

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

越光男先生, 谷洋海, 大門優, 森井雄飛 各博士

研究ターゲット

▶液体ロケットエンジン

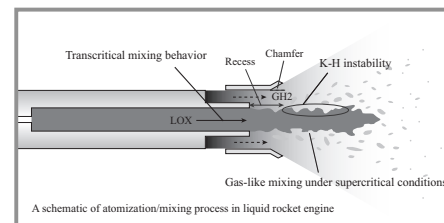
▶衛星スラスター

反応性熱流体现象



-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	<p>UNLINE DOUBLET (1 ON 1) UNLINE DOUBLET (2 ON 1)</p>	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	<p>LINE DOUBLET (1 ON 1)</p>	液/液 LOX/RP-1	H-1, F-1 engines
同軸型	<p>CONCENTRIC TUBE (WITHOUT SWIRLER)</p>	液/ガスor液/液 LOX/GH2, LOX/LH2, LOX/CH4	SSME, LE-7, LE-5 engines



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

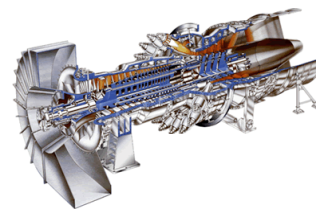
混合

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

Species	Formula	Weight	Order
H	H	1.008	1
OH	OH	17.003	2
H2O	H2O	18.015	3
H2	H2	2.016	4
O2	O2	31.999	5
O	O	15.999	6
HO2	HO2	33.012	7
H2O2	H2O2	34.015	8
CH4	CH4	16.043	9
C2H6	C2H6	30.070	10
C2H4	C2H4	28.054	11
C2H2	C2H2	26.038	12
CO	CO	28.010	13
CO2	CO2	44.010	14
NO	NO	30.006	15
NO2	NO2	46.005	16
HCO	HCO	29.018	17
HCN	HCN	26.038	18
N2	N2	28.014	19
N	N	14.007	20
N2O	N2O	44.013	21
NO2	NO2	46.005	22
NO3	NO3	69.006	23
HNO2	HNO2	47.003	24
HNO	HNO	31.002	25
CH3	CH3	15.023	26
CH2	CH2	14.027	27
CH	CH	13.023	28
C2	C2	24.026	29
C	C	12.011	30
CN	CN	26.027	31
C2N	C2N	39.046	32
C2O	C2O	38.034	33
C3	C3	36.041	34
C3H	C3H	37.045	35
C3H2	C3H2	38.049	36
C3H3	C3H3	39.053	37
C3H4	C3H4	40.057	38
C3H5	C3H5	41.061	39
C3H6	C3H6	42.065	40
C3H7	C3H7	43.069	41
C3H8	C3H8	44.073	42
C3H9	C3H9	45.077	43
C3H10	C3H10	46.081	44
C3H11	C3H11	47.085	45
C3H12	C3H12	48.089	46
C3H13	C3H13	49.093	47
C3H14	C3H14	50.097	48
C3H15	C3H15	51.101	49
C3H16	C3H16	52.105	50
C3H17	C3H17	53.109	51
C3H18	C3H18	54.113	52
C3H19	C3H19	55.117	53
C3H20	C3H20	56.121	54
C3H21	C3H21	57.125	55
C3H22	C3H22	58.129	56
C3H23	C3H23	59.133	57
C3H24	C3H24	60.137	58
