

NEXTfoam

CFD Engineering Consulting

넥스트폼(NEXTfoam)은 CFD 엔지니어링 서비스를 제공하는 회사입니다.

2023년 한국추진공학회 춘계학술대회

동축 제트 유동에서 MMH/NTO 접촉 자발 점화에 대한 수치 해석

정황희¹, 신재렬^{1*}, 채종원², 이복직³

¹(주)넥스트폼 기술연구소

²한국항공우주연구원 위성기술연구부

³서울대학교 항공우주공학과

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- 수치해석 시뮬레이션 & 결과
 - 1, 2D 대향류 해석
 - 2D 동축 제트 해석
- 결론 & 향후 연구

10N 저장성 이원추진제 추력기

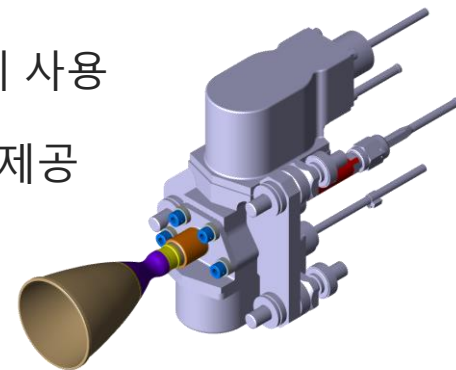
- 스페이스파이오니어 사업 : 우주전략기술 자립화 및 원천기술 확보

- 16개의 핵심 부품 기술 국산화 및 기술개발



- 저장성 이원추진제 추력기

- 연료(MMH)와 산화제(NTO)를 사용하는 이원추진제 추력기 개발
- 정지궤도위성, 달 착륙선 및 심우주 탐사선 등 다양한 임무에 사용
- 위성의 궤도 이동 및 자세제어에 필요한 속도증분(Del-V)을 제공
- 희귀합금(Pt/Rh of Pt/Ir) 금속 3D 프린팅을 이용하여 제작
- 추력기 설계/설계/해석/제작/공정/조립/시험 절차 수립
- 국산화를 통한 수립대체효과/비용 절감/사회경제적 수익 향상 기대

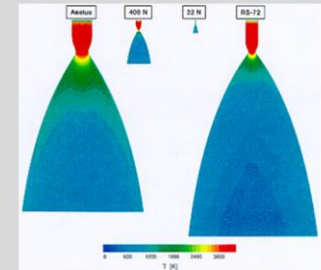


연구 목표

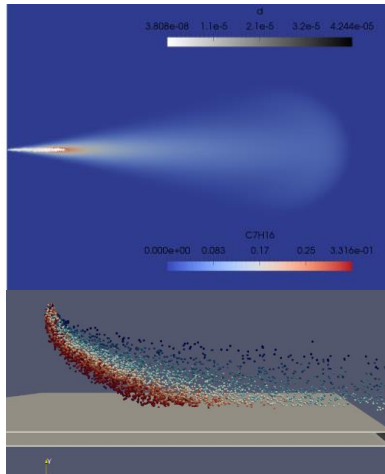
- 추력기 연소 해석 S/W 개발
 - MMH/NTO 반응 기구 개발
 - 연소 해석 솔버 개발
 - 사용자 GUI 환경 개발
 - 추력기 연소 해석

• ROCFLAM

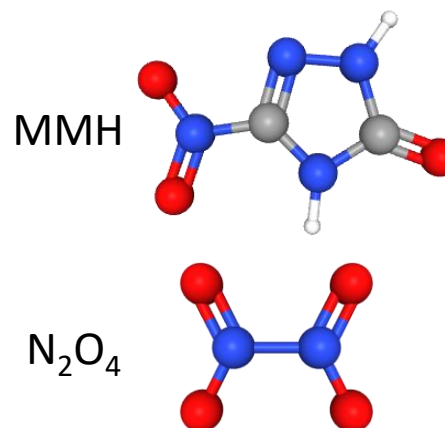
- Compressible -sub, trans and supersonic
 - 2D axisymmetric finite volume, SIMPLE algorithm
 - standard k-ε with wall function, 2 layer model
- Multi-gaseous species chemistry
 - Arrhenius, EDC, global chemistry
 - standard jannaf property data
- Lagrangian
 - droplet-to-wall interaction model
 - secondary droplet break-up
 - annular film cooling model
 - viscous heating species diffusion
 - heat conduction in solid wall



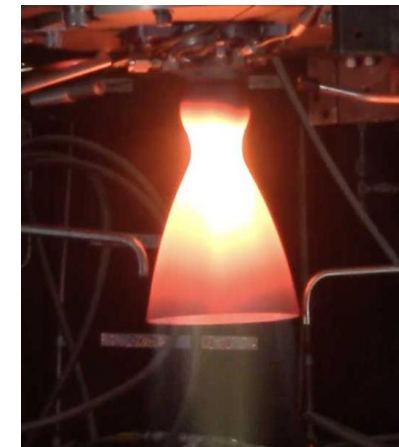
[Spray]



[Hypergolic chemistry]



[Conjugate Heat Transfer]



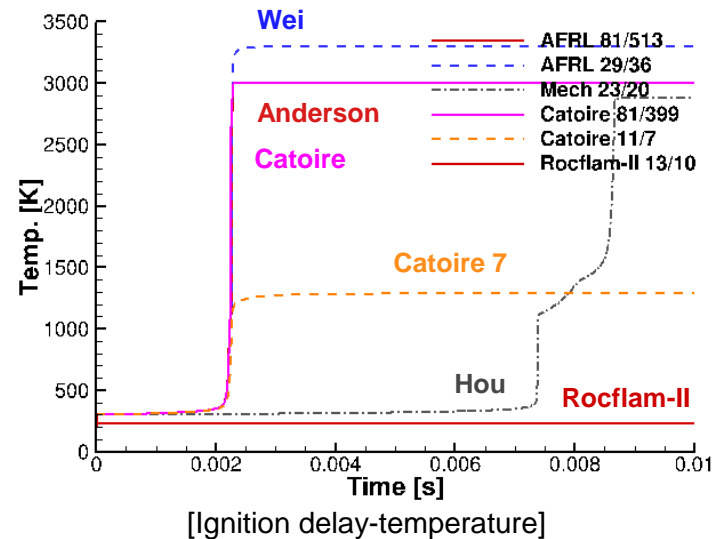
축소 매커니즘 개발

• 이전 연구자들의 매커니즘:

- Anderson(2010) : 81 화학종, 513 반응식
- Wei(2019) : 29 화학종, 36 반응식 (Anderson의 축소 모델)
- Hou(2018) : 23 화학종, 20 반응식
- Catoire : 81 화학종, 399 반응식
- Catoire(2004) : 11 화학종, 7 반응식 (Catoire의 축소 모델)
- RocFlam-II(1998) : 13 화학종, 10 반응식

```
constantProperty volume;  
fractionBasis mole;  
fractions  
{  
    CH3NHNH2    1;  
    N2O4        1.0275;  
    NO2         1.4725;  
}  
p              24200;  
T              298;
```

