



NEXTFOAM

CFD Engineering Consulting

The 11th Asian Joint Conference on Propulsion and Power

Numerical study of reacting flow for bi-propellant thrust

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- **Introduction**
 - Space Pioneer Program
 - Objective
- **Reduced Reaction Mechanism**
 - Development
 - Verification
- **10N Thruster Performance**
 - Numerical Method
 - Results & Analysis
- **Conclusion**

Introduction : Space Pioneer Program

- Space Pioneer: Localizing space core components
- Including 16 projects
- One of which: **Bi-propellant thruster** development

- Feature

Development of a binary propellant thruster using **fuel (MMH)** and **oxidizer (NTO)**

Used for various missions such as geostationary satellites, lunar landers, and deep space exploration

Provides velocity augmentation (ΔV) required for satellite orbit movement and attitude control

Manufactured using rare alloy (Pt/Rh or Pt/Ir) metal 3D printing

Establish thruster design/analysis/manufacture/process/assembly/test procedures

Establishment substitution effect/cost reduction/social and economic profit improvement expected through localization

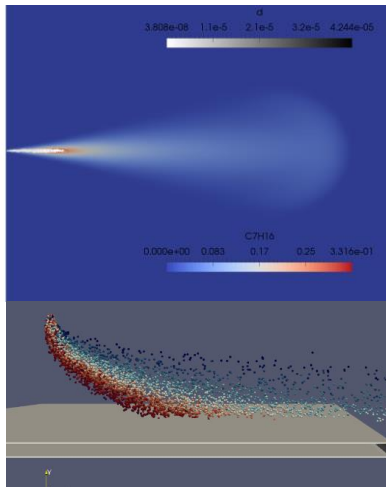


Responsible for development of combustion analysis software

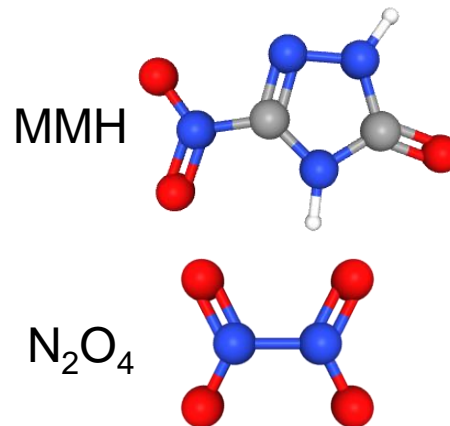
Introduction : Objective

- Development of **Combustion Analysis S/W** of Bipropellant Thruster
 - MMH/NTO reduced reaction mechanism
 - Combustion analysis solver

[Spray]



[Hypergolic chemistry]



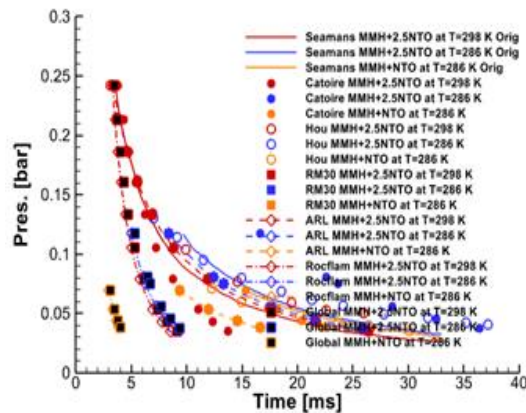
[Conjugate Heat Transfer]



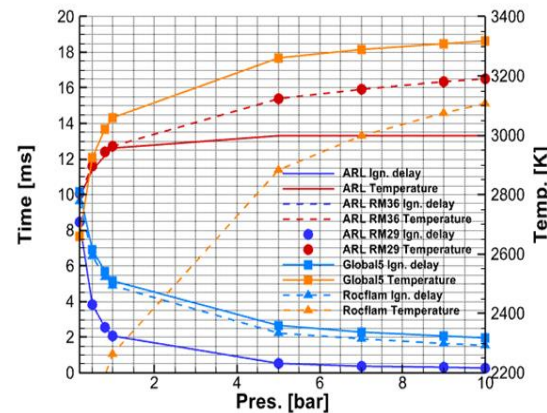
Reduced Mechanism Development

- Mechanism of previous research:

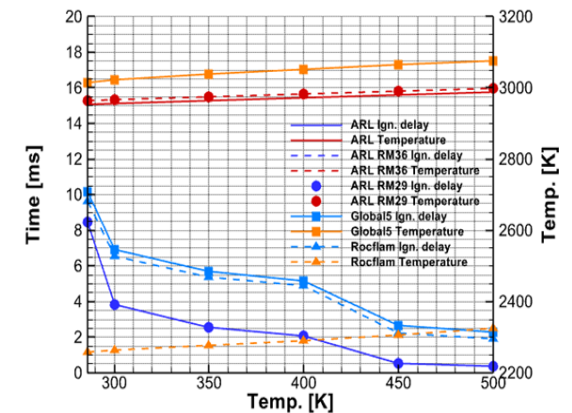
- Anderson(2010) : 81 species, 513 reactions
- Wei(2019) : 29 species, 36 reactions (Reduced model of Anderson)
- Hou(2018) : 23 species, 20 reactions
- Catoire : 81 species, 399 reactions
- Catoire(2004) : 11 species, 7 reactions (Reduced model of Catoire)
- RocFlam-II(1998) : 13 species, 10 reactions



[Ignition delay-pressure curve]



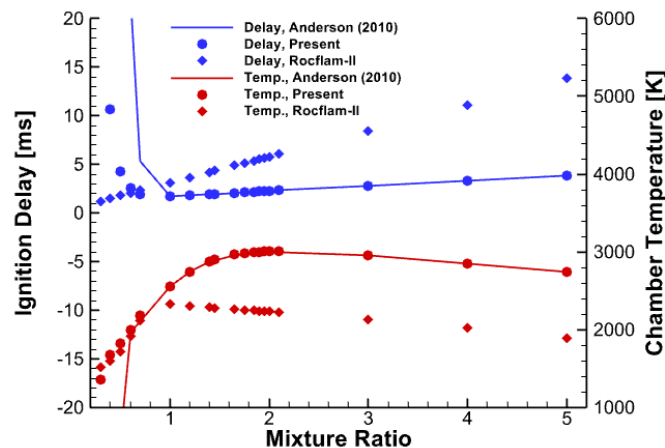
[pressure dependency(MR=1.65, 300K)]