C3H25	C3H25	61.141	59
C3H26	C3H26	62.145	60
C3H27	C3H27	63.149	61
C3H28	C3H28	64.153	62
C3H29	C3H29	65.157	63
C3H30	C3H30	66.161	64
C3H31	C3H31	67.165	65
C3H32	C3H32	68.169	66
C3H33	C3H33	69.173	67
C3H34	C3H34	70.177	68
C3H35	C3H35	71.181	69
C3H36	C3H36	72.185	70
C3H37	C3H37	73.189	71
C3H38	C3H38	74.193	72
C3H39	C3H39	75.197	73
C3H40	C3H40	76.201	74
C3H41	C3H41	77.205	75
C3H42	C3H42	78.209	76
C3H43	C3H43	79.213	77
C3H44	C3H44	80.217	78
C3H45	C3H45	81.221	79
C3H46	C3H46	82.225	80
C3H47	C3H47	83.229	81
C3H48	C3H48	84.233	82
C3H49	C3H49	85.237	83
C3H50	C3H50	86.241	84
C3H51	C3H51	87.245	85
C3H52	C3H52	88.249	86
C3H53	C3H53	89.253	87
C3H54	C3H54	90.257	88
C3H55	C3H55	91.261	89
C3H56	C3H56	92.265	90
C3H57	C3H57	93.269	91
C3H58	C3H58	94.273	92
C3H59	C3H59	95.277	93
C3H60	C3H60	96.281	94
C3H61	C3H61	97.285	95
C3H62	C3H62	98.289	96
C3H63	C3H63	99.293	97
C3H64	C3H64	100.297	98
C3H65	C3H65	101.301	99
C3H66	C3H66	102.305	100
C3H67	C3H67	103.309	101
C3H68	C3H68	104.313	102
C3H69	C3H69	105.317	103
C3H70	C3H70	106.321	104
C3H71	C3H71	107.325	105
C3H72	C3H72	108.329	106
C3H73	C3H73	109.333	107
C3H74	C3H74	110.337	108
C3H75	C3H75	111.341	109
C3H76	C3H76	112.345	110
C3H77	C3H77	113.349	111
C3H78	C3H78	114.353	112
C3H79	C3H79	115.357	113
C3H80	C3H80	116.361	114
C3H81	C3H81	117.365	115
C3H82	C3H82	118.369	116
C3H83	C3H83	119.373	117
C3H84	C3H84	120.377	118
C3H85	C3H85	121.381	119
C3H86	C3H86	122.385	120
C3H87	C3H87	123.389	121
C3H88	C3H88	124.393	122
C3H89	C3H89	125.397	123
C3H90	C3H90	126.401	124
C3H91	C3H91	127.405	125
C3H92	C3H92	128.409	126
C3H93	C3H93	129.413	127
C3H94	C3H94	130.417	128
C3H95	C3H95	131.421	129
C3H96	C3H96	132.425	130
C3H97	C3H97	133.429	131
C3H98	C3H98	134.433	132
C3H99	C3H99	135.437	133
C3H100	C3H100	136.441	134