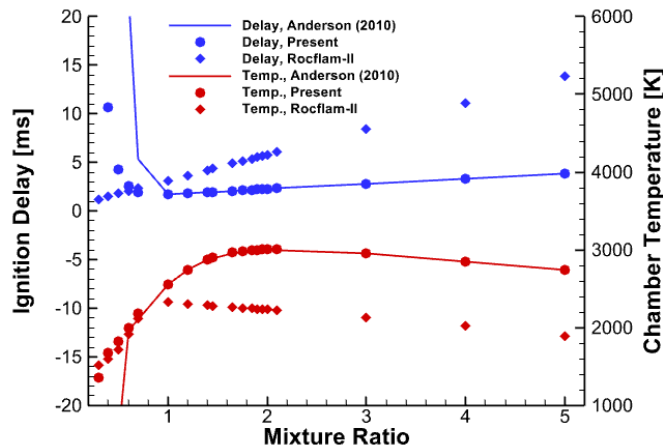
[Initial condition]



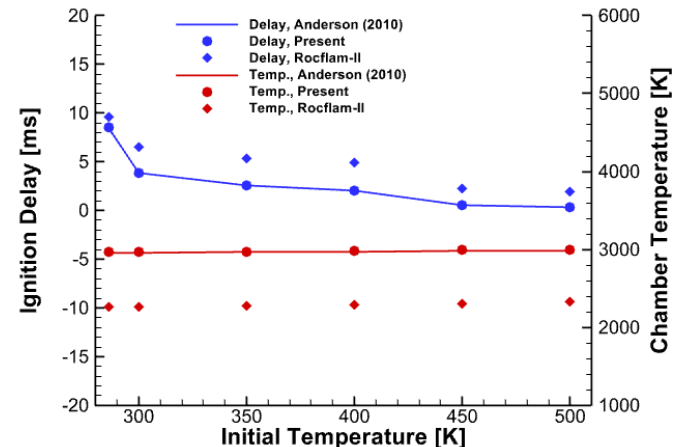
축소 매커니즘 개발

• 매커니즘 개발:

- NextFOAM(2022) : **31** 화학종, **29** 반응식 (=RM29)
 - Anderson 매커니즘을 기반으로 개발된 축소 매커니즘
 - 민간도 분석과 시행착오법을 사용하여 개발
 - **Anderson** 논문의 Arrhenius 변수 인용
 - 대부분의 화학 물성치는 **Burcat**의 가스 물성치 인용
 - HNNO 와 CH3O2H 가스 물성치는 **Marinov**의 가스 물성 인용
 - CH3NNH 가스 물성치 **Catoire**의 가스 물성 인용



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



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

축소 매커니즘 개발

• 29 단계 축소 반응식

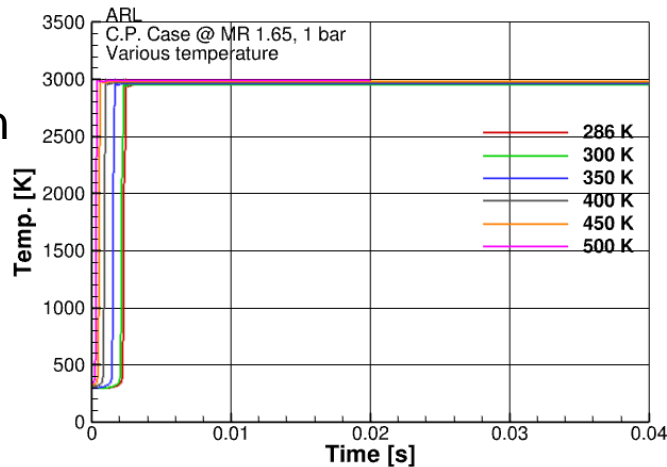
No.	Reaction	No.	Reaction
R1	$\text{N}_2\text{O}_4(+\text{M})=\text{NO}_2+\text{NO}_2(+\text{M})$	R16	$\text{H}+\text{OH}+\text{M}=\text{H}_2\text{O}+\text{M}$
R2	$\text{CH}_3\text{NHNH}_2=\text{CH}_3\text{NNH}+\text{H}_2$	R17	$\text{HCN}+\text{O}=\text{NH}+\text{CO}$
R3	$\text{CH}_3\text{NHNH}_2+\text{NO}_2=\text{CH}_3\text{NNH}_2+\text{HONO}$	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)

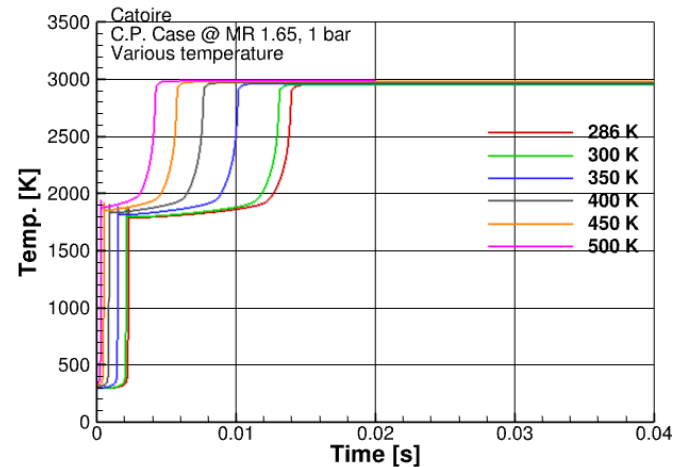
매커니즘 검증

• 0 차원 분석 (온도 의존성)

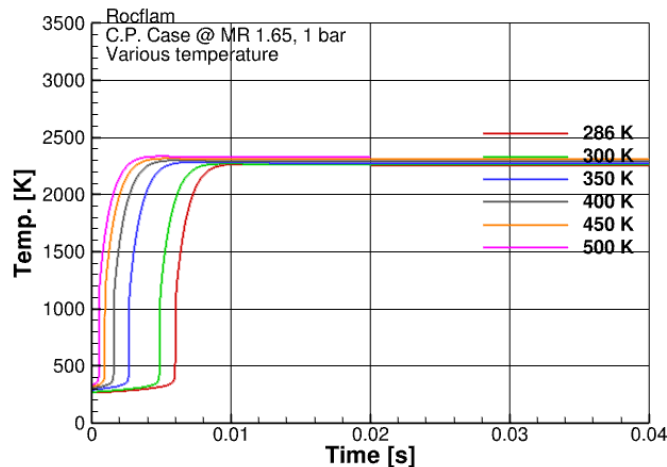
Anderson



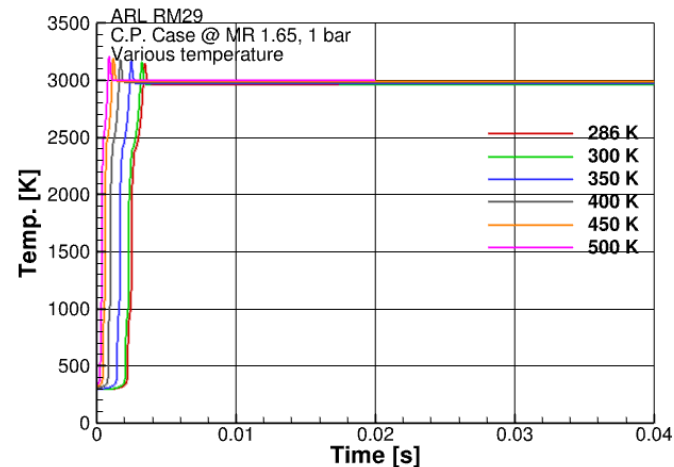
Catoire



Rocflam



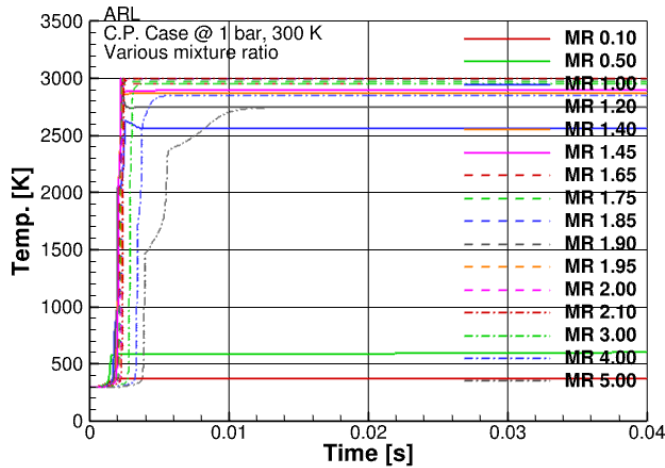
Present (RM29)



