Sep/20/2013, ロケット・宇宙機モデリングラボラトリーシンポジウム
Rocket and Spacecraft Modeling Laboratory, The University of Tokyo

反応性熱流動モデリングの研究

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謝辞
反応性熱流動グループ各位
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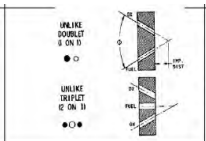
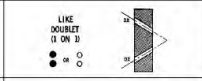
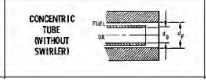
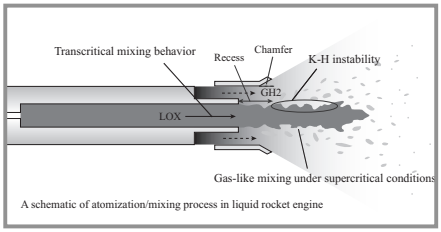
研究ターゲット

- 液体ロケットエンジン
- 衛星スラスター

反応性熱流体現象

-燃料と酸化剤が混合し，反応過程を経て，燃焼する熱流体場

異種衝突型		液／液 NTO/ヒドラジン自燃性二液推進薬	LEM ascent engine Delta launch vehicle Agena upper state Agena target vehicle
同種衝突型		液／液 LOX/RP−1	H − 1, F − 1engines
同軸型		液／ガスor液／液 LOX/GH2, LOX/LH2, LOX/CH4	SSME, LE−7, LE−5engines



A schematic of atomization/mixing process in liquid rocket engine

エンジン開発における問題点

- 振動燃焼（低周波，高周波不安定）
- 壁面熱流束（フィルムクーリング，構造）
- 過渡特性（定格作動点以外での運用）
- 形状効果

いずれにおいても未だ予測/評価が困難

-既存手法/モデルの限界

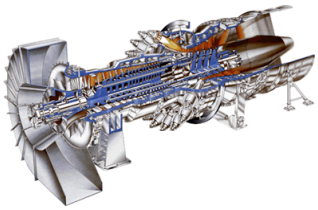
-燃焼解析技術の発展の必要性

「非定常」の「流体混合現象」「燃焼現象」「化学反応」がキーとなる

非定常 **混合** **燃焼** **化学反応**

一般的な燃焼流の課題

- 高効率かつクリーンな燃焼技術（超希薄燃焼など）
- 多様化する燃料
- 燃焼振動（不安定性）
- 壁面近傍の熱環境予測



流れに基づく燃焼制御から化学反応機構の理解に基づく燃焼制御へ

非定常 **混合** **燃焼**

スワール，タンブル

化学反応機構

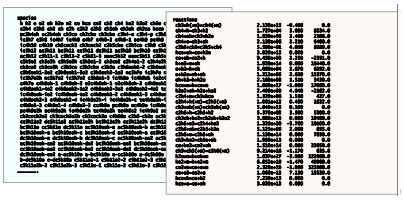
詳細反応を考慮した反応性流体解析技術の必要性

燃焼流シミュレーションの課題

詳細反応を考慮した反応性流体解析は可能か？

- 詳細反応機構の自動生成が既に可能

  e.g., KUCRS, LLNL-CMLS, GRI-mech, Leeds



KUCRS（三好先生）http://www.frad.t.u-tokyo.ac.jp

数百数千の化学種，数万の化学反応

- 詳細反応機構の非定常流体解析への組み込み
  - 化学反応/燃焼に関する解析モデルの簡略化：総括反応，EBU，Flamelet，G-equation
  - 未だ，水素（8化学種程度）に限られることが多い：デトネーション
  - ラージエディシミュレーション（LES）の場合：整合性あるモデル化

