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Application of Detailed Chemical Kinetics to Combustion Instability Modeling

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Challenges of Combustion Instability

Combustion instability is an organized, oscillatory motion in a combustion chamber sustained by combustion.

CI caused a four year delay in the development of the F-1 engine used in the Apollo program

> 2000 full scale tests

> $400 million for propellants alone (2010 prices)

Irreparable damage can occur in less than 1 second.

Damaged engine injector faceplate caused by combustion instability

"Combustion instabilities have been observed in almost every engine development effort, including even the most recent development programs"

– JANNAF Stability Panel Draft (2010)

Prior Work – Kinetics Used

- **Simulations:**
  1) 3D real geometry
  2) Unsteady
  3) Long run-times
  4) Coupled physics
- **1- 4 have forced the use of simplified kinetics**
  - Global reactions

$$CH_4 + 2\,O_2 \longrightarrow 2\,H_2O + CO_2$$

$$2\,CH_4 + 3\,O_2 \longrightarrow 2\,CO + 4\,H_2O$$
$$2\,CO + O_2 \longleftrightarrow 2\,CO_2$$

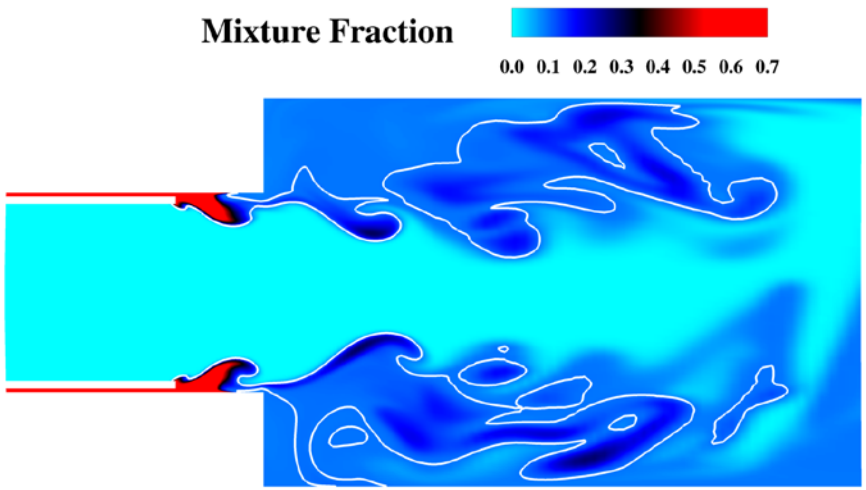
$$2\,CH_4 + O_2 \longrightarrow 2\,CO + 4\,H_2$$
$$CH_4 + H_2O \longrightarrow CO + 3\,H_2$$
$$2\,H_2 + O_2 \longleftrightarrow H_2O$$
$$CO + H_2O \longleftrightarrow CO_2 + H_2$$

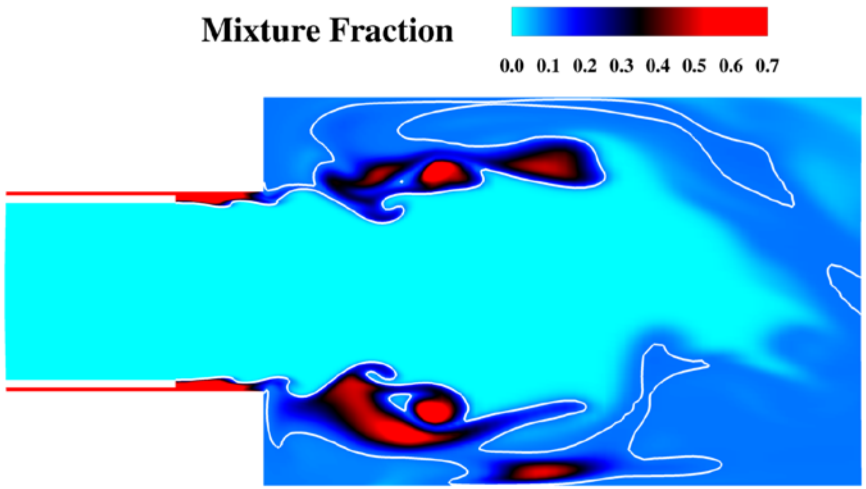
Complex Flowfield

Global mechanisms can be tuned but have limited parameters to adjust

The flowfields contains widely varying parameters, making tuning to operating conditions difficult at best

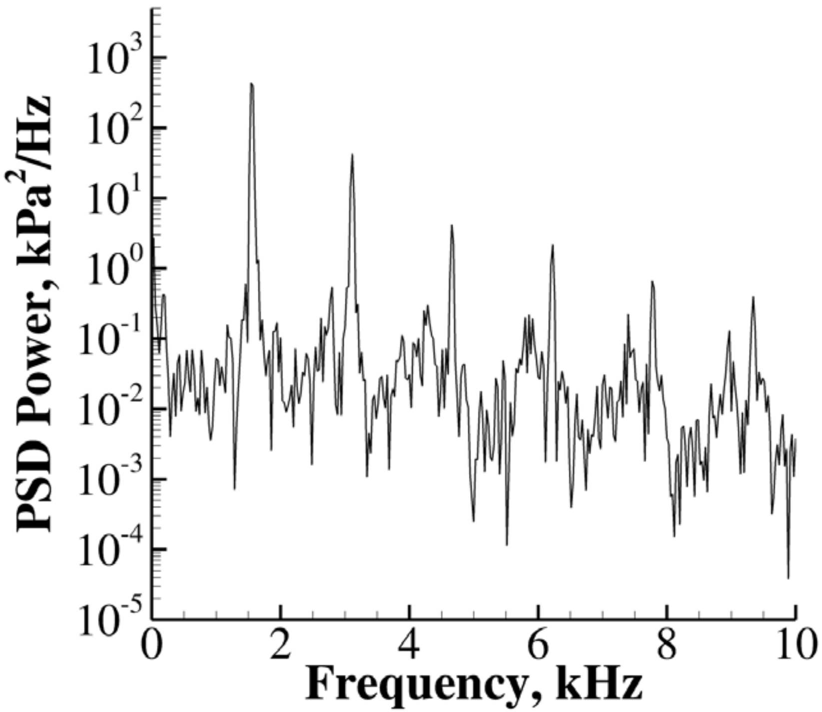
Mixture fraction for the same operating condition at different times



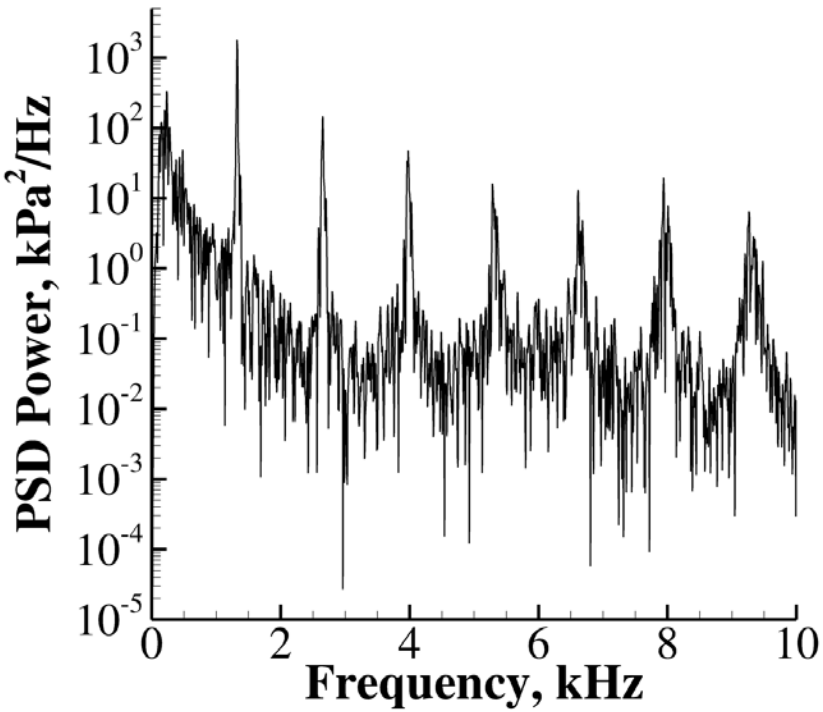


Single Step Results

Simulation



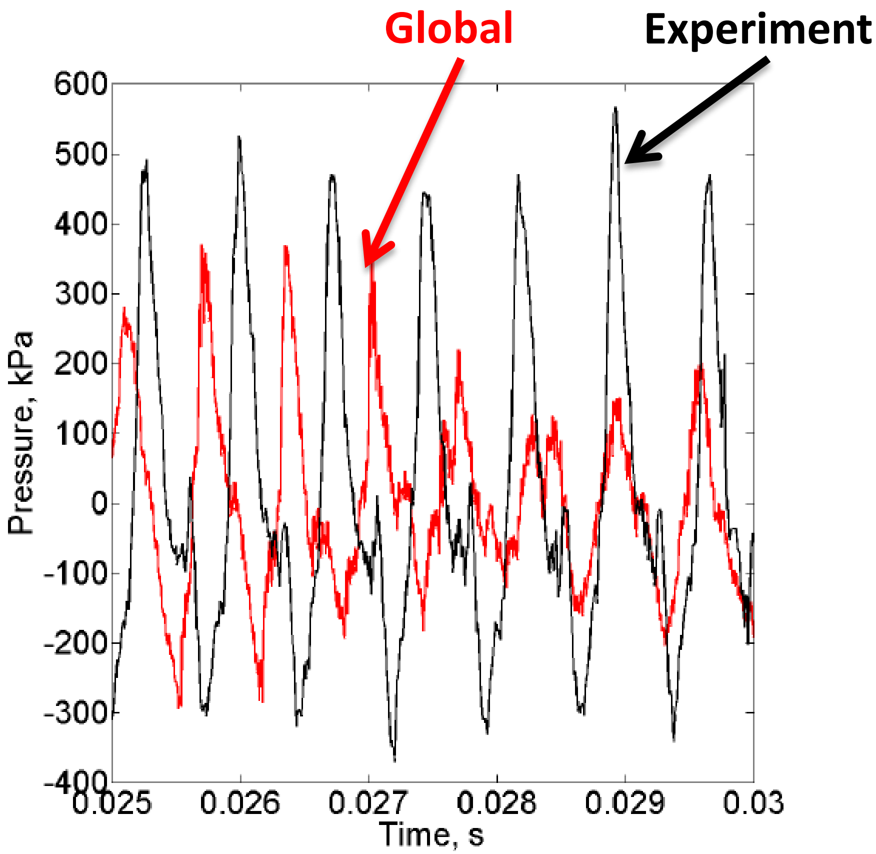
Experiment

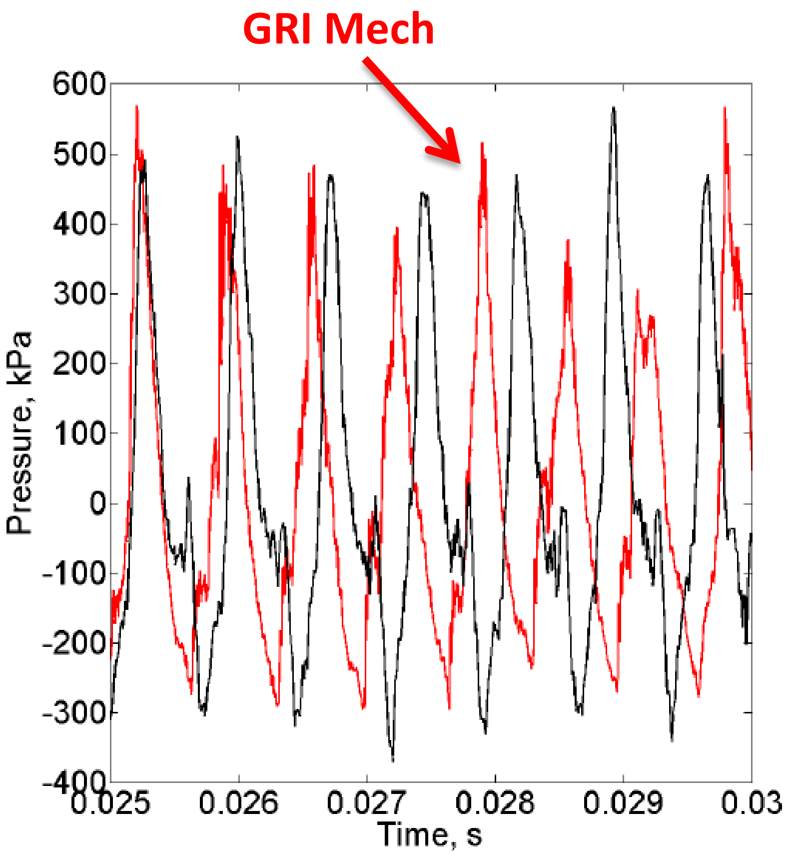


Amplitudes under predicted by 10%,
Frequencies over predicated by 15% (or more)