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 : $\Delta t = O(1) \sim O(-14)$ -- wide range of timescale

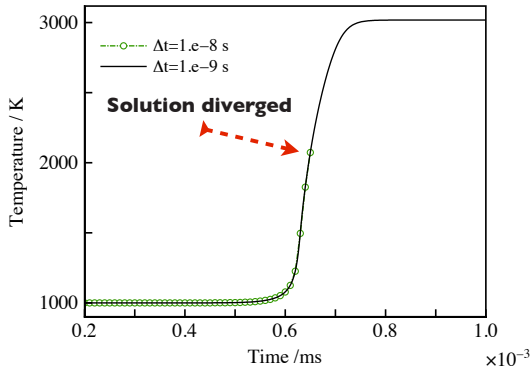
$$\begin{aligned} dY_k/dt &= \dot{\omega}_k/\rho \\ dT/dt &= - \sum e_k \dot{\omega}_k / (\rho c_v) \end{aligned}$$

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

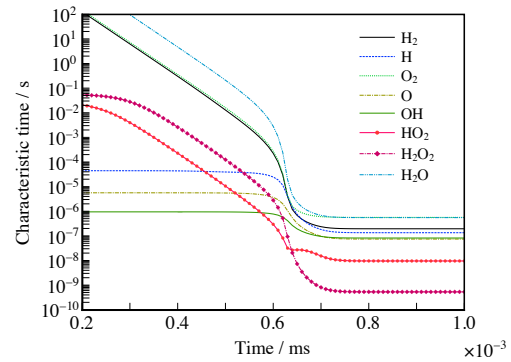
Stiffness in combustion problems

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



Temperature history of 0-D H_2/O_2 ignition problem

❖ Euler explicit method used for time integration



Characteristic time behavior of each species

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

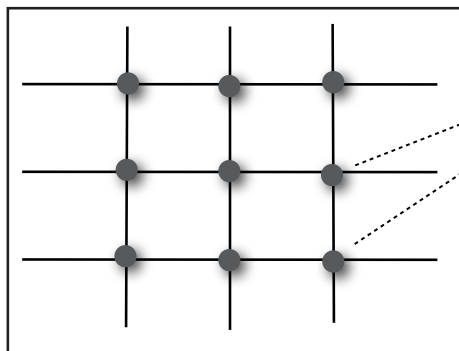
Use of implicit method:VODE

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

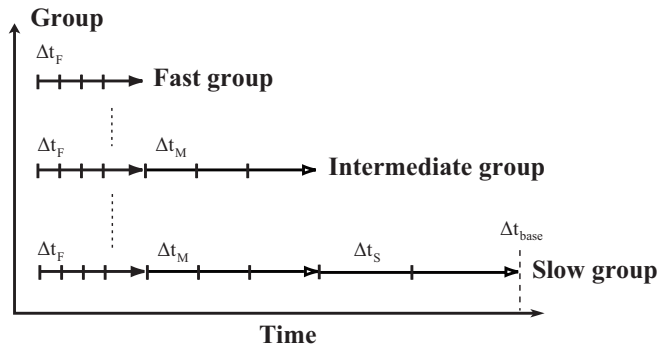


Each grid point has different information:
Start-up cost required

- 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



$$\frac{dY_s}{dt} = \frac{\dot{\omega}_s}{\rho},$$

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

Schematic of MTS

- The characteristic time

$$\tau_k = \frac{Y_k}{D_k},$$

- The time step size determined as

$$N_k = \max\{0, \lfloor \log_{10} \left(\frac{\Delta t_{base}}{\tau_k} \right) \rfloor\} + 1, \quad \Delta t_{N_i} = \beta \frac{\Delta t_{base}}{10^{N_i-1}},$$

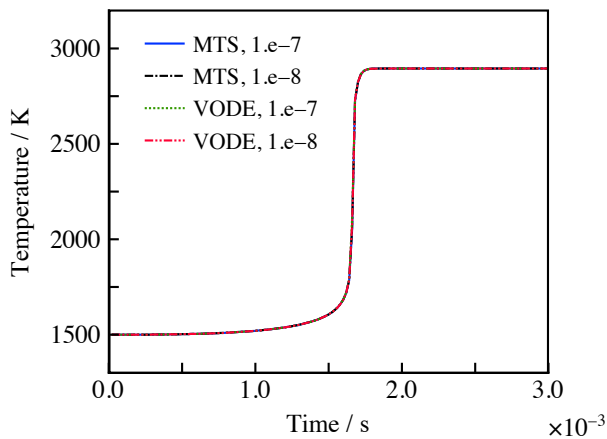
- The time integration

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

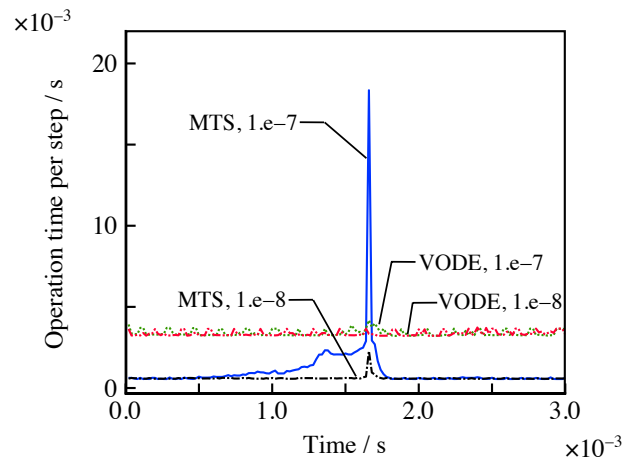
$$T^{(m+1)} = T^{(m)} - \Delta t_{N_i} \frac{\sum_{s=1}^N e_k^{(m)} \dot{\omega}_k^{(m)}}{\rho^n c_v^{(m)}},$$

