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

PI: Mirko Gamba

Co-I: Venkat Raman

Alex Feleo, Joshua Shepard
Supraj Prakash, Caleb Van Beck

Department of Aerospace Engineering
University of Michigan

DOE NETL Review November 8-10, 2021

Work presented here is based on work supported by DOE NETL/UTSR program under Award No. DOE FE0031228 and FE0031773 with Dr. Mark Freeman as Program Monitor

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 RDE 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 RDE

Objectives and tasks

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

Objective 1
Low-loss injector based RDEs for methane/syngas operation at elevated pressure/temperature

- **Task 2.1**
  Effect of stratification/fuel composition on detonation structure
- **Task 2.2**
  Injector design for minimizing parasitic/commensal combustion
- **Task 2.3**
  Develop design rules for performance and scalability

Objective 2
Stability and operability characteristics of RDEs at fixed and transient conditions

- **Task 3.1**
  Operating map of RDEs and transition between different operating conditions
- **Task 3.2**
  Stability of system to perturbations in boundary and/or operating conditions
- **Task 3.3**
  Develop design rules for operability and stability for integrated systems

Objective 3
Develop tools for quantitative diagnostics, estimation of performance, and design optimization

- **Task 4.1**
  Development of validated quantitative tools for estimating pressure gain based on measurements
- **Task 4.2**
  Imaging-based quantification of RDE losses
- **Task 4.3**
  Development of AI-based accelerated models for long term computations
- **Task 4.4**
  Development of CFD-based design tool using Bayesian optimization

AIR INLET / FUEL INJECTOR DESIGN

FIXED AND TRANSIENT OPERATION & PERFORMANCE

METHODS DEVELOPMENT

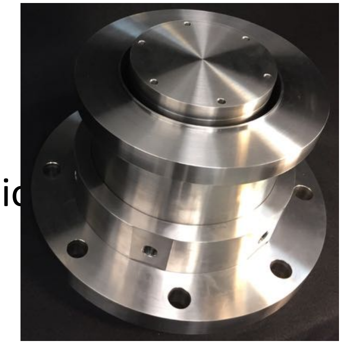
ADVANCING PHYSICAL UNDERSTANDING SOURCES OF GAIN AND LOSS
&
INVESTIGATING REALIAZABLE GAIN IN FIXED AND TRANSIENT CONDITIONS

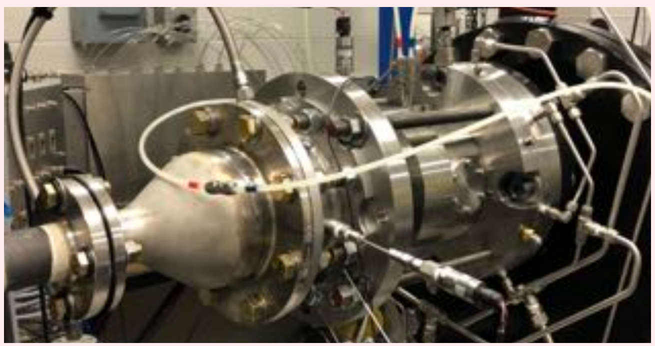
Outline

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

RDE experimental infrastructure at U-M

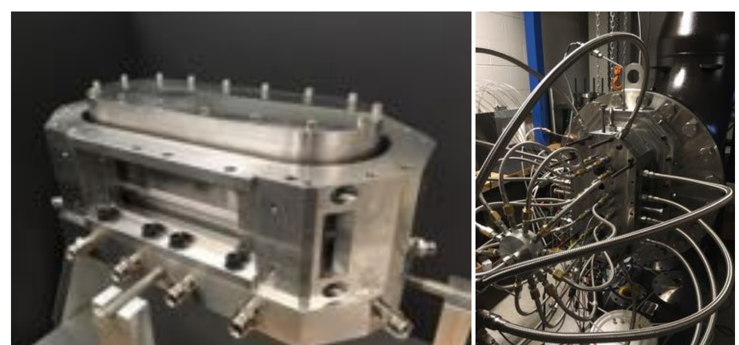
- **Modular baseline RDE**
  - Developed under previous projects
  - Operational with H2/Air, various flow rates and equivalence ratic
  - Operation for multi-component fuels
  - Able to generate transient operation (flow rates, equivalence ratio, composition)





