Pressure Gain, Stability, and Operability of Methane/Syngas Based RDEs Under Steady and Transient Conditions

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Outline

- **Programmatic overview and introduction to the problem**
- Experimental activities
- Computational activities

Overarching objectives

- **Objective 1:**
  Develop and demonstrate a low-loss fully axial injection concept, taking advantage of stratification effects to alter the detonation structure and position the wave favorably within the combustor

- **Objective 2:**
  Obtain stability and operability characteristics of an RDC at fixed and transient operating conditions, and determine performance rules for full-scale operations

- **Objective 3:**
  Develop quantitative metrics for performance gain, as well as quantitative description of the loss mechanisms through a combination of diagnostics development, reduced-order modeling, and detailed simulations

Expected outcomes: RDE physics advancements

- **Outcome 1 –** A comprehensive study of the stability and operability of high AAR designs under engine-relevant conditions
- **Outcome 2 –** A low-loss inlet design with optimal placement of detonation wave to promote efficiency gain
- **Outcome 3 –** Methods for estimating effective pressure gain realized
- **Outcome 4 –** A suite of computational tools for modeling full-scale RDEs, including an AI-based acceleration for long duration simulations
- **Outcome 5 –** Demonstration of efficiency improvement (gain) using a ~~methane/syngas mixture~~ hydrogen RDE

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- Computational activities

Two aspects of interest

Operability

&

Performance

- Power density & robustness
- Thermodynamic performance (gain)

Overarching goal:
Develop and describe a pathway towards achieving positive pressure gain through analysis of individual loss mechanisms

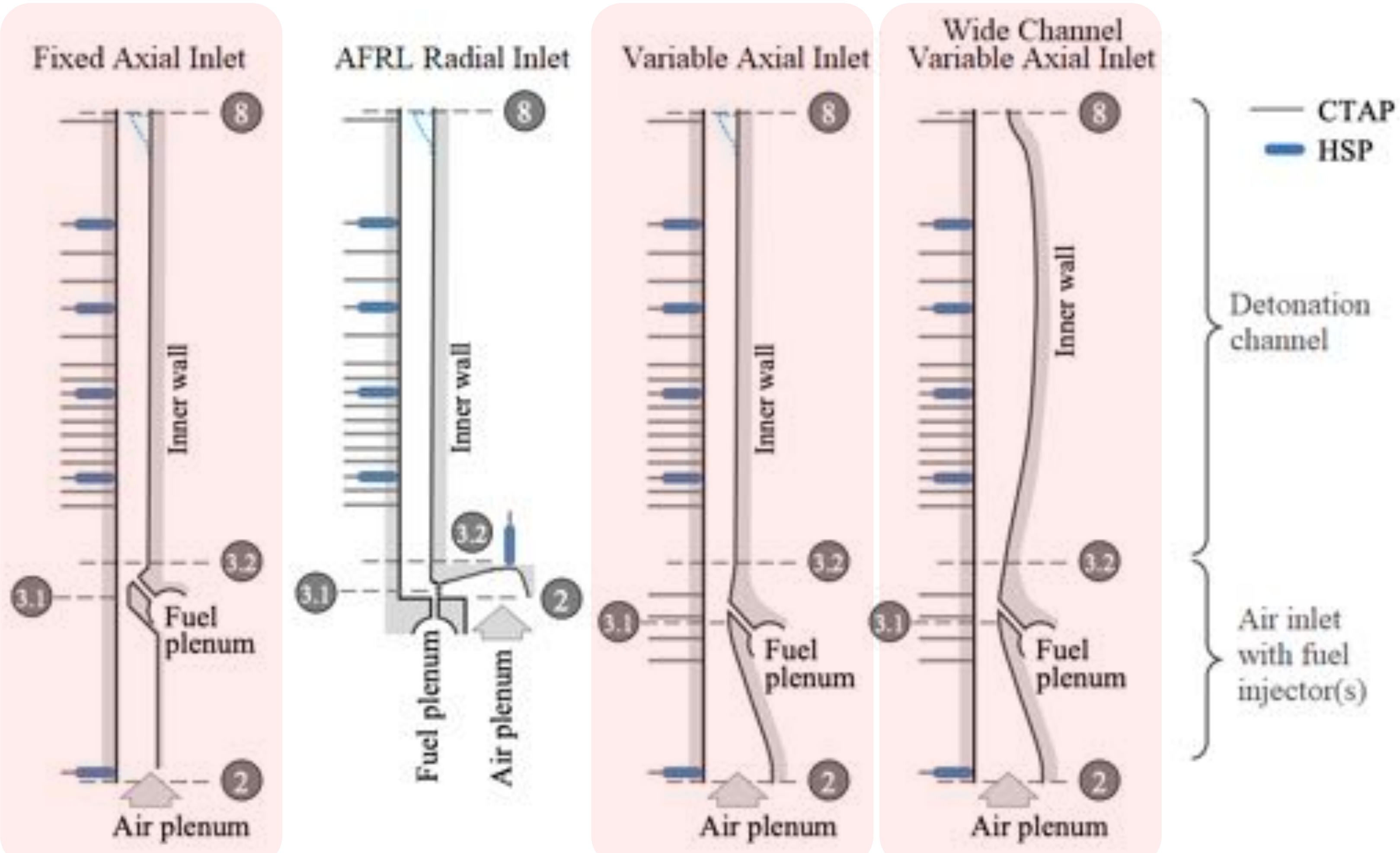
Credit: Joshua Shepard

Our contribution for the year

- Improved performance measurements on RDC
  - Iterative process to reduce uncertainties on thrust measurements
  - Conducted uncertainty analysis to identify measurement limitations
  - Conducted parametric study of the effect of operating conditions and design on performance (thrust and pressure gain)
  - This has built on our past RDC systems and experience
- Developed a Bayesian inference framework for assessing (estimating) losses in RDCs
  - Extends our past efforts on direct measurement
  - We will now apply this tool to correlate deflagration losses to performance
- Continued the investigation of pressure gain and losses in RDCs
  - A new loss mechanism has been identified
  - Performed a loss analysis on RDC performance

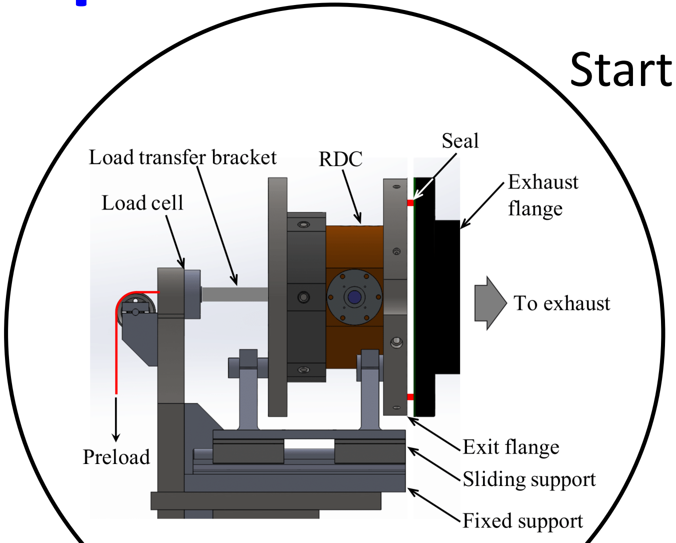
We have built on existing hardware

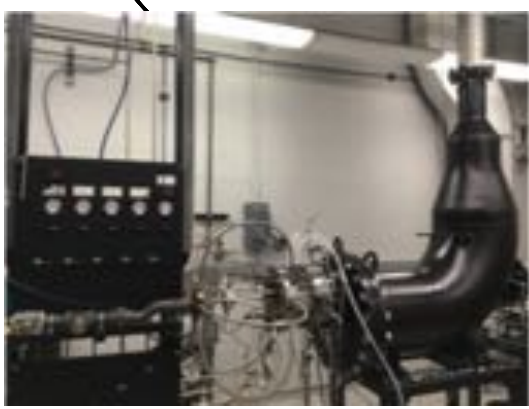
- We have focused on hydrogen-air mixtures to be aligned with program directions
- We have focused on extracting quantitative information on performance and losses/gain



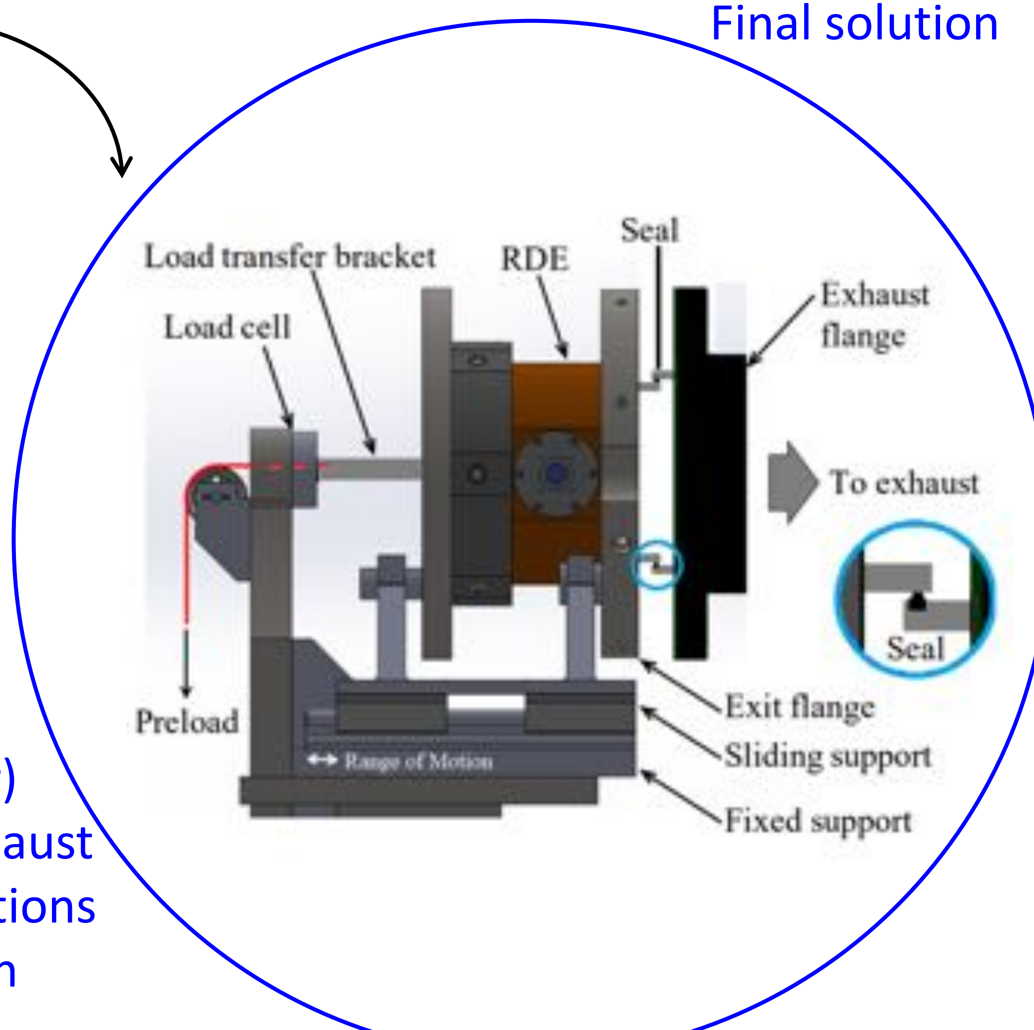
Improvements on thrust measurements

Starting point





Final solution

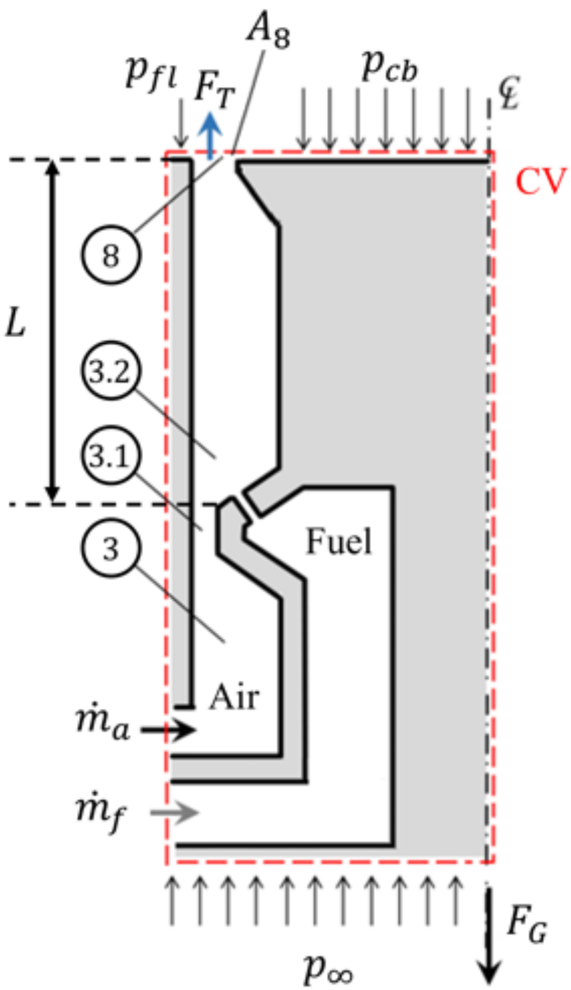


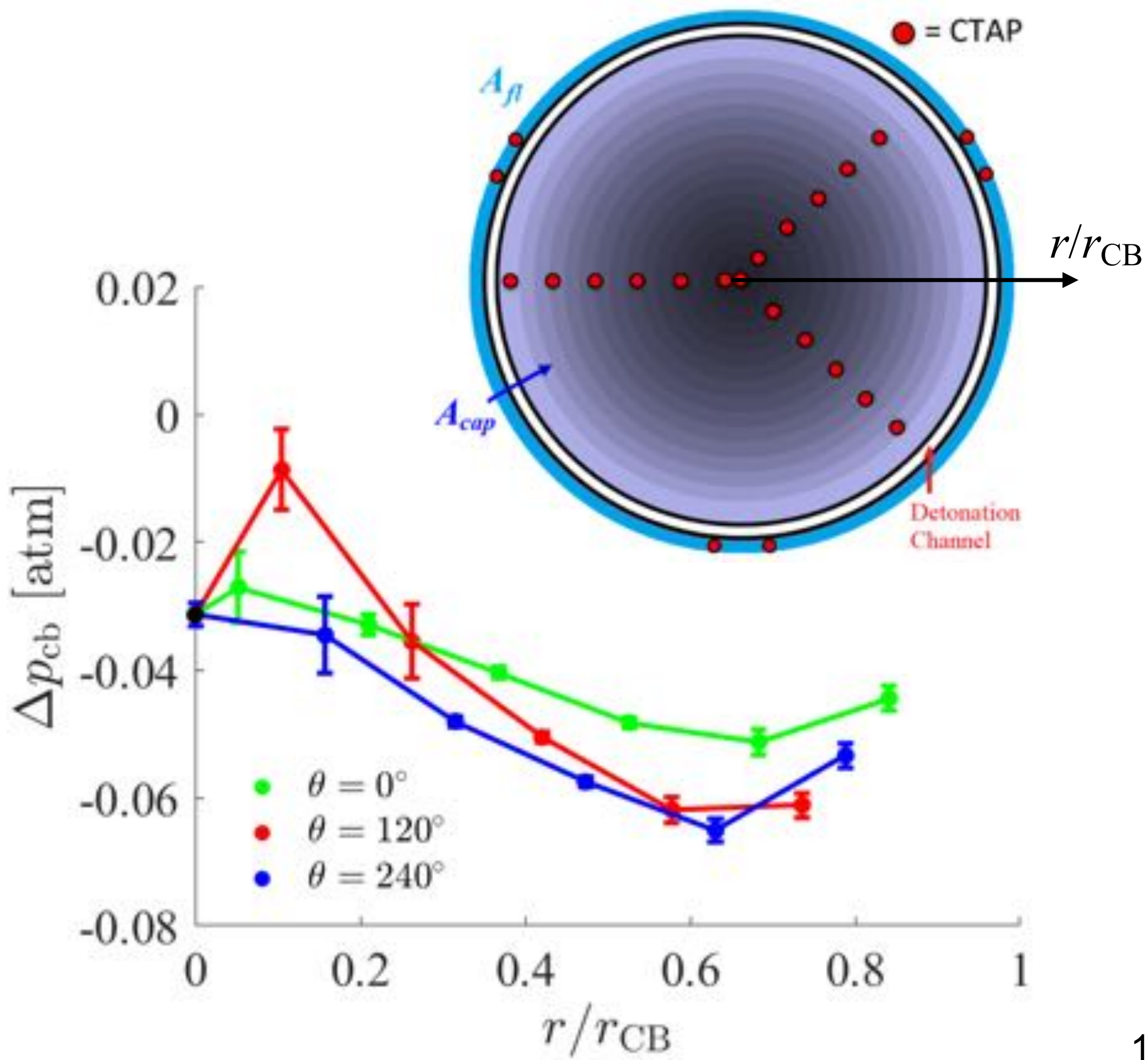
Modifications:

- Routing of inlet lines (fuel and air)
- Low-friction, slip fit flange on exhaust
- Minimize base pressure contributions
- Improve base pressure estimation

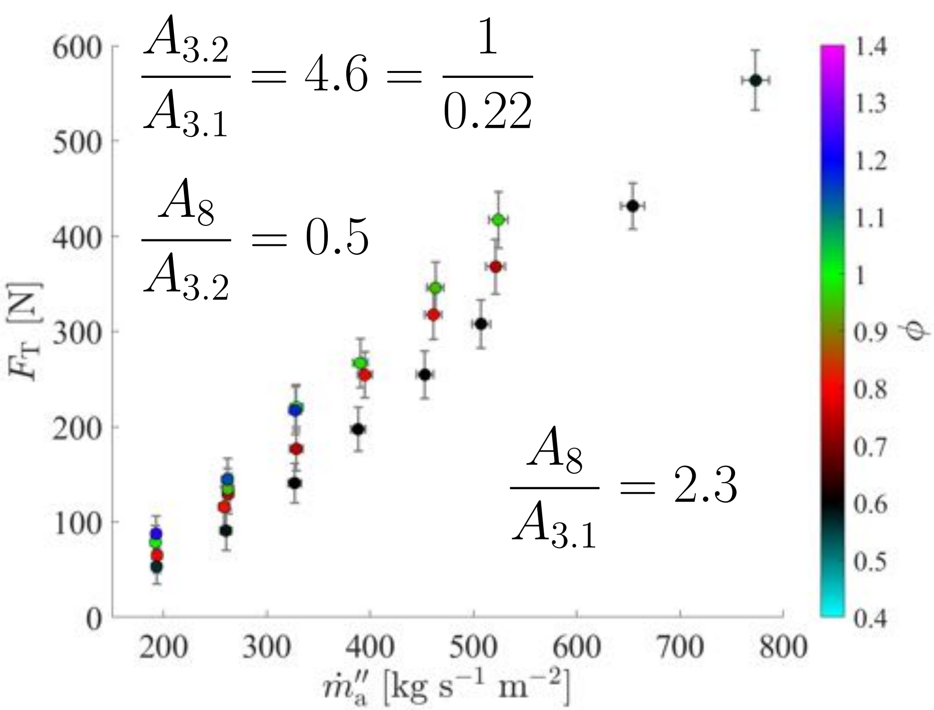
Detailed uncertainty analysis of thrust measurements

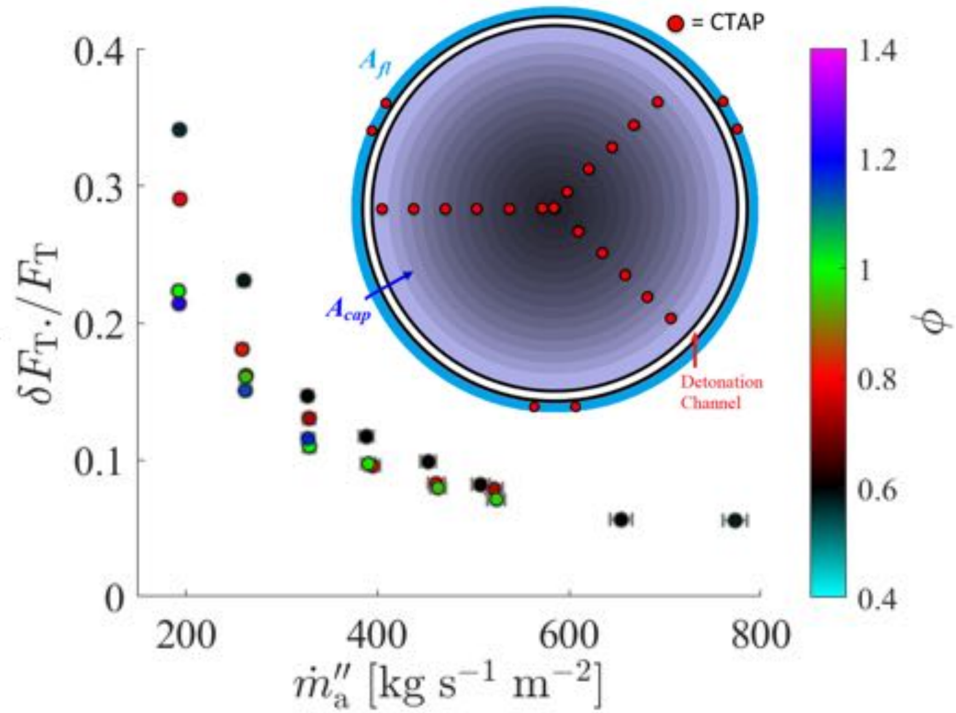
$$F_{\mathrm{T}} = F_{\mathrm{G}} - \int_{A_{\mathrm{cb}}} (p_{\mathrm{cb}} - p_{\infty})\mathrm{d}A_{\mathrm{cb}} - \int_{A_{\mathrm{fl}}} (p_{\mathrm{fl}} - p_{\infty})\mathrm{d}A_{\mathrm{fl}}$$