Why difficult

Two main issues for introducing detailed chemical kinetics into CFD

1. Stiffness of reactions

- Reaction : Δt=O(1)~O(-14) -- wide range of timescale

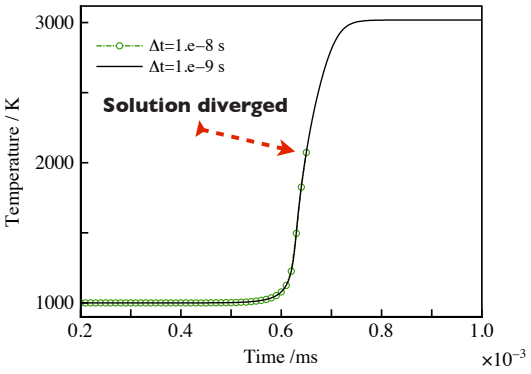
$$dY_k/dt = \dot{\omega}_k/\rho$$
$$dT/dt = -\sum e_k \dot{\omega}_k/(\rho c_v)$$

2. Massive number of the species-mass equations

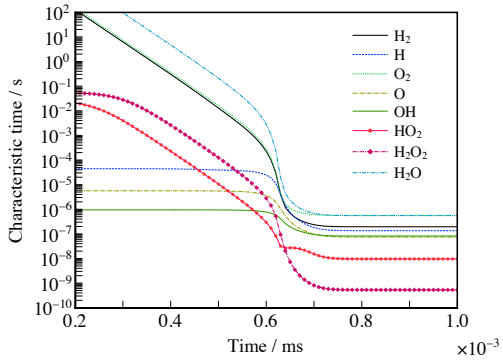
- Proportional to the number of species considered, possibly over 1000 species
- Time-consuming calculations of transport properties for mixture

Stiffness in combustion problems

- Stiffness: difference between maximum and minimum eigenvalues
- H_2/O_2 = 2.0/1.0, T=1000 K, p = 0.1 atm



Temperature history of 0-D H_2/O_2 ignition problem



Characteristic time behavior of each species

❖**Euler explicit method used for time integration**

$$\tau_k = \frac{X_k}{D_k} \quad \text{where} \quad \omega_k = C_k - D_k$$

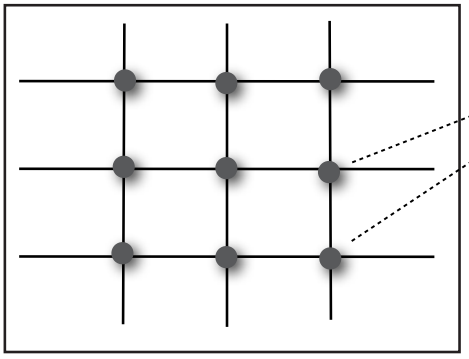
Use of implicit method:VODE

Brown, P.N., G.D. Byrne, and A.C. Hindmarsh, Vode - a Variable-Coefficient Ode Solver. *Siam Journal on Scientific and Statistical Computing*, 1989. 10(5):1038-1051.

- We have useful and powerful packages for stiff system, e.g., VODE, RADAU5

  This is not happened in multidimensional case, i.e., when coupling with CFD

The powerfulness of ODE limited to 0-D problem

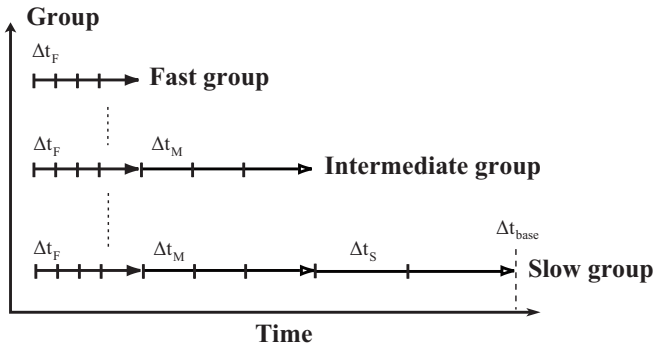


Each grid point has different information:
Start-up cost required

- CPU time would be proportional to at least the square of the number of species: N^2