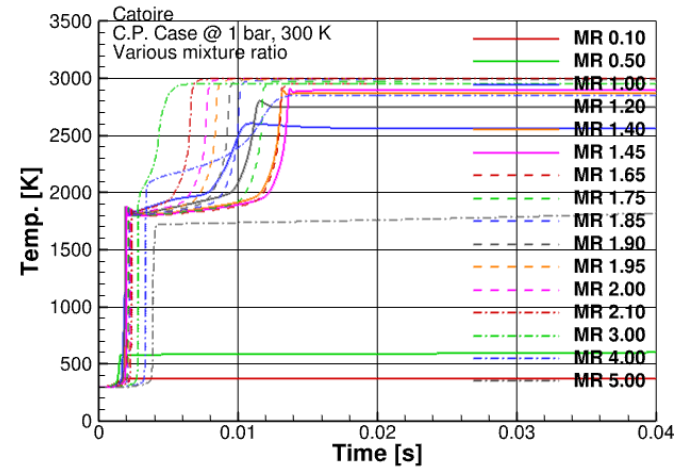
매커니즘 검증

• 0 차원 분석 (혼합 비율 의존성)

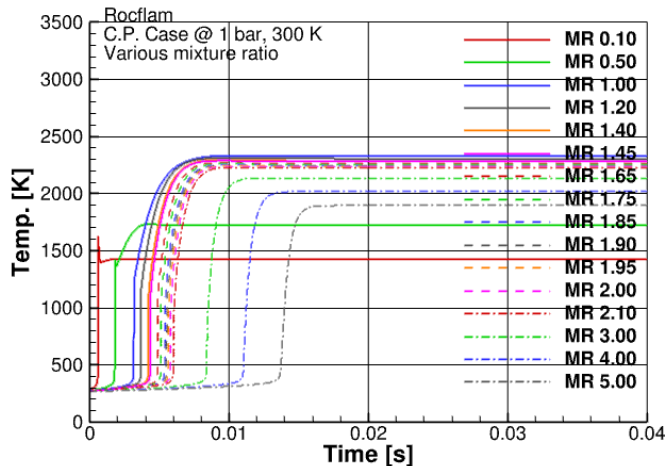
Anderson



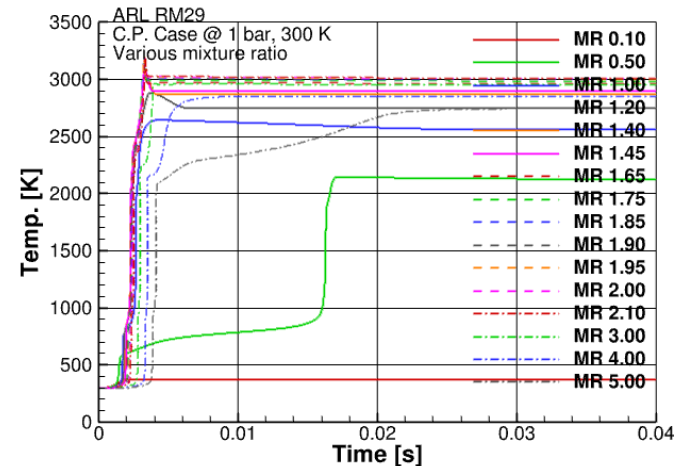
Catoire



Rocflam



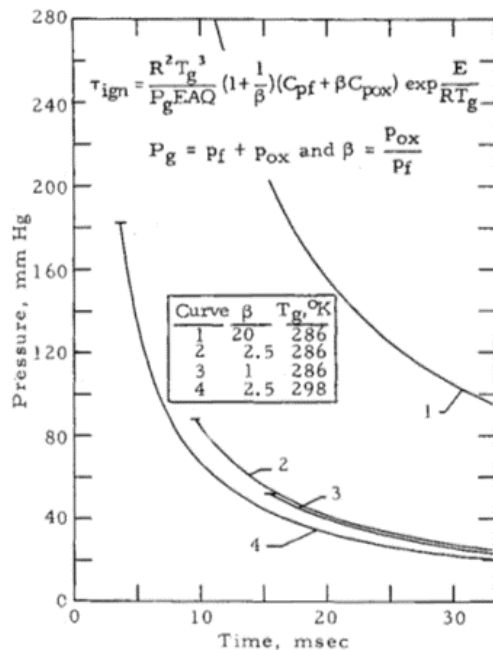
Present (RM29)



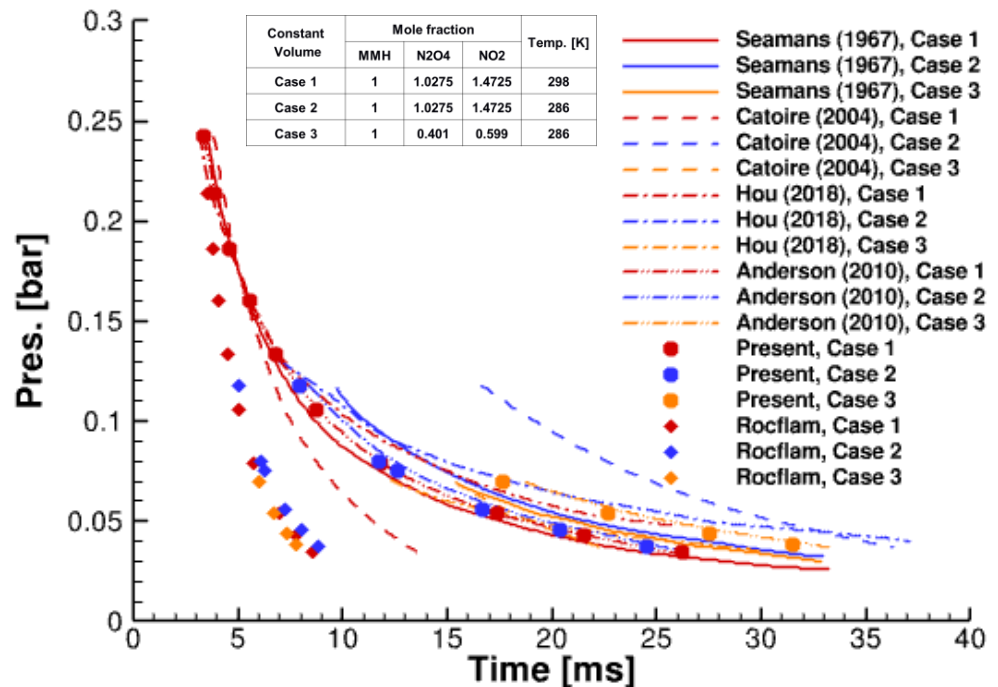
매커니즘 검증

• 0 차원 분석 (압력 의존성)