Two-dimensional Study

2D study showed substantial improvement in amplitudes with detailed kinetics, BUT, 2D predictions were always worse compared with 3D





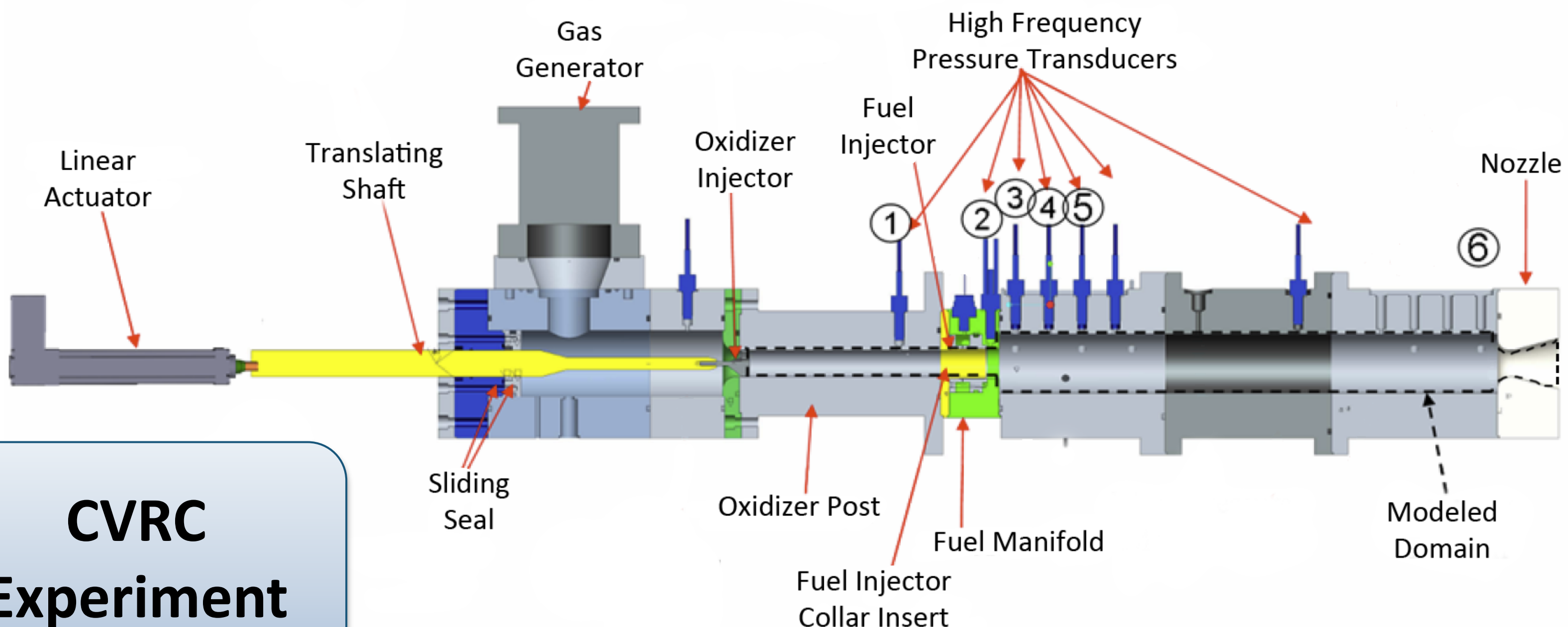
Sardeshmukh et al. 2015

Current Work: Detailed kinetics in 3D

	Global	Detailed GRI-1.2
Number of reactions	1	177
Number of species	4	31
Number of cores	960	21,600
Core hours per ms	11,520	259,200

Extremely Expensive!

22.5× more than Global



CVRC Experiment

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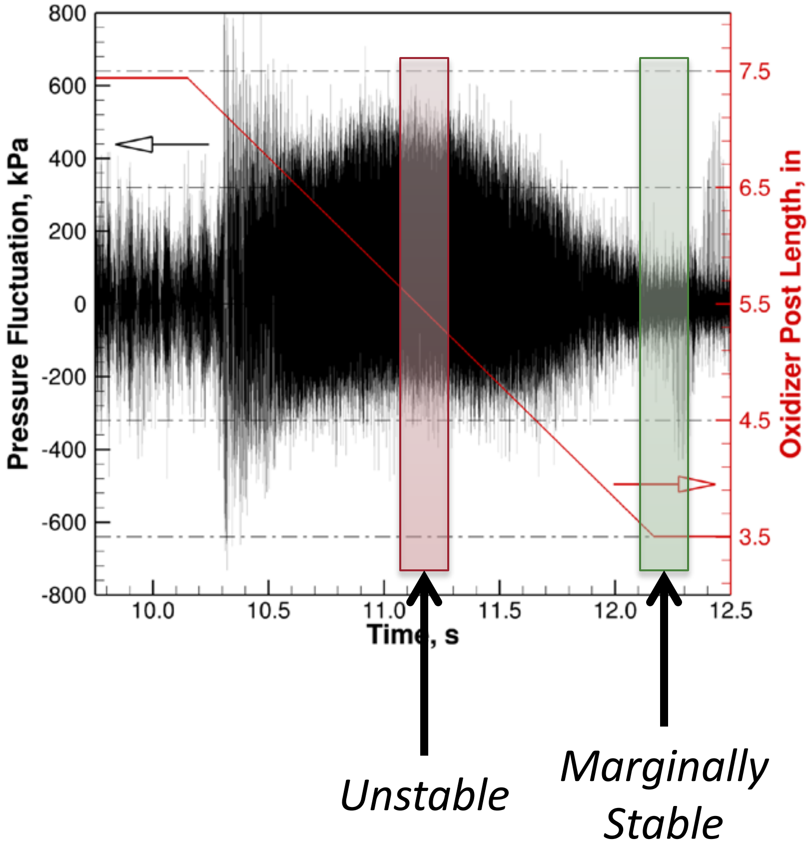
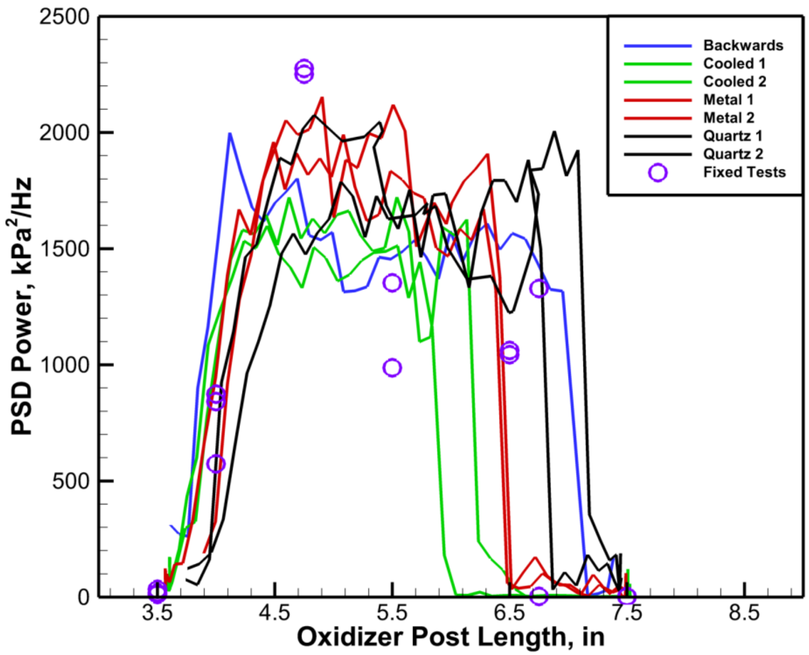
Experimental Results