A dynamic multi-time scale (MTS) method

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



Schematic of MTS

$$\frac{dY_s}{dt} = \frac{\dot{\omega}_s}{\rho},$$
$$\frac{dT}{dt} = -\frac{\sum_{s=1}^{N} e_s \dot{\omega}_s}{\rho c_v},$$

- The characteristic time $\tau_k = \frac{Y_k}{D_k},$

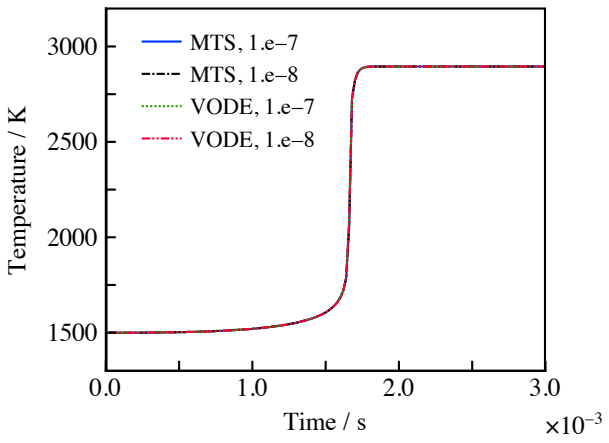
- The time step size determined as $N_k = \max\{0, \lfloor \log_{10}\left(\frac{\Delta t_{base}}{\tau_k}\right) \rfloor\} + 1, \qquad \Delta t_{N_i} = \beta \frac{\Delta t_{base}}{10^{N_i - 1}},$

- The time integration

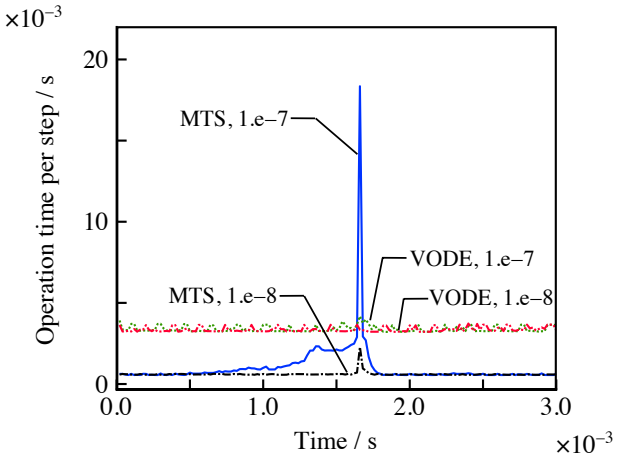
$$Y_k^{(m+1)} = Y_k^{(m)} + \Delta t_{N_i} \frac{\dot{\omega}_k^{(m)}}{\rho^n},$$
$$T^{(m+1)} = T^{(m)} - \Delta t_{N_i} \frac{\sum_{s=1}^{N} e_k^{(m)} \dot{\omega}_k^{(m)}}{\rho^n c_v^{(m)}},$$

Comparison between MTS and VODE

- CH_4/Air, equivalent ratio=1.0, p=1.0 atm, T=1500 K
- Detailed performance of MTS and VODE presented



Temperature profiles



Performance of MTS and VODE: operation time

CPU time comparison

- Computations on iMac, Intel Core i7 (2.93 GHz)

/Air	species #	initial pressure	initial temperature	Δt_{base} 1.e-7 s		Δt_{base} 1.e-8 s	
				save* / %	VODE/MTS s	save* / %	VODE/MTS s
CH_4	68	1	1500	67.2	102 33	83.24	1009 169
		10	1300	54.42	103 47	82.93	1021 174
nC_4H_{10}	146	1	1300	61.18	168 65	90.4	1637 157
		10	1100	61.41	203 78	91.1	1941 172
nC_7H_{16}	373	1	1300	83	893 152	95.99	8128 326
		10	1100	86.24	1064 146	96.6	9507 322