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



[Seamans results]



[Ignition delay-pressure curve]

1 차원 수치 해석

• 1 차원 대향류 화염 해석 - CANTERA

- T. Hayashi(2019, *C&F* 201, 244-251)
- 120 화학종 & 907 반응식

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

[Hayashi results]

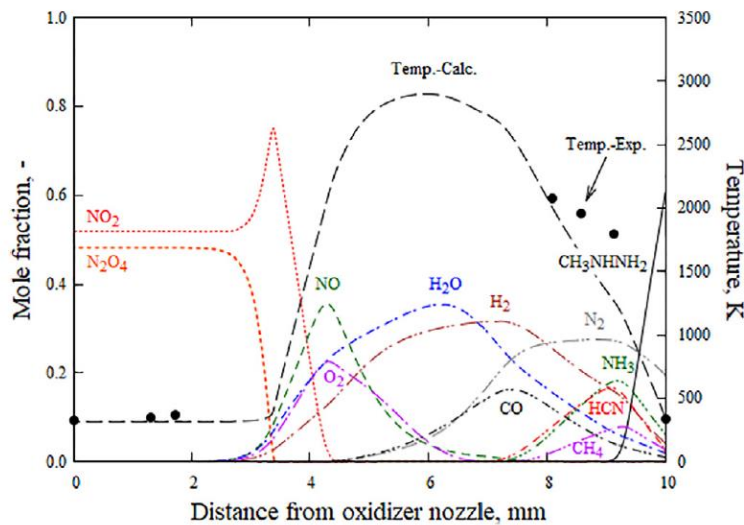
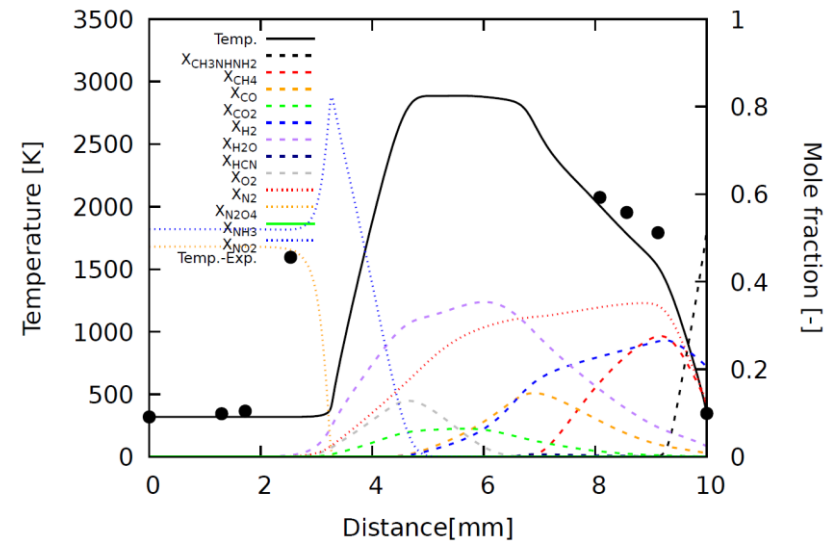


Fig. 9. Axial distribution of temperature and major species obtained by CANTERA for MMH/NTO combustion. (Dots indicate temperature measured by thermocouple).

[Present results]



2 차원 수치 해석

- 2 차원 대향류 연소 해석 - OpenFOAM

[Hayashi experimental results]

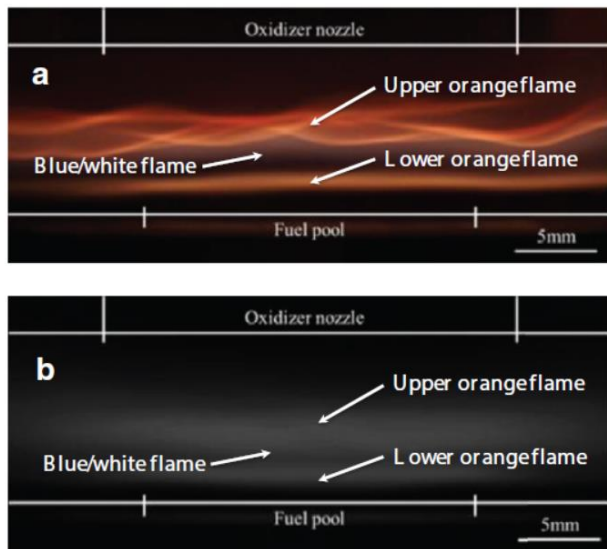
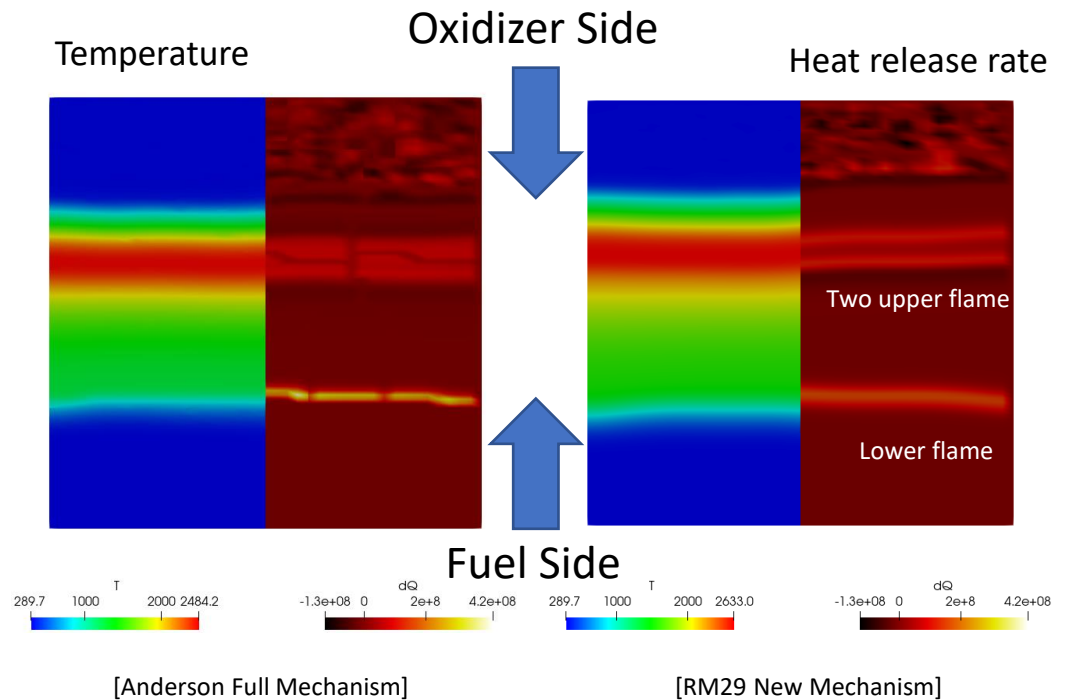


Fig. 6. Broad band photograph of MMH-NTO flame and averaged image of MMH-NTO flame (a) instantaneous image, (b) averaged image of 3000 frames in grayscale. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)



• Hiroumi Tani, PCI (2015)

- Hypergolic ignition and flame structures of hydrazine/nitrogen tetroxide co-flowing plane jets

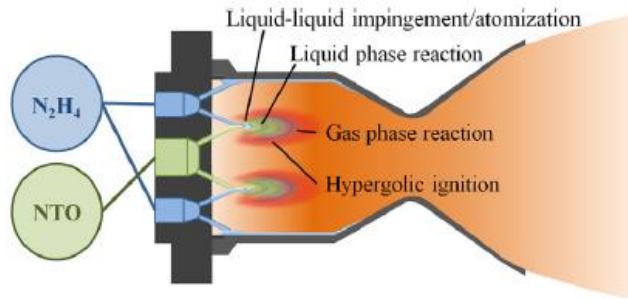


Fig. 1. Schematics of complicated multi-physics phenomena in N_2H_4/NTO bipropellant thrusters.