Unsteady pressure for a translating test

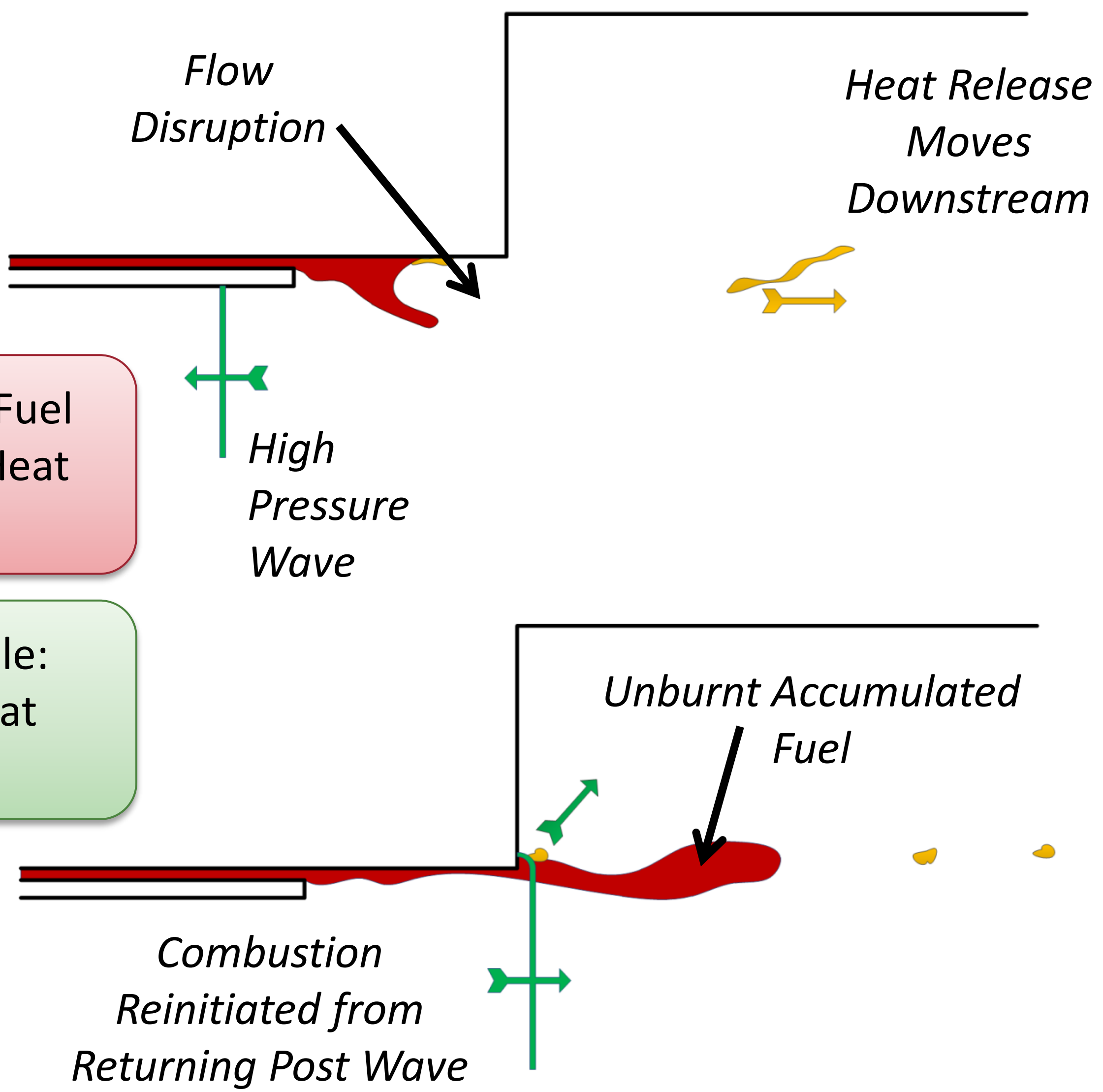


PSD power for the first mode



Harvazinski et al. 2013

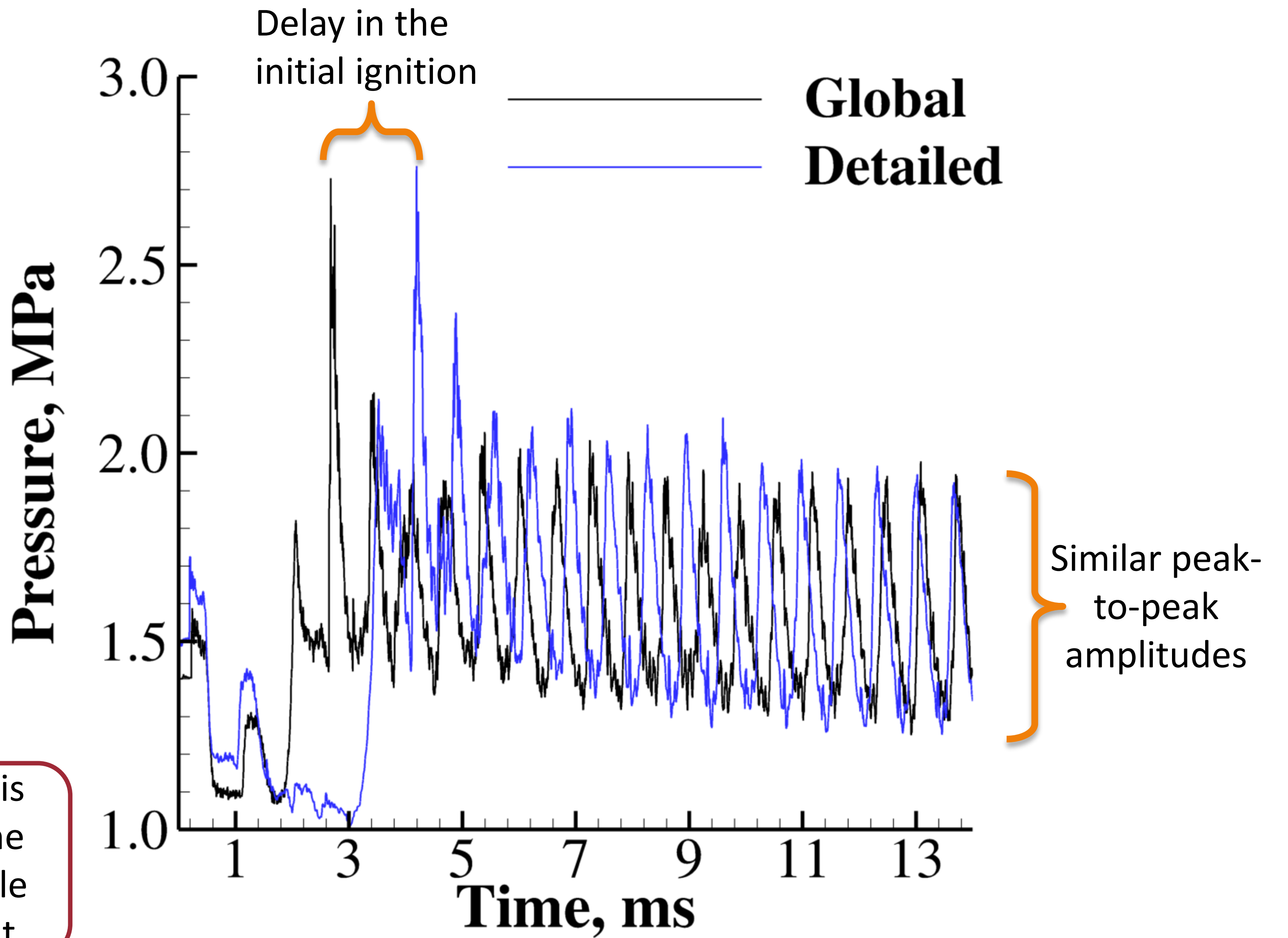
Instability Mechanism



Unstable: Cyclic Fuel Disruption and Heat Release

Marginally Stable: Continuous Heat Release

Unstable Operating Point



A similar delay is observed for the marginally stable operating point

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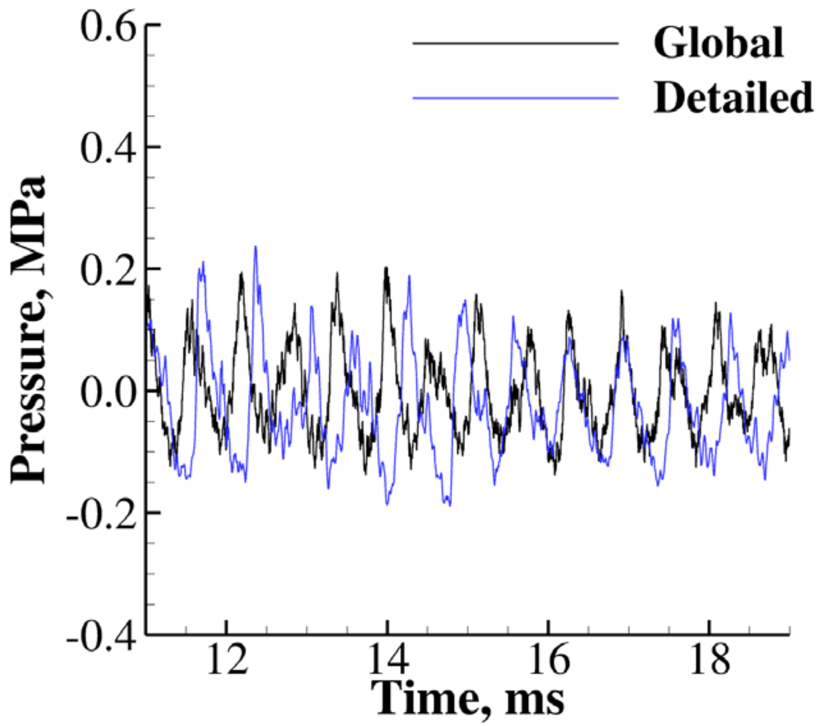
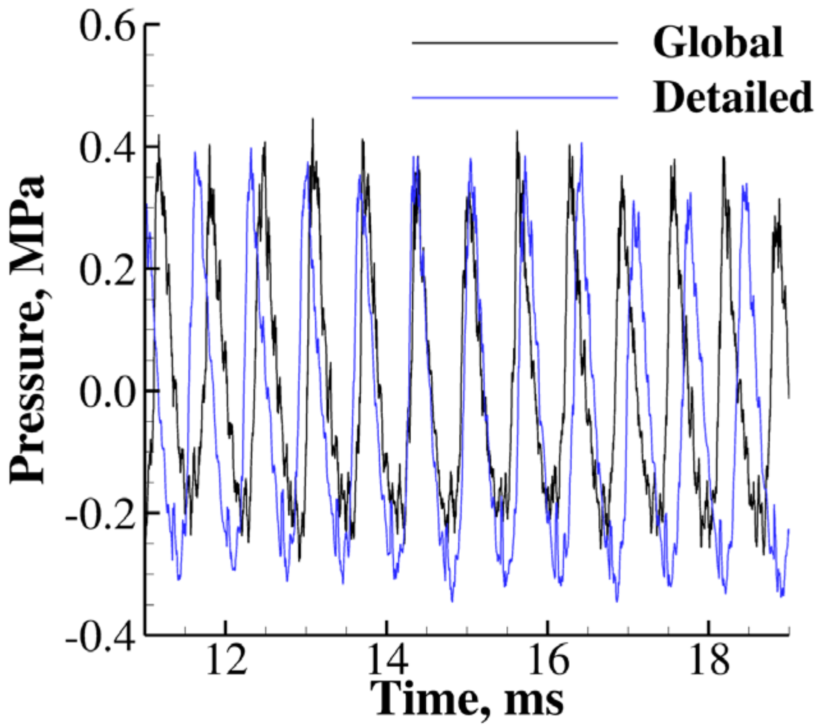
Fluctuating Pressure

Marginally Stable



More cycle to cycle variability

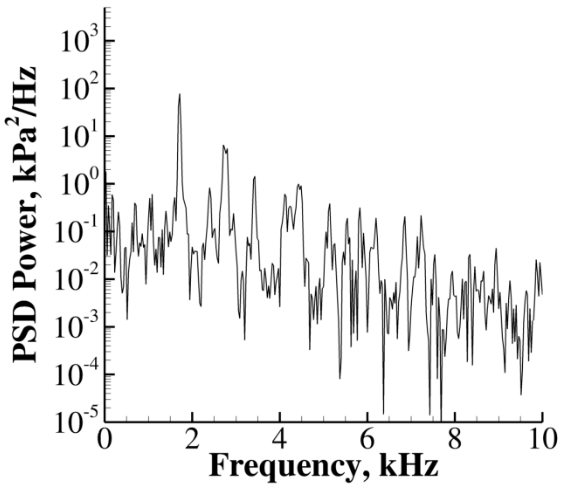
Unstable



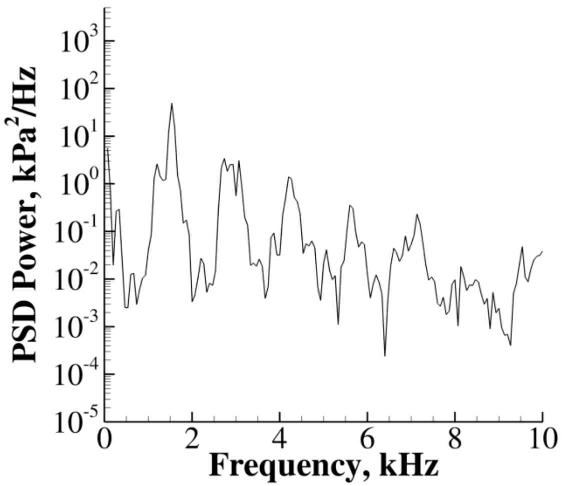
Steep-fronted waves

PSD Analysis – Marginally Stable

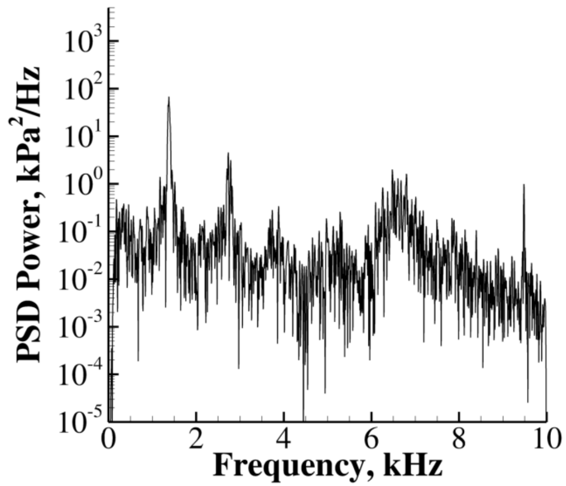
Global



Detailed



Experiment



Global simulation – 40 ms (35 ms of data used for analysis)
Detailed Simulation – 20 ms (15 ms of data used for analysis)