*(VODE-MTS)/VODE*100

New explicit method based on MTS: αMTS

- Idea based on MTS (Gou et al.) and αQSS (Mott et al.)
- Euler method used in the original MTS replaced

$$\frac{dY_k}{dt} = \frac{\dot{\omega}_k}{\rho} = q_k - p_k Y_k$$

$$q_k = \frac{C_k}{\rho}, \quad p_k = \frac{D_k}{\rho Y_k}$$

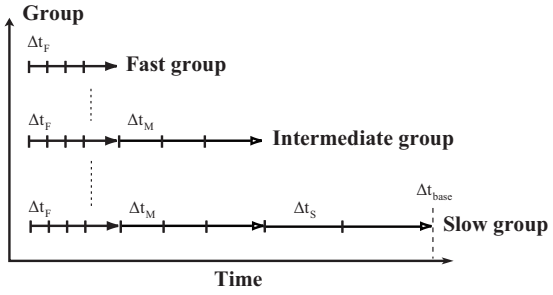
$$Y_k(t) = Y_k^{(0)} e^{-p_k t} + \frac{q_k}{p_k}\left(1 - e^{-p_k t}\right)$$

$$Y_k^{(m+1)} = Y_k^{(m)} e^{-p_k^{(m)} \Delta t_{N_i}} + \frac{q_k^{(m)}}{p_k^{(m)}}\left(1 - e^{-p_k^{(m)} \Delta t_{N_i}}\right)$$

$$= Y_k^{(m)} + \frac{\Delta t_{N_i}\left(q_k^{(m)} - p_k^{(m)} Y_k^{(m)}\right)}{1 + \alpha_k^{(m)} p_k^{(m)} \Delta t_{N_i}}$$

$$Y_k^{(m+1)} = Y_k^{(m)} + \Delta t_{N_i} \frac{\dot{\omega}_k^{(m)}}{\rho^n}$$

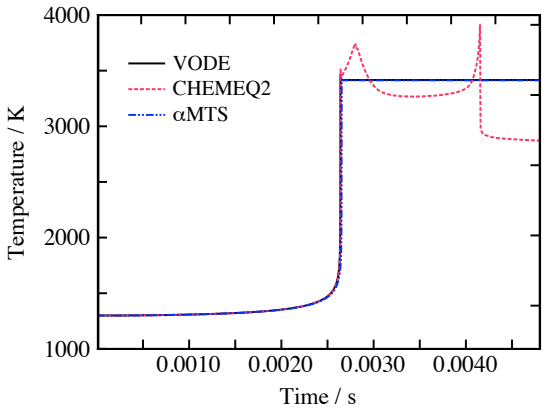
▸Multi-stage Runge-Kutta methods not work



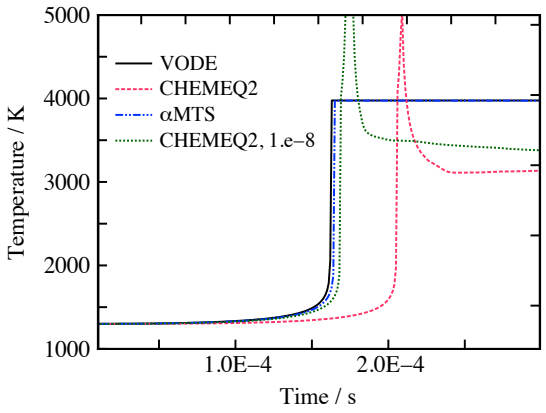
▸Applied to the time integration form in MTS

Performance of new αMTS

- CH_4/O_2, equivalent ratio=1.0, p= 1 and 20 atm, T=1300 K
- The original MTS fails for the conditions
- The time step size: 1.e-7 s