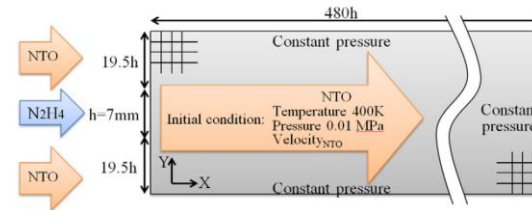
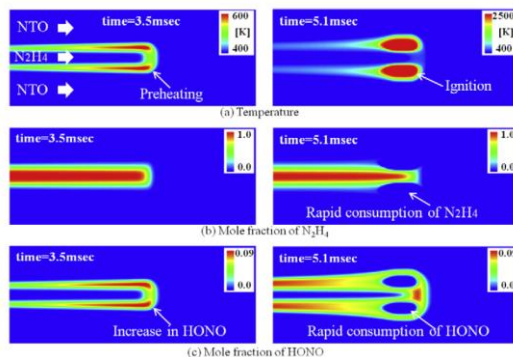


Fig. 2. Computational domain, boundary and initial conditions.

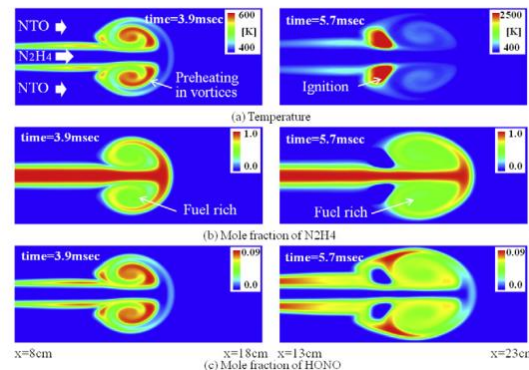
Table 1
Injection conditions.

	Pressure	Temperature	Velocity N_2H_4	Velocity NTO (m/s)	Mole fractions of NO_2 and N_2O_4
Case 1	0.01 MPa	400 K	50 m/s	50	0.990:0.010
Case 2	↓	↓	↓	30	↓
Case 3	↓	↓	↓	70	↓

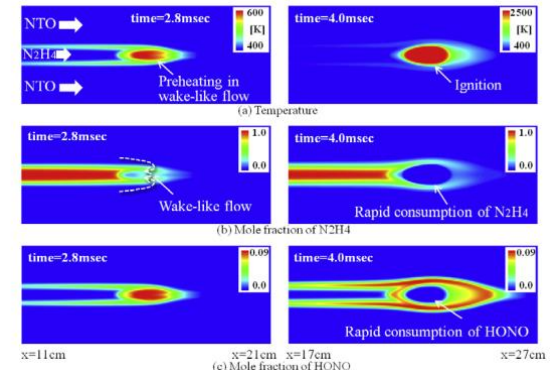
[NTO velocity - 30 m/s]



[NTO velocity - 50 m/s]



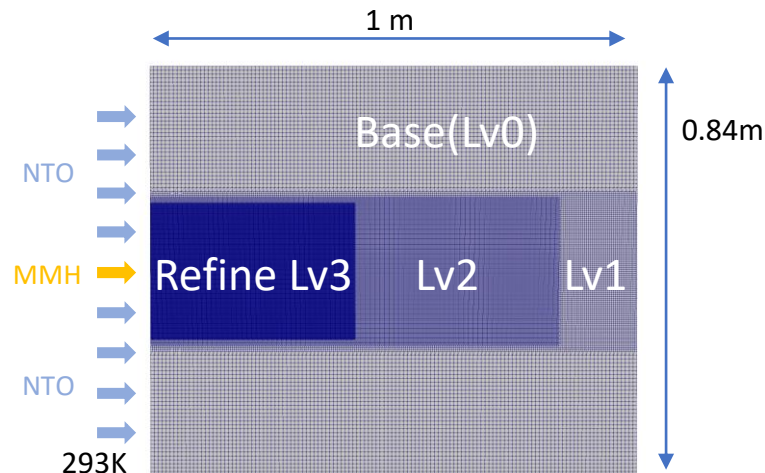
[NTO velocity - 70 m/s]



동축 제트 유동 해석

- 격자

- 격자 도구: snappyHexMesh(OpenFOAM)
- 격자 수: 17.5 만 셀
- 격자 크기: 1 mm (fine region)



- 경계조건

- symmetry
- non-reflecting outlet

	Velocity _{MMH}	Velocity _{NTO}
Case1	50 [m/s]	30 [m/s]
Case2		50 [m/s]
Case3		70 [m/s]

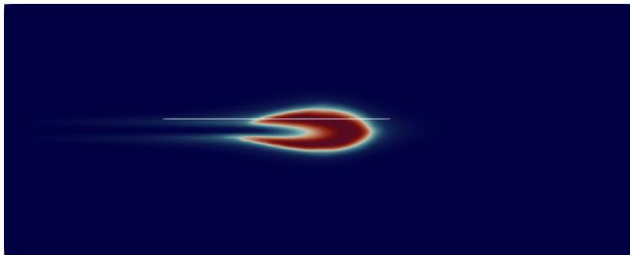
- 해석 솔버: reactingPimpleCentralFoam

- 연소 및 화학 반응이 있는 압축성 유동에 대한 압력 기반 semi implicit 솔버

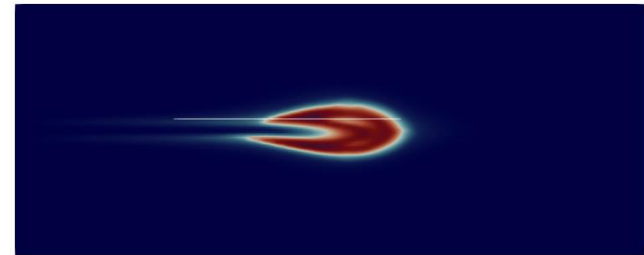
동축 제트 유동 해석

- 접축 자발 점화 및 화염 구조
 - 급격한 온도 상승 구간 (2.7 ms ~ 3.0 ms)