Comparison between MTS and VODE

- CH₄/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	83.24	1009
					33		169
		10	1300	54.42	103	82.93	1021
					47		174
nC ₄ H ₁₀	146	1	1300	61.18	168	90.4	1637
					65		157
		10	1100	61.41	203	91.1	1941
					78		172
nC ₇ H ₁₆	373	1	1300	83	893	95.99	8128
					152		326
		10	1100	86.24	1064	96.6	9507
					146		322

*(VODE-MTS)/VODE*100

New explicit method based on MTS: α MTS

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

$$\frac{dY_k}{dt} = \frac{\dot{\omega}_k}{\rho}$$

$$= q_k - p_k Y_k$$

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

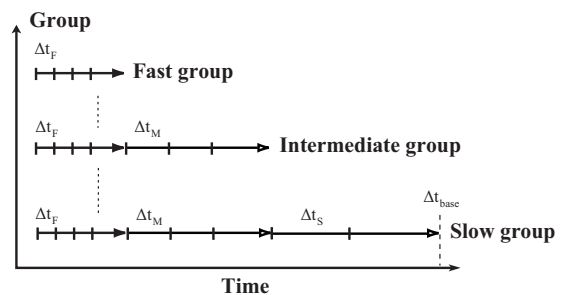
$$Y_k(t) = Y_k^{(0)} e^{-p_k t} + \frac{q_k}{p_k} (1 - e^{-p_k t})$$

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

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

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

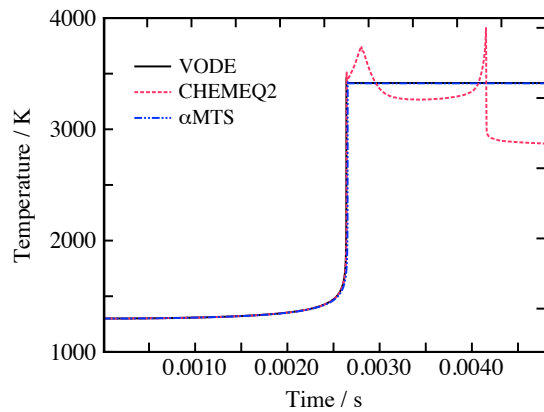
► Multi-stage Runge-Kutta methods not work



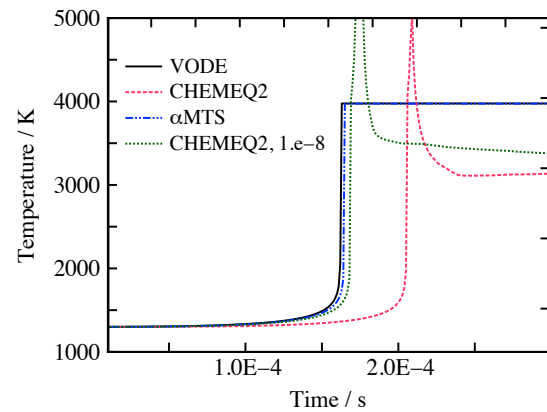
► Applied to the time integration form in MTS

Performance of new α MTS

- 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



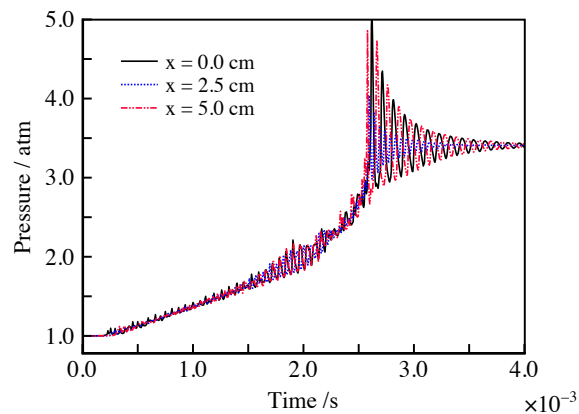
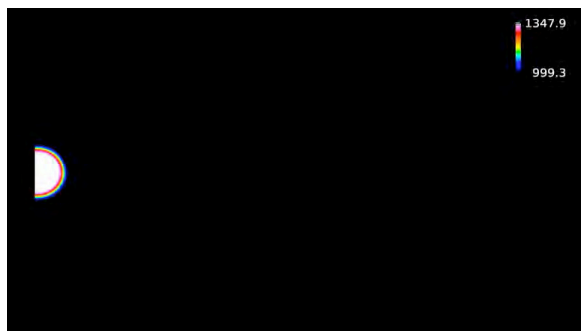
Temperature profiles in $p = 20$ atm