Temperature profiles in p = 1 atm



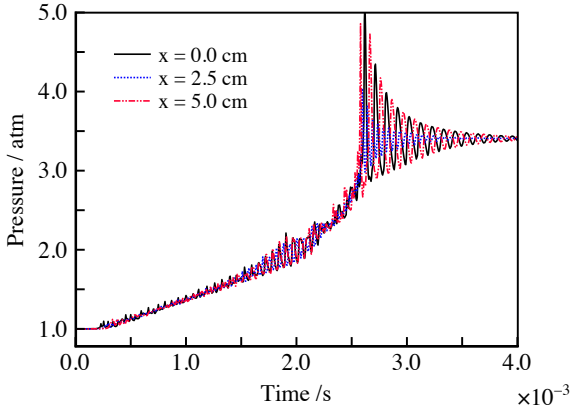
Temperature profiles in p = 20 atm

A faster method with a different concept

- Extend Robust Explicit Numerical Algorithm (ERENA)
  - 森井，寺島，越，清水，第51回燃焼シンポジウム，12月5日（木）

End-gas auto ignition for an example

- n-C_4H_{10}/O_2/Ar premixed gas (Φ=1.0)
- 113 species & 426 reactions mechanism



Pressure histories at three different locations

CPU time comparison on 1-D reactive flow simulation

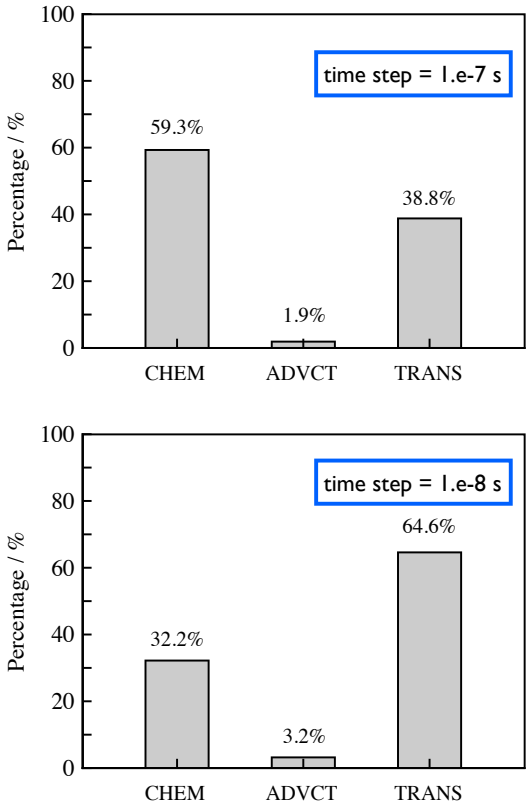
- Computations on Intel Core i7-3960X (3.3 GHz)

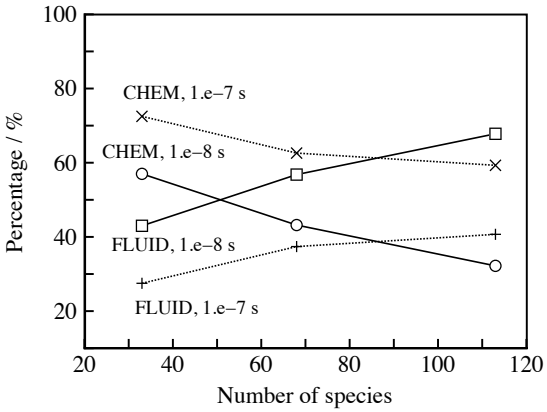
	species #	1.e-7 s		1.e-8 s	
		Save / %	MTS/VODE	Save / %	MTS/VODE
CH_4/O_2/Ar	68	60.5	3077/7791	70	20412/67837
n-C_4H_{10}/O_2/Ar	113	59.3	7626/18762	71.5	46566/163137

*(VODE-MTS)/VODE*100

Chemistry or Fluid

• n-$C_4H_{10}/O_2/Ar$ (113 species)