Detailed Comparison

Marginally Stable

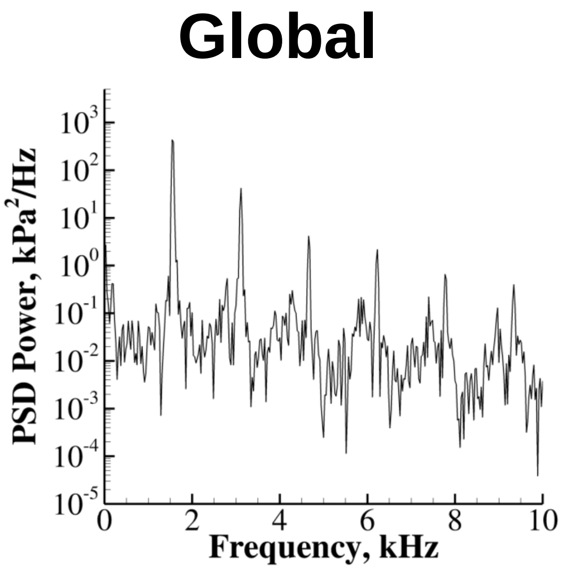
Mode	Experiment			Global			Detailed		
	f, Hz	p'_{ptp}, kPa	f_i/f_1	f, Hz	p'_{ptp}, kPa	f_i/f_1	f, Hz	p'_{ptp}, kPa	f_i/f_1
1	1379	121.70	1.00	1714	129.54	1.00	1533	146.65	1.00
2	2734	5.86	1.98	3428	20.57	1.98	2733	73.12	1.78
3	3882	16.03	2.82	4429	27.57	2.58	4200	36.37	2.74

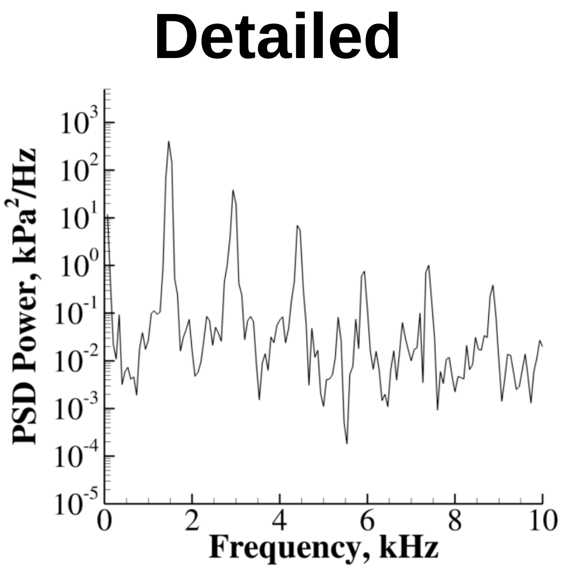
Error in the frequency is reduced from 20% to 11%

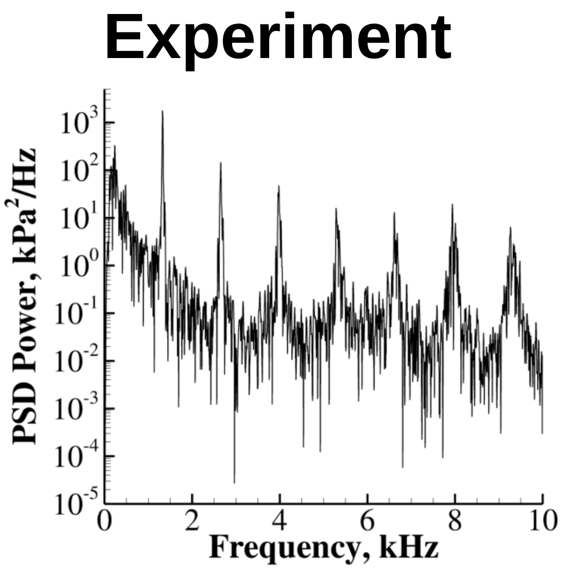
Error in 1st mode amplitude goes from 6% too high to 18% too high

Amplitudes of the harmonic also show an increase

PSD Analysis - Unstable







Global simulation – 40 ms (35 ms of data used for analysis)
Detailed Simulation – 20 ms (15 ms of data used for analysis)

Detailed Comparison

Unstable Stable

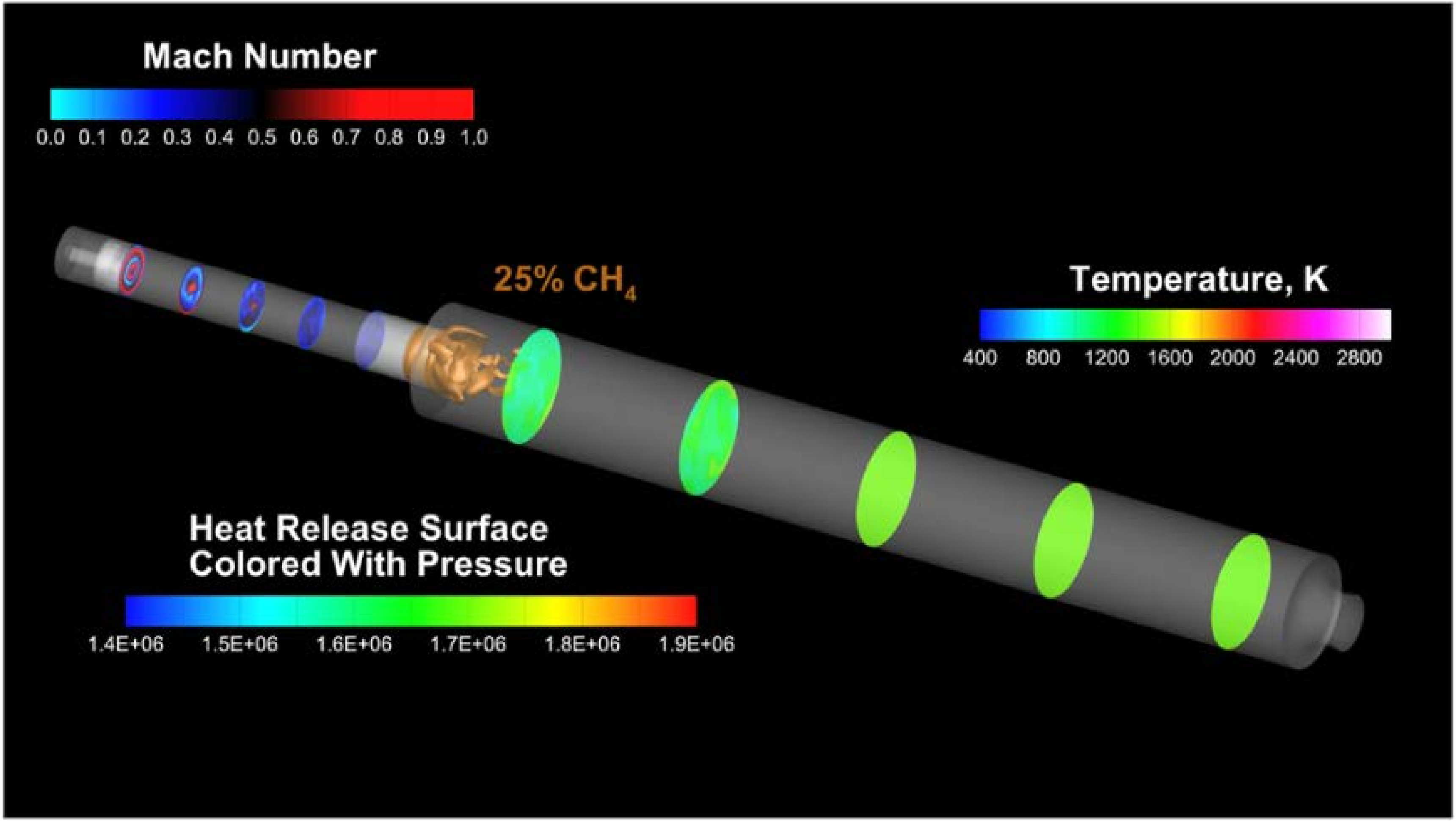
Mode	Experiment			Global			Detailed		
	f, Hz	p'_{ptp}, kPa	f_i/f_1	f, Hz	p'_{ptp}, kPa	f_i/f_1	f, Hz	p'_{ptp}, kPa	f_i/f_1
1	1324	387.15	1.00	1543	349.10	1.00	1467	416.79	1.00
2	2655	89.29	2.01	3114	87.55	2.01	2933	130.41	2.00
3	3979	46.37	3.01	4629	36.25	3.00	4400	64.88	3.00

Error in the frequency is reduced from 15% to 10%

Error in 1st mode amplitude goes from 10% too low to 7% too high

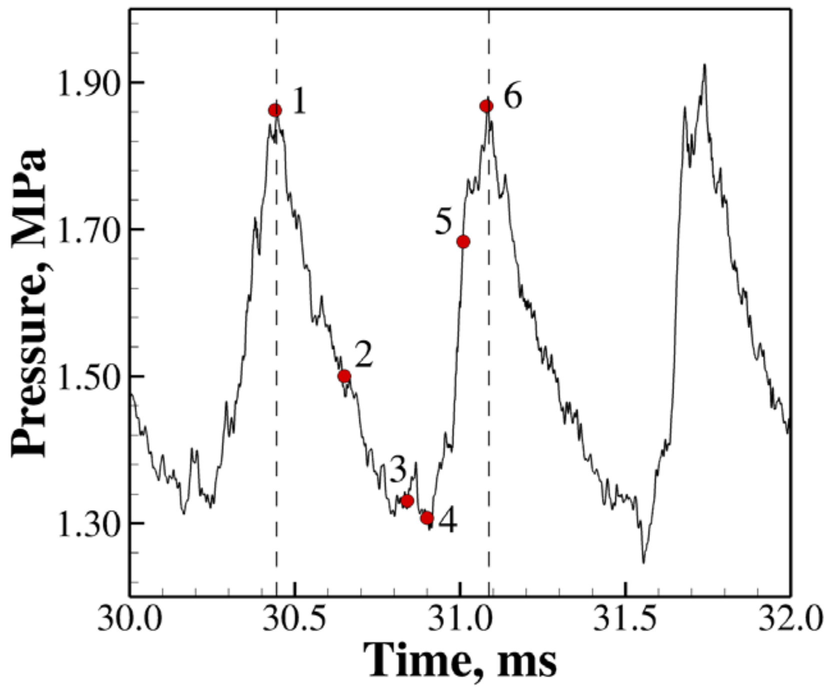
Amplitudes of the harmonic also show an increase

