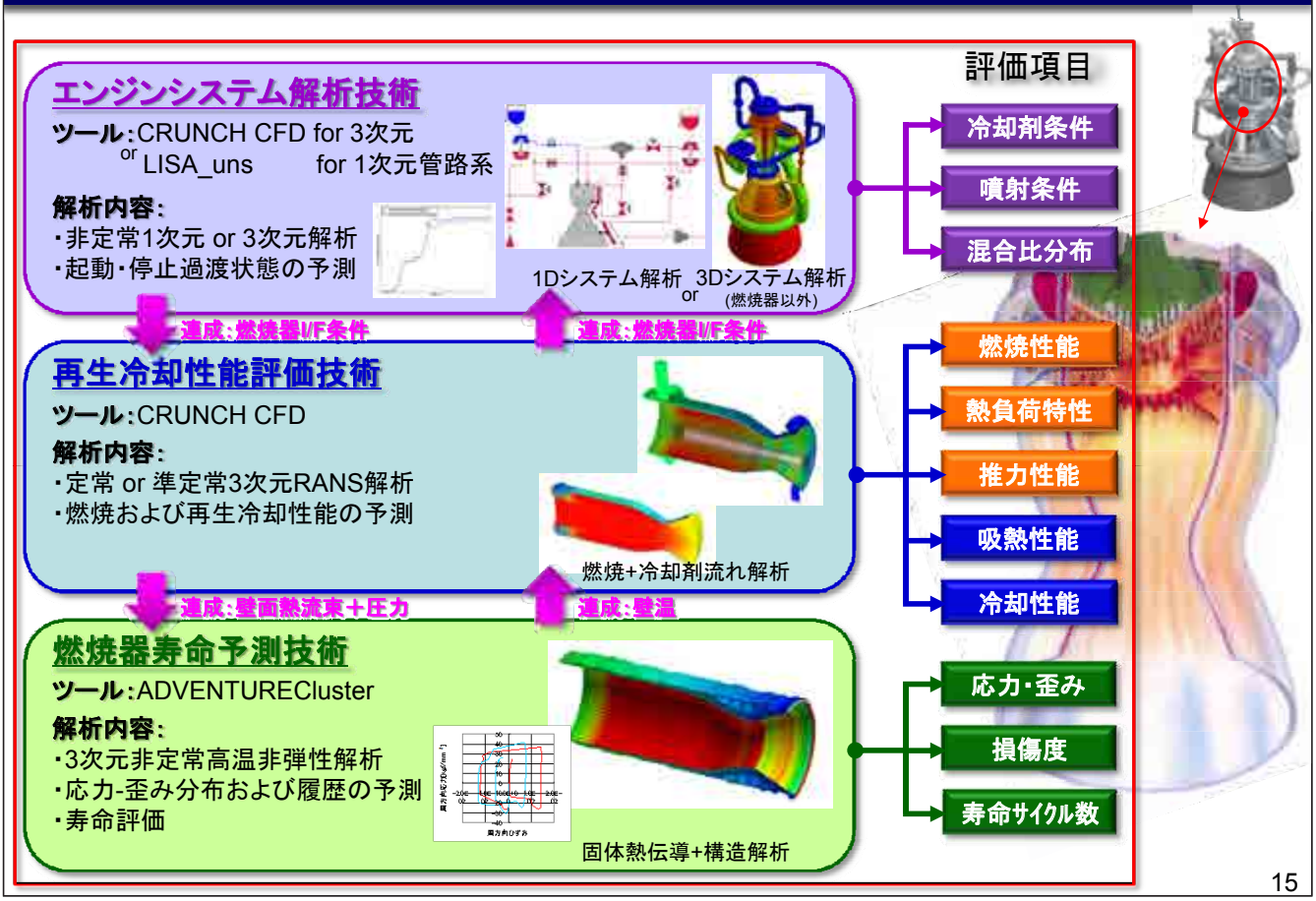
燃焼器性能・寿命評価技術; 目指す解析ツールのイメージ



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