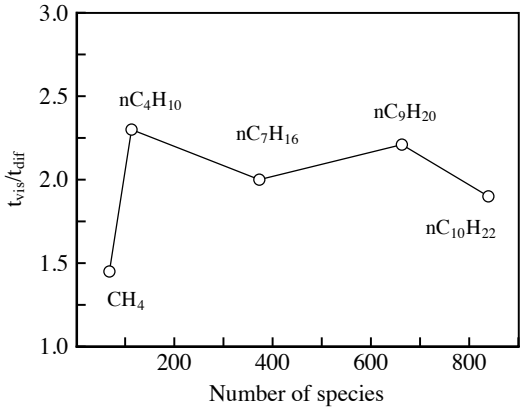


Scaling of the computational times for CHEM and FLUID with three reaction mechanisms

Note: chemistry is always time-consuming with VODE

Mixture of transport properties

•Attention needed in detailed chemistry simulations



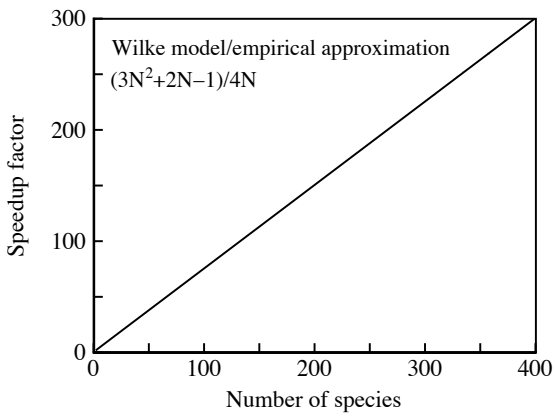
Comparison between costs of viscosity and diffusion coefficients

• Method of Wilke (1950)

$$\mu_m = \sum_{i=1}^{N} \frac{\mu_i}{\sum_{j\neq i}^{N} \frac{X_j}{X_i}\phi_{ij}}$$

• An empirical approximation (~10% error)

$$\mu_m = \frac{1}{2}\left[\sum_{i}^{N} X_i\mu_i + \left(\sum_{i}^{N}\frac{X_i}{\mu_i}\right)^{-1}\right]$$



Comparison between costs of Wilke model and an empirical approximation

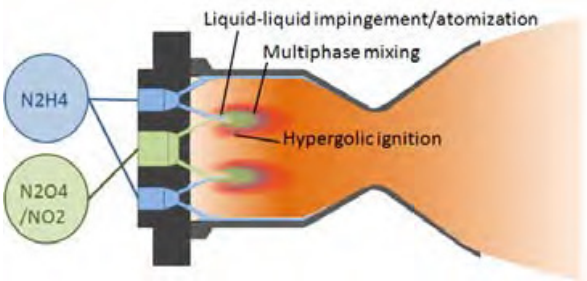
Ongoing work on diffusion coefficients

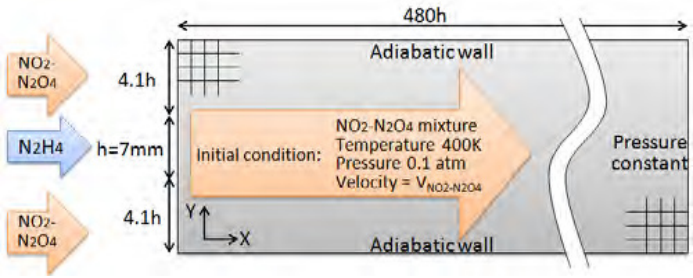
- Care for diffusion coefficients computations still remains; species bundling ?
- Correspondingly, the number of species-mass equations could be reduced in CFD ?