Detailed uncertainty analysis of thrust measurements





- High-quality measurements have been acquired, but uncertainties are still large
- Uncertainty due to base pressure correction are minimized, but still significant
- Importance of proper base pressure accounting has been highlighted
  - Sufficient instrumentation and optimal distribution is needed
  - Errors due to integration from set of discrete pressure measurements
  - Analysis conducted but not shown here

Pressure gain evaluated using the concept Equivalent Available Pressure (Kaemming & Paxson, 2018)

Unity exit Mach number: $\widetilde{p}_8 = \dfrac{F_{\mathrm{T}} + p_\infty A_8}{A_8\left(1+\gamma_8\right)}$

$$\mathrm{EAP} = \widetilde{p}_{\mathrm{t},8} = \widetilde{p}_8 \left(\frac{\gamma_8+1}{2}\right)^{\frac{\gamma_8}{\gamma_8-1}}$$

$$\mathrm{PG} = \frac{\mathrm{EAP}}{p_2} - 1$$

Non-unity exit Mach number:

$$\widetilde{p}_8 = \frac{F_{\mathrm{T}} + p_\infty A_8}{A_8\left(1+\gamma_8 M_{8,\mathrm{z}}^2\right)}$$

$$M_{8,\mathrm{z}} = \frac{\dot{m}_{\mathrm{T}}\sqrt{R_8 T_8}}{p_8 A_8 \sqrt{\gamma_8}}$$

Assumptions on (p_8,T_8); measurements under way

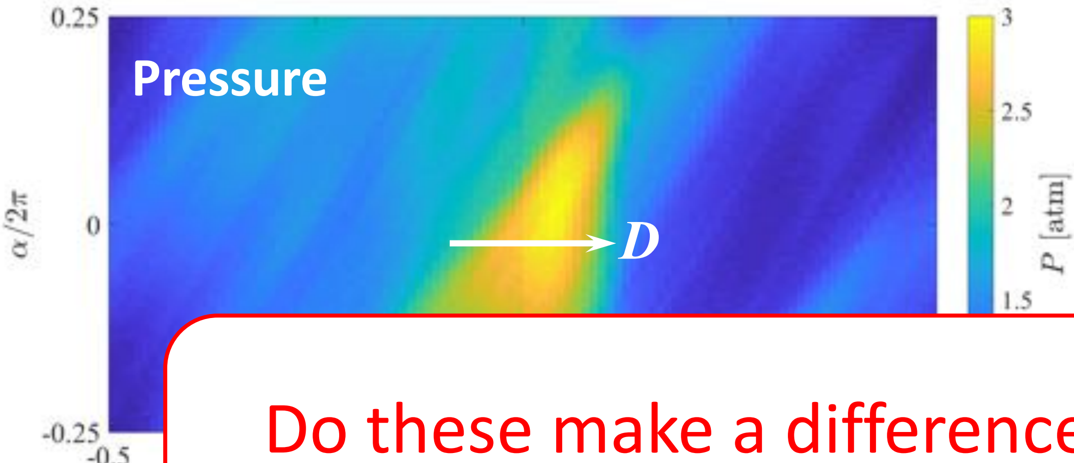
$$\mathrm{EAP}(M_{8,\mathrm{z}}) = \widetilde{p}_8 \left(1+\frac{\gamma_8-1}{2}M_{8,\mathrm{z}}^2\right)^{\frac{\gamma_8}{\gamma_8-1}}$$

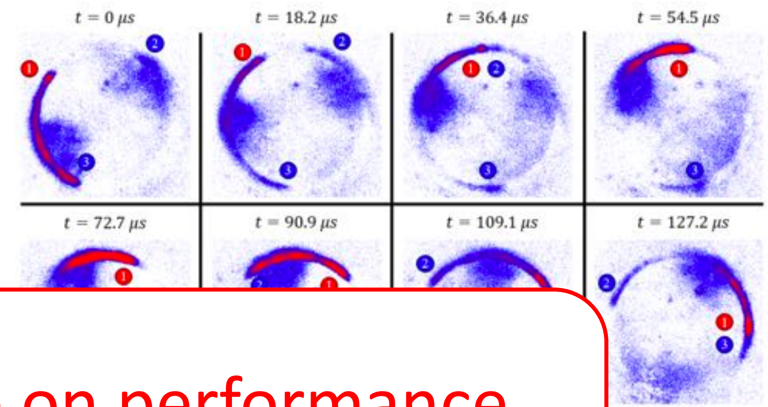
$$= \left(\frac{F_{\mathrm{T}}}{A_8}+p_\infty\right)\frac{\left(1+\frac{\gamma_8-1}{2}M_{8,\mathrm{z}}^2\right)^{\frac{\gamma_8}{\gamma_8-1}}}{\left(1+\gamma M_{8,\mathrm{z}}^2\right)}$$

$$\mathrm{PG_M} = \frac{\mathrm{EAP}(M_{8,\mathrm{z}})}{p_2} - 1$$

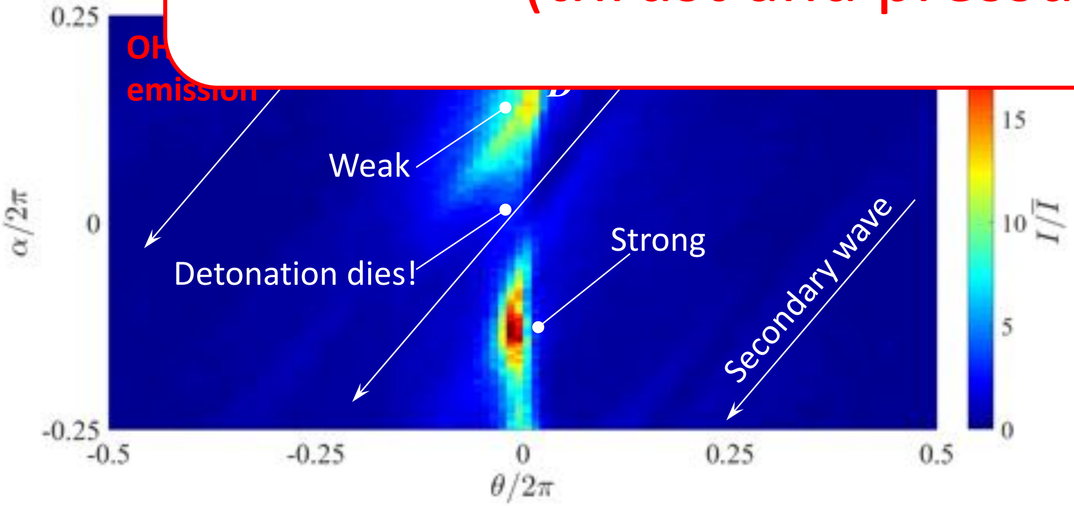
From the past: Multiple competing (secondary) waves couple and suppress detonation wave

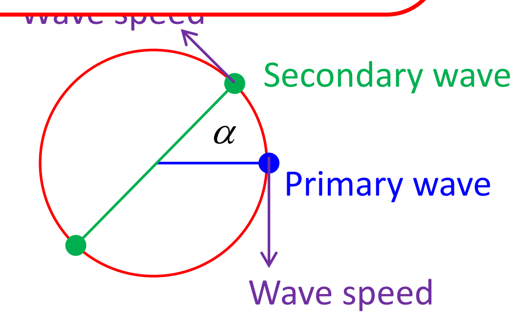
Phase-average distribution conditional to separation between detonation and secondary wave



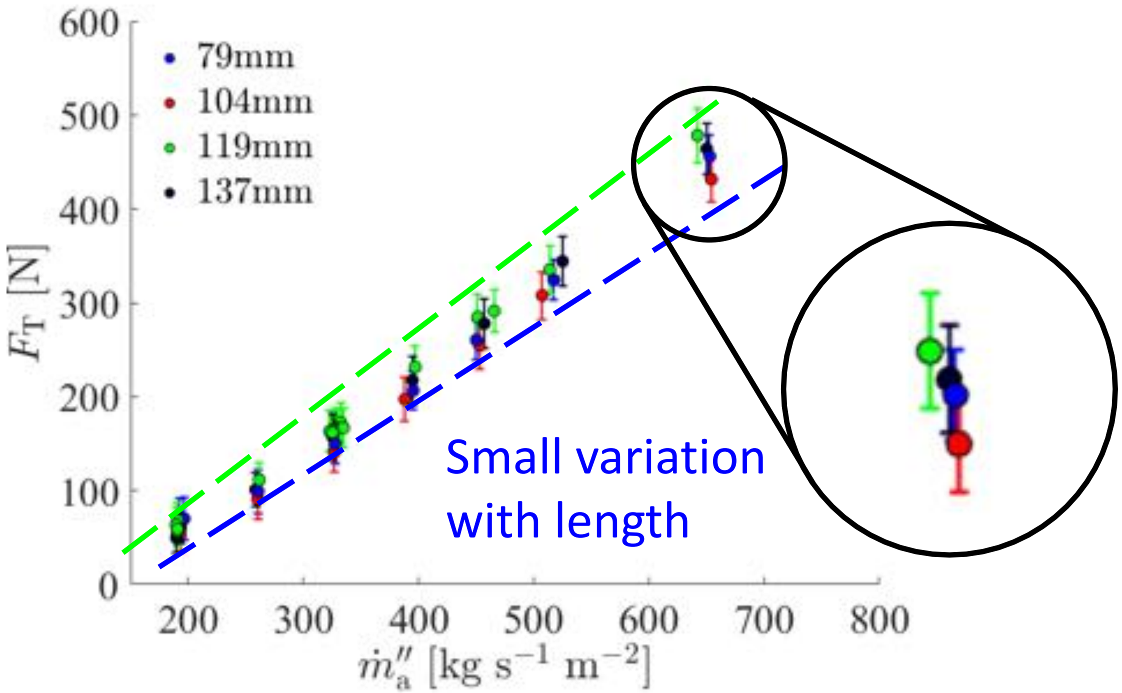


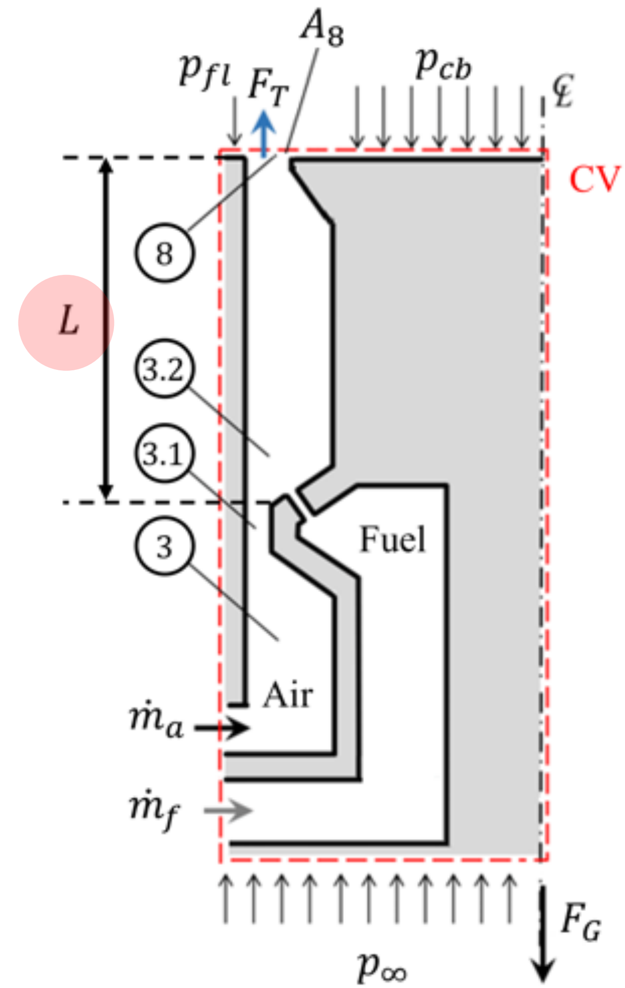
Do these make a difference on performance (thrust and pressure gain)?





Effect of combustor length, same inlet/exit



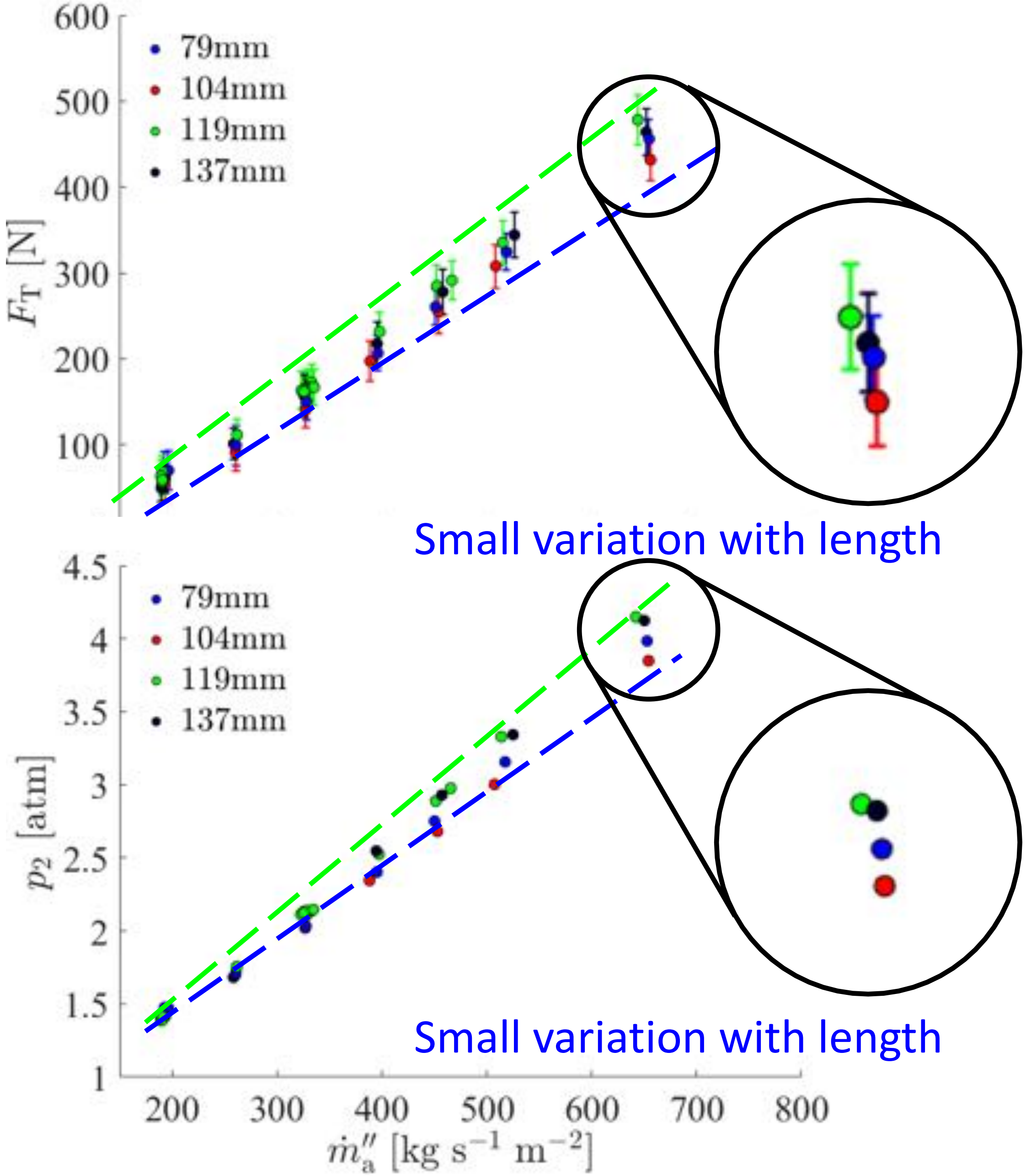


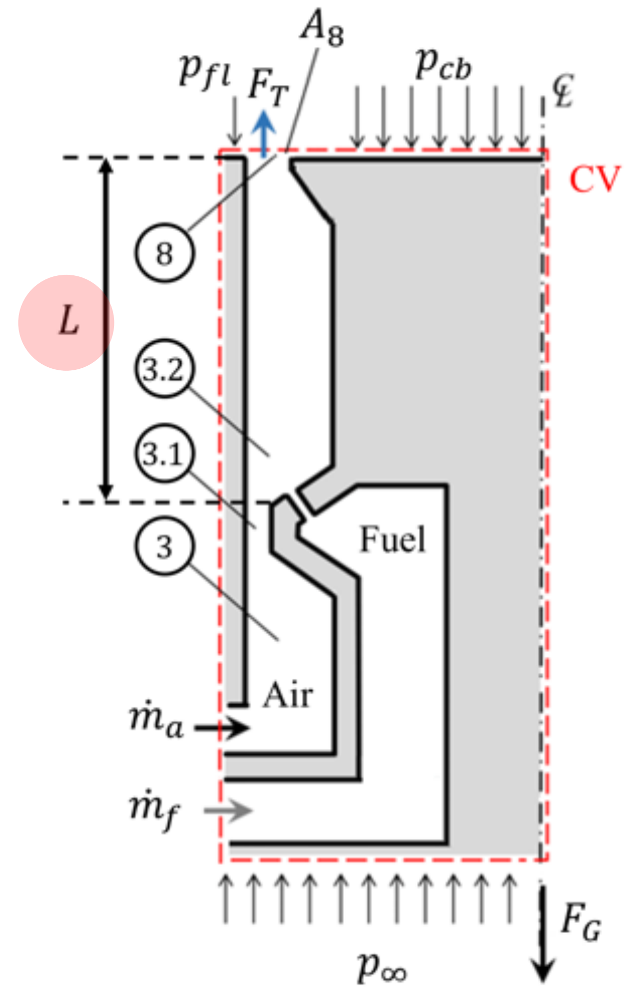
With length changing, there are changes in:

- Number
- Speed
- Strength of detonation wave

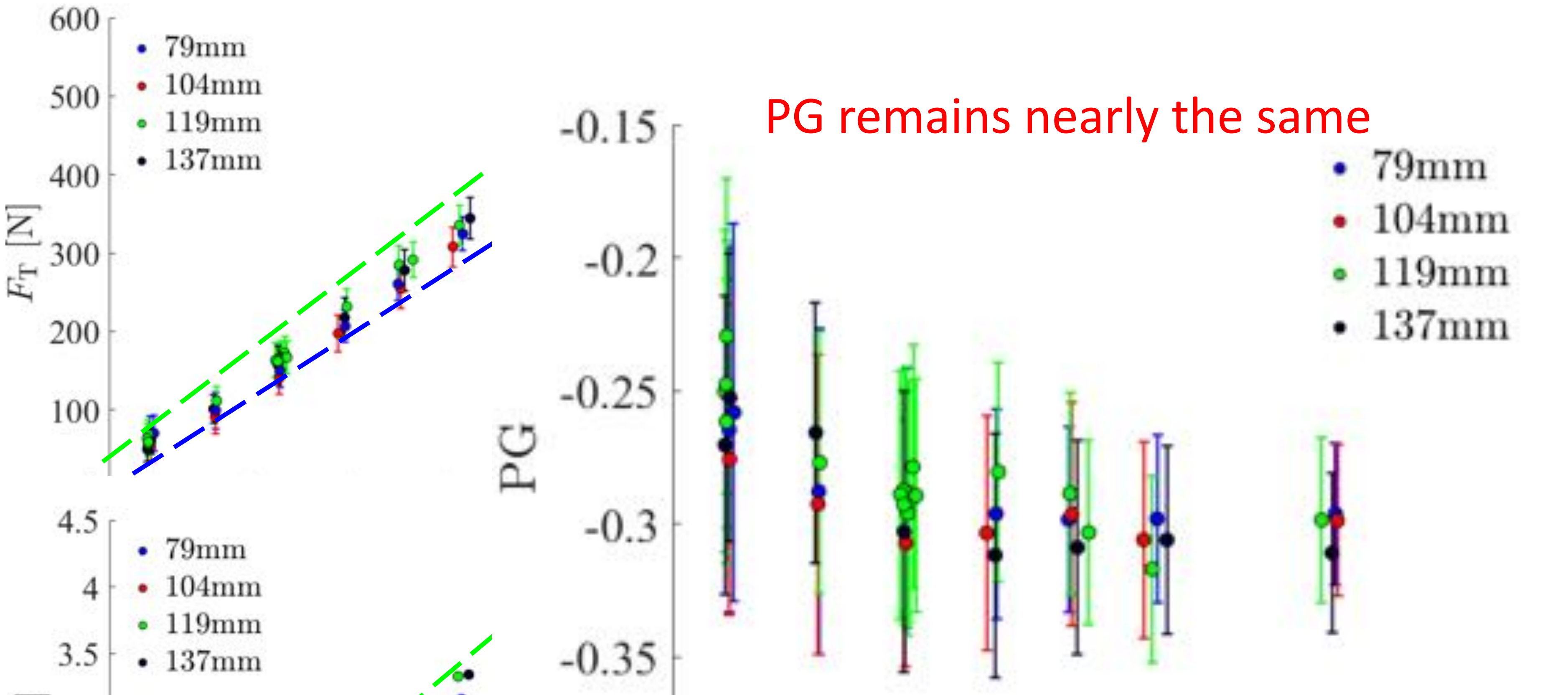
Mode of operation and dynamics are drastically different