Detailed Results - Unstable

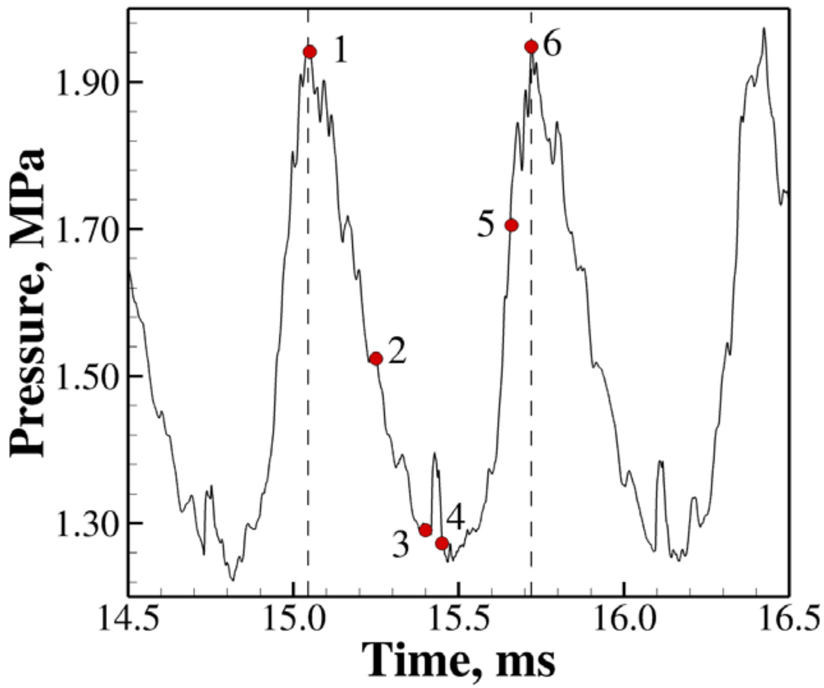


Detailed Cycle Evaluation

Global



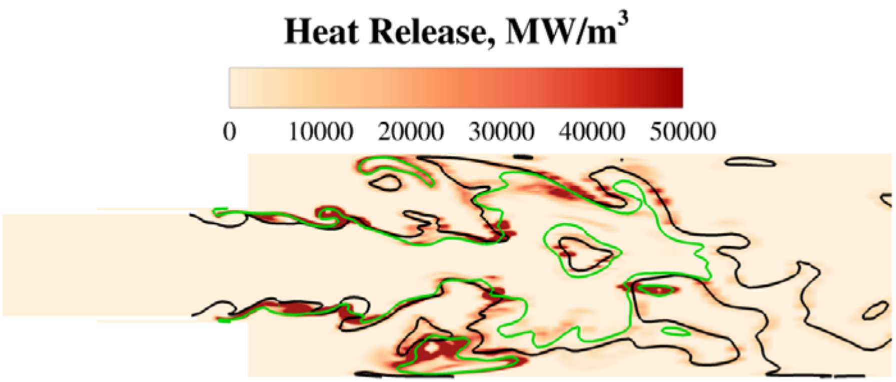
Detailed



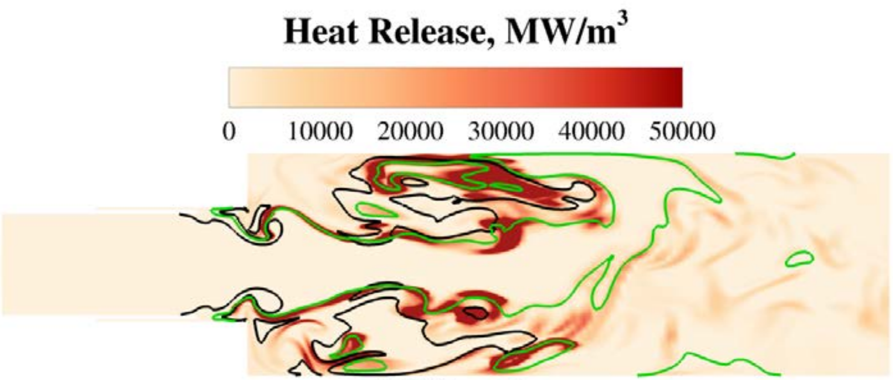
Time 1

Global

Detailed



(b) Time 1.



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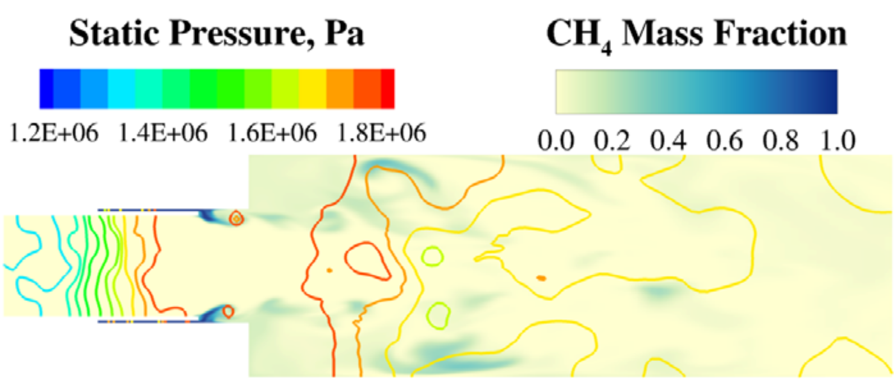

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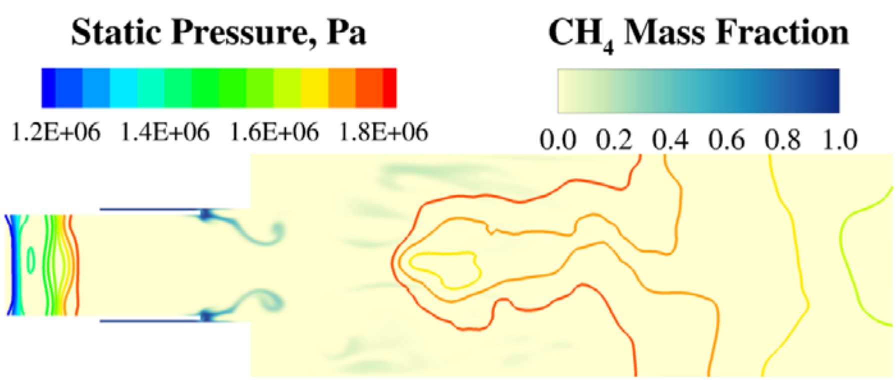
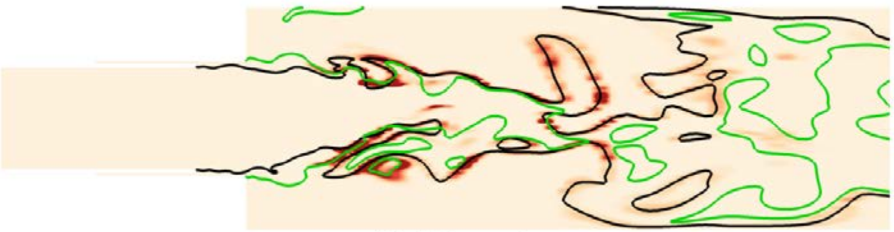


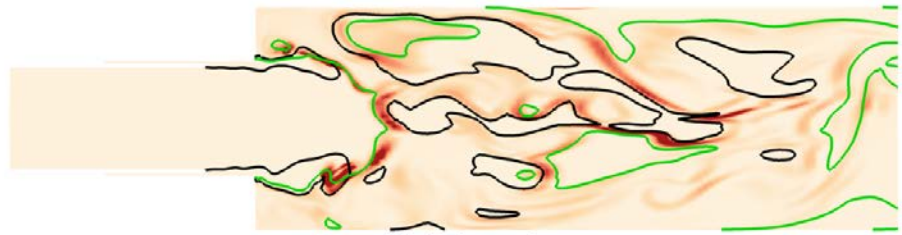
(a) Time 1.

Time 2

Global | Detailed



(d) Time 2.



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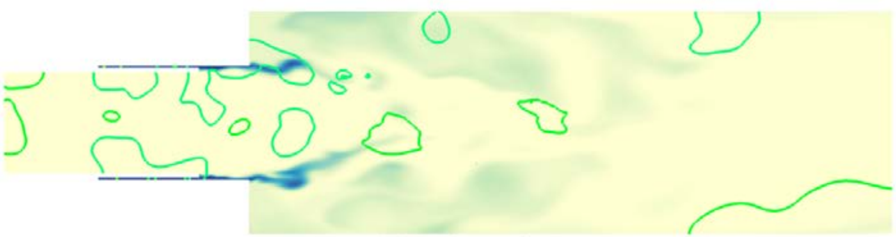


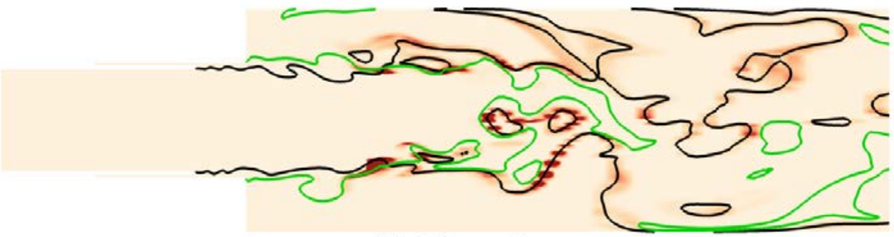
(c) Time 2.

(c) Time 2.

Time 3

Global

Detailed



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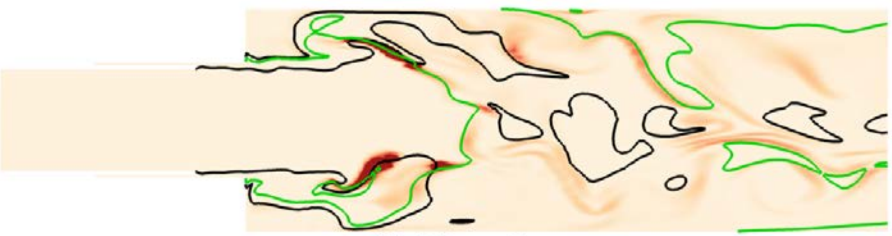
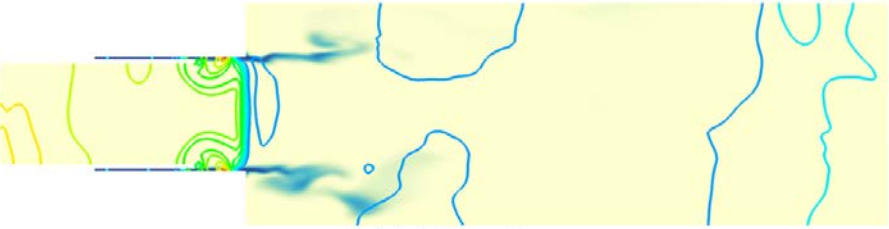


(f) Time 3.

(e) Time 3.

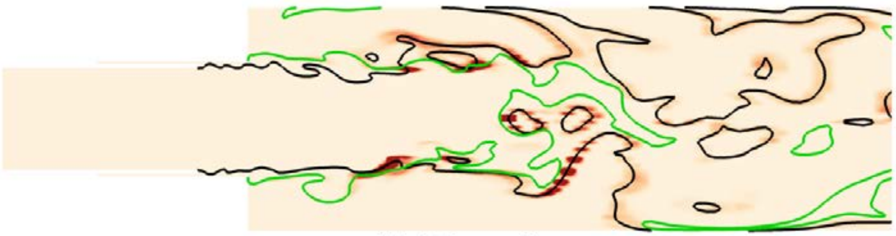


(e) Time 3.