For corporation of large detailed chemistry into CFD, care must be taken of calculation parts which require computational time of N^2

Hydrazine combustion simulations in 2-D

- Application of our reactive flow simulation code with detailed chemistry to space propulsion
- Ongoing work

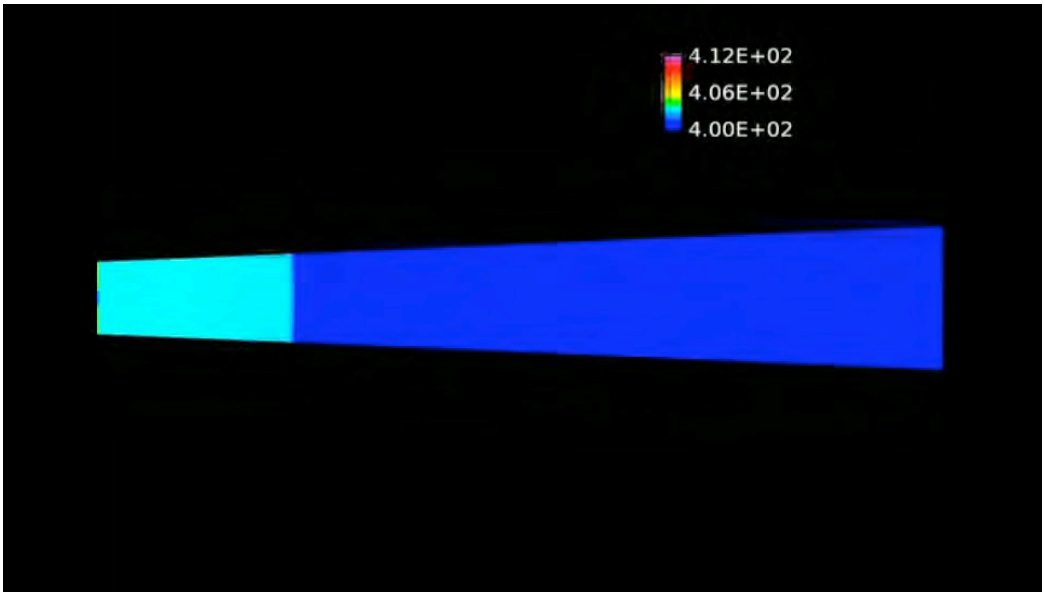




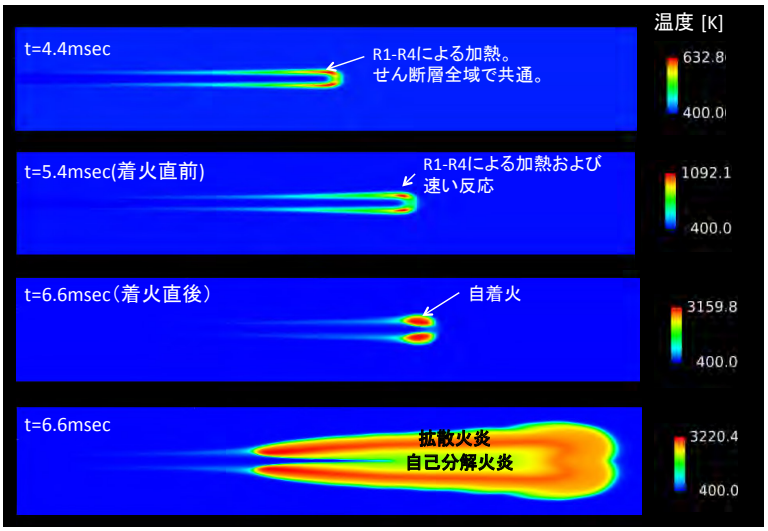
Numerical methods

- Fluid (a compressible N-S equations)
  - HLLC/HLL hybrid solver (Kim et al., 2009) for numerical flux
  - 3rd-order accuracy (MUSCL) with Minmod limiter
  - Central differencing for viscous, heat source, and diffusion terms
  - TVD Runge-Kutta method for the time integration (3rd-order accuracy)
- Chemical reaction (internal energy and volume are constant)
  - ERENA (Morii et al., 2013) for the time integration
  - A detailed mechanism of N_2H_4 (Daimon et al., 2013a, 2013b): 39 species and 261 reactions