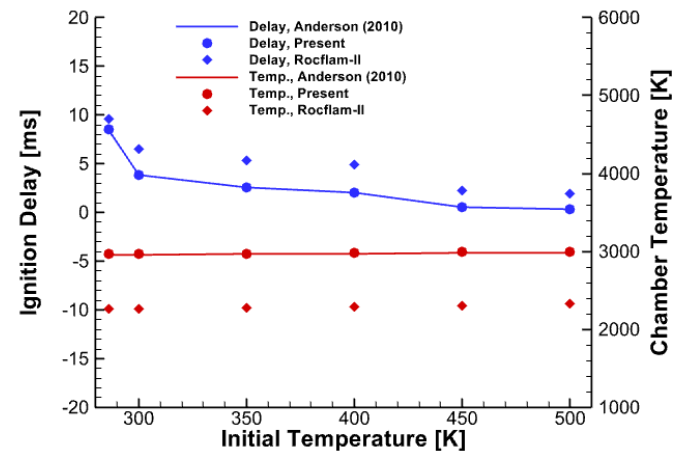
[Temperature dependency(MR=1.65, 1bar)]

Reduced Mechanism Development

- New mechanism:
 - NextFOAM(2022) : **31** species, **29** reactions
 - reduced mechanism of Anderson's full chemistry
 - developed using try and error method
 - cites Arrhenius parameter from **Anderson's** study
 - cites mostly from **Burcat's** gas property
 - cites from **Marinov's** gas property HNNO and CH3O2H
 - cites from **Catoire's** gas property CH3NNH



[Dependency of mixture ratio(1bar, 300K)]



[Dependency of initial temperature(1bar, MR=1.65)]

Reduced Mechanism Development

- Reaction equations of 29 reaction steps

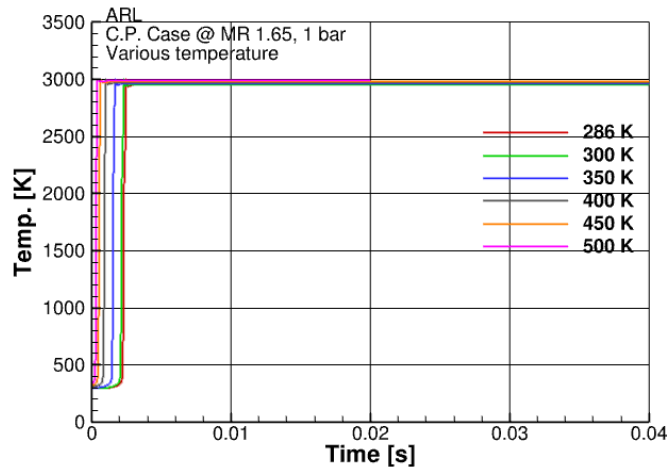
No.	Reaction	No.	Reaction
R1	$\text{N}_2\text{O}_4(+\text{M})=\text{NO}_2+\text{NO}_2(+\text{M})$	R16	$\text{H}+\text{OH}+\text{M}=\text{H}_2\text{O}+\text{M}$
R2	$\text{CH}_3\text{NHNH}_2=\text{CH}_3\text{NNH}+\text{H}_2$	R17	$\text{HCN}+\text{O}=\text{NH}+\text{CO}$
R3	$\text{CH}_3\text{NHNH}_2+\text{NO}_2=\text{CH}_3\text{NNH}_2+\text{HONO}$	R18	$\text{N}+\text{H}_2=\text{NH}+\text{H}$
R4	$\text{CH}_3\text{NNH}_2+\text{NO}_2=\text{CH}_3\text{NNH}+\text{HONO}$	R19	$\text{N}+\text{NO}=\text{N}_2+\text{O}$
R5	$\text{CH}_3\text{NNH}+\text{NO}_2=\text{CH}_3\text{NN}+\text{HONO}$	R20	$\text{NO}+\text{H}=\text{N}+\text{OH}$
R6	$\text{CH}_3\text{NNH}+\text{CH}_3=\text{CH}_4+\text{CH}_3\text{NN}$	R21	$\text{H}+\text{CH}_3(+\text{M})\rightleftharpoons\text{CH}_4(+\text{M})$
R7	$\text{CH}_3\text{NN}=\text{CH}_3+\text{N}_2$	R22	$\text{H}+\text{CH}_4\rightleftharpoons\text{CH}_3+\text{H}_2$
R8	$\text{NO}+\text{OH}(+\text{M})=\text{HONO}(+\text{M})$	R23	$\text{OH}+\text{CH}_4\rightleftharpoons\text{CH}_3+\text{H}_2\text{O}$
R9	$\text{HONO}+\text{OH}=\text{H}_2\text{O}+\text{NO}_2$	R24	$\text{OH}+\text{CH}_2\text{O}\rightleftharpoons\text{HCO}+\text{H}_2\text{O}$
R10	$\text{NO}_2+\text{H}=\text{NO}+\text{OH}$	R25	$\text{CH}_3+\text{NO}\rightleftharpoons\text{HCN}+\text{H}_2\text{O}$
R11	$\text{NO}_2+\text{O}=\text{NO}+\text{O}_2$	R26	$\text{CH}_4+\text{NO}_2=\text{CH}_3+\text{HONO}$
R12	$\text{HCO}+\text{M}=\text{H}+\text{CO}+\text{M}$	R27	$\text{CH}_3+\text{NO}_2=\text{CH}_3\text{O}+\text{NO}$
R13	$\text{CO}+\text{OH}=\text{CO}_2+\text{H}$	R28	$\text{CH}_3\text{O}+\text{NO}_2=\text{CH}_2\text{O}+\text{HONO}$
R14	$\text{O}+\text{H}_2=\text{OH}+\text{H}$	R29	$\text{CH}_3\text{O}+\text{NO}_2(+\text{M})=\text{CH}_3\text{ONO}_2(+\text{M})$
R15	$\text{OH}+\text{OH}=\text{H}_2\text{O}+\text{O}$		