- **Fully-axial, enhanced RDE**
  - Operational, designed for improved operation
    - Management of non-ideal behaviors
  - Transient operation
  - Undergoing redesign to extend transient operation

- **Optical RDE (Race-Track RDE)**
  - Operational
  - Equivalent to 12” round RDE
  - Used for flowfield measurements under RDE relevant conditions

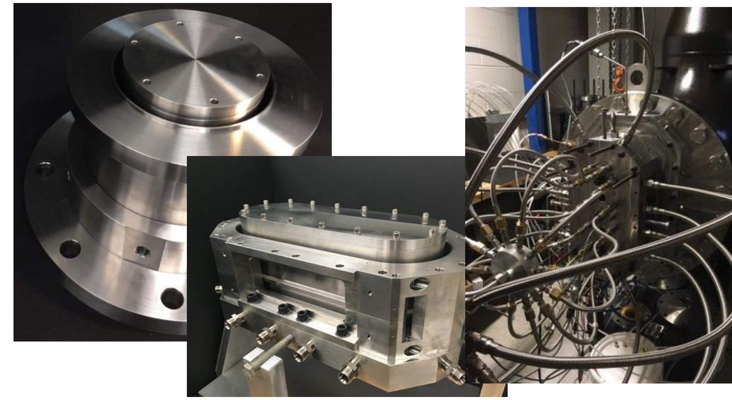


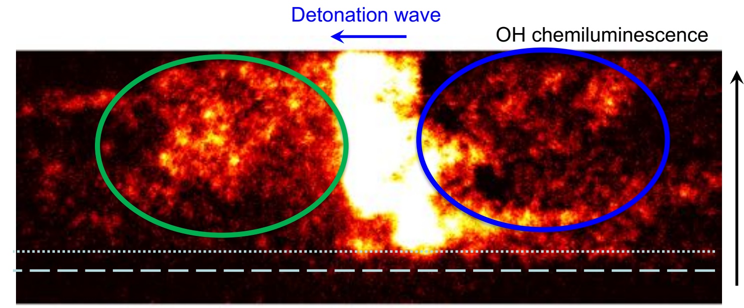
Our contribution for the year

- **Continued the investigation of H_2/CO_2 and H_2/CH_4 mixtures**
  - We have built from last year's work
  - Focus on secondary wave suppression, and modification of secondary combustion
- **Investigated inlet temperature effects on H_2/air operation**
  - Identified changes in stability properties
  - Mode of operation changes as inlet temperature increases
    - From stable single wave to slapping wave
  - We need to refine some of the analysis tools for slapping wave modes
- **Continued the investigation of pressure gain and losses in RDCs**
  - Some improvements on thrust measurements made, more in preparation
- **Characterized and investigate new axial air inlet RDC configuration at different inlet area ratios**
  - Focus for today's discussion
- **Investigated the response properties of the air inlet**
  - Developed a one-dimensional model to describe the propagation of disturbances into the air plenum

From the past: impact of combustion losses

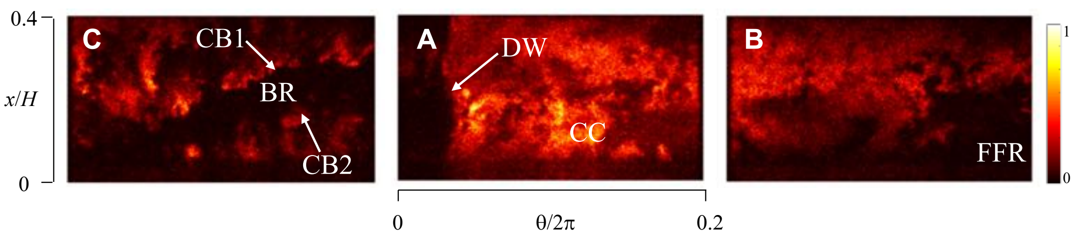
- **Develop and investigated an axial air inlet design**
  - Operation
  - Performance (based on thrust)
- **Investigated and identified non-ideal effects as limiting processes**
  - Deflagration losses
  - Parasitic/commensal combustion
- **Based on what learnt, we have redeveloped a 2nd generation axial air inlet design**
  - Designed to managed some of the losses