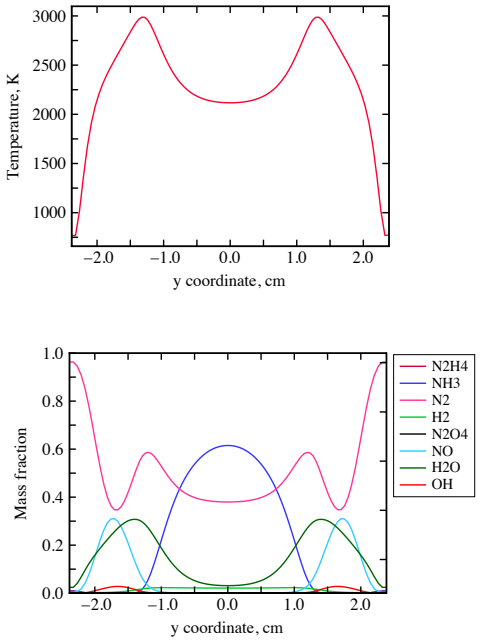
An animation from 2-D simulations



Dynamics and flame structure of hydrazine combustion



Sequence of ignition and flame dynamics



Temperature and mass fractions of several species at a sectional line

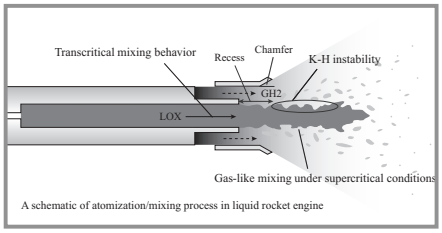
- 谷，寺島，大門，越，第51回燃焼シンポジウム，12月5日（木）

Turbulent combustion modeling for LES

- Need to be addressed in the future
- Developing a model suitable to the fluid/chemistry splitting method

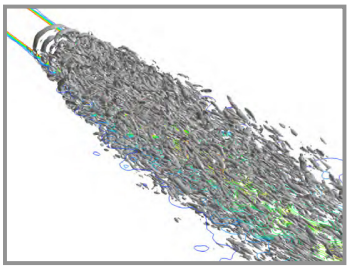
High-pressure and Cryogenic fluid modeling for LRE

- 液体ロケットエンジン噴射器・燃焼室の「超臨界圧」「極低温」流体混合　→　燃焼



A schematic of atomization/mixing process in liquid rocket engine

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = \nabla \cdot (\varrho_\rho \nabla \rho),$$
$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u} + p\boldsymbol{\delta} - \boldsymbol{\tau}) = \nabla \cdot (\varrho_\rho (\boldsymbol{u} \otimes \boldsymbol{g}) \nabla \rho),$$
$$\frac{\partial p}{\partial t} + \boldsymbol{u} \cdot \nabla p = -\rho c^2 \nabla \cdot \boldsymbol{u} + \frac{\alpha_p}{c_v \beta_T} \left(\frac{1}{\rho} \nabla \cdot (\boldsymbol{\tau} \cdot \boldsymbol{u} - \boldsymbol{q}) \right),$$
$$p = \frac{RT}{V - b_{srk}} - \frac{a_{srk}\alpha(T)}{V^2 + b_{srk}V}$$



- AIAA J. (2012), J. Computational Physics (2012), Computers & Fluids (2013), J. Propulsion & Power (2013)
- AIAA Paper 2011-3955 (2011), 2013-712 (2013), EUCASS (2013)

Directions

I.大規模詳細反応機構を組み込むことが可能な反応性流体解析のフレームワークの提案

- 効率的かつ堅牢な時間積分法
- 輸送係数の効率的な取扱い（拡散係数）
- 化学種移流拡散方程式の縮退

I.乱流燃焼モデル（on LES）

- 分離解法に適したモデル

I.反応性流体解析と超臨界圧解析技術との融合

- 高圧（極低温噴射）燃焼

I.燃焼不安定性の解析技術構築

- 大規模解析からの縮退モデルの可能性

I.反応を含む熱境界層の解析