- decomposition of NTO (R1)
- decomposition of MMH (R2); the path $\text{MMH}\rightarrow\text{CH}_3\text{NNH}_2\rightarrow\text{CH}_3\text{NNH}\rightarrow\text{CH}_3\text{NN}\rightarrow\text{CH}_3$ (R3–R7)
- conversions between HONO, NO, and NO₂ (R8–R12)
- important reactions of CH₄ chemistry; the path $\text{CH}_3\rightarrow\text{CH}_3\text{O}\rightarrow\text{CH}_2\text{O}\rightarrow\text{HCO}\rightarrow\text{CO}\rightarrow\text{CO}_2$ (R13–R29)

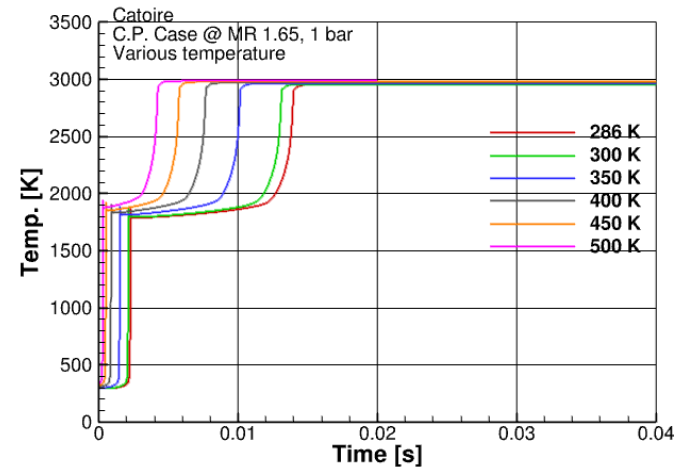
Mechanism Verification

- 0D analysis (temperature dependency)

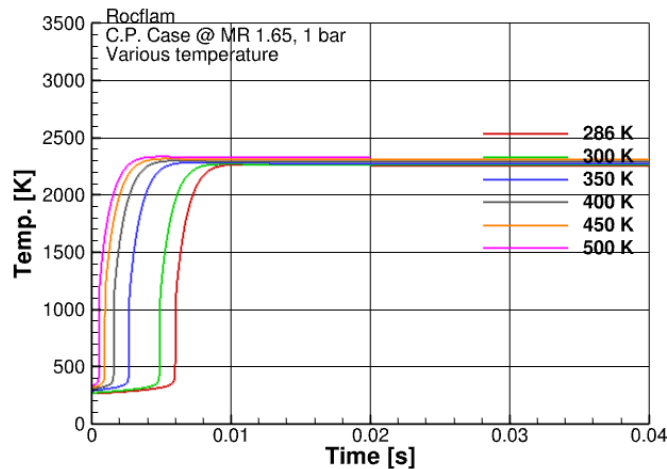
Anderson



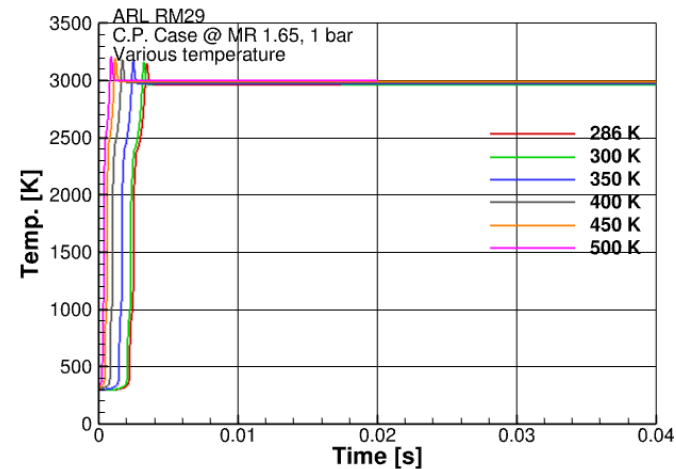
Catoire



Rocflam



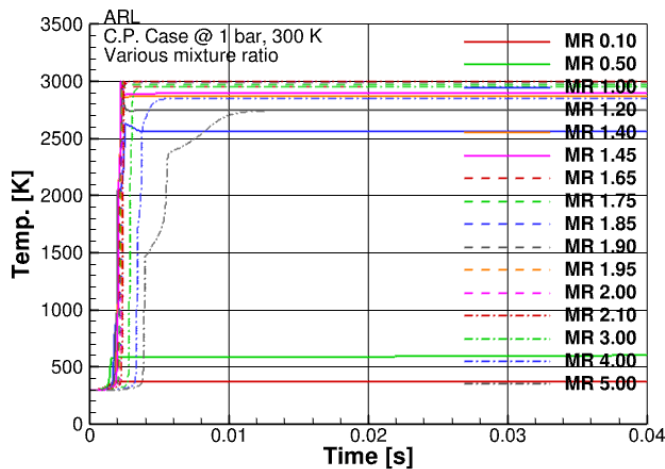
Present
(RM29)



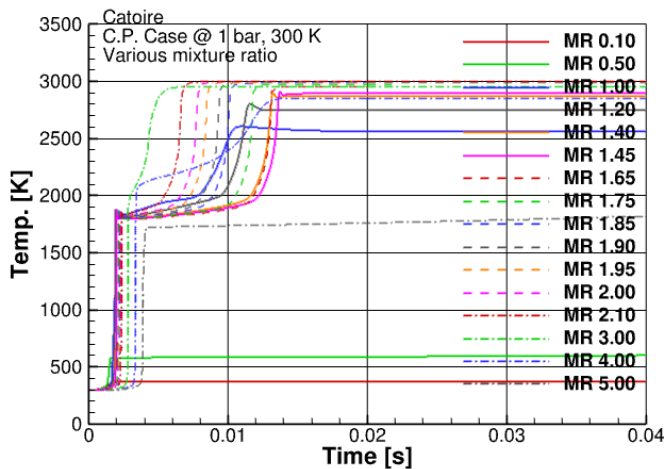
Mechanism Verification

- 0D analysis (mixture ratio dependency)