Effect of combustor length, same inlet/exit

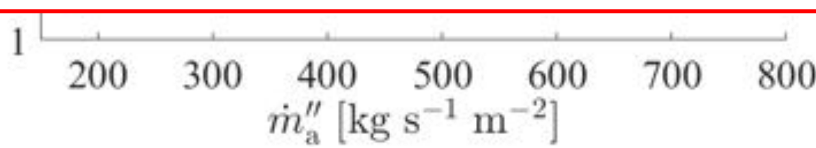




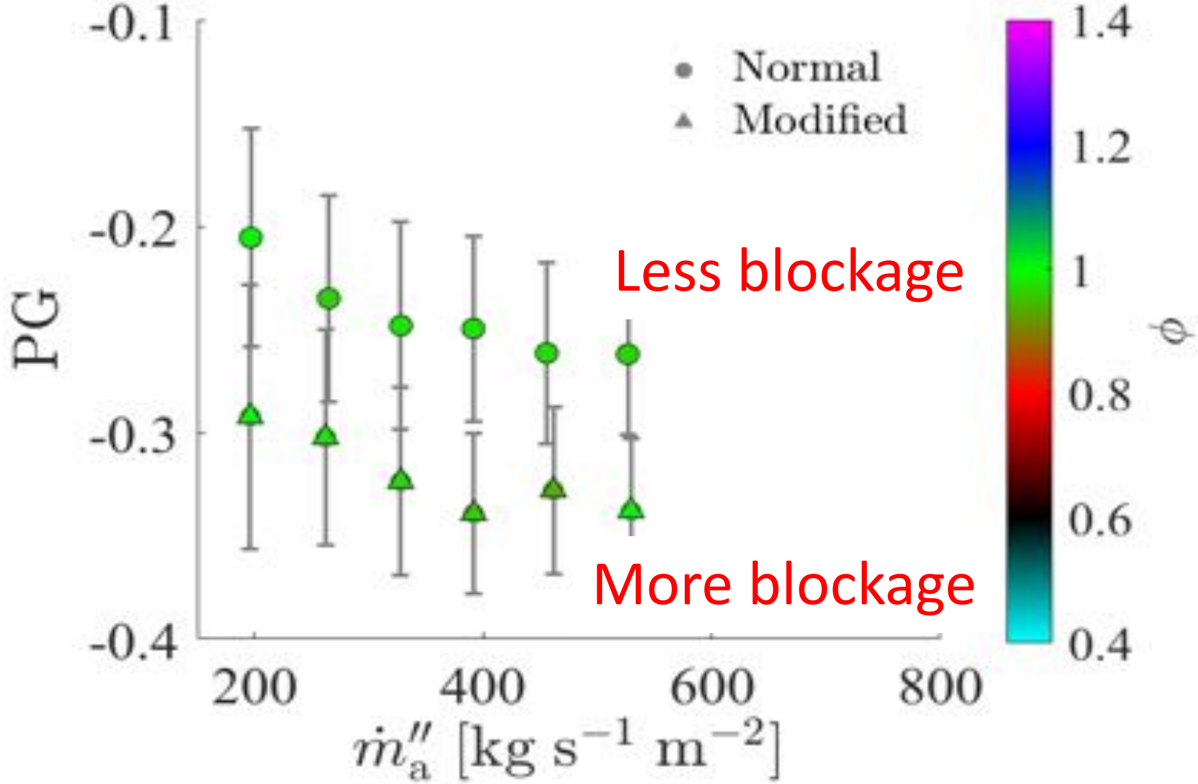
Effect of combustor length, same inlet/exit

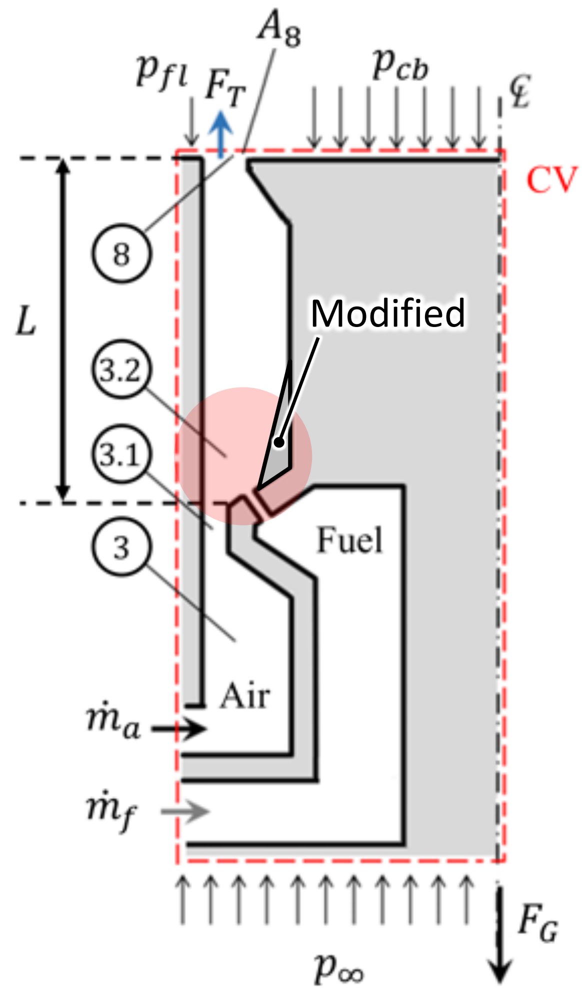


Pressure gain (performance) is mostly insensitive to many details of detonation and secondary waves, and operating mode



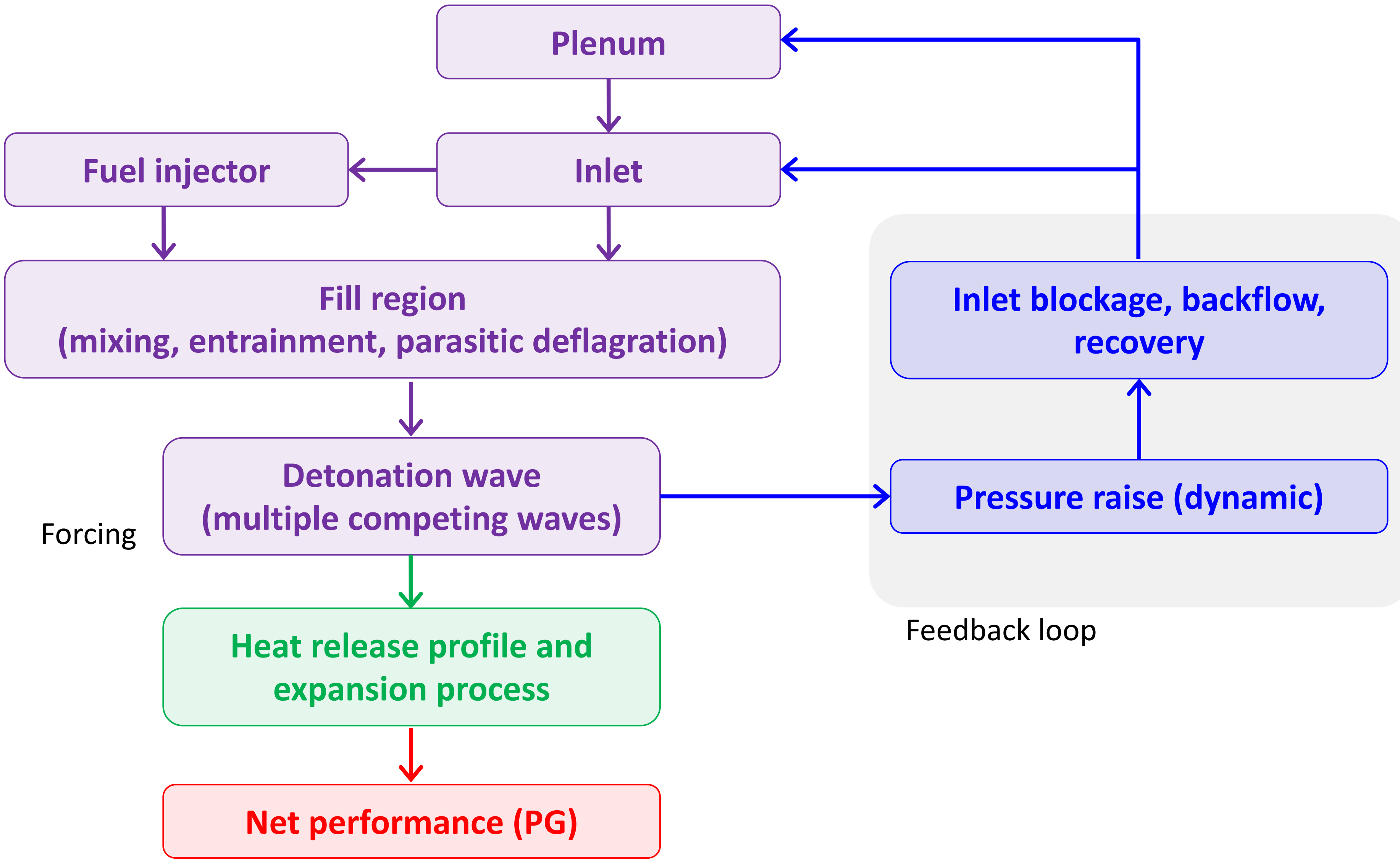
Effect of inlet design, same operating conditions



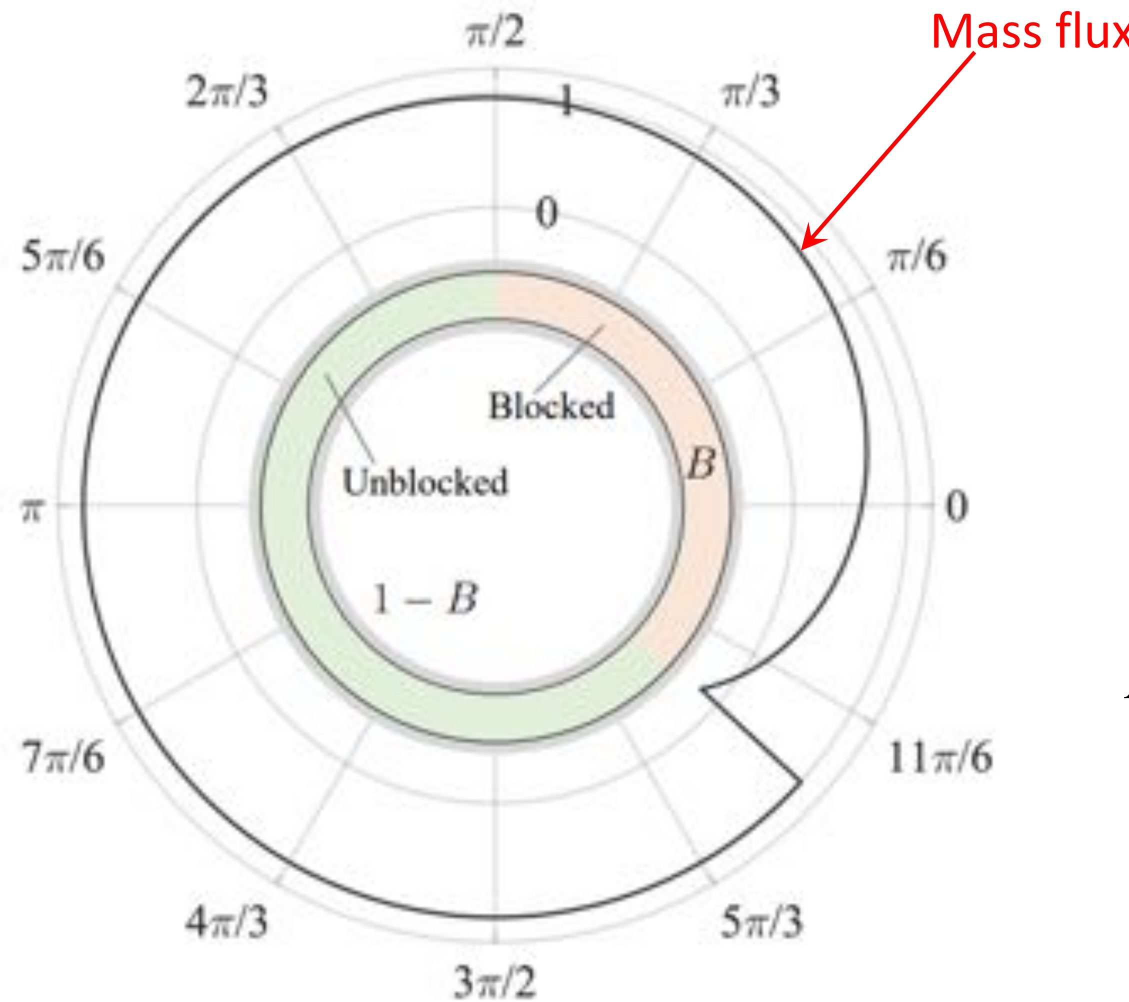


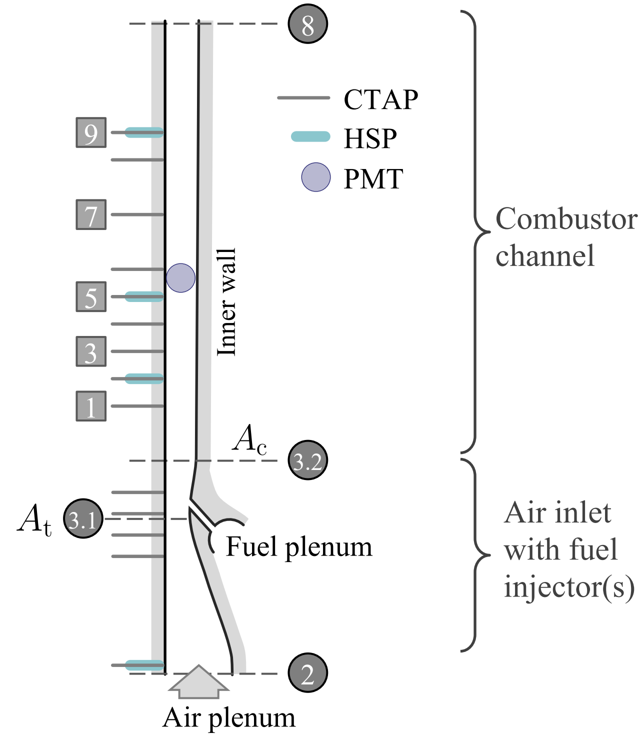
- This results from plenum/inlet/combustor coupling
- Modified design promotes blockage and possibly back-flow, which induce an increase in plenum pressure (fixed $\dot{m}''_a$)

Results reinforce the concept of plenum/inlet/coupling, affecting overall performance



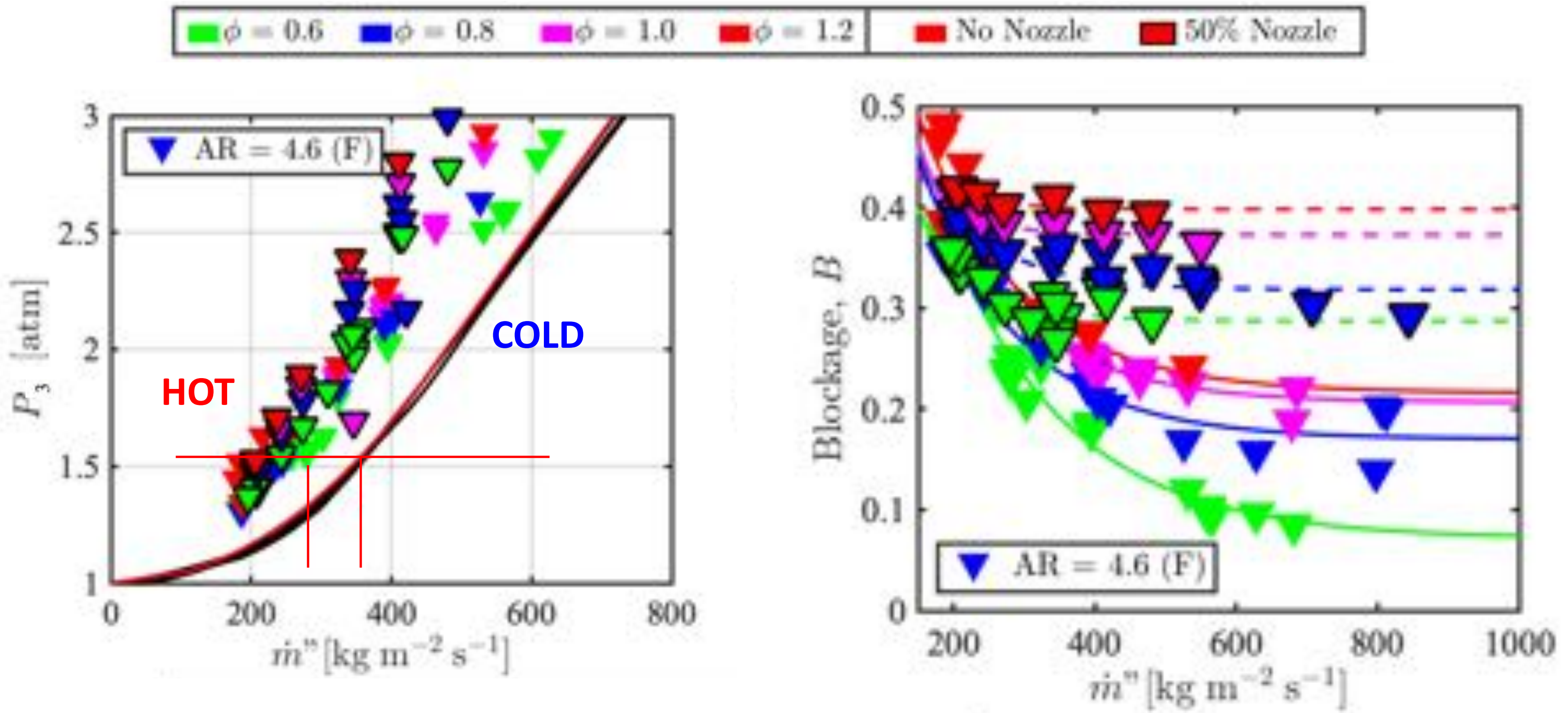
Concept of inlet blockage fraction (B)





- Binary representation, but in reality blockage is a dynamic process

Concept of inlet blockage fraction (B)