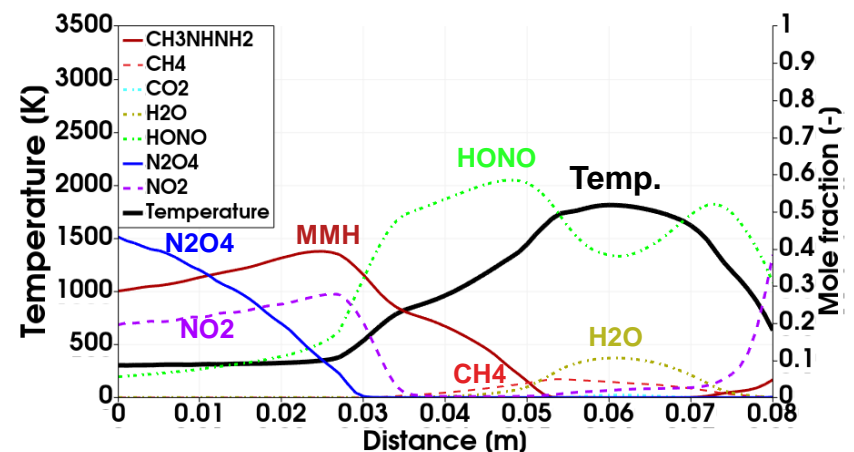
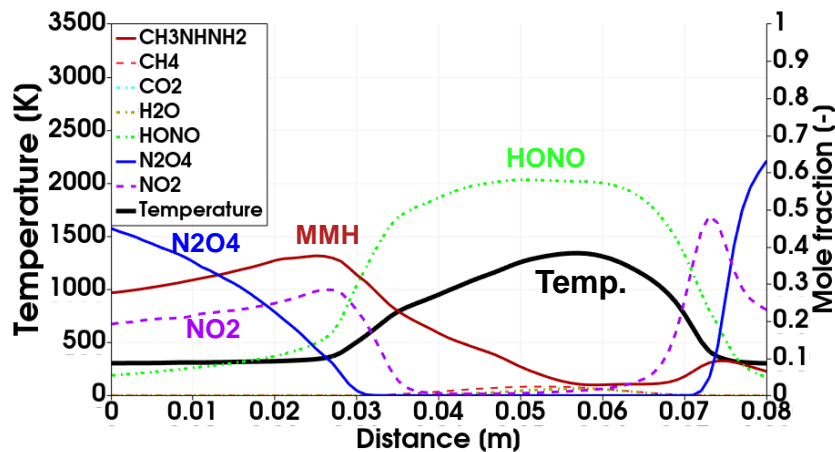
Time: 0.0027 sec



Time: 0.0028 sec



HONO

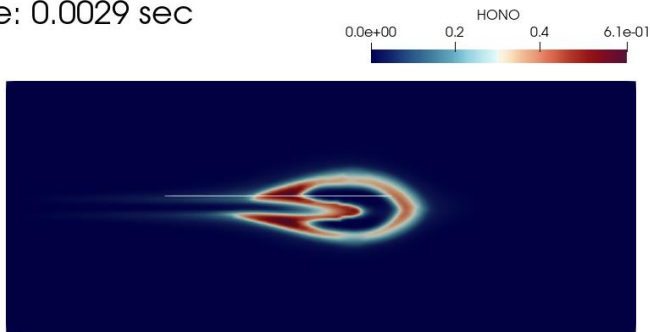


동축 제트 유동 해석

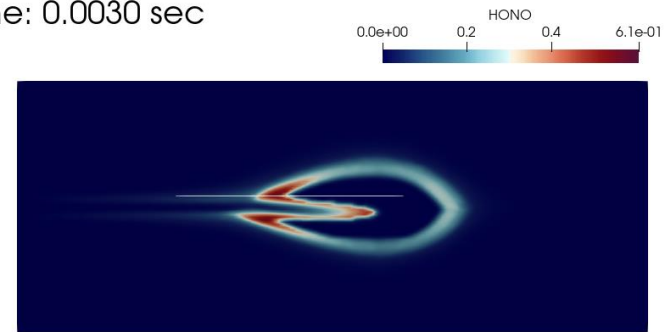
• 접축 자발 점화 및 화염 구조

• 급격한 온도 상승 구간 (2.7 ms ~ 3.0 ms)

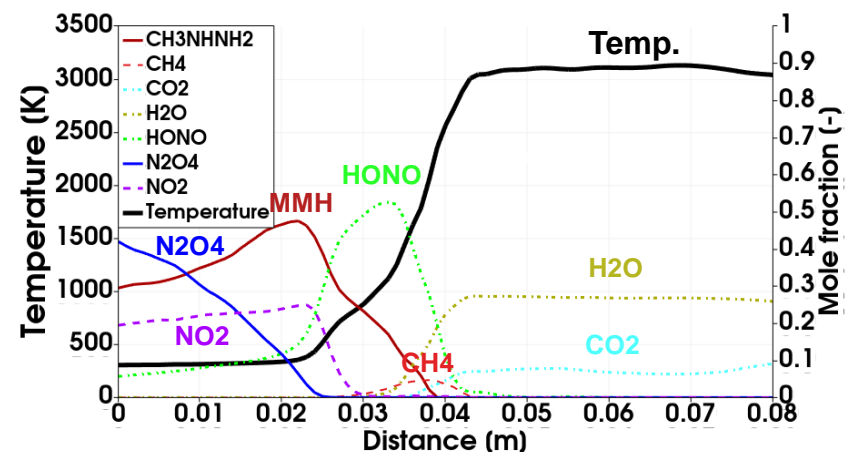
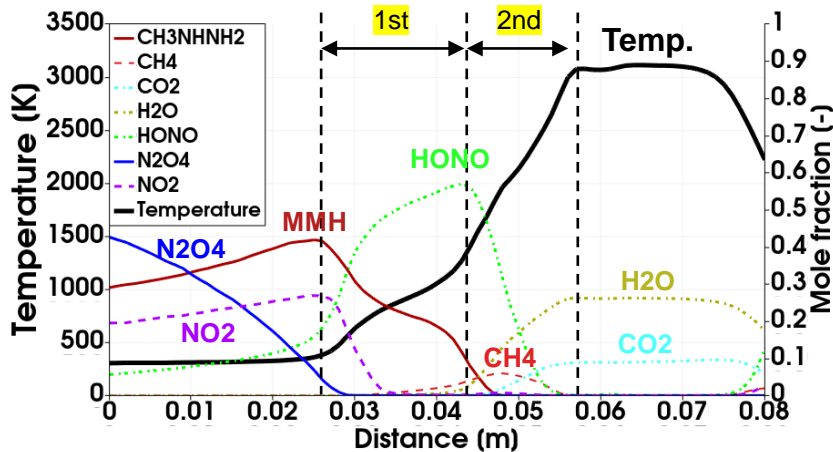
Time: 0.0029 sec



Time: 0.0030 sec



HONO

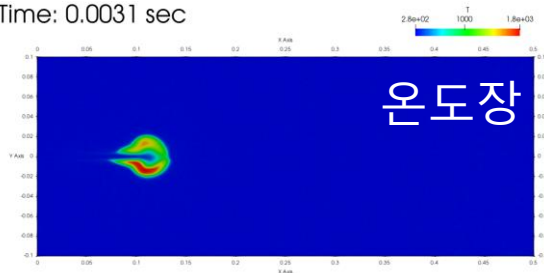


동축 제트 유동 해석

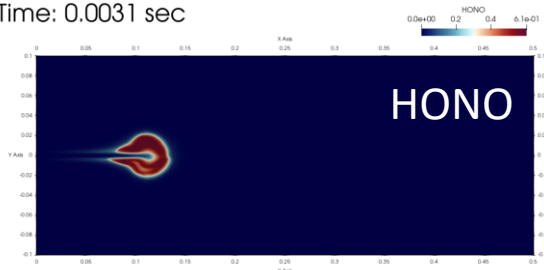
• 시뮬레이션 결과 (점화 시점)