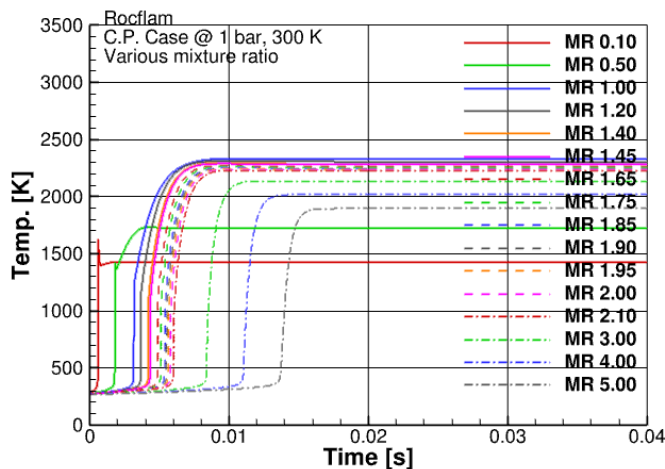
Anderson



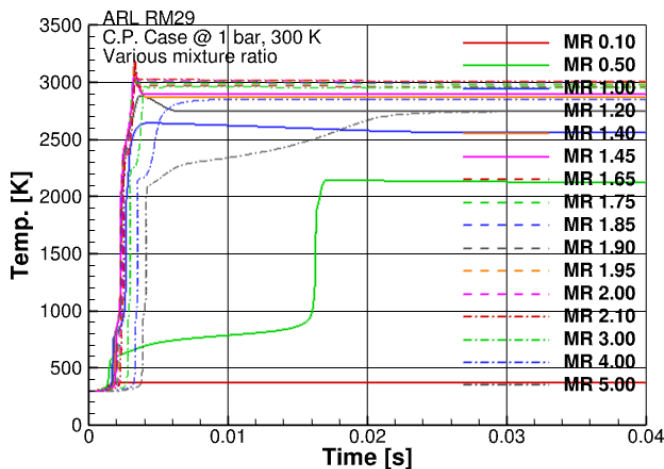
Catoire



Rocflam

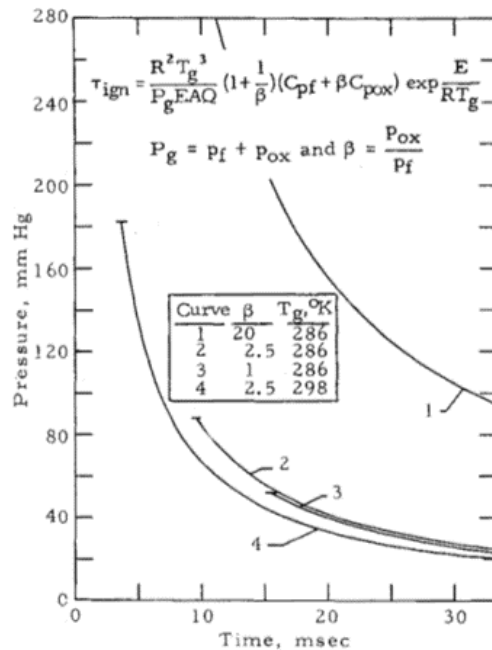


Present
(RM29)

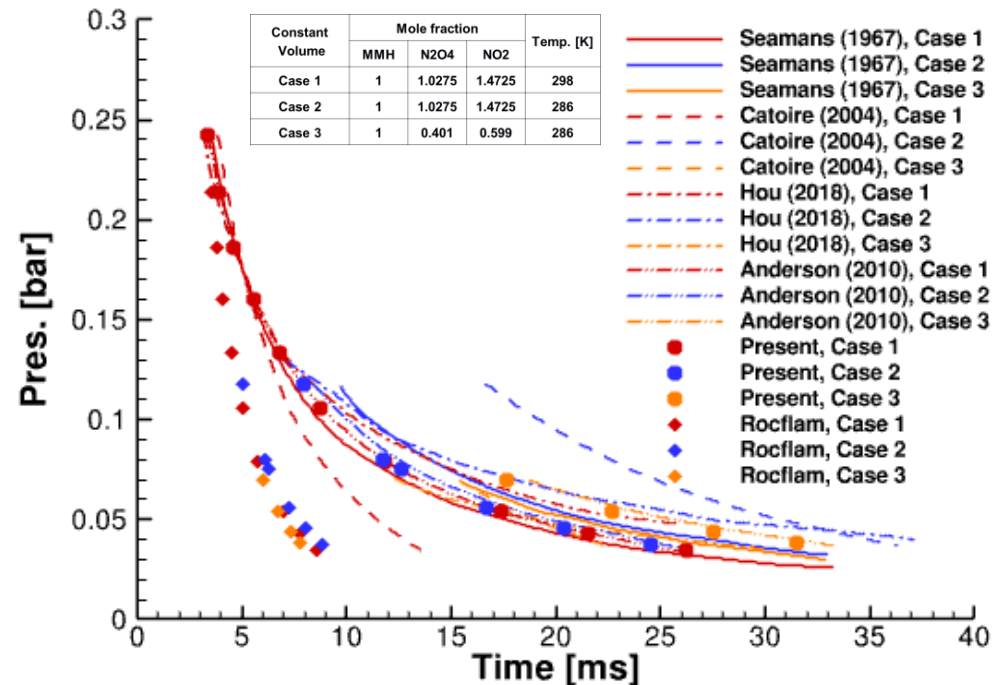


Mechanism Verification

- 0D analysis (low pressure dependency)
 - T.F. Seamans(1967, *AIAA Journal* 5(9), 1616-1624)
 - Explain the spontaneous ignition process of MMH/NTO



[Seamans results]



[Ignition delay-pressure curve]

Mechanism Verification

- Cantera – 1D diffusion flame

- J. Hayashi(2019, *Combustion and Flame* 201, 244-251)

Table 2

Calculation conditions of the axisymmetric one-dimensional steady state counterflow pool flame.