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-C₄H₁₀/O₂/Ar premixed gas ($\Phi=1.0$)
- 113 species & 426 reactions mechanism



Pressure histories at three different locations

CPU time comparison on 1-D reactive flow simulation

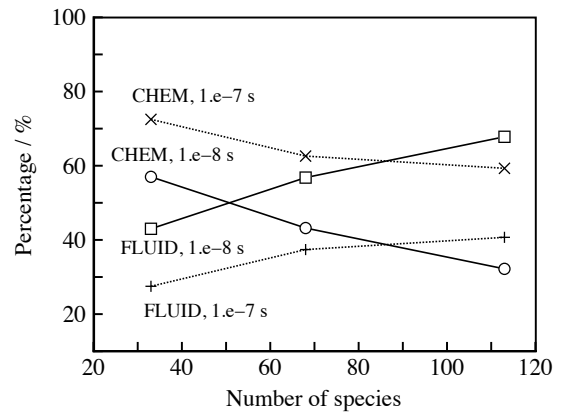
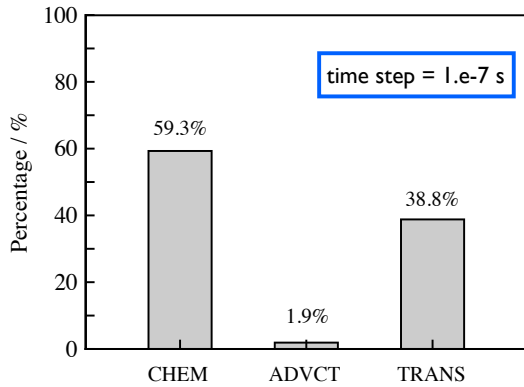
- Computations on Intel Core i7-3960X (3.3 GHz)

	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 ₄ H ₁₀ /O ₂ /Ar	113	59.3	7626/18762	71.5	46566/163137

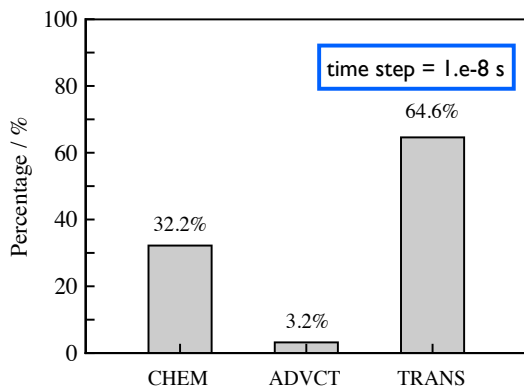
*(VODE-MTS)/VODE*100

Chemistry or Fluid

• n-C₄H₁₀/O₂/Ar (113 species)



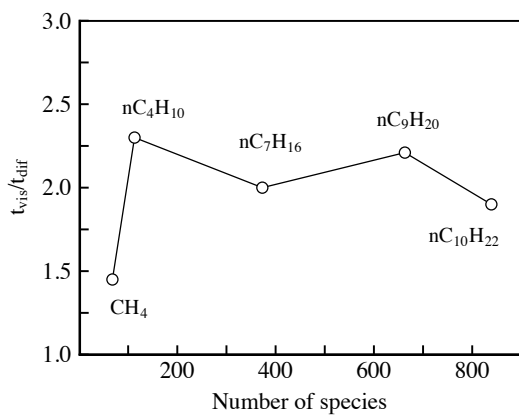
Scaling of the computational times for CHEM and FLUID with three reaction mechanisms