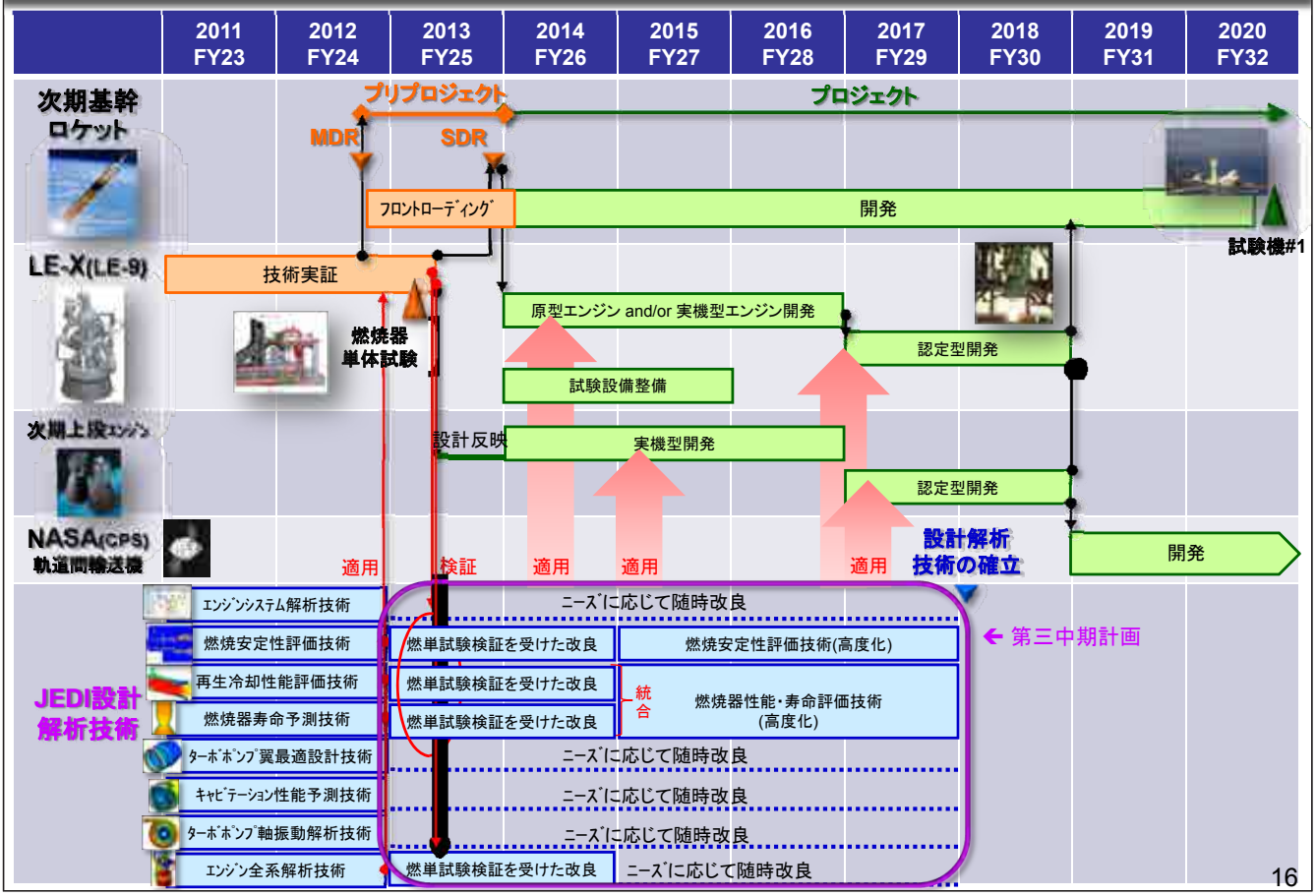
JAXA宇宙輸送ミッションへの貢献



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