Time 4

Global

Detailed



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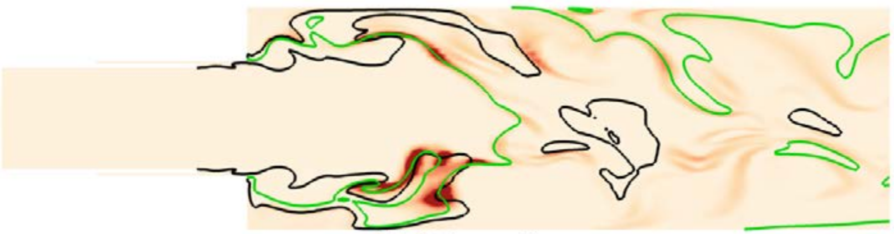

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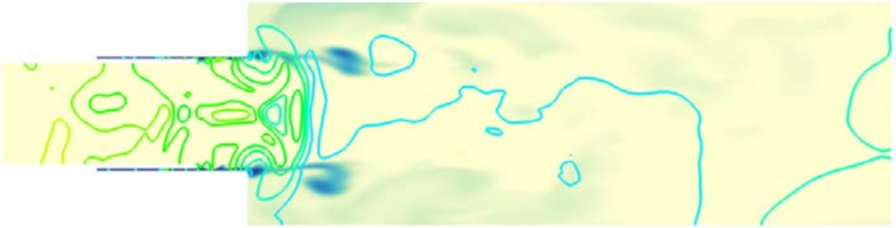

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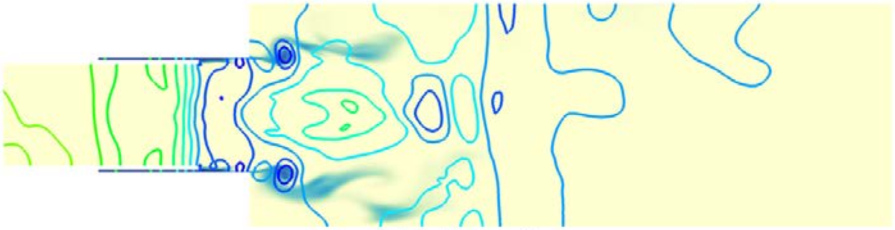
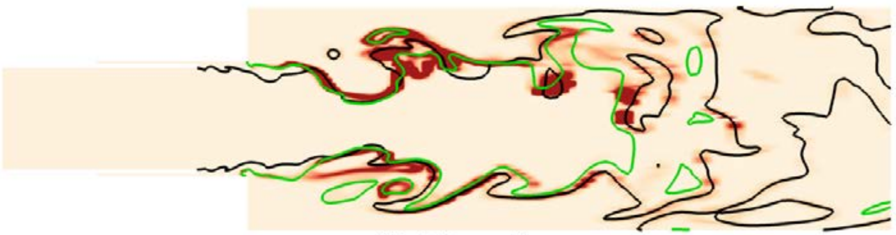


(g) Time 4.

Time 5

Global

Detailed



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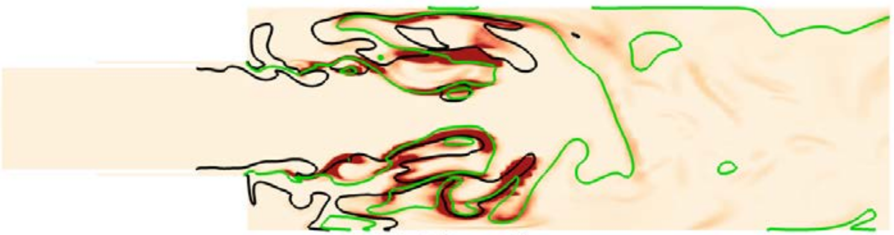

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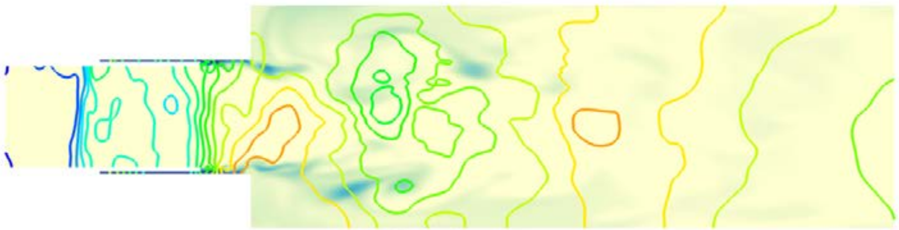

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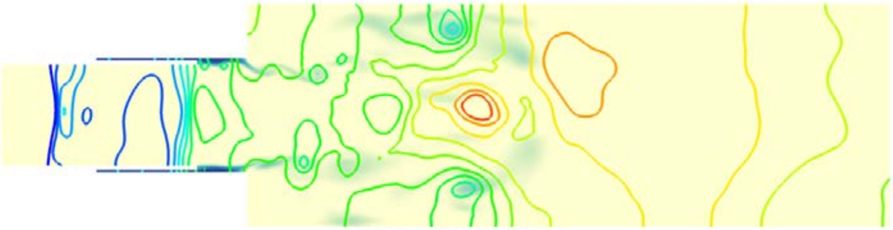
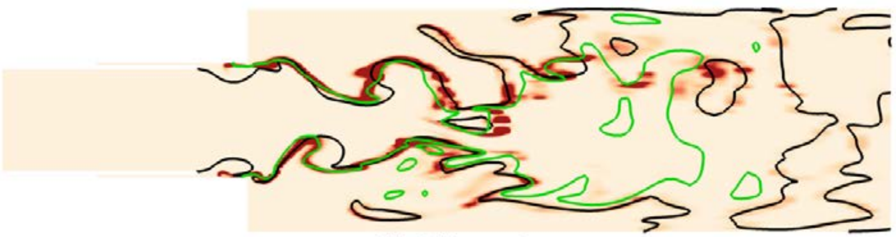


(i) Time 5.

Time 6

Global



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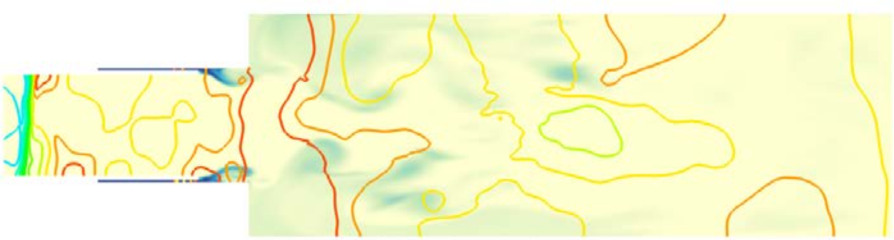

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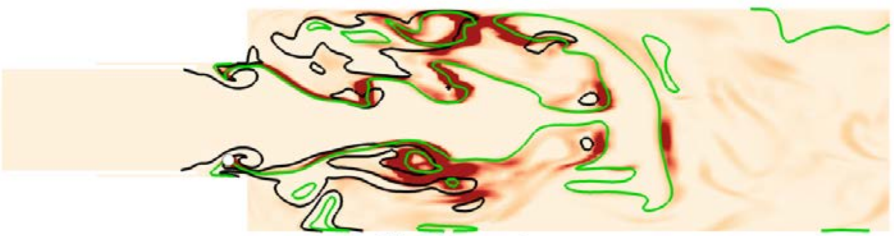
Detailed



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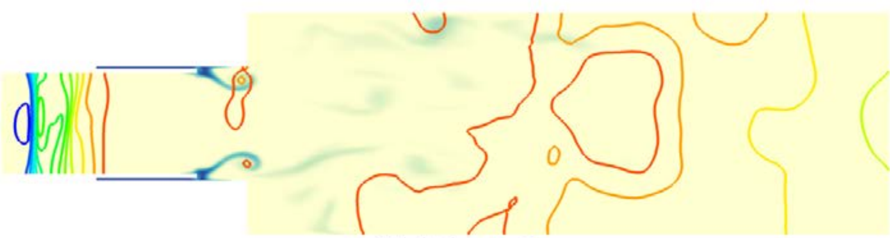
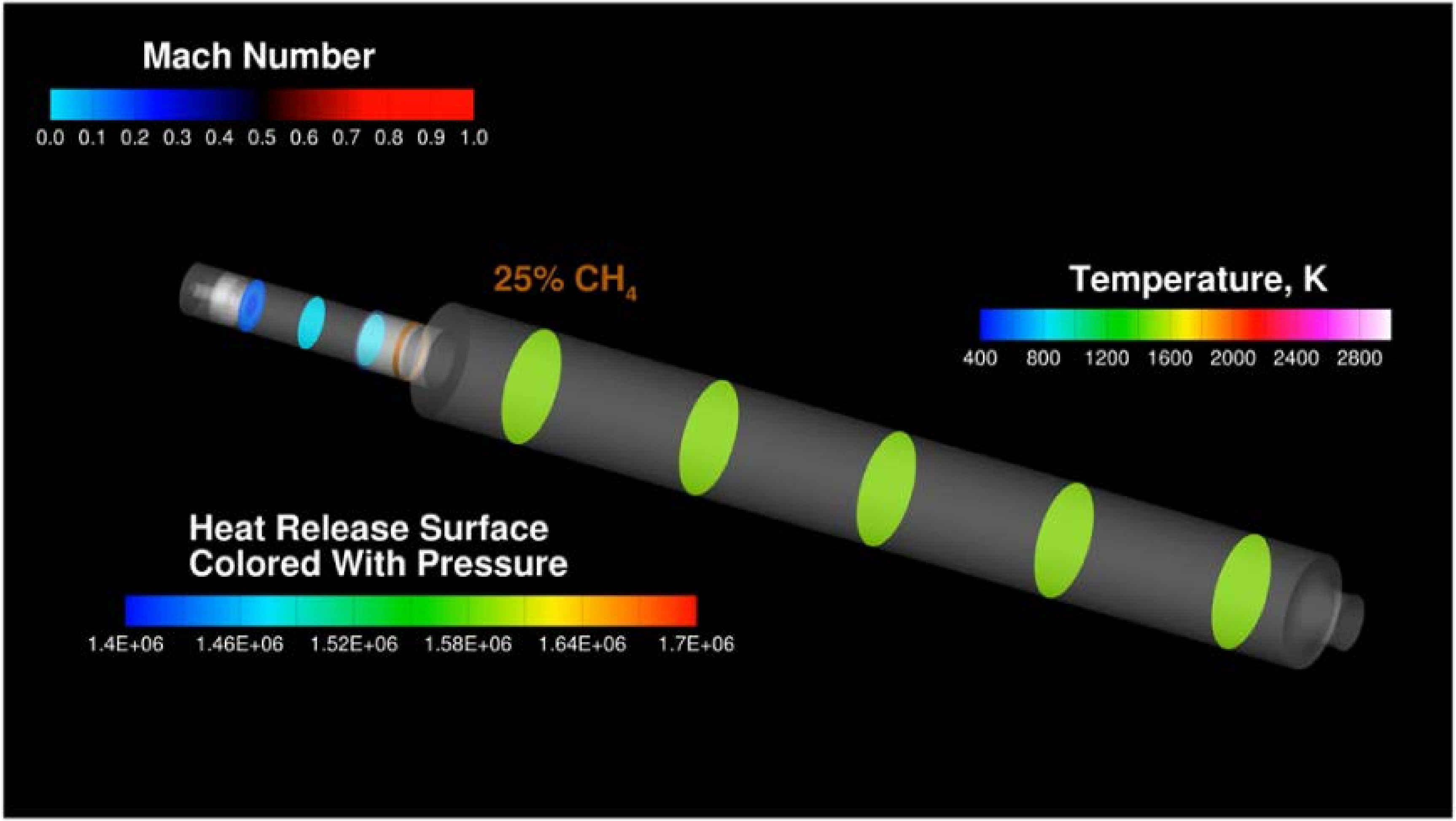


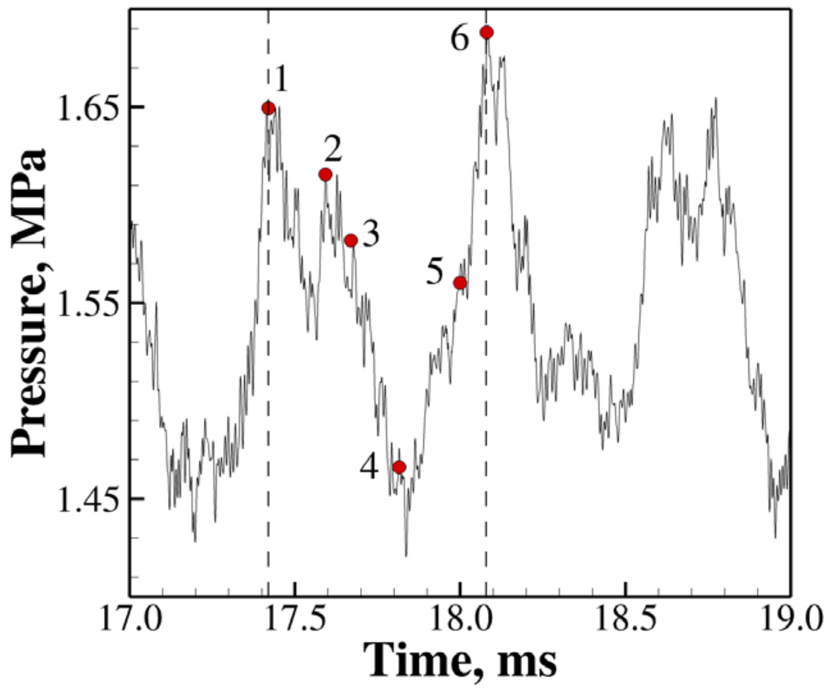
(k) Time 6.