Case 1 (30m/s)

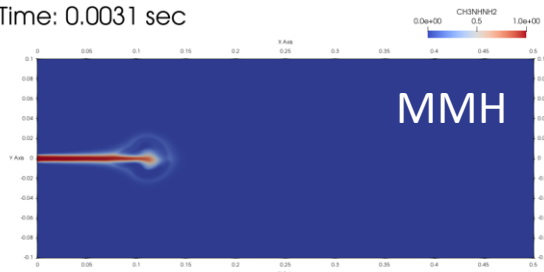
Time: 0.0031 sec



Time: 0.0031 sec

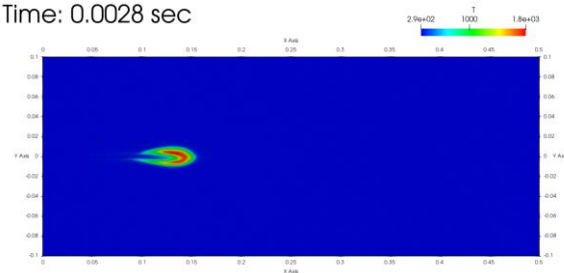


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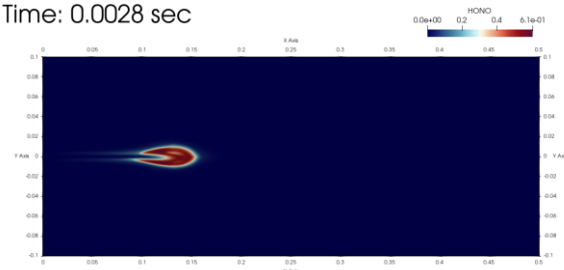


Case 2 (50 m/s)

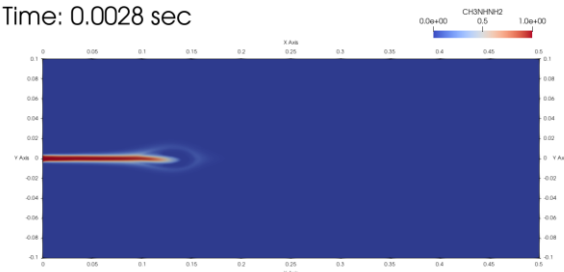
Time: 0.0028 sec



Time: 0.0028 sec

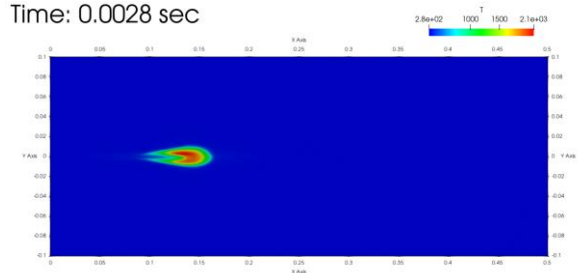


Time: 0.0028 sec

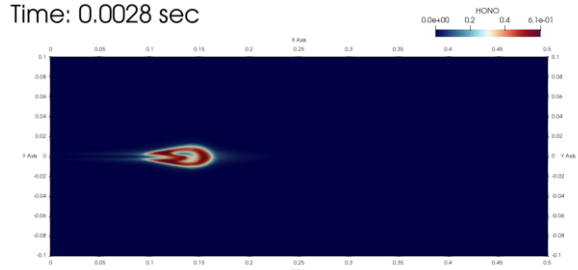


Case 3 (70 m/s)

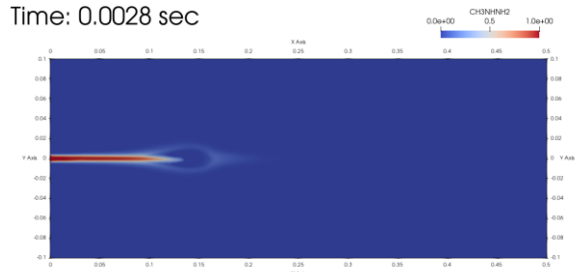
Time: 0.0028 sec



Time: 0.0028 sec



Time: 0.0028 sec

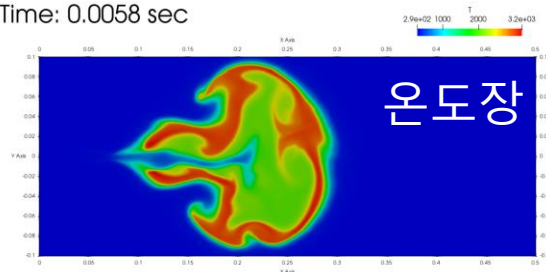


동축 제트 유동 해석

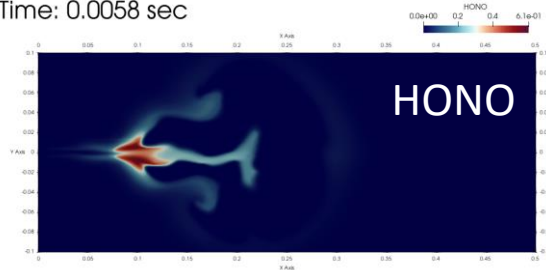
- 시뮬레이션 결과 (점화 이후)

Case 1 (30m/s)

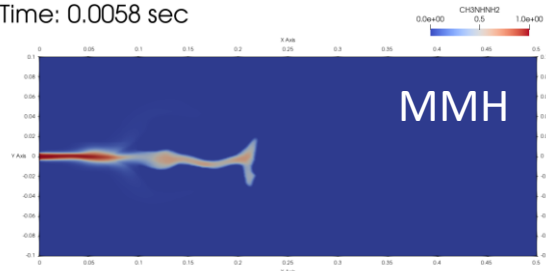
Time: 0.0058 sec



Time: 0.0058 sec

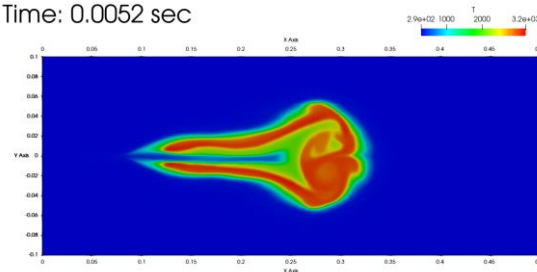


Time: 0.0058 sec

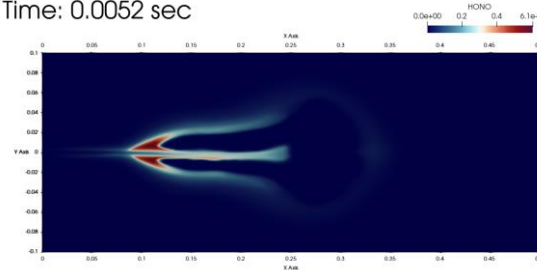


Case 2 (50 m/s)