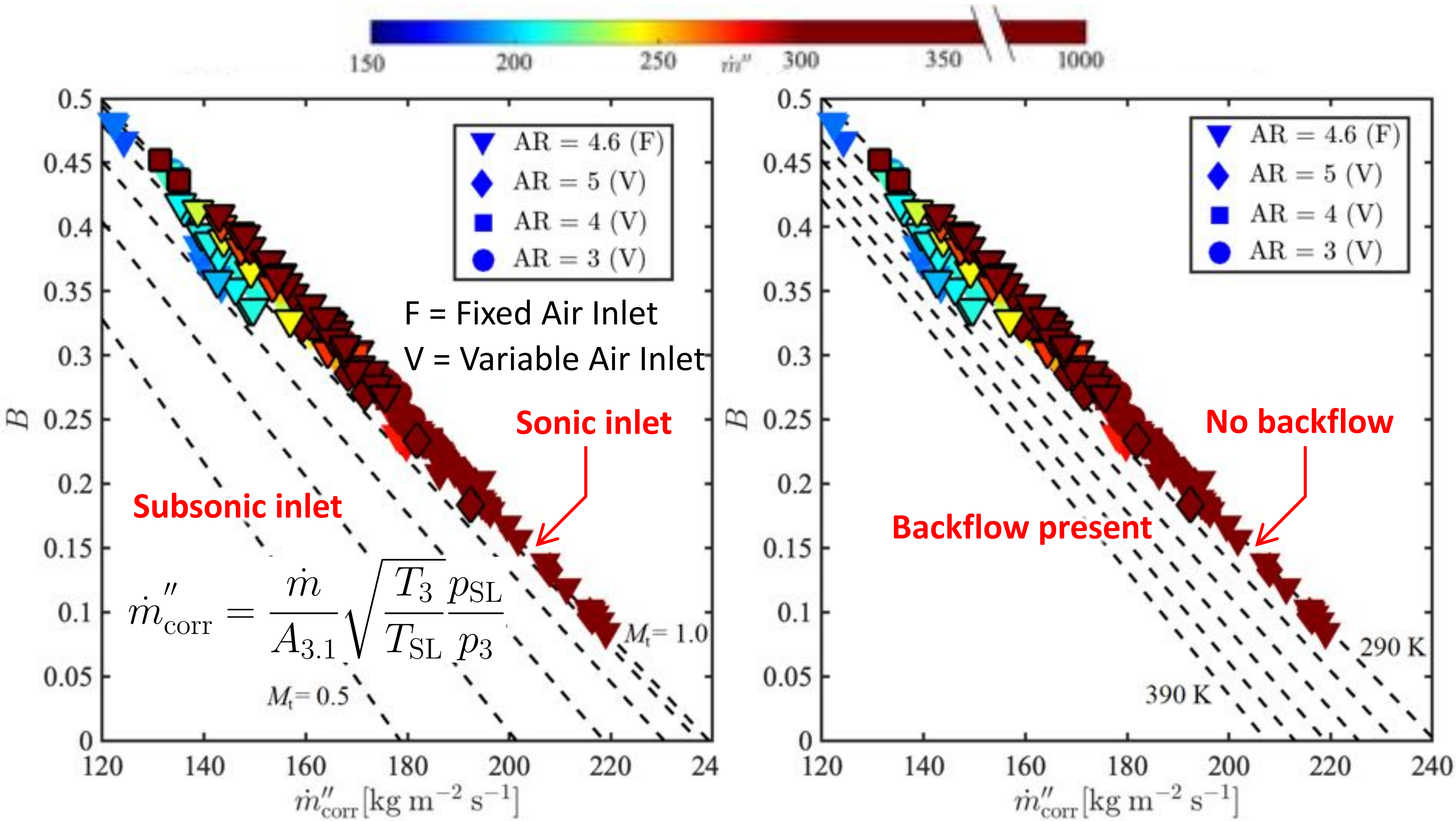
$$B = 1 - \frac{\dot{m}''_{\mathrm{Hot}}}{\dot{m}''_{\mathrm{Cold}|P_3,\mathrm{Hot}}}$$

Mass flow rate for hot flow at a given plenum pressure

Mass flow rate for a cold flow at the same plenum pressure of that of the hot flow

Inlet blockage fraction scales with corrected mass flux

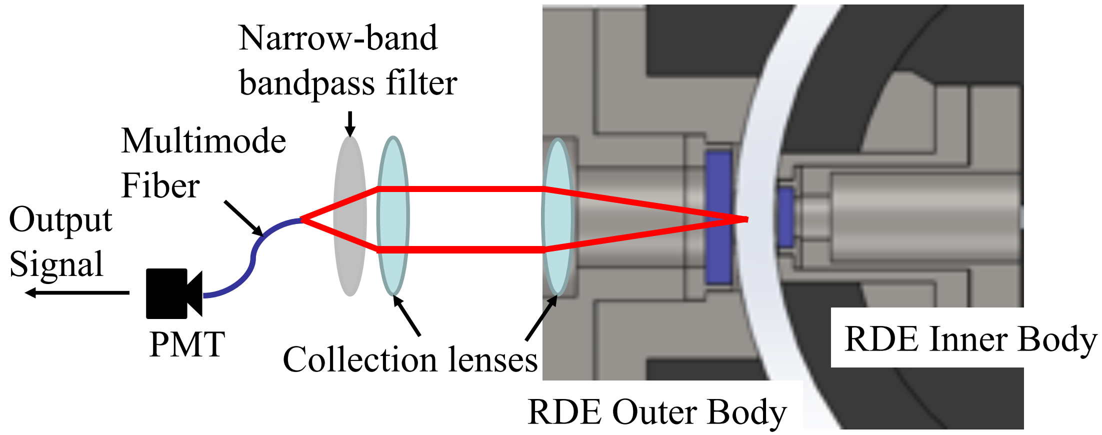
Data presented from all UM data from last 3 years

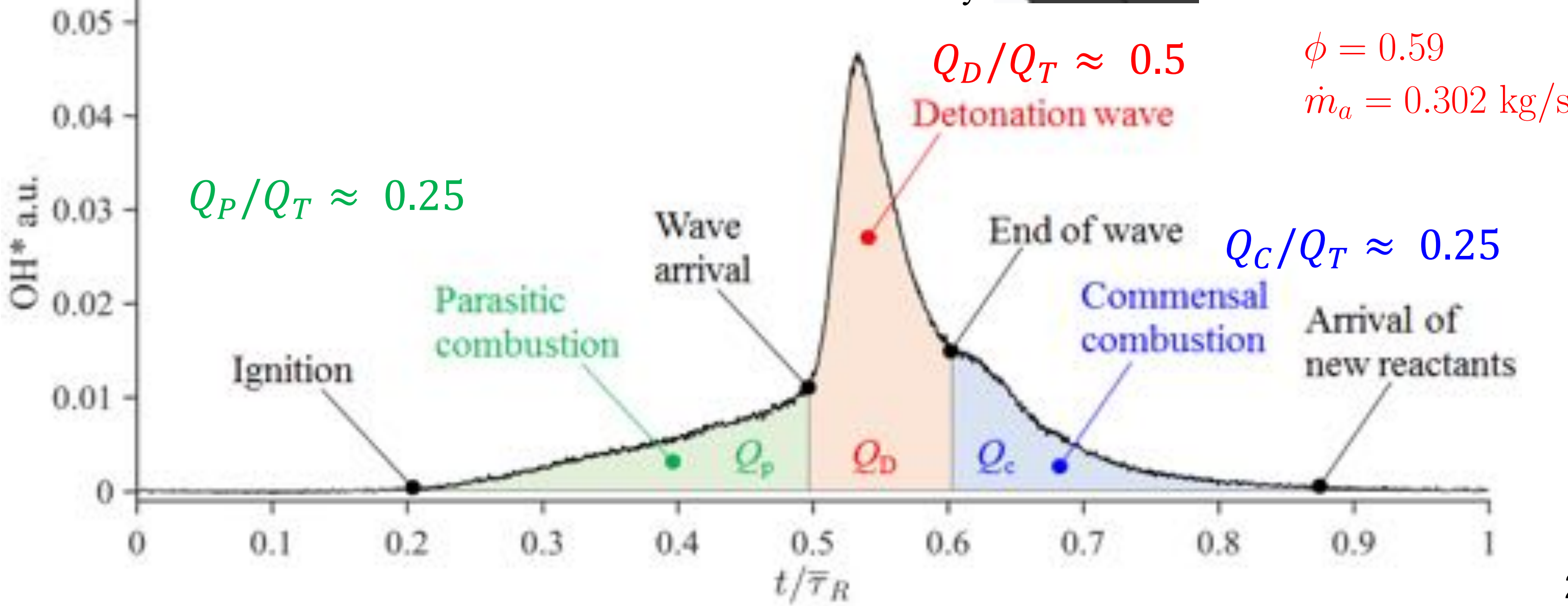


- All operating conditions have sonic inlet with possibly some backflow
- Blockage can be predicted given corrected mass flux

From the past: estimate of deflagration fractions

- Fraction of deflagration (parasitic / commensal) and detonation heat release fractions estimated from OH* chemiluminescence (at a fixed point)





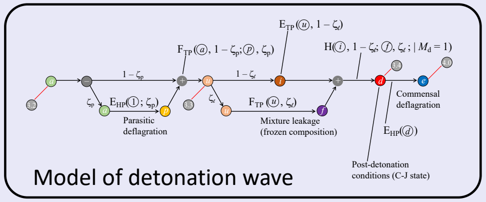
Bayesian inference framework for indirect assessment of losses

Known input (operating conditions $\mathbf{Y}$)

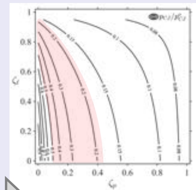
Unknown input (model parameters $\mathbf{X}$)

$\mathbf{X} = \{\zeta_\mathrm{p}, \zeta_\ell, \ldots\}$

(Losses)



$\mathbf{Z} = \mathcal{M}(\mathbf{Y};\mathbf{X})$



Output ($\mathbf{Z}$)

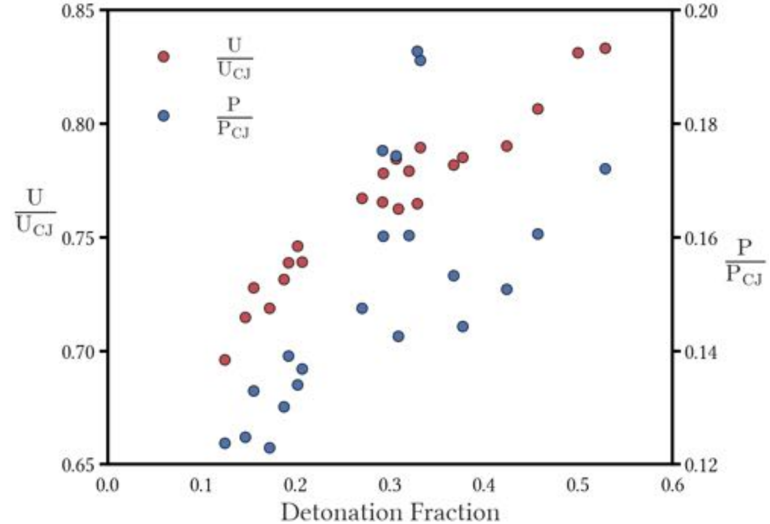
$\mathbf{Z} = \left\{W, \frac{p_\mathrm{d}}{p_\mathrm{u}}, \ldots\right\}$

ζ_p – Fraction of fuel consumed by deflagration upstream of wave (parasitic)

ζ_ℓ – Fraction of mixture escaping detonation wave; leaked fuel fraction

Bayes' rule: $\mathcal{P}(\mathbf{X}|\mathbf{D}) = \frac{\mathcal{P}(\mathbf{D}|\mathbf{X})\mathcal{P}(\mathbf{X})}{\mathcal{P}(\mathbf{D})}$ Posterior distribution of model parameters

Data (measurements): $\mathbf{D} = \left\{W, \frac{p_\mathrm{d}}{p_\mathrm{u}}, \ldots\right\}_\mathrm{m}$

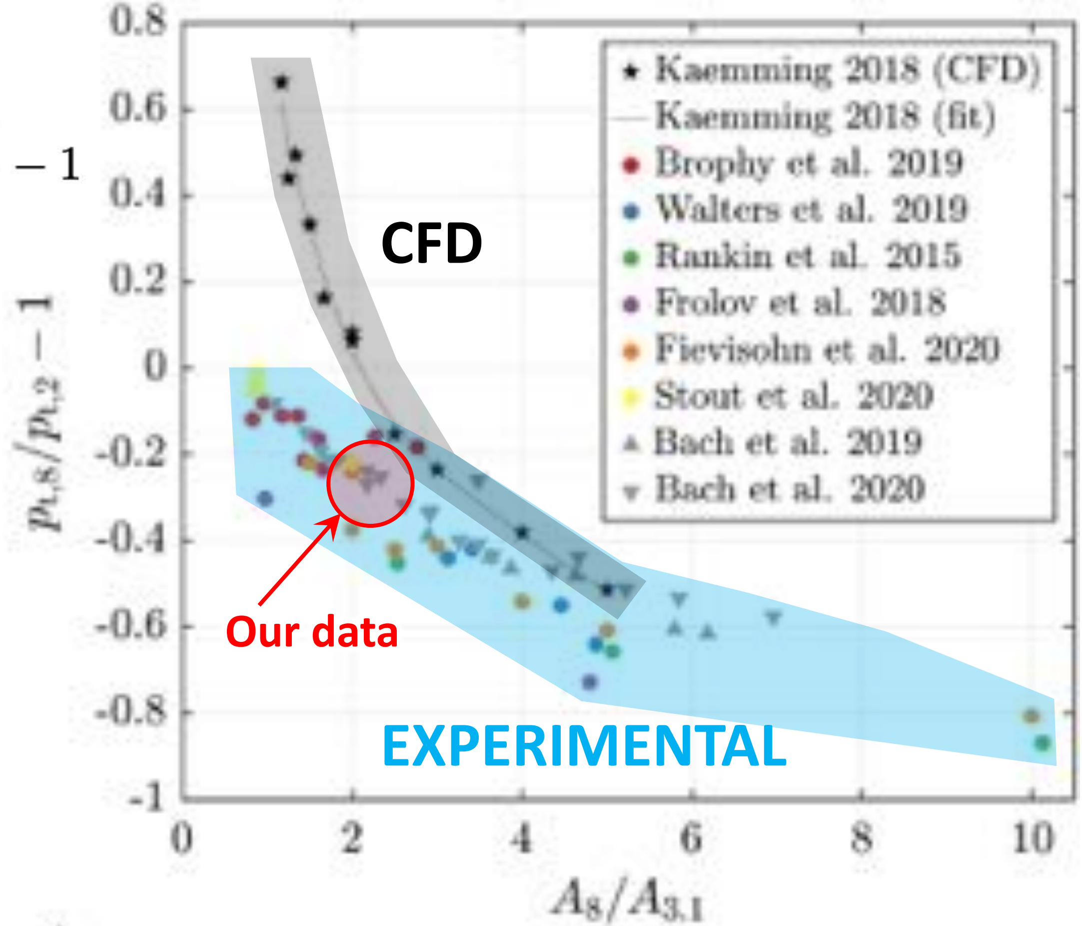


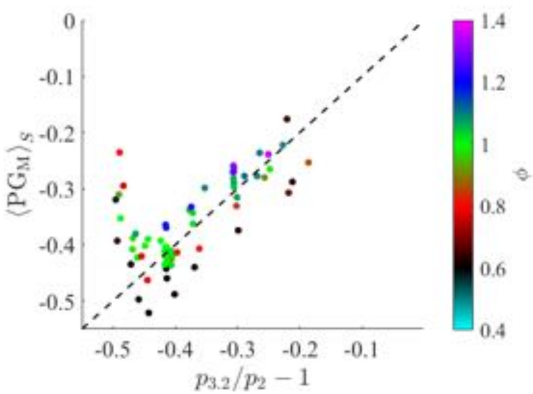
$\zeta_\mathrm{D} = (1-\zeta_\mathrm{p})(1-\zeta_\ell)$

- Builds on our prior experimental estimates based on OH* chemiluminescence emission
- Use this tool to correlate parasitic and detonation fractions (and other losses) with secondary wave characteristics and performance metrics (thrust, pressure gain, etc.), including effect of RDC geometry (inlet design, detonation chamber length/shape) and degree of inlet blockage

O'gain, where art thou: analysis of losses and gains

$$\mathrm{PG} = \frac{\mathrm{EAP}}{p_2} - 1$$



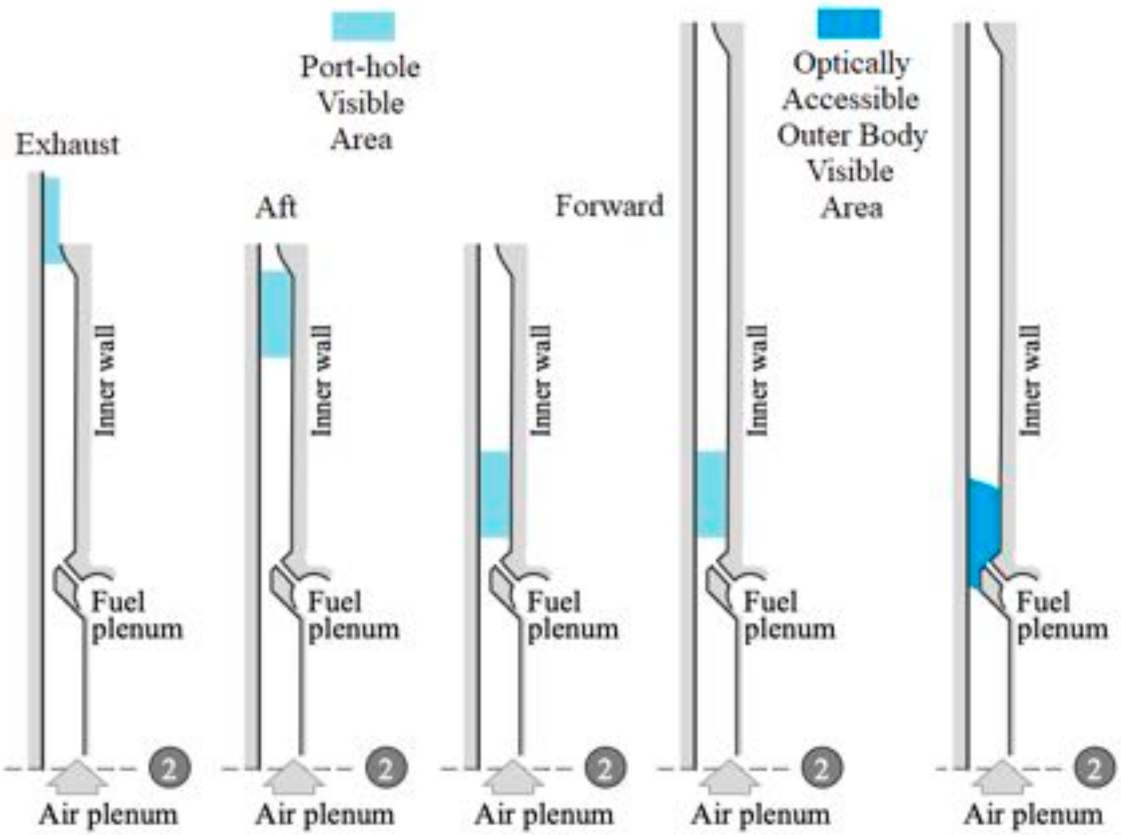


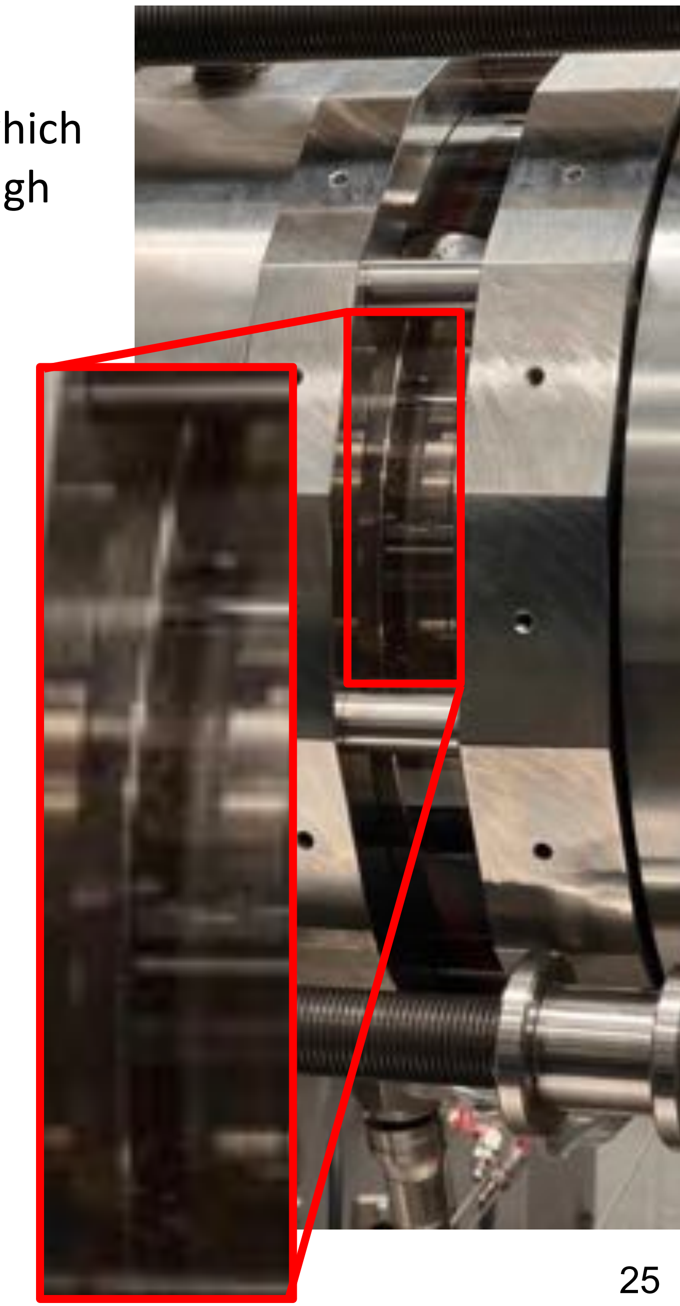
- Why all measurements nearly collapse?
- Why such a a large deviation from theory?
- Are we missing something here? (e.g., additional phenomena / loss mechanism)
- Is PG as typically defined a meaningful measure of benefit?