Note: chemistry is always time-consuming with VODE

Mixture of transport properties

• Attention needed in detailed chemistry simulations



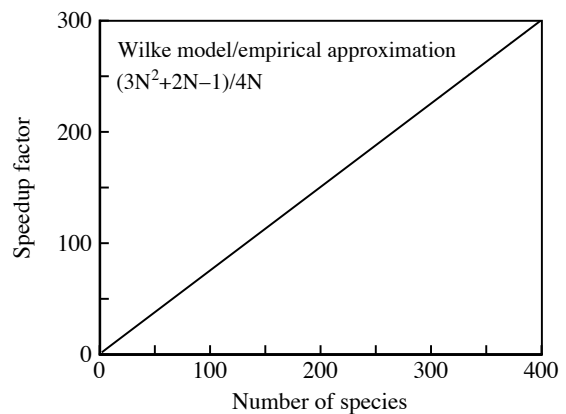
Comparison between costs of viscosity and diffusion coefficients

• 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

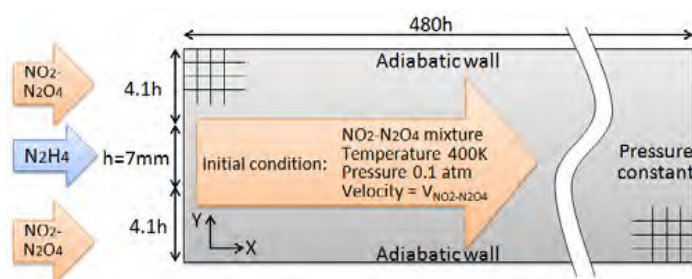
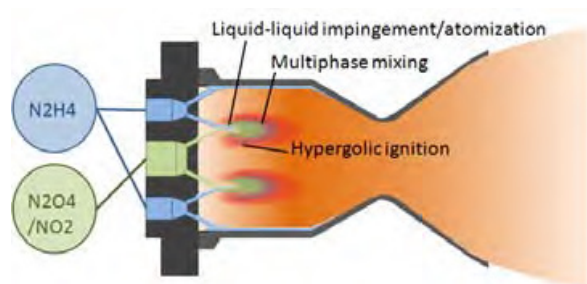
Ongoing work on diffusion coefficients

- 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

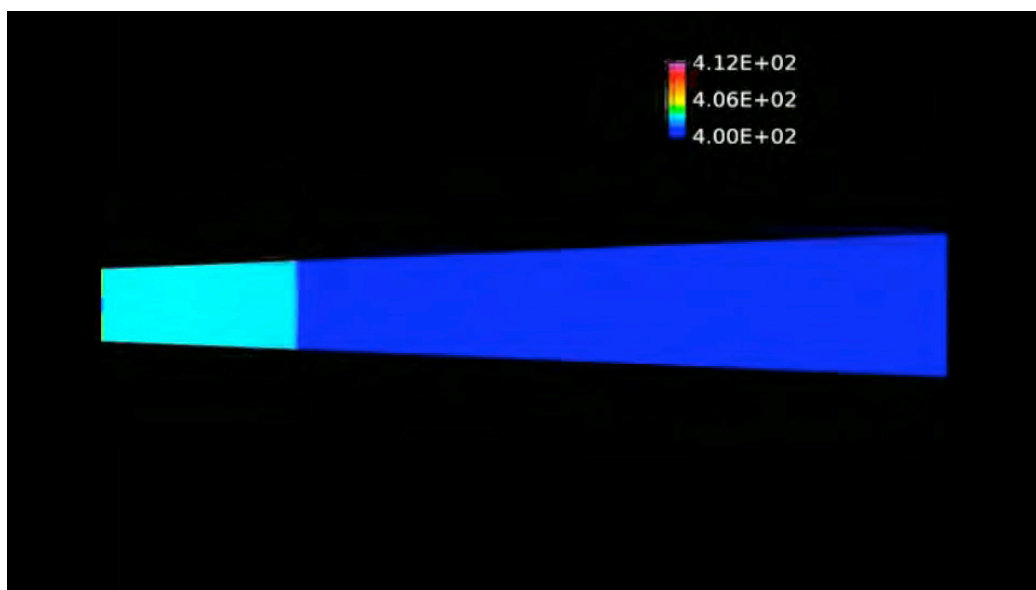
▶ Fluid (a compressible N-S equations)