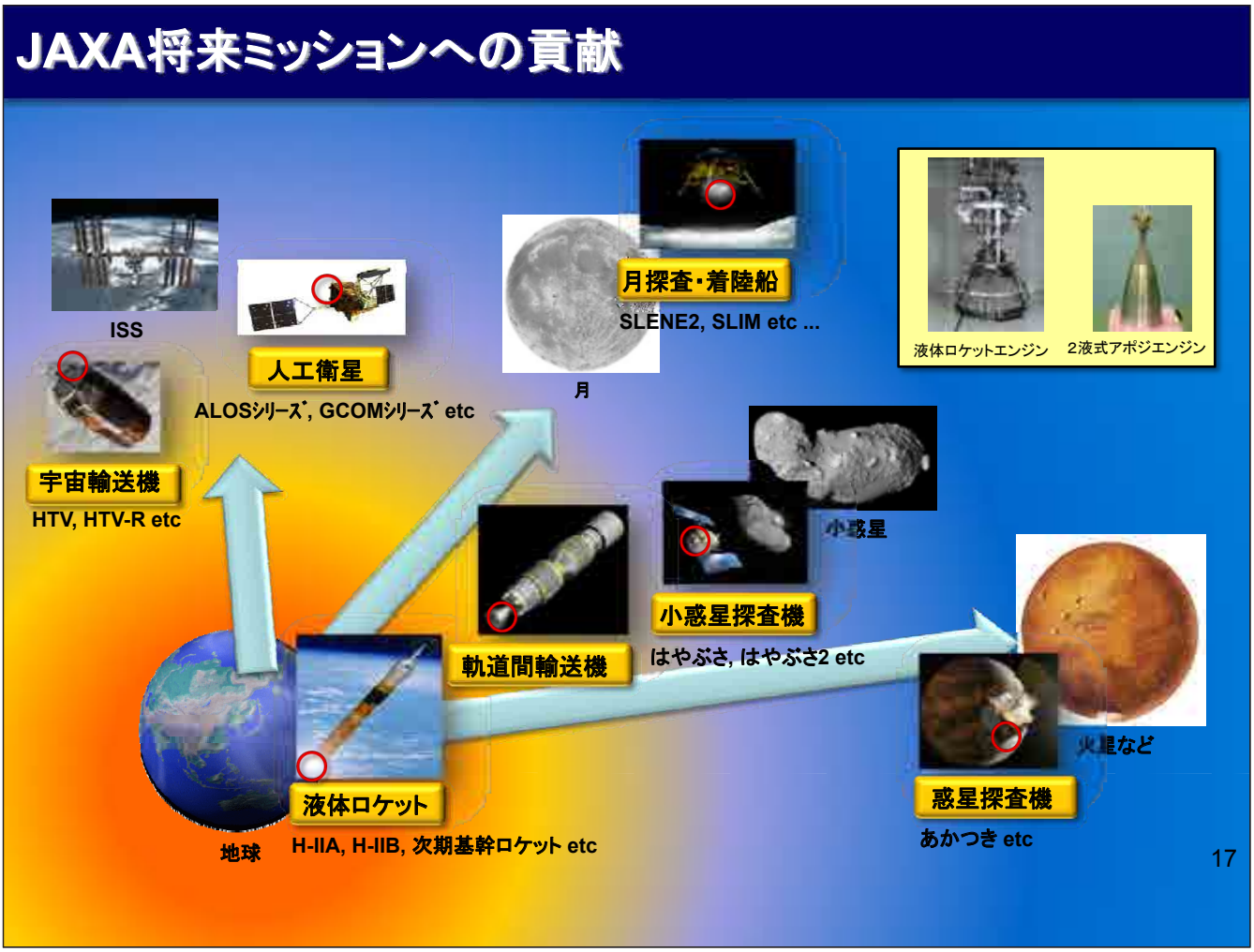
JAXA将来ミッションへの貢献



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