From: Bach, E. *et al.* (2022). *AIAA Journal*, 1-12.

Initial investigation of fill region dynamics

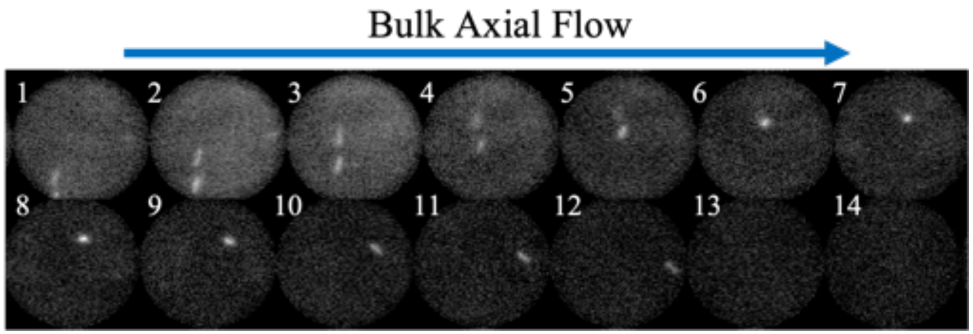
- Particle tracking (PT) of (hot) luminescent particles
  - Introduced iron oxide particles within air supply system which were tracked through 19 mm diameter port-hole or through optically accessible outer body



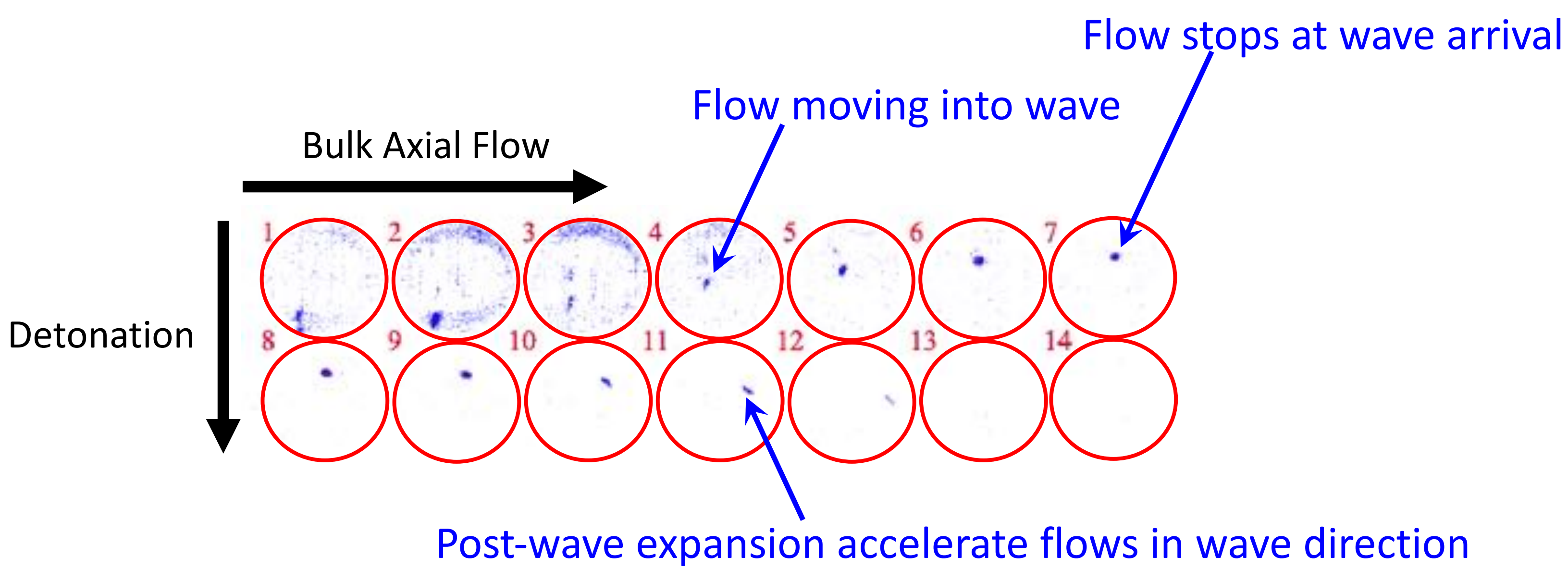


Fill region dynamics

- From high-speed (70 kHz, 10 μs integration) movies of luminous particles seeded into flow

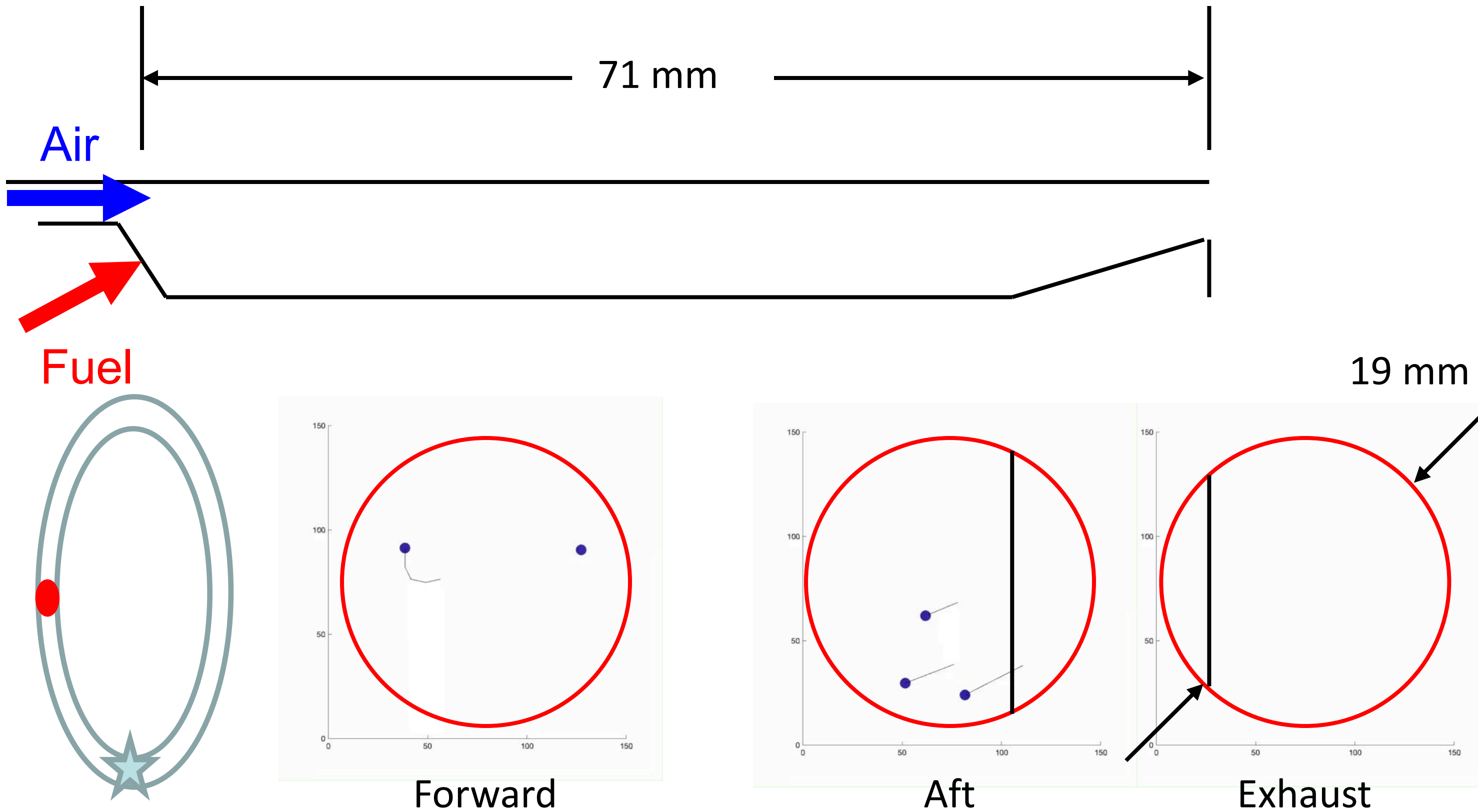


Sequence of images taken through port-hole



Fill region dynamics

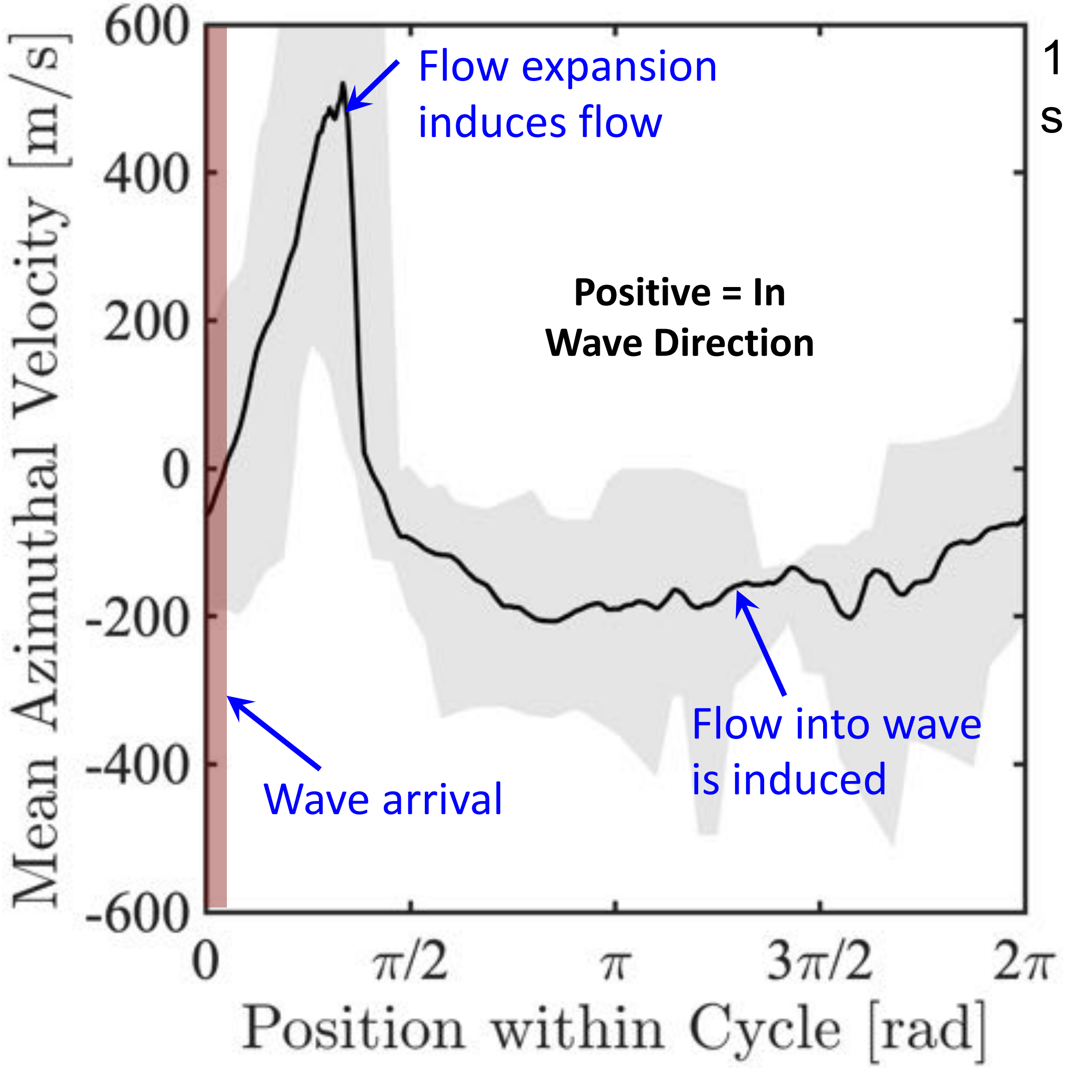
- Tests conducted with FAI configuration at 150 g/s, ϕ=0.8
  - Data from 3 discrete tests shown at right
  - Individual luminescent particles tracked to form 2-D characterization of RDE flow field
- Additional tests conducted varying inlet air mass flow and equivalence ratio



Aft Looking Forward View of Approximate Wave Position

Scale 2:1

Example of phase-averaged velocity profile in fill region



150 g/s, ϕ = 1
single wave operation

Fill region dynamics: this is not new!

- Wave-inflow first highlighted in modeling efforts of Nordeen[1]
- Partially corroborated experimentally by Andrus in pre-mixed ethylene/air RDE[2]

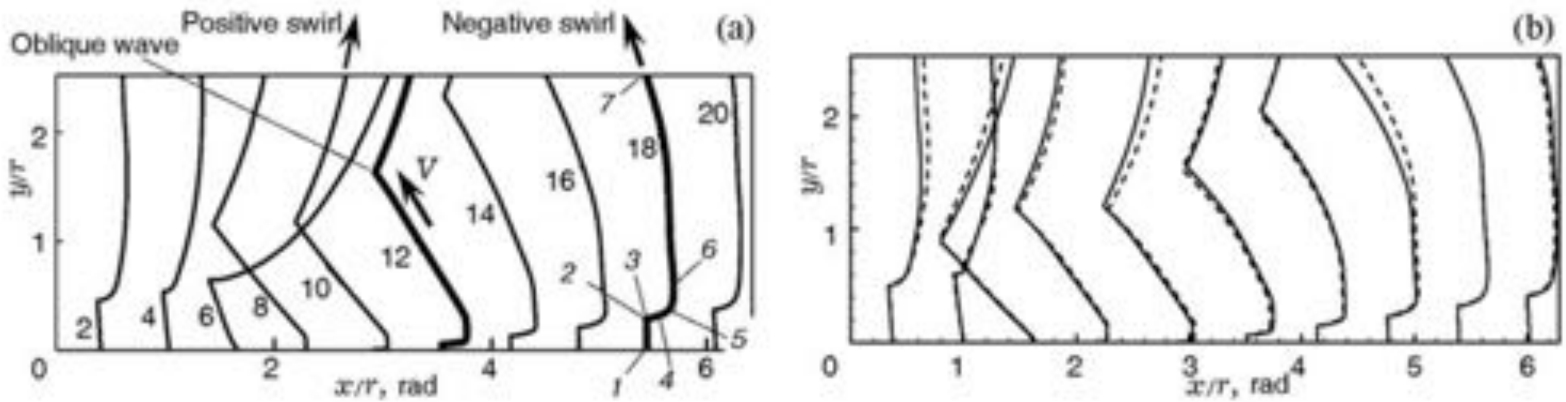
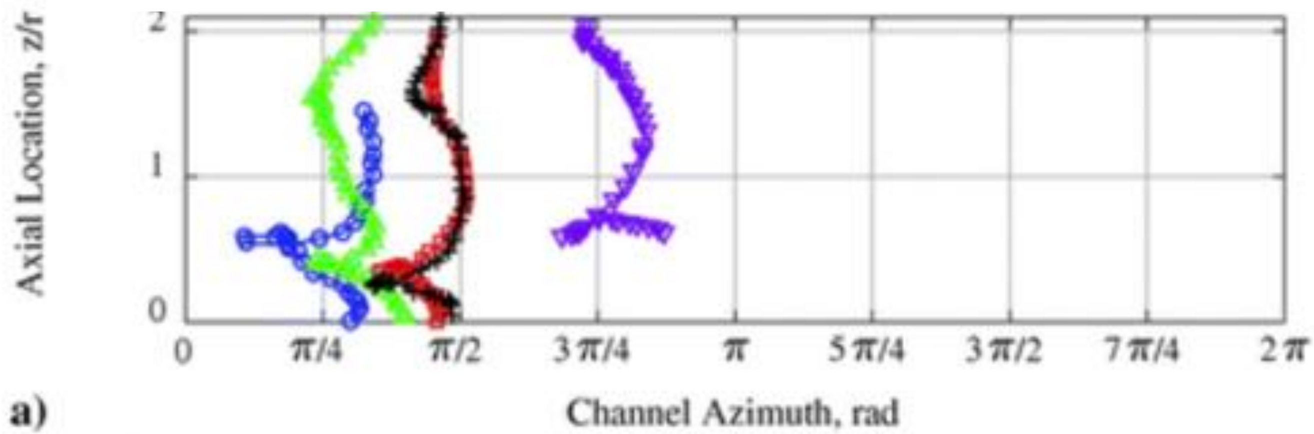


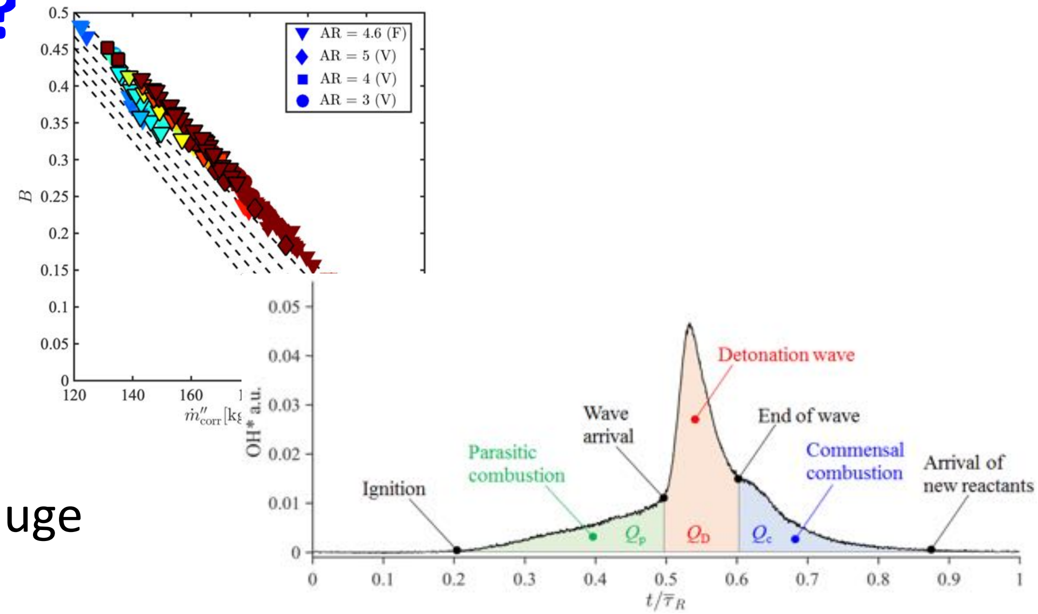
Figure 2.8: Fluid parcel flow pathlines: (a) time-averaged simulation in the laboratory frame of reference; (b) time-accurate particle traces (dashed curves) versus the time-averaged pathlines (solid curves). From Nordeen *et al.* [5]



[1]Craig Nordeen, Douglas Schwer, Fred Schauer, John Hoke, Thomas Barber, and Baki Cete- gen. Divergence and mixing in a rotating detonation engine. In *51st AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition*. Paper No. AIAA- 2013-1175, Jan 2013.

[2]Ionio Andrus, Marc Polanka, Paul King, Fred Schauer, and John Hoke. Experimentation of premixed rotating detonation engine using variable slot feed plenum. *Journal of Propulsion and Power*, 33(6):1448–1458, 2017.

So, what happens here?



- **In addition to:**
  - Pressure loss across the inlet
  - Inlet blockage
  - Inlet backflow
  - Parasitic combustion (which has huge impact on wave characteristics)
  - Fuel leakage (incomplete heat release at the wave)
- **Does an inlet swirl exist?**
- **Potential consequences:**
  - Flow in the direction of the detonation wave is induced (azimuthal flow)
  - Induced azimuthal flow competes with gain across detonation wave (induced flow is zero)
  - Induced flow facilitates entrainment and parasitic combustion, potentially the onset of secondary wave

Possible link between effect of deflagration losses and inlet swirl on reduction of available energy

Loss mechanism		Effect on available energy
Parasitic deflagration	→	Pressure raise across wave
Fuel leakage across wave	→	Sensible enthalpy raise
Inlet swirl into wave	→	Induced KE “gain”

Equivalent state that gives available energy

We are starting this approach and analysis now, and it will be the focus for the next year.