	Oxidizer	Fuel
Composition [mole fraction]	$\text{NO}_2:\text{N}_2\text{O}_4 = 0.52:0.48$	MMH
Temperature [K]	318.75	346.76 ^a
Flow rate [g/s]	0.21	0.024 ^a

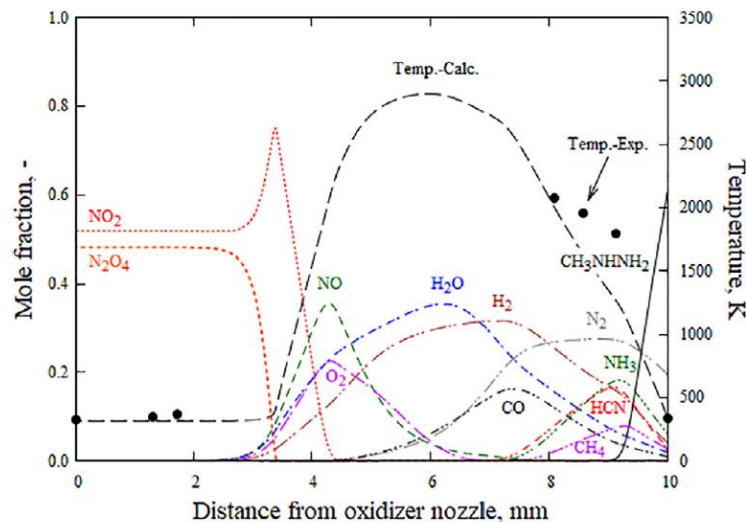
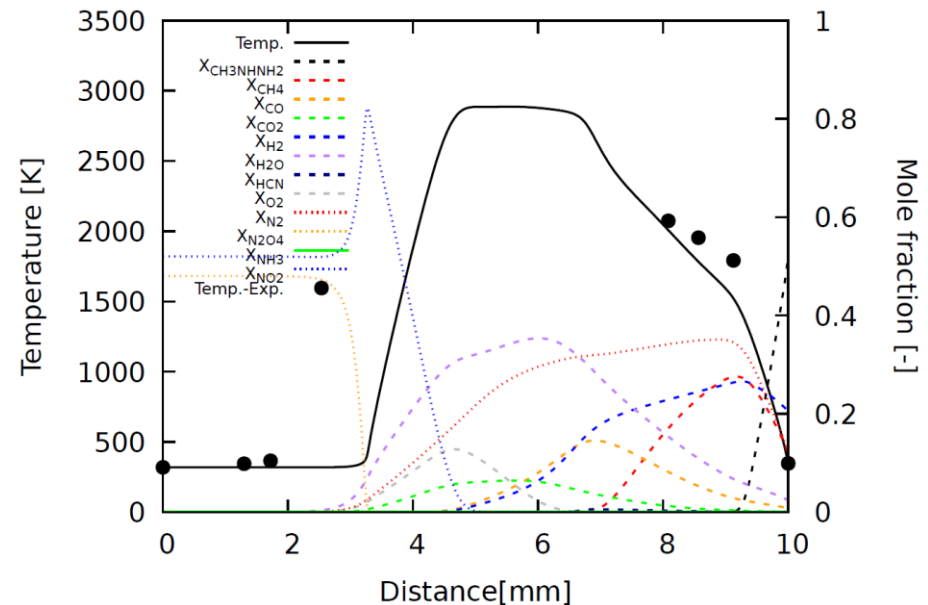


Fig. 9. Axial distribution of temperature and major species obtained by CANtera for MMH/NTO combustion. (Dots indicate temperature measured by thermocouple).

Present result



Mechanism Verification

- OpenFOAM – 2D counter flow
 - J. Hayashi(2019, *Combustion and Flame* 201, 244-251)

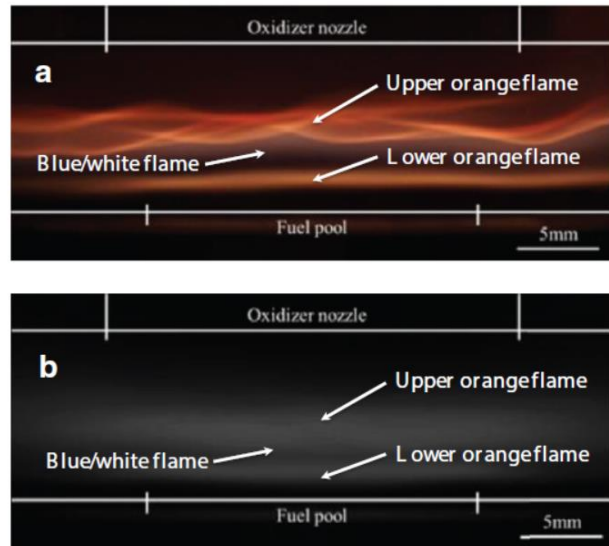
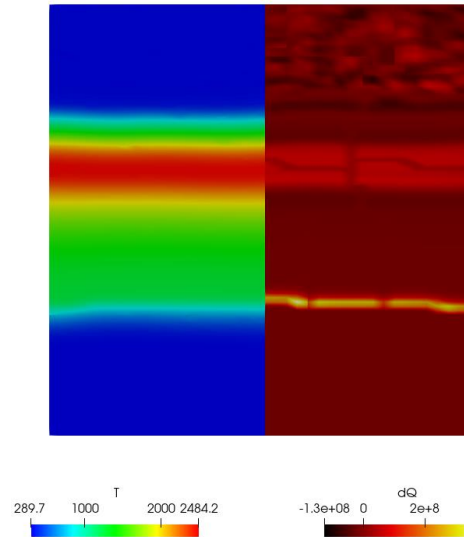
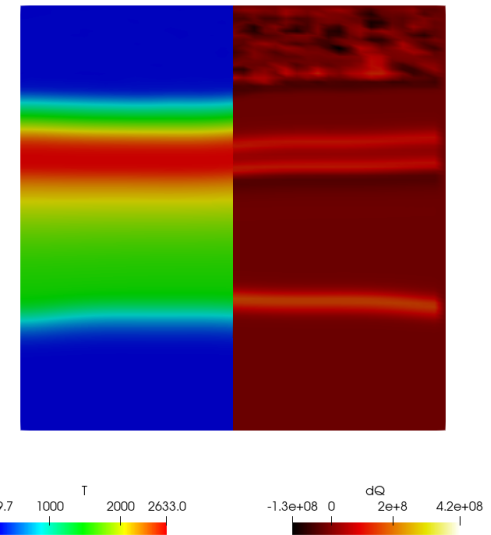