Detailed Results – Marginally Stable



Detailed Cycle Evaluation

Global



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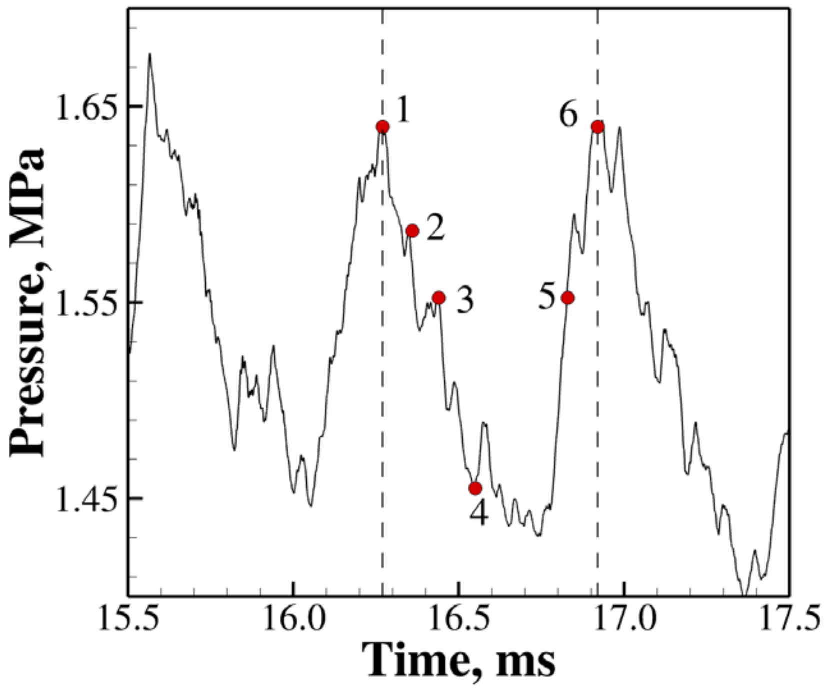
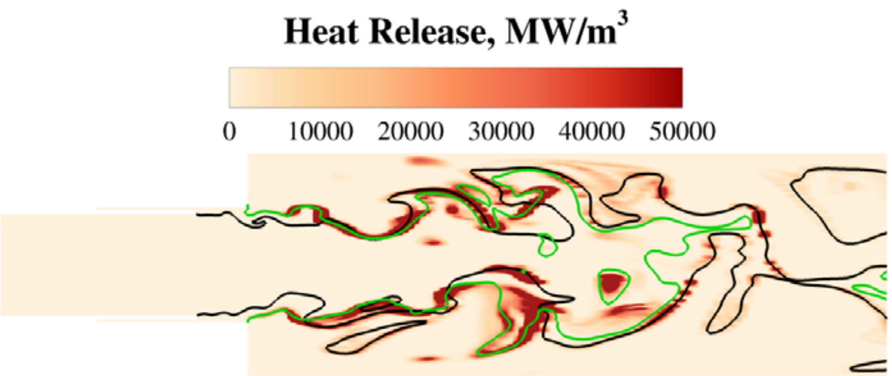


Time 1

Global

Detailed



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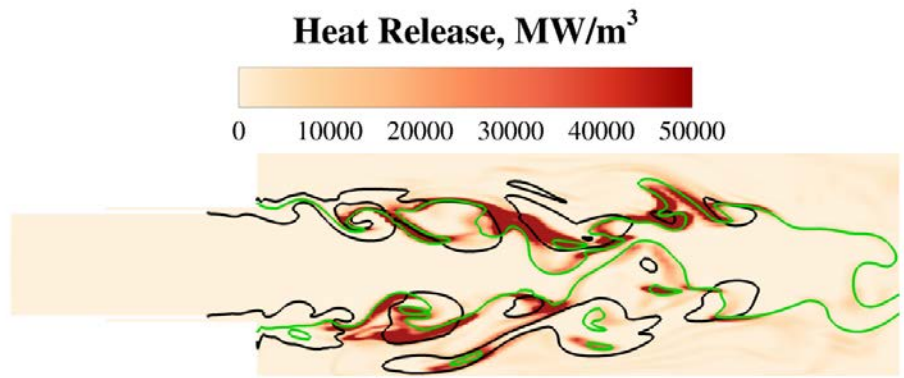

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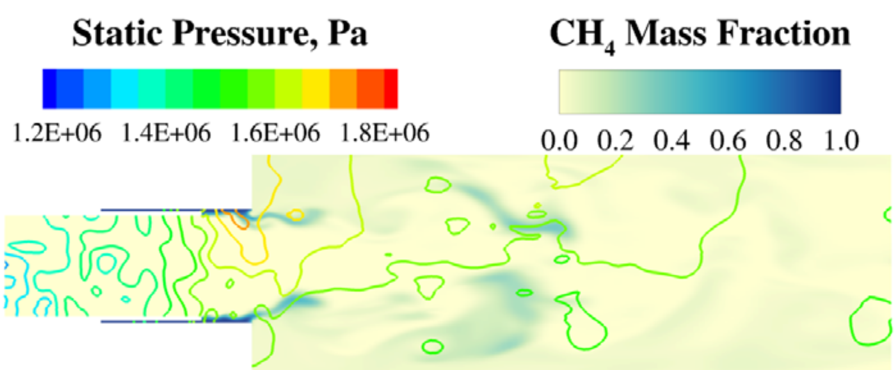

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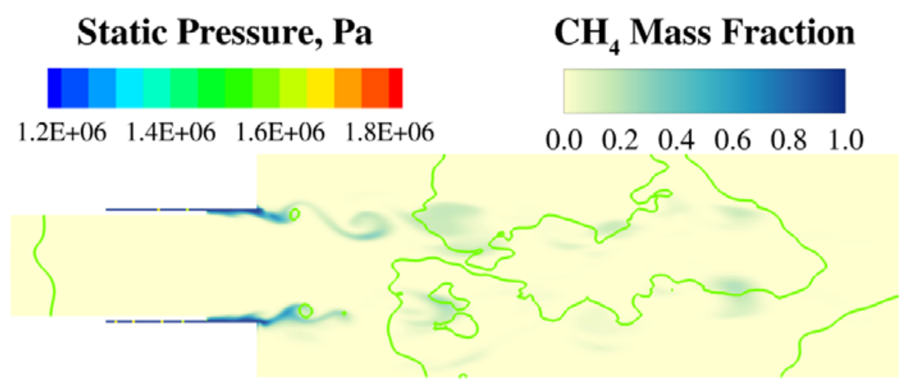
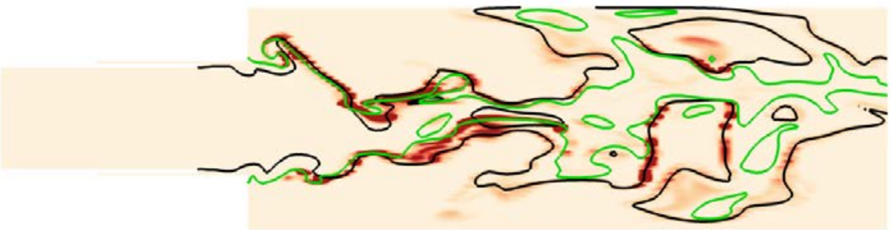


(a) Time 1.

Time 2

Global

Detailed



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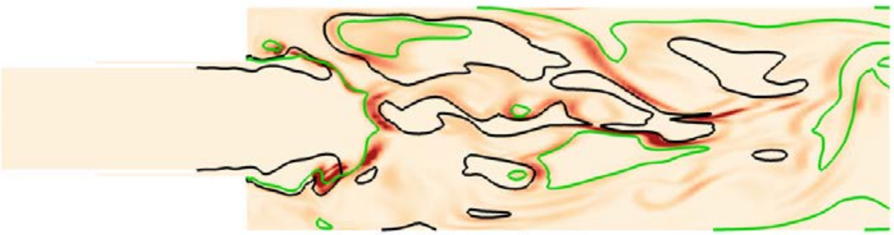

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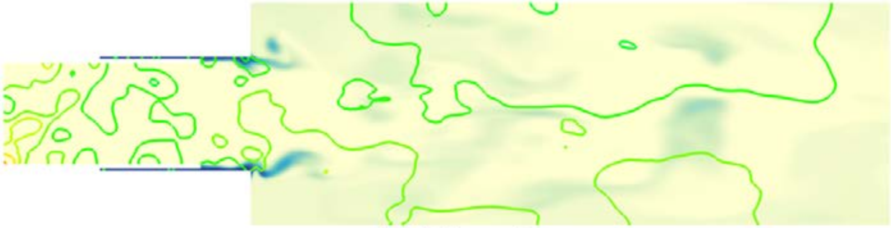

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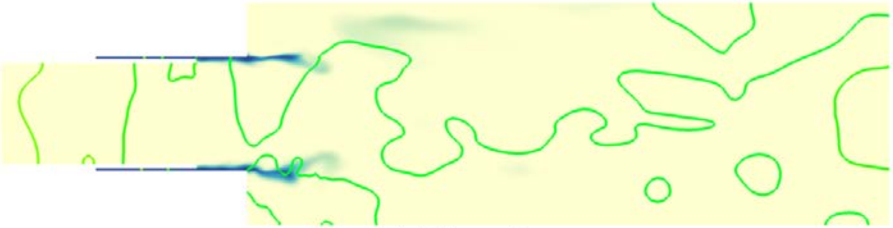
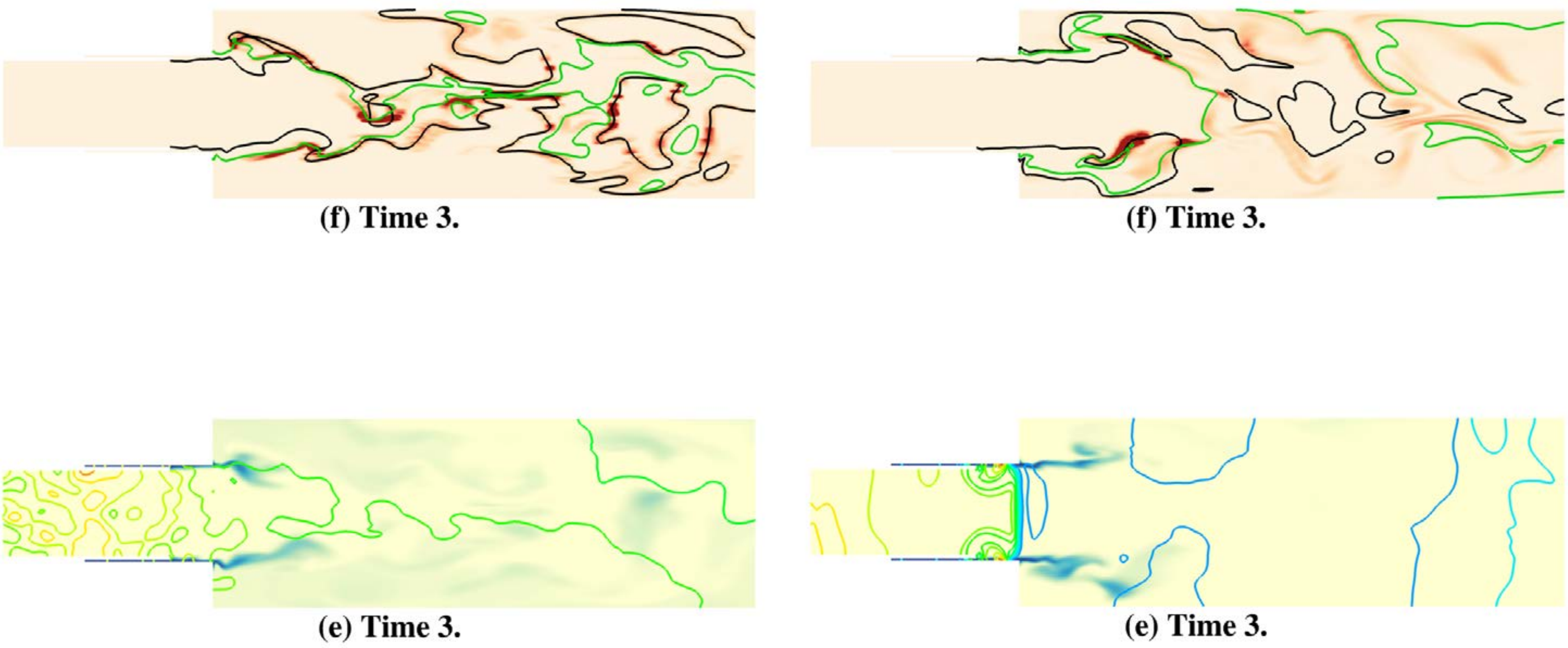