Our contribution and conclusions

- Improved performance measurements on RDC
  - We are now able to begin answer some of the questions we posed in the past:
    - How does deflagration affect PG?
    - How do secondary wave affect PG?
    - Loss/gain budget analysis, and impact of operating conditions and design
- Developed a Bayesian inference framework for assessing (estimating) losses in RDCs
  - Extends our past efforts on direct measurement
  - We will now apply this tool to correlate deflagration losses to performance
- Identified the possibility of inlet swirl to exist in our inlets
  - Additional loss mechanisms is present, but we need to investigate its source and effective impact on wave characteristics and overall performance
- We are starting to look at how performance could be evaluated (in addition to PG), by looking at available energy arguments
  - Will allow to further the loss analysis on RDC performance
  - Provide an alternative framework to evaluate the effective benefits

Outline

- Programmatic overview and introduction to the problem
- Experimental activities
- **Computational activities**

Computational Modeling for Prediction of RDE Performance and Emissions

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Venkat Raman

University of Michigan, Ann Arbor
Department of Aerospace Engineering

Objectives

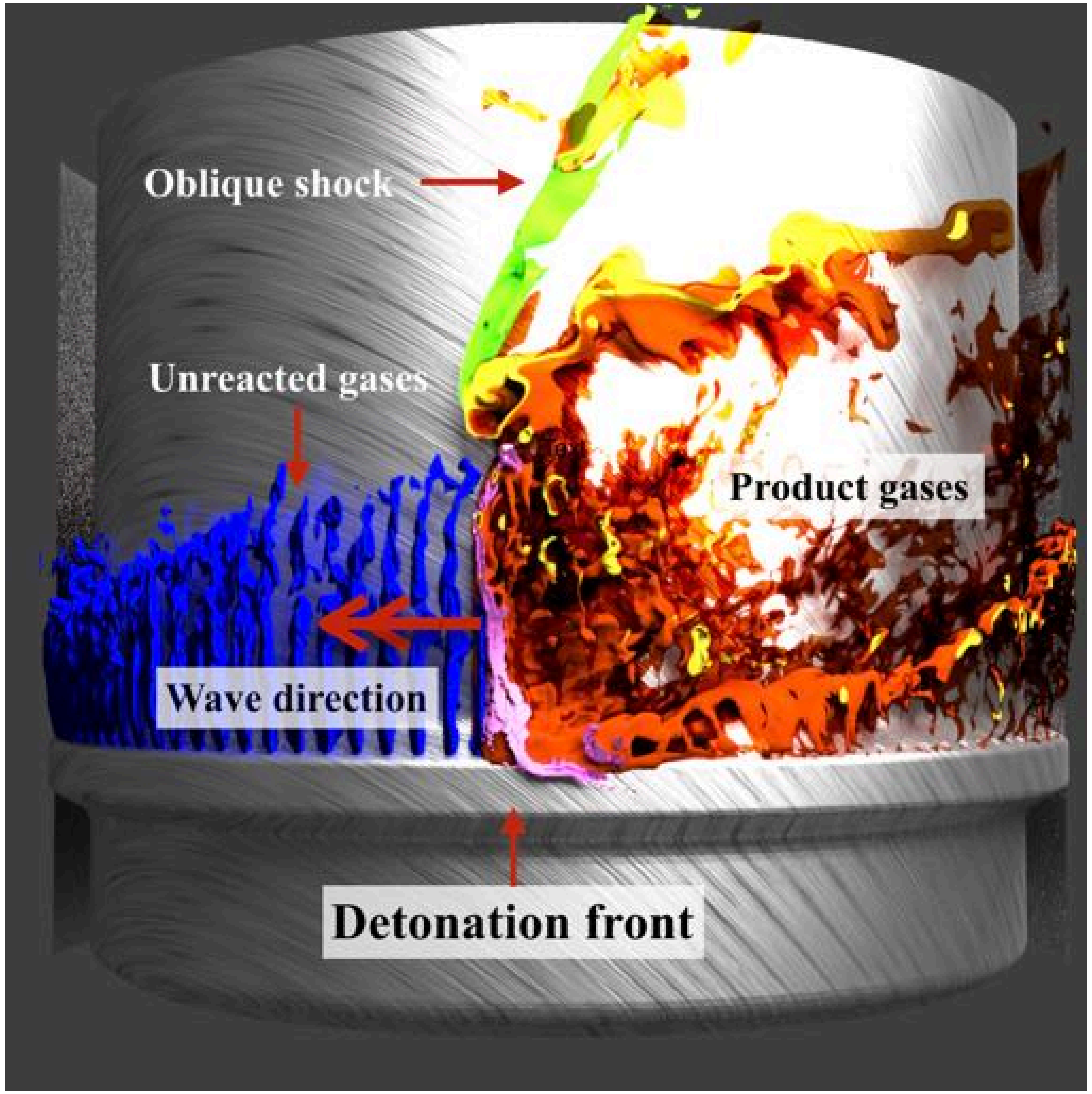
- **Main goal: Develop a predictive computational framework for predicting performance and emissions from RDE**

- **Tasks**
  - ➡ High-fidelity simulation of NOx emissions and impact of design
  - ➡ Multi-fidelity framework for performance prediction

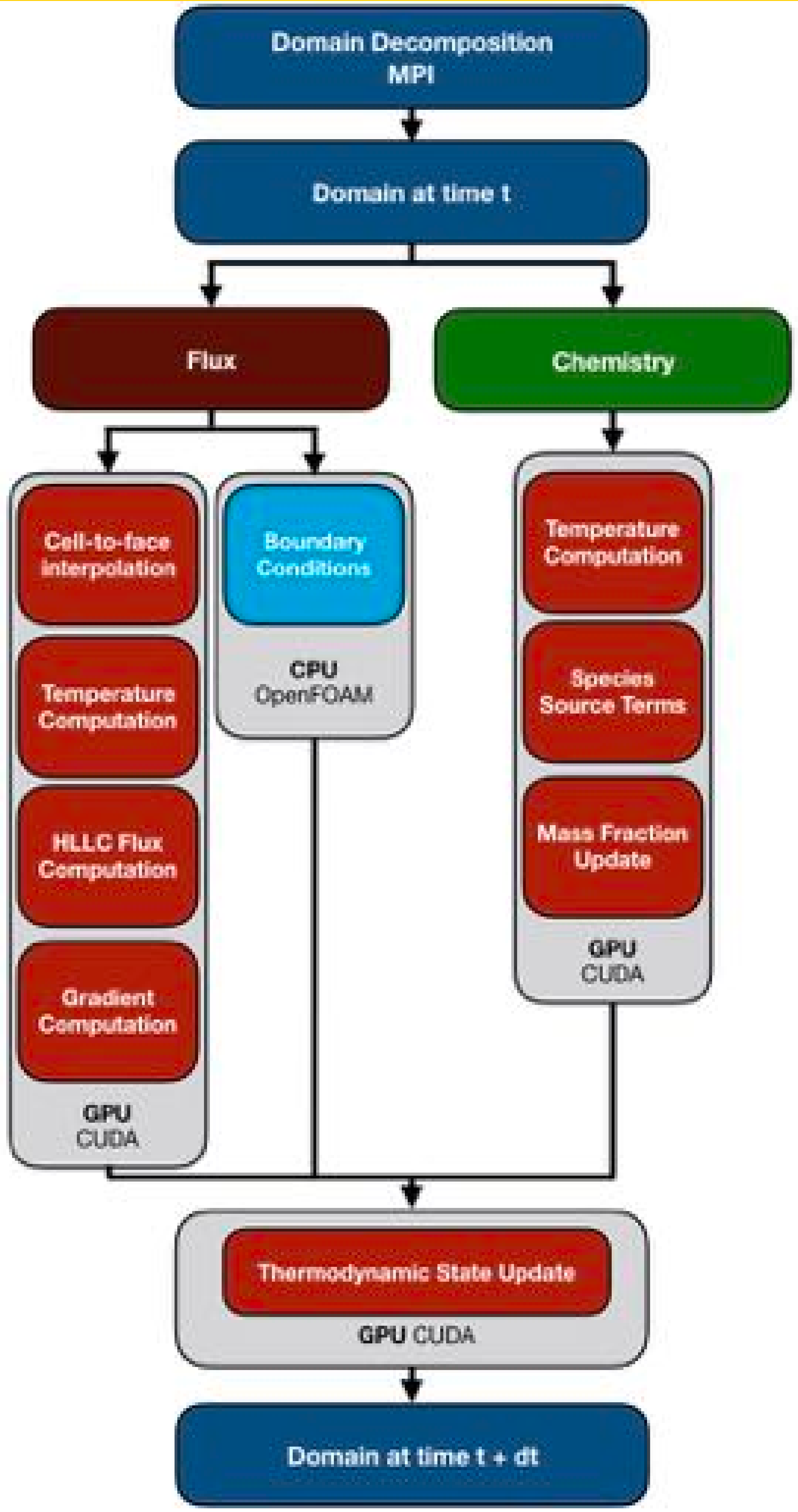
3D RDE Simulation Setup: Solver

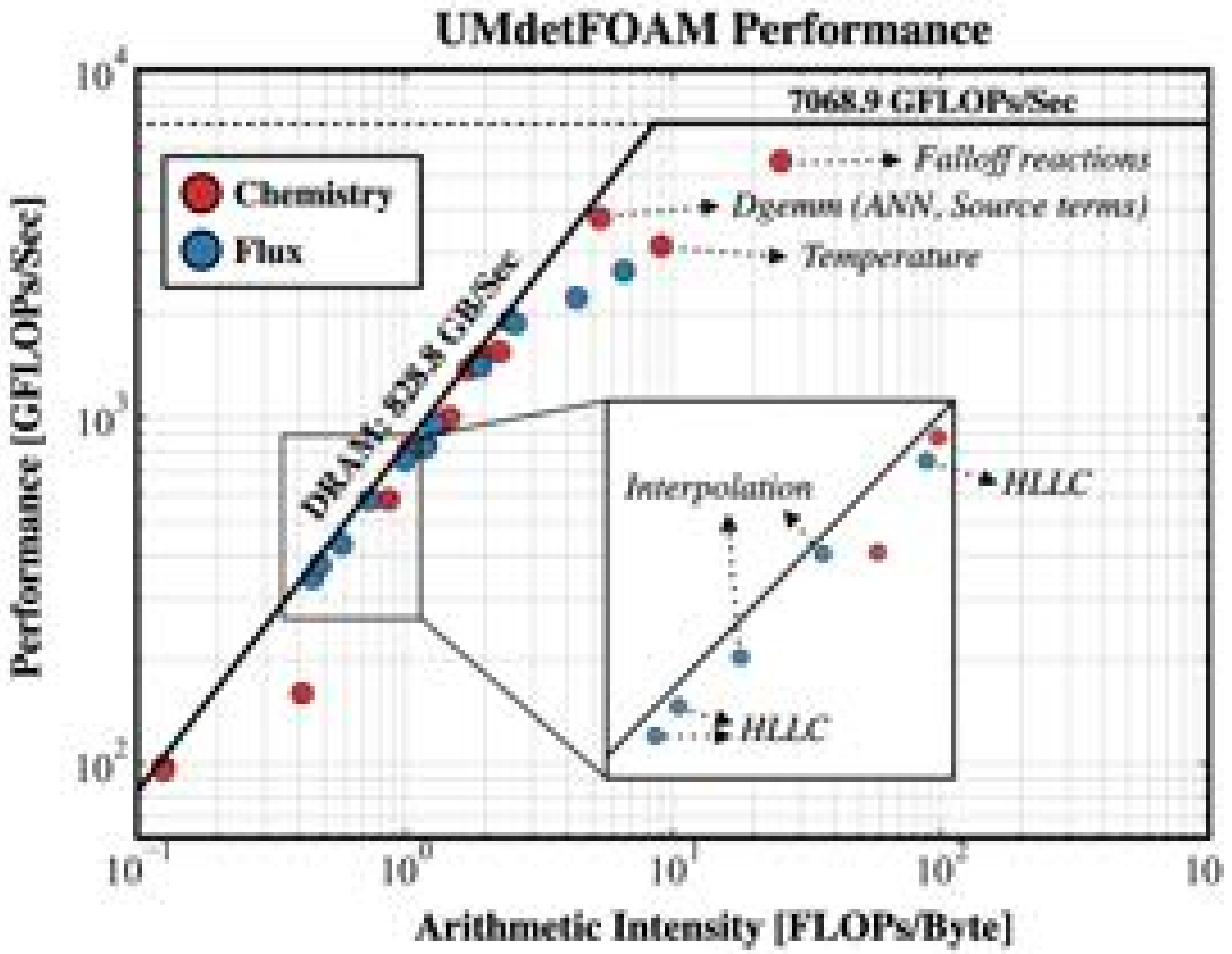
- **OpenFOAM + Cantera = UMdetFOAM**
  - ➡ Compressible flow solver for *full* Navier-Stokes equations
  - ➡ Finite Volume Method (FVM)
    - Unstructured grid for complex geometries
    - HLLC + MUSCL (2nd order) spatial scheme
    - KNP diffusion scheme
    - 2nd order Runge Kutta for temporal scheme
  - ➡ CUDA-based GPU offloading
  - ➡ Detailed/skeletal chemical kinetics through user-specified model
    - GPU-based chemistry library (Barwey *et al*. 2021)
  - ➡ High-fidelity approach -> No turbulence models

Instantaneous snapshot of UM AAI geometry using UMdetFOAM



Solver overview



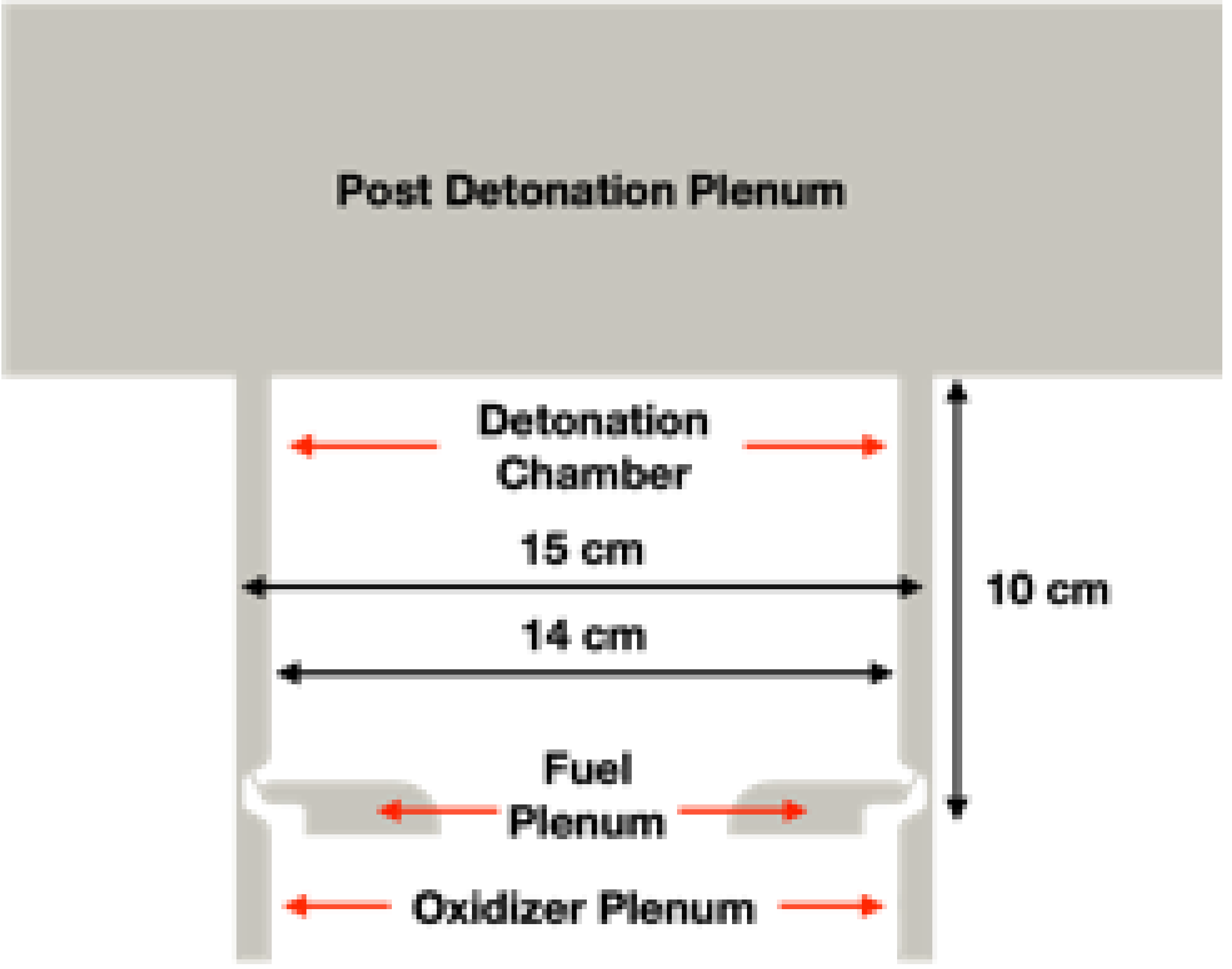


- **Near theoretical limit for computational efficiency**
- ***Order of magnitude* reduction in solver time to solution**

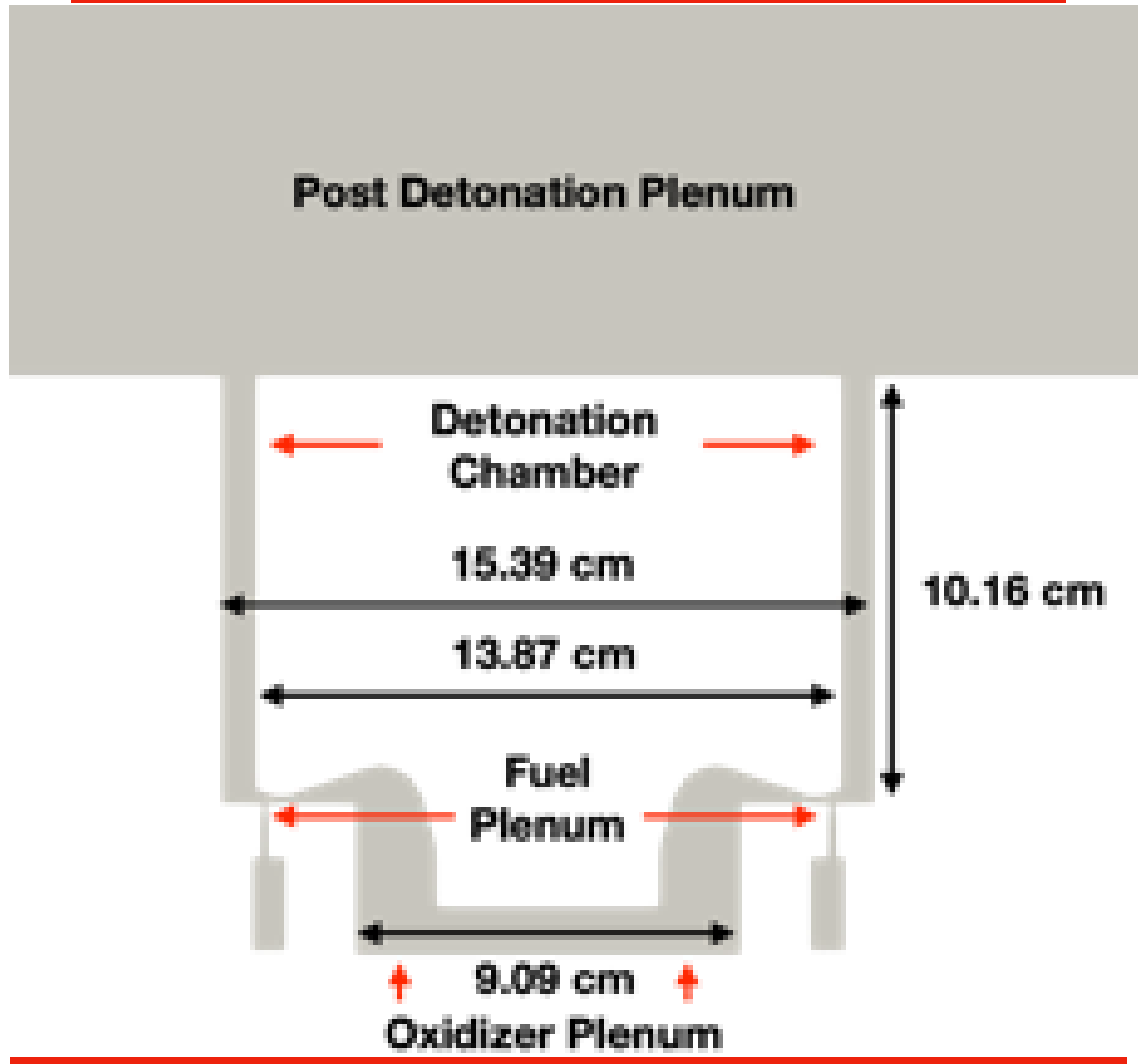
3D RDE Simulation Setup: Cases Studied

- Geometries
  - ➡ UM Axial Air Inlet (AAI)
    - 100 μm - injector region
    - 200 μm - up to 4 cm in detonation chamber
    - Roughly 25 million control volumes
  - ➡ AFRL Radial Air Inlet (RAI)
    - 200 μm - detonation chamber
    - Roughly 48 million control volumes
- Boundary Conditions
  - ➡ Constant Mass Flow Rate
  - ➡ Adiabatic, No-Slip Walls
- H_2-Air-NO_x combustion
  - ➡ Modified Jachimowski Chemistry Mechanism [Wilson et al, 1992]
- 2.48 ms Simulation Time
  - ➡ Roughly 10 Wave Cycles
  - ➡ Started from quasi-steady state achieved with H_2-Air combustion