Fig. 6. Broad band photograph of MMH-NTO flame and averaged image of MMH-NTO flame (a) instantaneous image, (b) averaged image of 3000 frames in grayscale. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

Anderson Mechanism



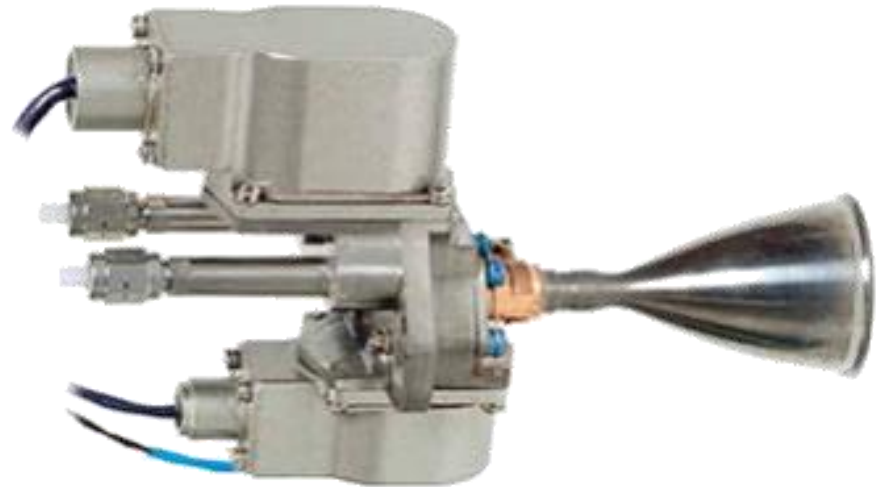
Present mechanism



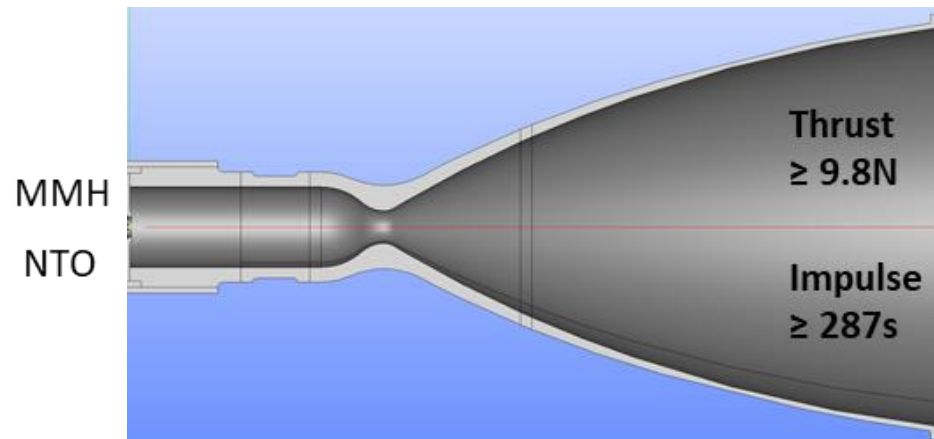
10N Thruster Performance

- **Target performance**

- Vacuum thrust $\geq 9.9 \text{ N} \pm 0.2 \text{ N}$
- Vacuum specific impulse $\geq 287 \text{ s}$



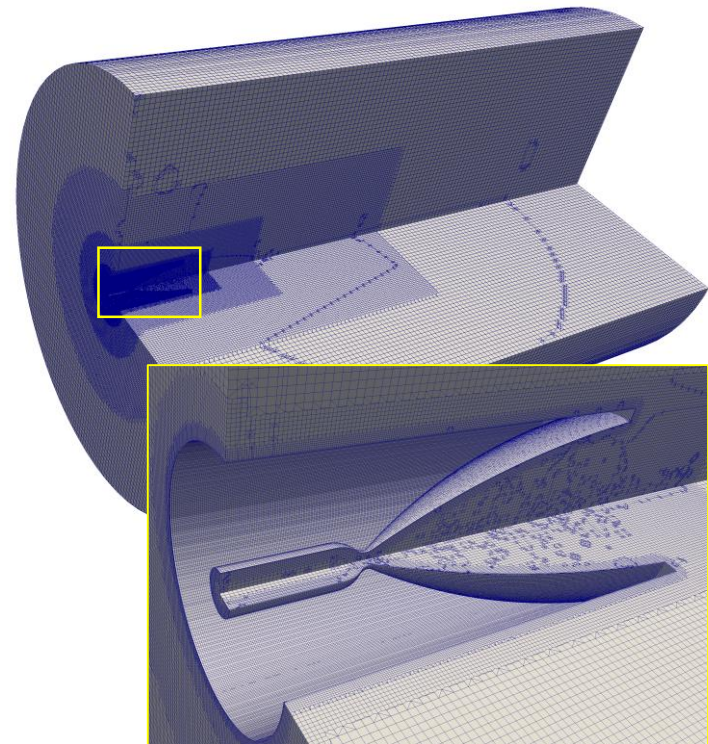
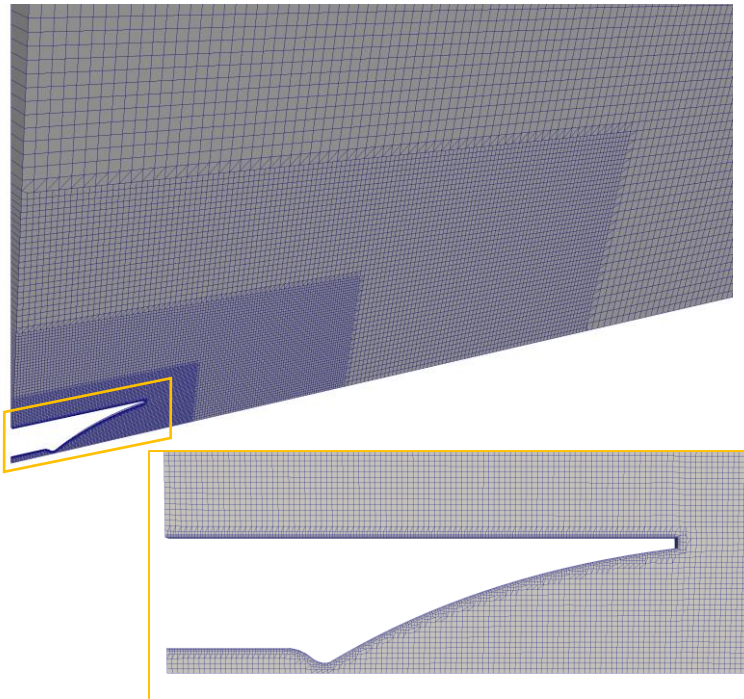
[10N Biprop Thruster S10-18]