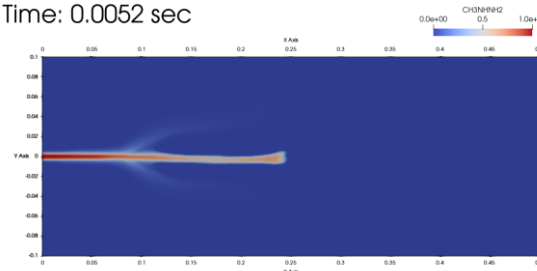
Time: 0.0052 sec



Time: 0.0052 sec

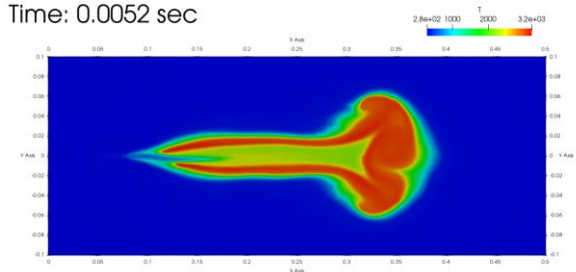


Time: 0.0052 sec

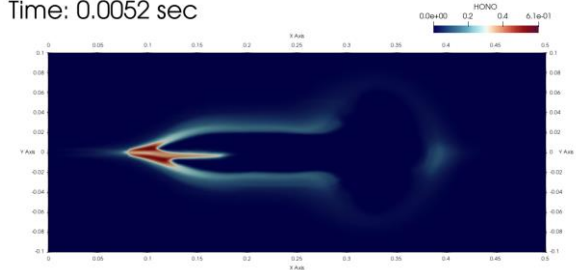


Case 3 (70 m/s)

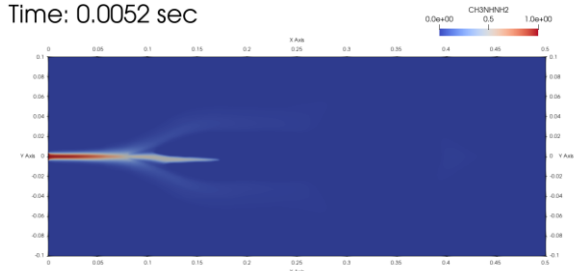
Time: 0.0052 sec



Time: 0.0052 sec



Time: 0.0052 sec



- Anderson의 매커니즘을 기반으로 MMH/NTO 반응에 대한 34 화학종, 29 반응식을 갖는 축소된 매커니즘(RM29) 개발하였다.
- 매커니즘 검증을 통해 축소된 매커니즘(RM29)이 Anderson의 full chemistry 와 비교하여 점화지연, 온도 의존성, 혼합 비율 의존성, 압력 의존성이 비슷한 결과를 나타내는 것을 확인하였다.
- 대향류 해석을 통해 참조논문의 해석결과보다 실험 결과에 근접한 온도 분포와 삼중 화염의 존재를 수치해석으로 확인하였다.
- MMH/NTO의 접촉 과정에서 HONO이 생성되면서 preheatin이 되고 약 1500K 이 넘어가면 HONO이 급격히 소모되고 CH₄ 연소반응에 의해 온도가 3000K 으로 상승하는 것을 확인하였다.

• 표면 필름-증발 모델 연구

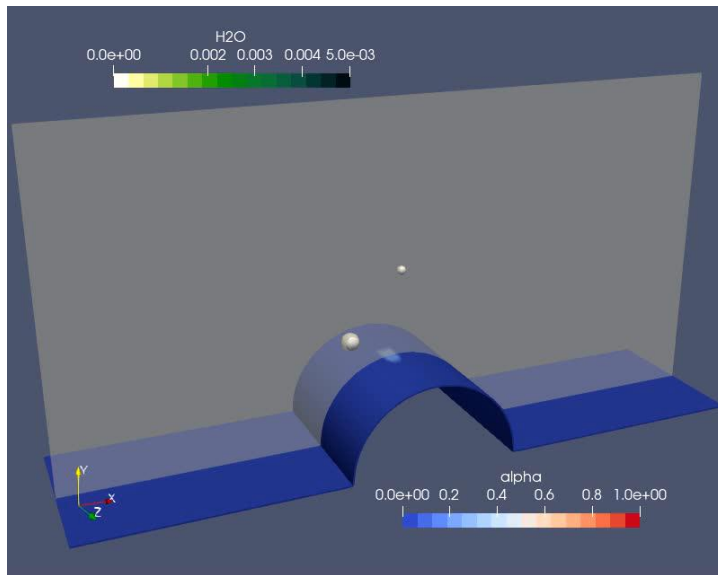
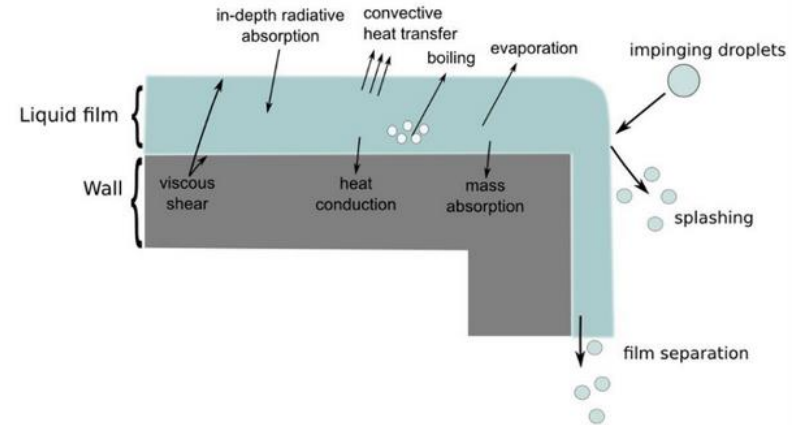
- Film Liquid Evaporation

• Spray: thermoSurfaceFilm

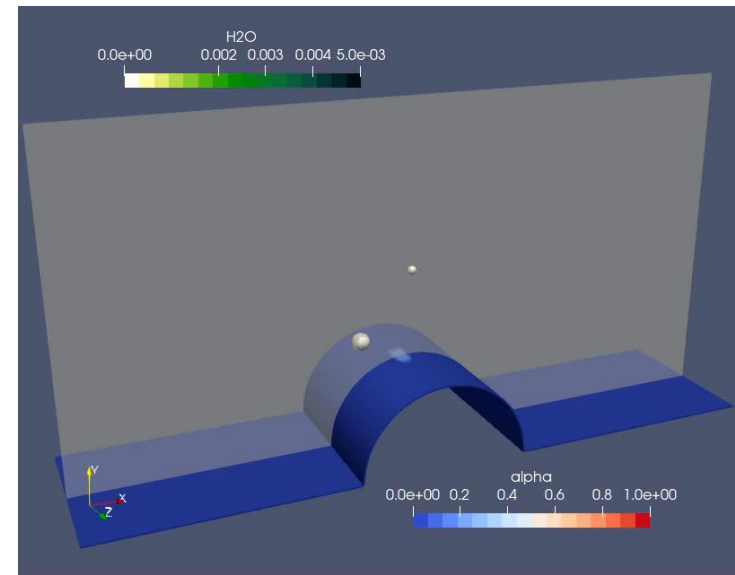
✓ Interaction type: absorb

• Film region: thermoSingleLayer

✓ Phase change for mass transfer



[Evaporation off]



[Evaporation On]

Thank you for your attention.