Configuration	Case #	$\dot{m}_{air}$ [g/s]	$\dot{m}_{fuel}$ [g/s]	Phi
UM AAI	1	404.2	11.9	1.01
AFRL RAI	2	320	9.3	1
	3	630	18.0	1
	4	860	25.0	1



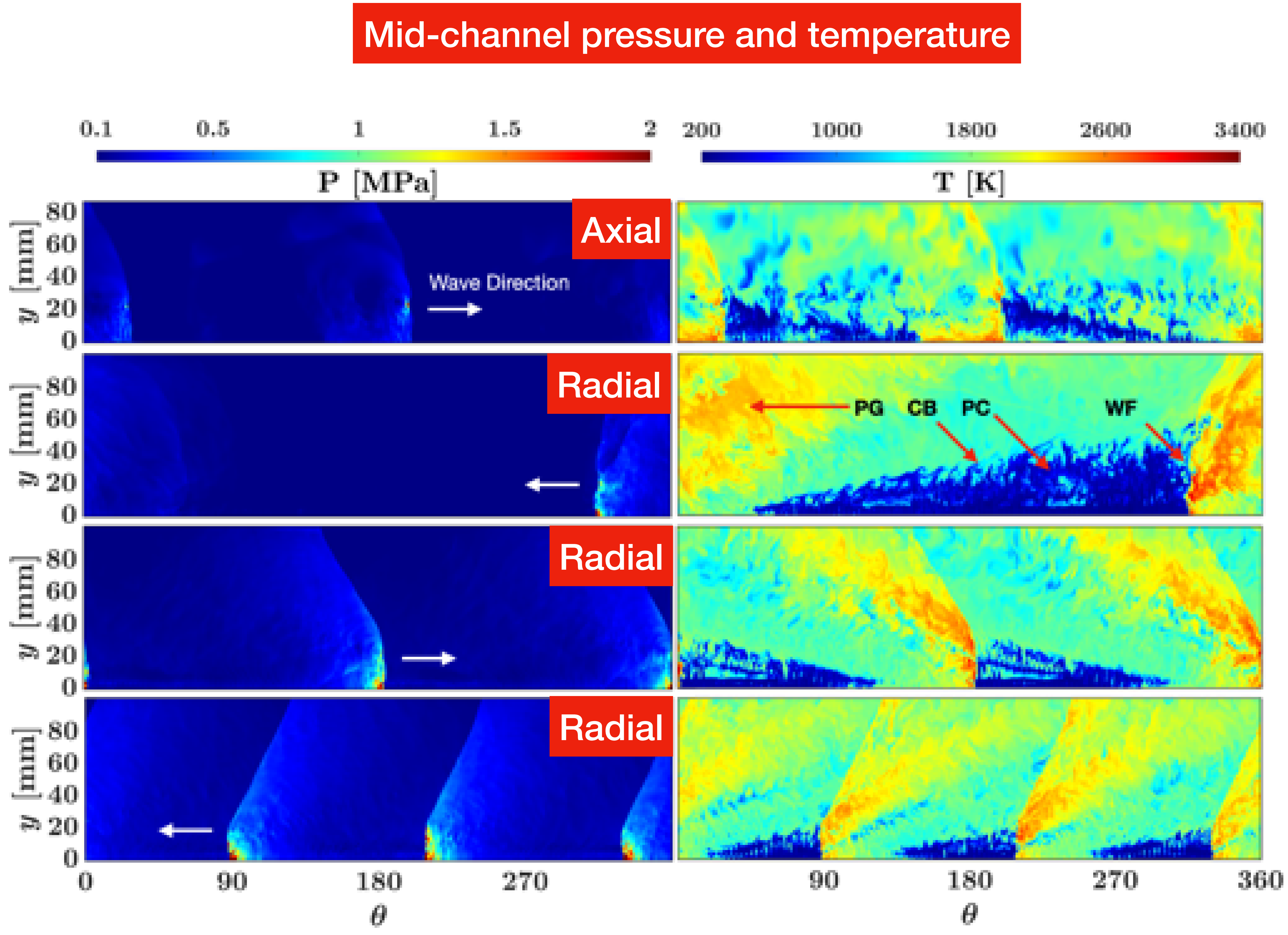
UM Axial Air Inlet Geometry



AFRL Radial Air Inlet Geometry

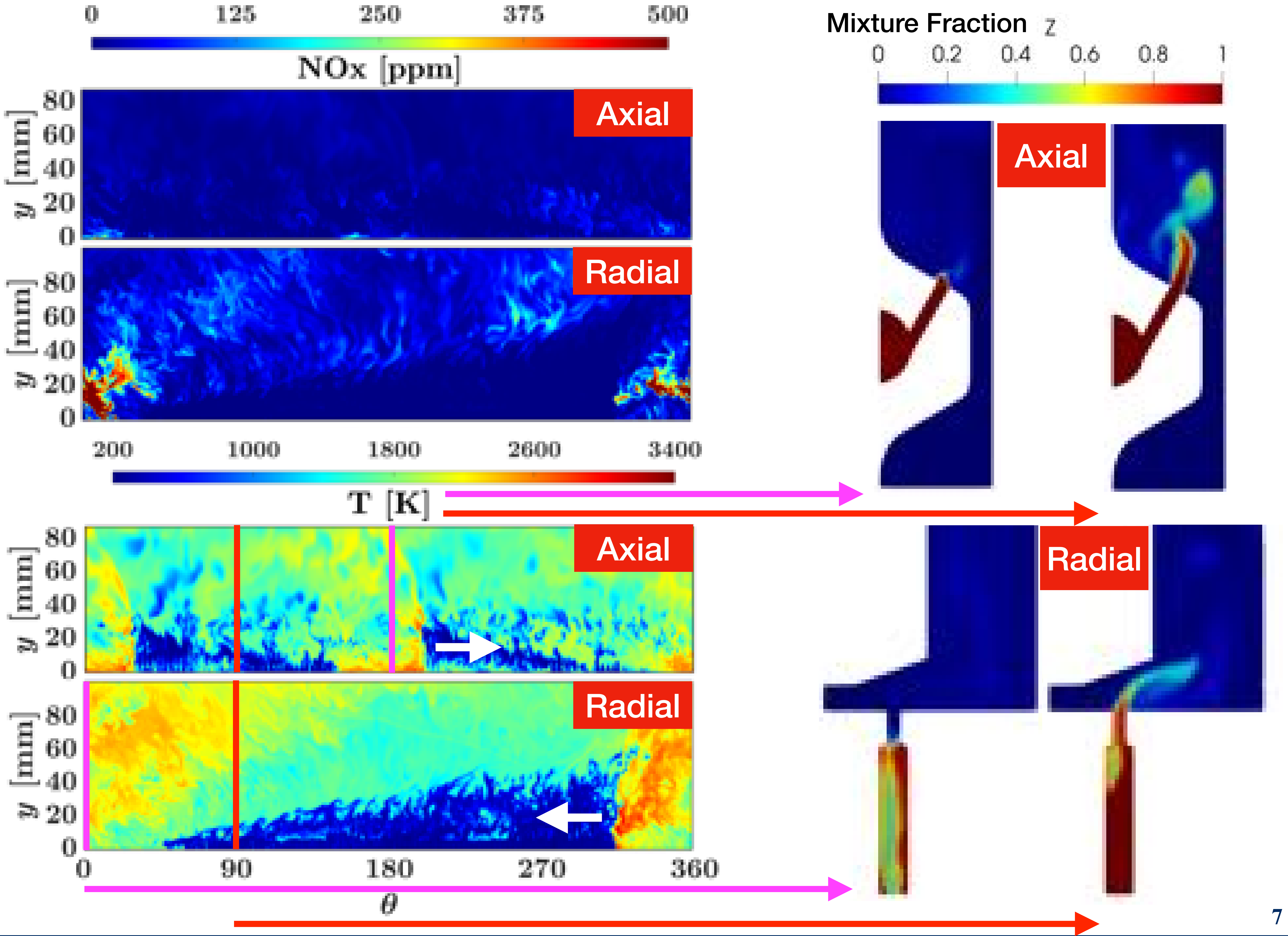
RDE Flow Characteristics

- **Detonation Structure in RDEs**
  - ➡ PG - Product Gases
  - ➡ CB - Contact Burning
  - ➡ PC - Parasitic Combustion
  - ➡ WF - Wave Front
- **Generally more structured refill region in RAI RDE**
  - ➡ Refill height reduced with increasing mass flow rate
  - ➡ High temperature region reduction
- **Temporary blockage of injectors due to waves**



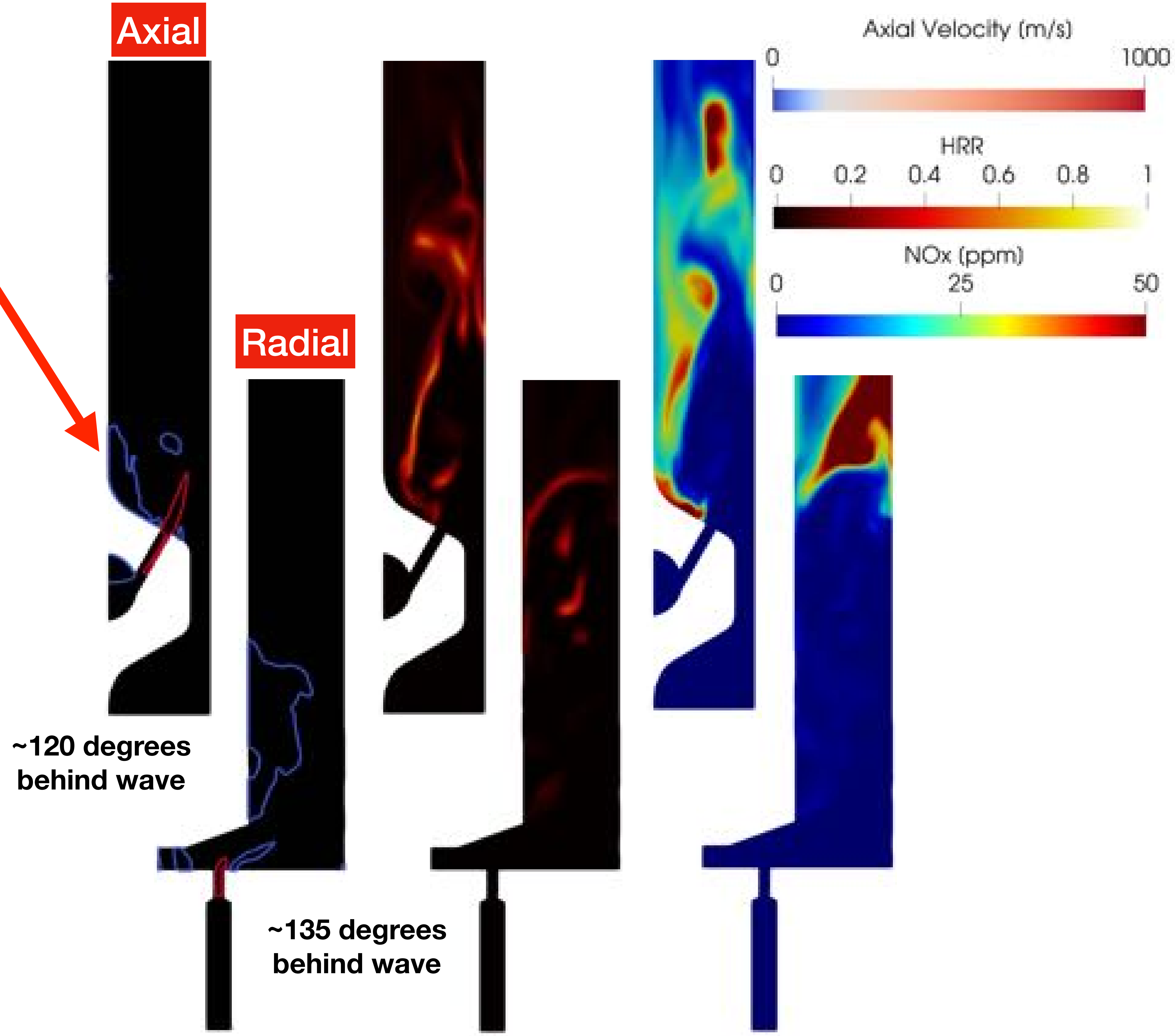
NO_x Formation Patterns Between Geometries Contd.

- **NO_x follows different patterns in Axial and Radial geometries**
  - ➡ Axial Air Inlet:
    - Faster fuel recovery
  - ➡ Radial Air Inlet:
    - Stronger waves
    - Higher temperatures
    - Similar to 2D ideal RDE NO_x patterns from [Schwer et al, 2016]

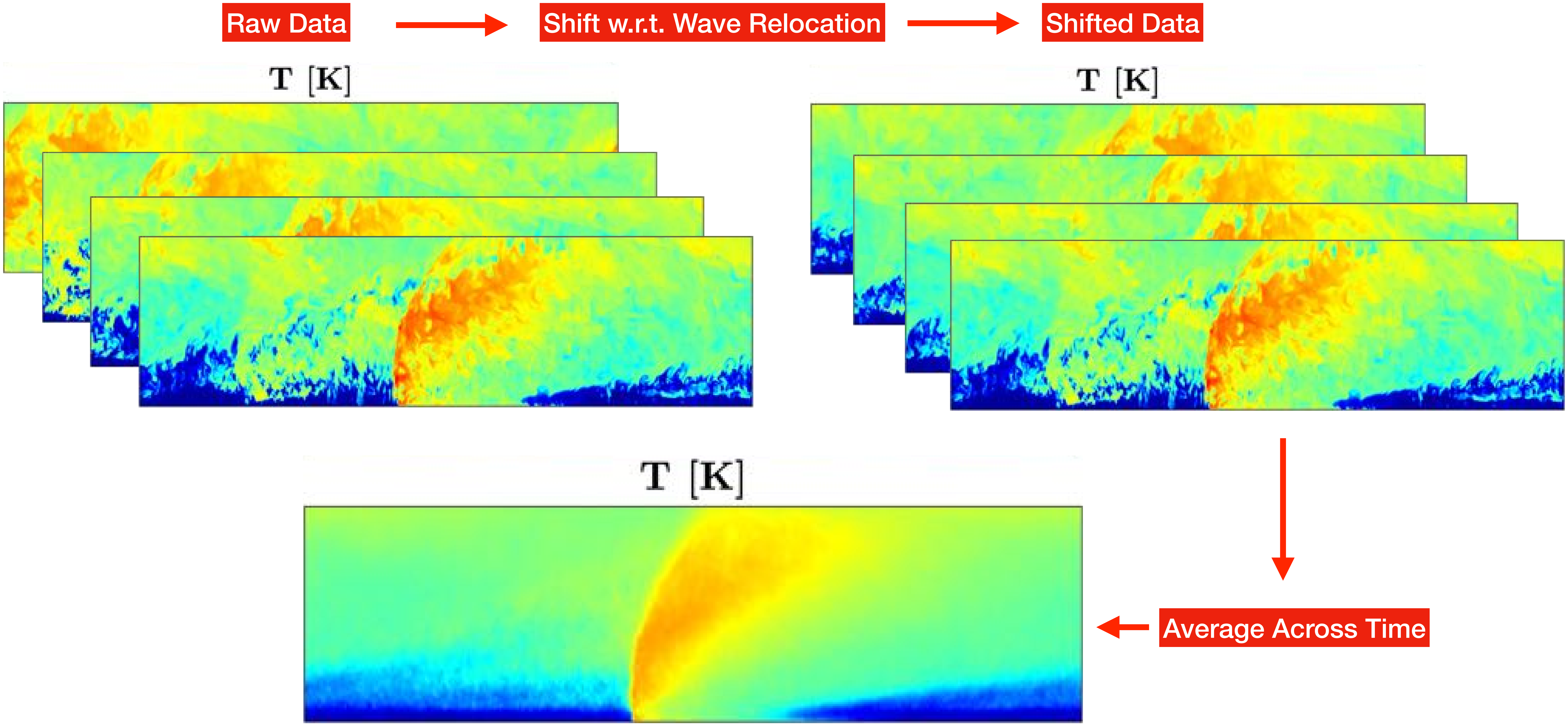


NO_x Formation Patterns Between Geometries Contd.

- **Parasitic combustion in refill region caused by recirculation of hot gases**
  - ➡ Heat release near chamber bottom in Axial Air Inlet RDE causes pre-ignition of fresh mixture
- **NO_x is extremely sensitive to temperature**
  - ➡ High NO_x formation near inner wall near injectors in Axial Air Inlet RDE
  - ➡ Axially delayed recirculation in Radial Air Inlet RDE
- **Why is more NO_x produced in the Radial Air Inlet RDE then?**