[Section view of thruster]

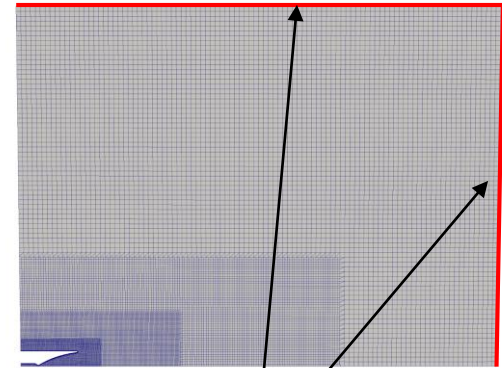
10N Thruster Performance

- **Mesh generation**– snappyHexMesh(unstructured)
- 2D axis symmetry mesh
 - 25,000 cells
- 3D mesh
 - 5,440,000 cells



10N Thruster Performance

- Solver: pimpleCentralFoam (OpenFOAM)
 - pressure-based semi-implicit compressive viscous fluids
- Turbulent model: k- ω SST
- Single species non-reacting analysis
- Initial conditions
 - Chamber pressure: 9 bar
 - Chamber temperature: 3163.25 K
 - Ambient pressure: 5 mbar
 - waveTransmissive boundary condition



waveTransmissive B.C.

10N Thruster Performance

- **Non-reflecting** boundary condition
 - waveTransmissive B.C.

Non-reflecting B.C.

Time: 0.0000 sec



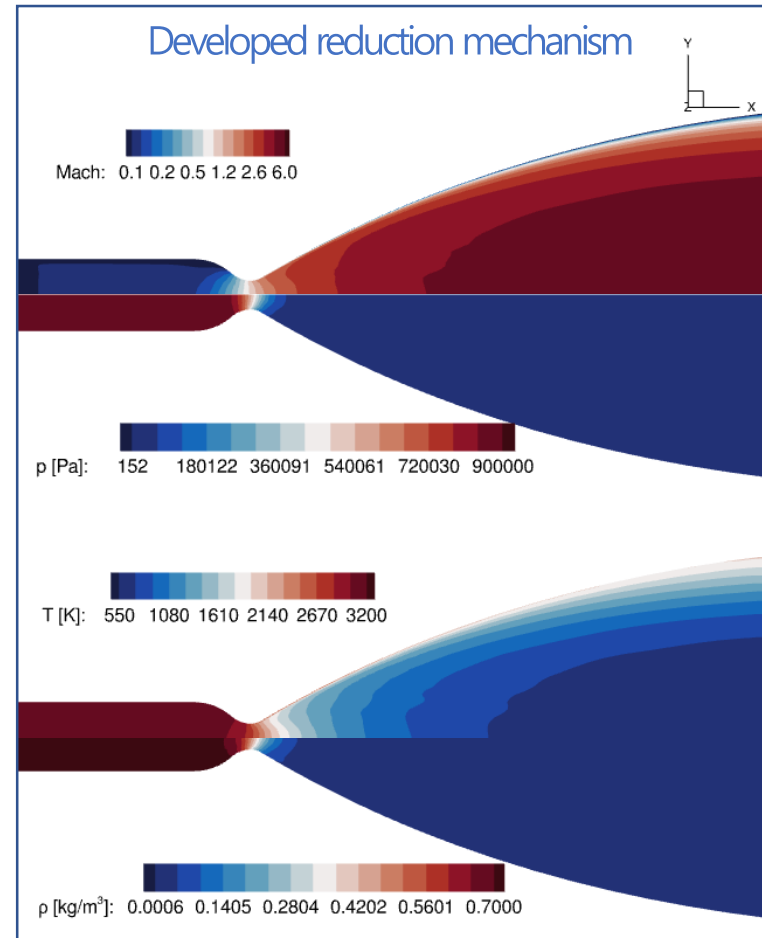
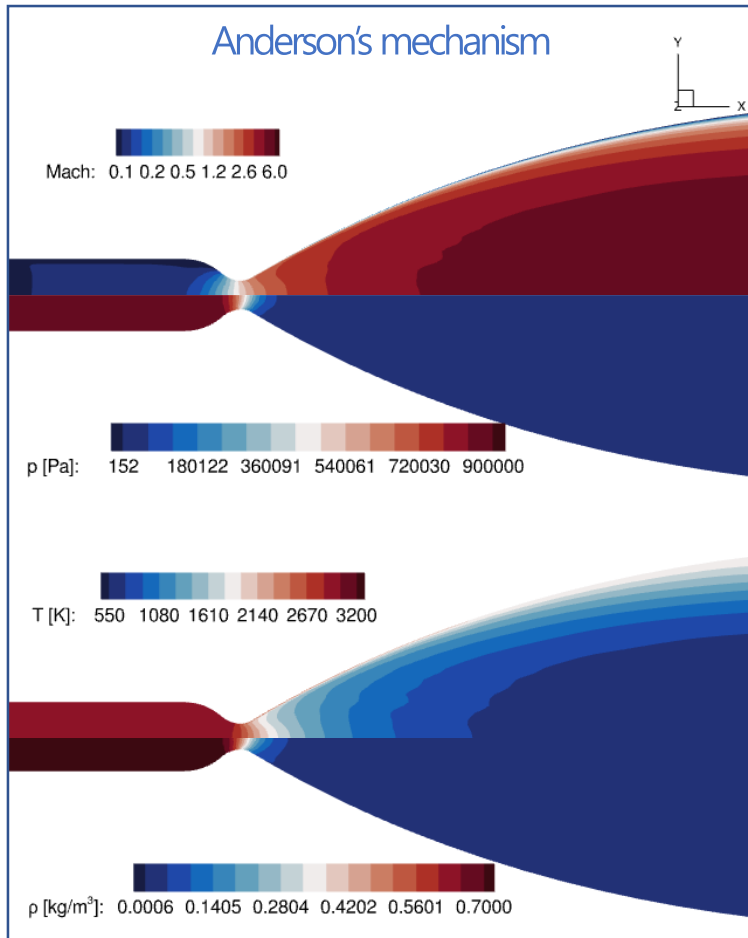
Reflecting B.C.