(c) Time 2.

Time 3

Global

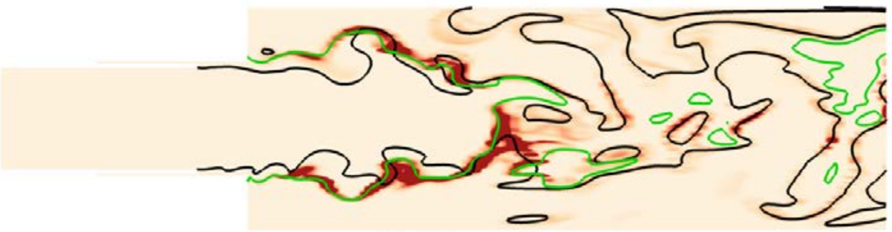
Detailed



Distribution A: approved for public release; distribution unlimited.

Time 4

Global | Detailed



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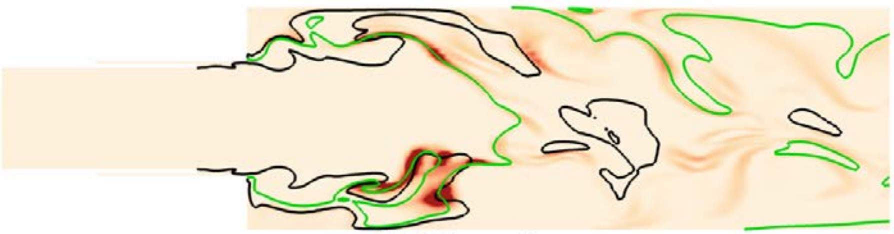

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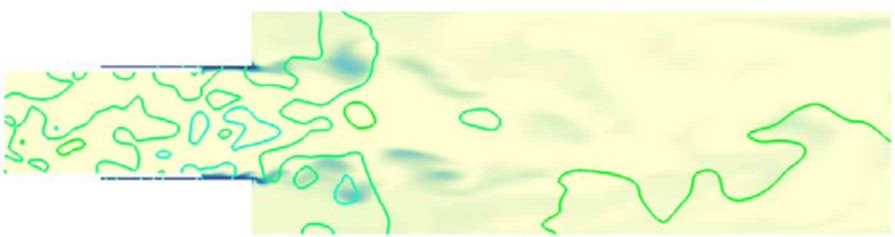

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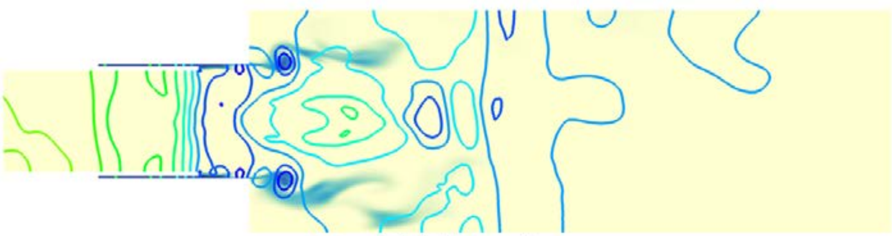
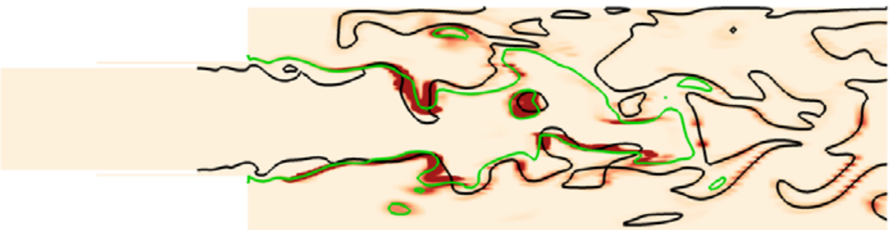


(g) Time 4.

Time 5

Global



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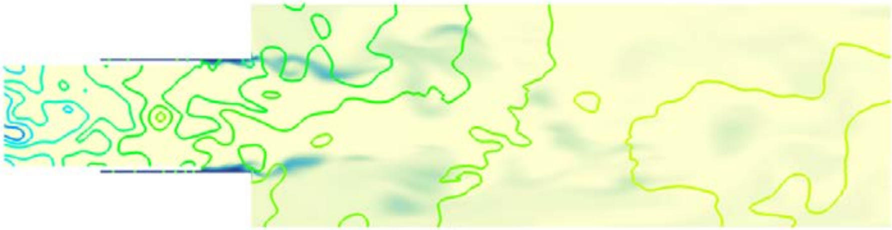
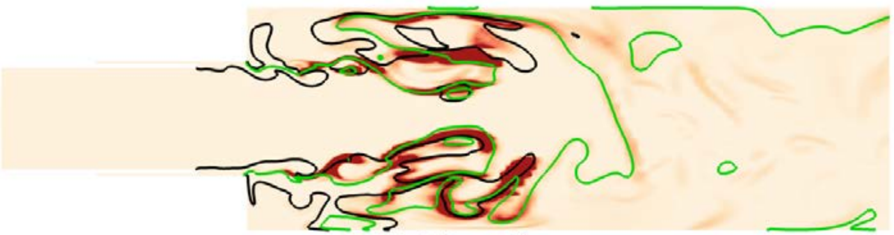


(i) Time 5.

Detailed



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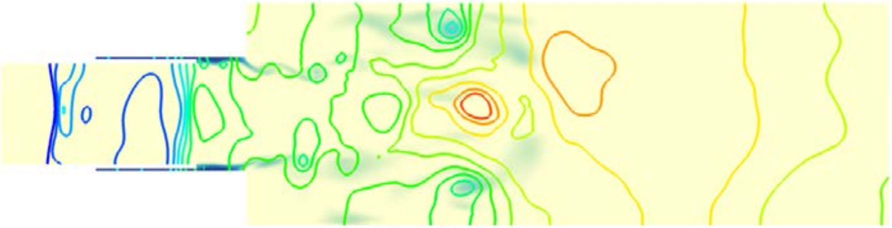
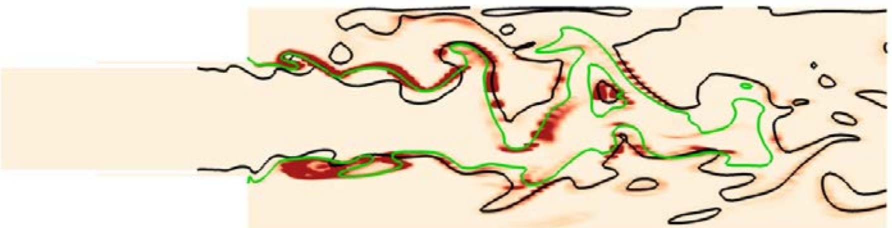


(i) Time 5.

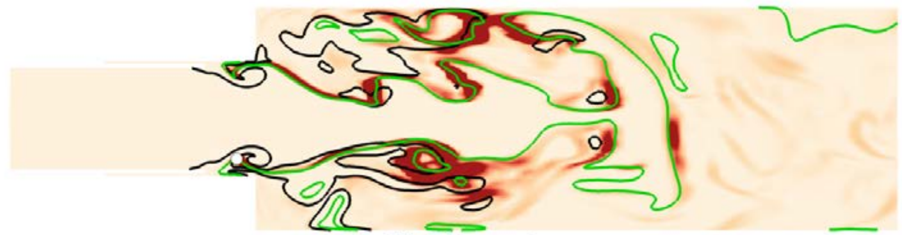
Time 6

Global

Detailed



(l) Time 6.



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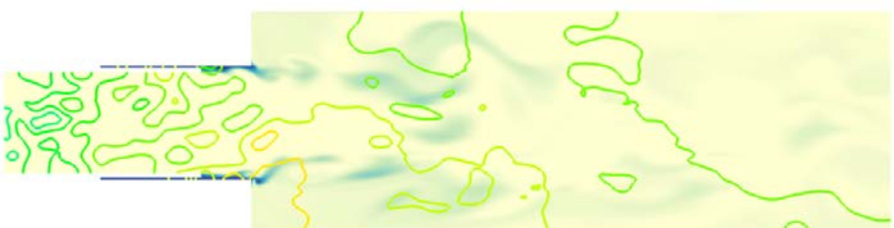

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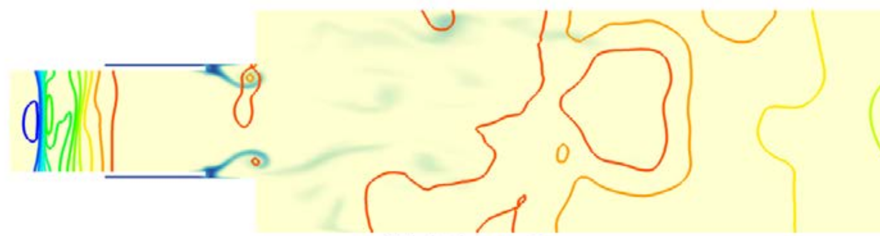

(k) Time 6.

Summary and Conclusions

- **A comparison of global and detailed kinetics mechanisms was completed for two operating conditions of a rocket injector**
- **Detailed kinetics showed higher amplitudes and lower frequencies**
  - Frequencies still do not match experimental values, heat transfer is the remaining unknown
- **The cyclic heat release of the unstable case was predicted by both mechanisms**

Summary and Conclusions

- **Similar results between both mechanisms suggest that in this configuration:**
  - The flow is mixing dominated
  - The coupling between pressure and heat release is captured sufficiently by the global mechanism
  - Differences in the heat release locations is a secondary effect and does not drive the instability
- **The prior improvement observed in the 2D simulations suggests that the poor ability to predict mixing in 2D is the key problem, not the simplicity of the kinetics.**

Questions

Acknowledgments

All computing resources were provided by the DoD high performance computing modernization program. Substantial resources for the detailed chemistry simulations were obtained through the TI-14 and TI-15 Capability Applications Project, Phase II.