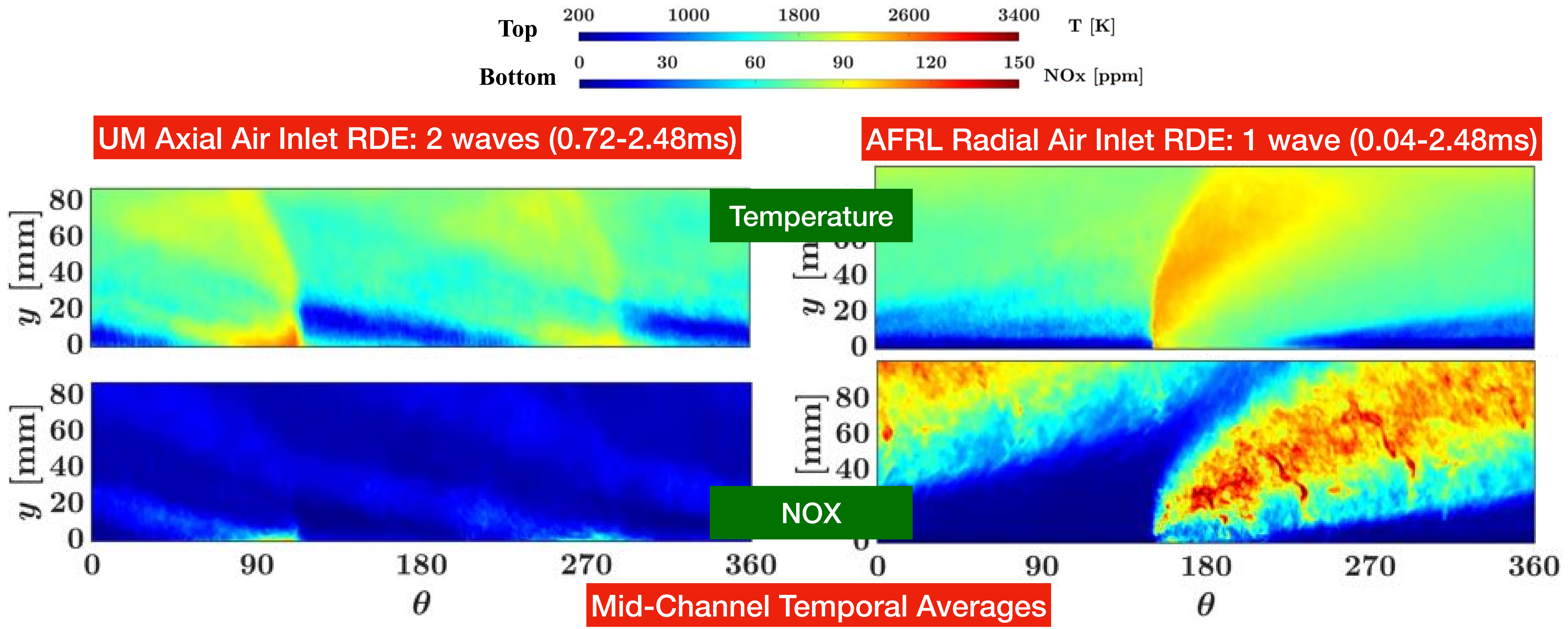


Temporally Averaged Spatial Quantities in RDEs



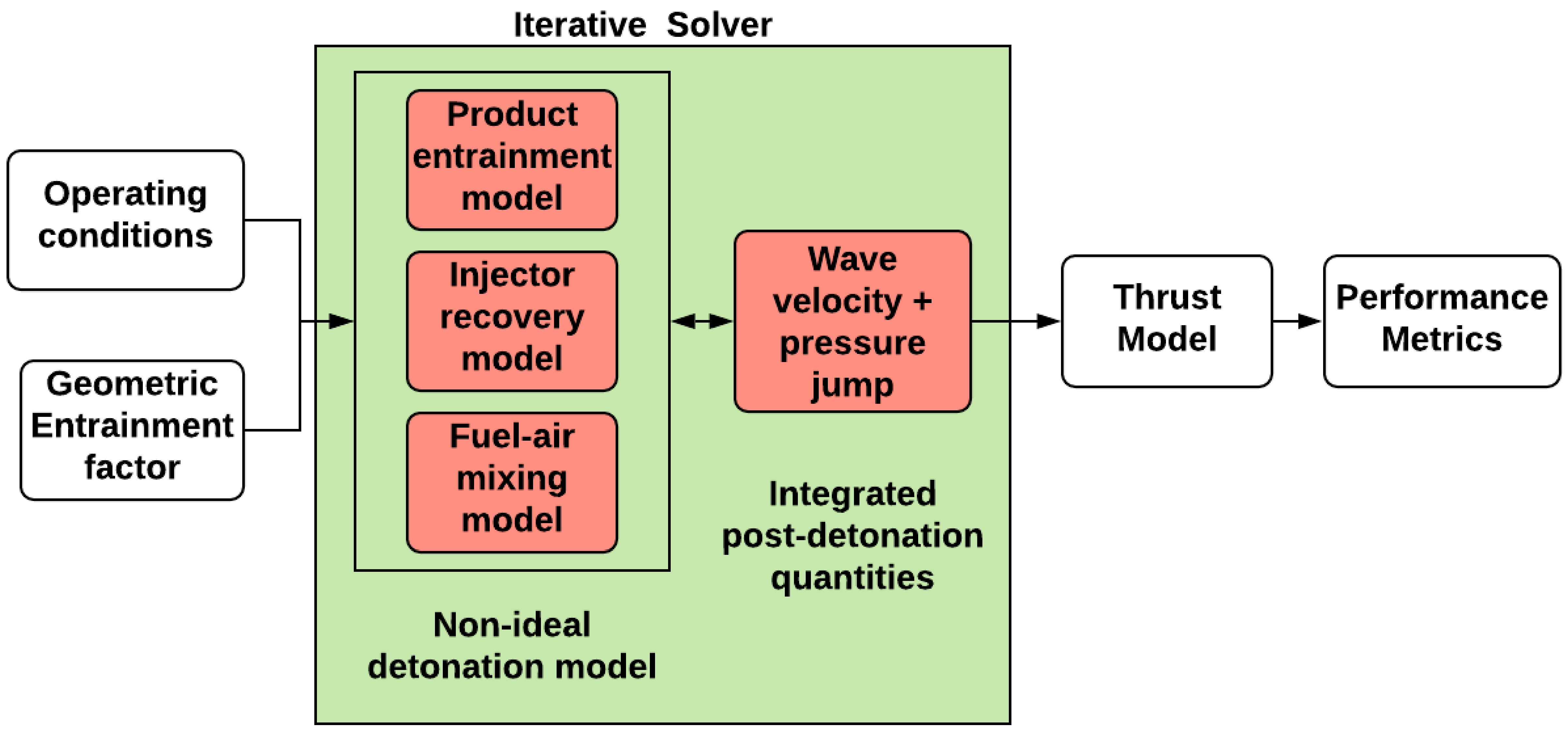
NO_x Formation Patterns Between Geometries Contd.

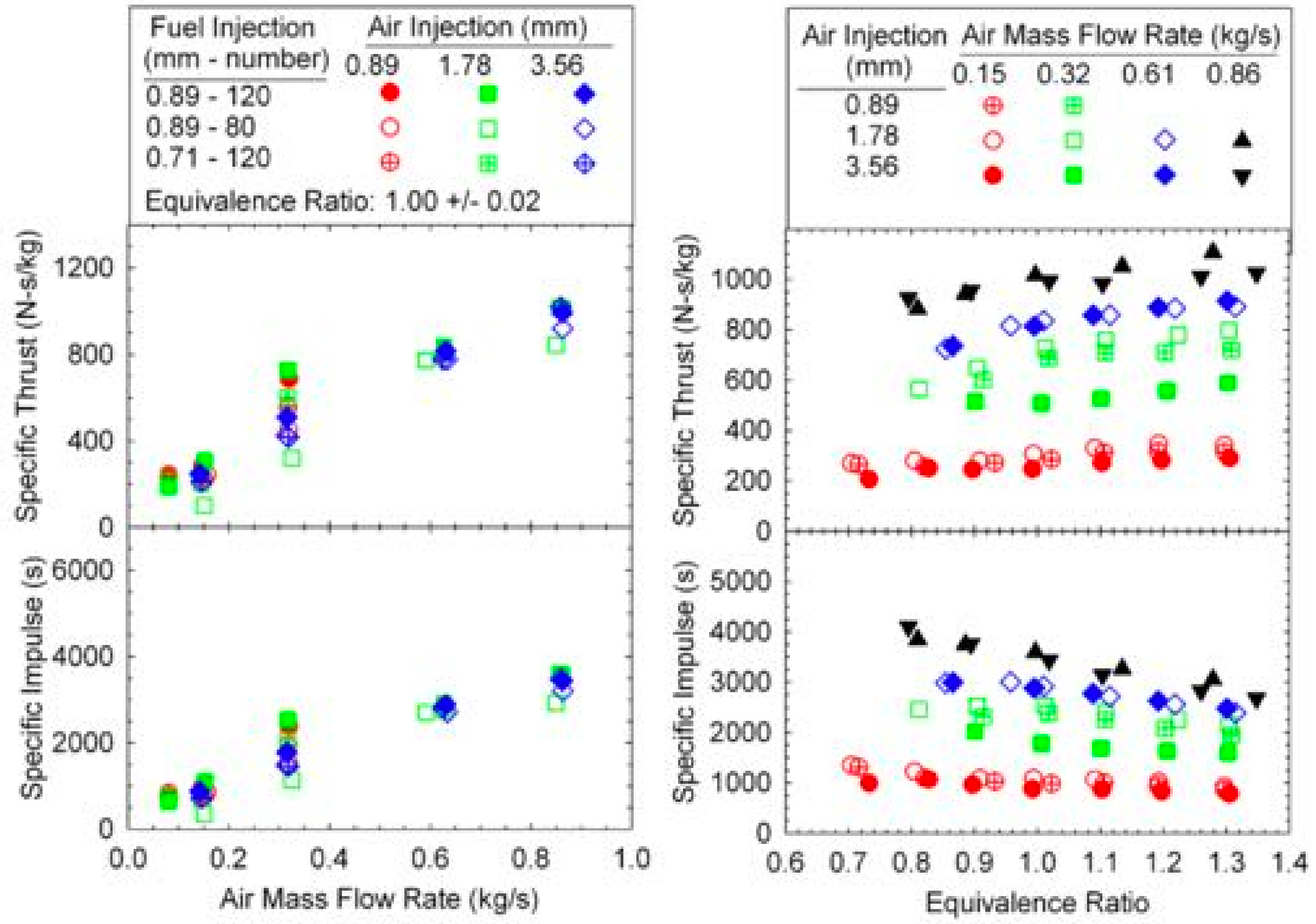
- **Parasitic combustion is only one loss mechanism, not the entire story of combustion within the RDE**
- **Broader post-detonation high temperature region in Radial Air Inlet RDE lends to greater NO_x production**
  - ➡ Axial Air Inlet RDE does show high temperatures, but with smaller exposure



Beyond CFD

- Full scale CFD is not always the solution
  - ➡ Time consuming, not fully reliable
- Need for combining multiple data points
  - ➡ Experiments
  - ➡ High-fidelity simulations
  - ➡ Multiple configurations, fuels and conditions
- Design optimization tools needed
  - ➡ Rapid estimation of performance





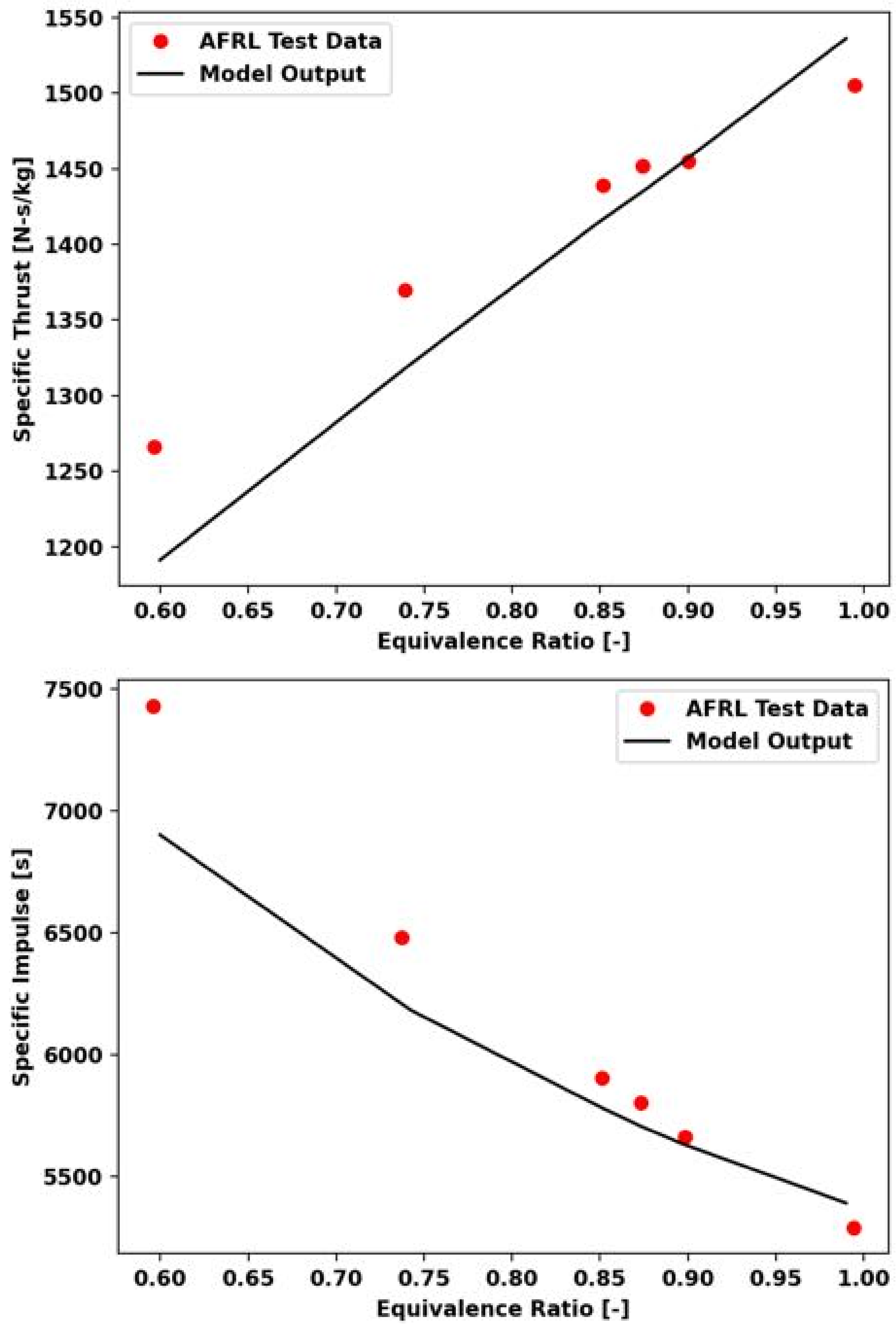
RDE model for performance estimation

- **Reduced order model of Kaemming et al. (2017)**
  - ➡ Inlet, thermodynamics, and exit models
- **Inlet model: time-varying flow rate**
  - ➡ $\tau_{drop} = \alpha/\tau_{factor} \rightarrow k = -\,ln(1-b)/\tau_{drop}$
  - ➡ $P_{3.4}(t)/P_{3.2} = 1 + [(P_2/P_1)_{Det} - 1]e^{-kt}$
  - ➡ $\dfrac{\dot{w}_{inlet}(t)}{dA_{inj}} = f\left(M_{inj}\left(P_{3.4}(t)\right)\right)$
  - ➡ $V_{refresh}(t) = \dfrac{\dot{w}(t)}{\rho A_{eff}}$
  - ➡ Preburning: $\dot{w}_{deflag} = \int \dot{w}(t)\dfrac{V_{flame}}{V_{refresh}}dt$
  - ➡ $\dot{w}_{det} = \int \dot{w}(t)dt - \dot{w}_{deflag}$
  - ➡ Detonation height: $h_{det} = \int V_{refresh}(t) - V_{flame}dt$
- **Thermodynamic cycle: 3 streams**
  - ➡ (a) detonation, (b) detonation + shock, (d) mixture of deflagration + detonation
  - ➡ Flow mixing parameterized - $f(h_{det})$

RDE model for performance estimation cont'd

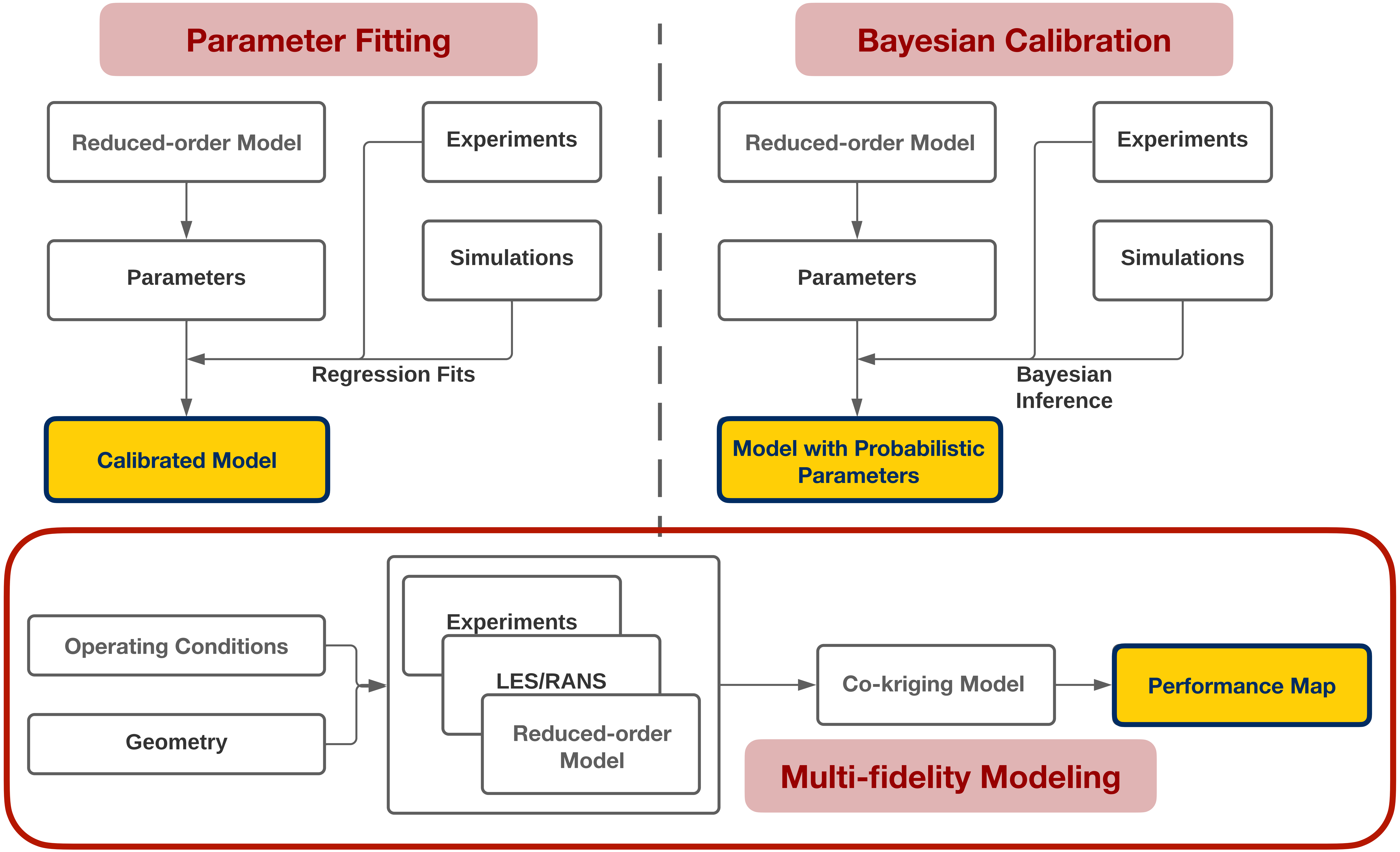
- **Exit model: flow distortion**
  - ➡ 3 streams contribute to $\dot{w}_{exit,total}$
    - Weighting is $f(h_{det})$
  - ➡ Choked flow at exit
    - $\delta = \dfrac{V_{8,max} - V_{8,min}}{V_{8},avg}$ ⟵ **Sound speed**
    - $M(x) = \delta x + (1 - \delta/2)$
  - ➡ Flow distortion:
    - $\dfrac{\dot{w}}{\dot{w}*} = f\big(M(x), \gamma\big)$
- **$P_{3.2}$ iterated such that $\dot{w}_{inlet} = \dot{w}_{exit}$**

- **Validated on AFRL RDE test data**
  - Nominal model parameters
  - Not "expertly tuned"
- **Model is low-fidelity solution in modeling framework**



Multi-fidelity framework

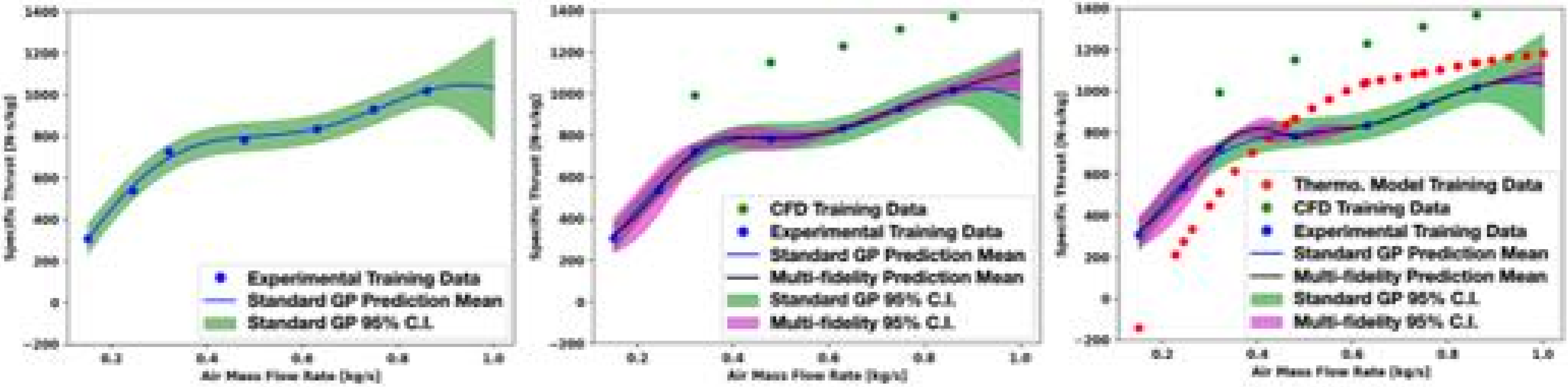
- **Integrate models of multiple levels of fidelity (performance tools, experiments, simulations) to create performance map**
  - ➡ Model calibration is difficult and not universal
  - ➡ Use nominal model parameters and account for model error



Multi-fidelity using multiple levels cont'd

- **Fits using different number of fidelity levels were generated to demonstrate multilevel multi-fidelity framework**

  ➡ Additional fidelity levels produce predictions with increasingly tight confidence bounds



Conclusions (Computational Modeling)

- **High-fidelity simulations to reliably predict performance developed and demonstrated**
  - ➡ Heterogeneous solver
  - ➡ High scalability
  - ➡ Ability to use detailed chemical kinetics
- **NOx emission most sensitive to structure of post-detonation region**
- **Performance prediction using data assimilation developed**
  - ➡ Sparse use of experimental and high-fidelity simulation data
  - ➡ Estimates performance surface, can be used to perform optimization

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Nonidealities in Rotating Detonation Engines

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Keywords

rotating detonation engine, pressure gain combustion, detonation wave, unsteady mixing, secondary combustion, deflagration loss, multiple competing waves, secondary waves

Abstract

A rotating detonation engine (RDE) is a realization of pressure-gain combustion, wherein a traveling detonation wave confined in a chamber provides shock-based compression along with chemical heat release.