Time: 0.0000 sec



10N Thruster Performance analysis

- Flow analysis using the developed reduction mechanism



10N Thruster Performance analysis

- Performance

- Chamber condition MR=1.65, 9 bar and Initial chamber condition for computing

Chamber Condition	Anderson (2010)	Present (RM29)	Rocflam-II	CEA2
CO	0.17840	0.18308	0.09843	0.17635
CO2	0.07982	0.07246	0.20547	0.08339
H2	0.01531	0.01565	0.02707	0.01536
H2O	0.28936	0.27411	0.18383	0.29272
N2	0.41750	0.41605	0.39710	0.41810
T [K]	3000	3180.61	3075.61	3051.41
Density [kg/m ³]	0.74	0.69	0.71	0.72

species unit: mass fraction

- Nozzle performance comparison

※ Frozen shows maximum performance

※ Equilibrium shows minimum performance

※ Non-Equilibrium shows realizable performance

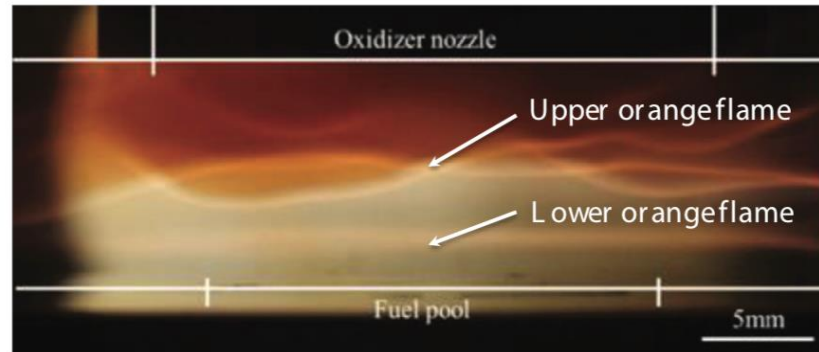
At Exit	CEA2		Anderson (2010)	Present (RM29)	Rocflam-II
Reaction	Equilibrium	Frozen	Non-Eq	Non-Eq	Non-Eq
Isp [s]	336	327	326	339	331
Ivac [s]	345	334	330	343	335
F [N]	10.95	10.62	10.17	10.22	10.21
Mach	5.55	6.04	5.84	5.86	5.82
p [Pa]	293	224	159	152	162
T [K]	707.00	517.78	549.95	581.06	567.93
Density [kg/m ³]	1.0442×10 ⁻³	1.0746×10 ⁻³	0.7188×10 ⁻³	0.6381×10 ⁻³	1.3009×10 ⁻³

Conclusion

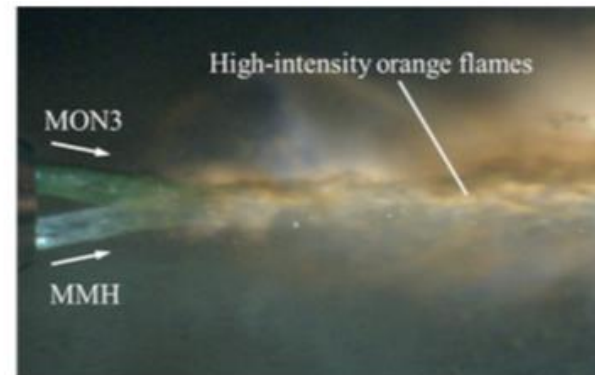
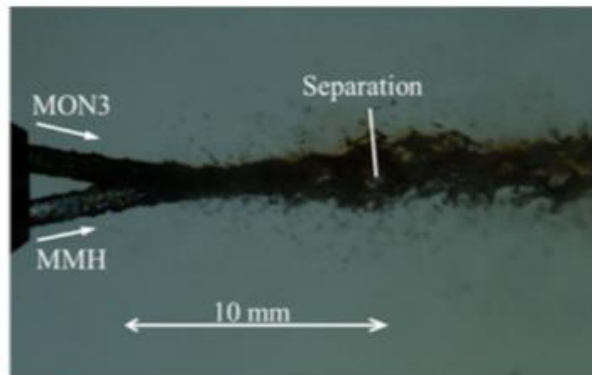
- The developed mechanism was reduced to 34 species and 29 reactions based on Anderson's mechanism.
- The reduced mechanism(RM29) showed performance comparable to full chemistry analysis(Anderson's).
- The nozzle performance analysis satisfied the design performance by applying RM29.
(thrust $\geq 10\text{N}$, specific impulse $\geq 287\text{ s}$)

Future work

- Identification of combustion characteristics of bi-propellant



- Analysis of bi-propellant atomization and injection trajectory



Japan Aerospace Exploration Agency(JAXA), Japan, 2017

Thank you for your attention.