- 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)

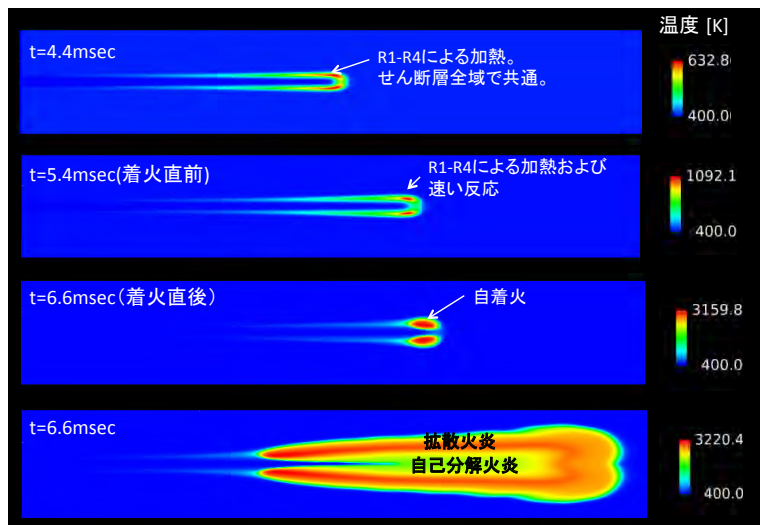
▶ Chemical reaction (internal energy and volume are constant)

- 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

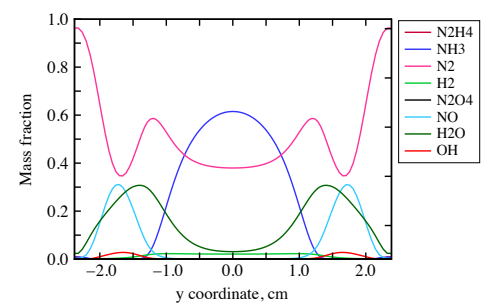
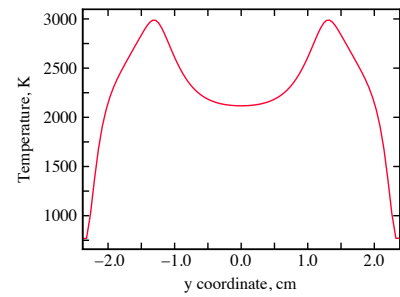
An animation from 2-D simulations



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)

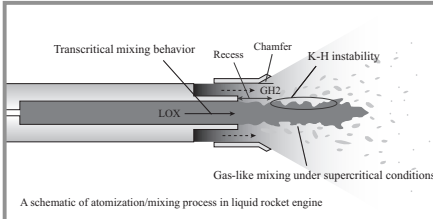
Turbulent combustion modeling for LES

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

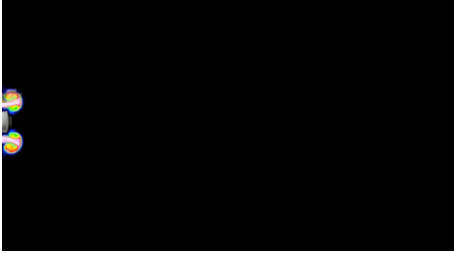
High-pressure and Cryogenic fluid modeling for LRE

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





A schematic of atomization/mixing process in liquid rocket engine



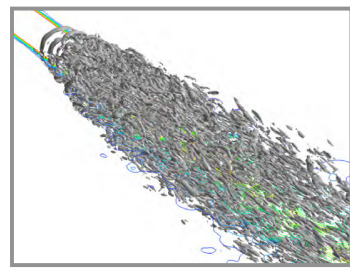
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \nabla \cdot (\rho \nabla \rho),$$

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

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

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

- 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. 乱流燃烧モデル (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) 燃烧

I. 燃烧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