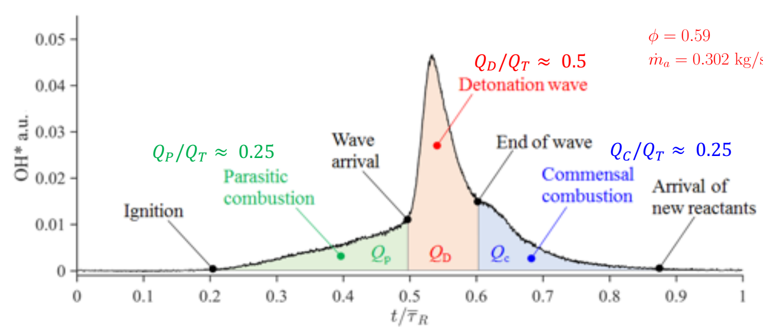




Parasitic combustion
- Combustion before arrival of wave
- Heat released before the detonation wave does not support it
- Mixture is heated and vitiated

Commensal combustion
- Combustion trailing the wave
- Heat released after the detonation wave does no have an impact on it
- Consequence of mixture leakage



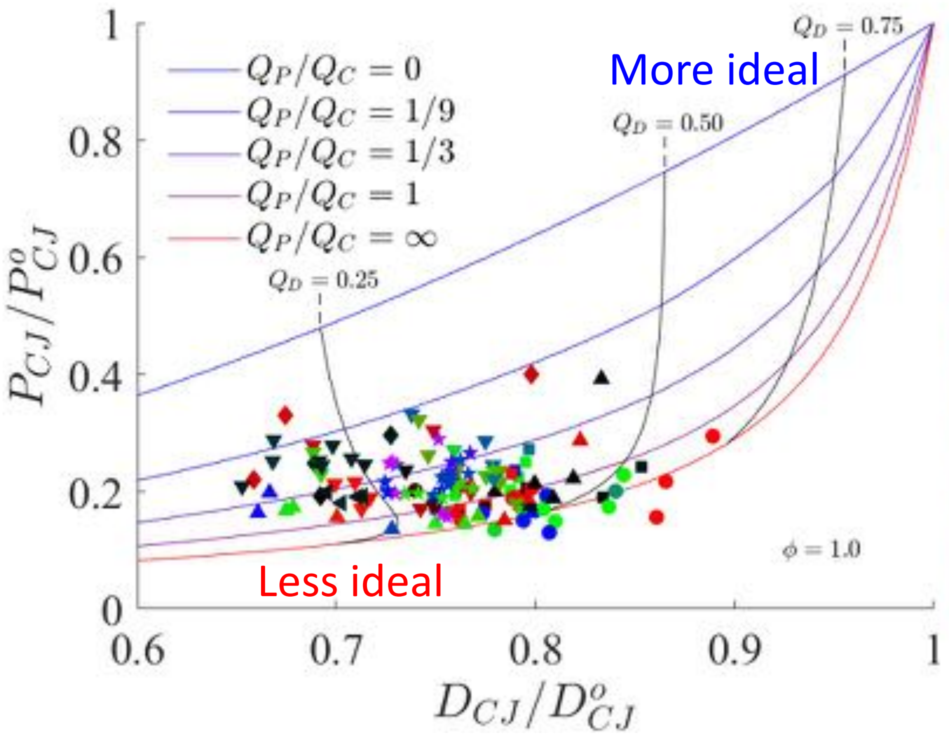


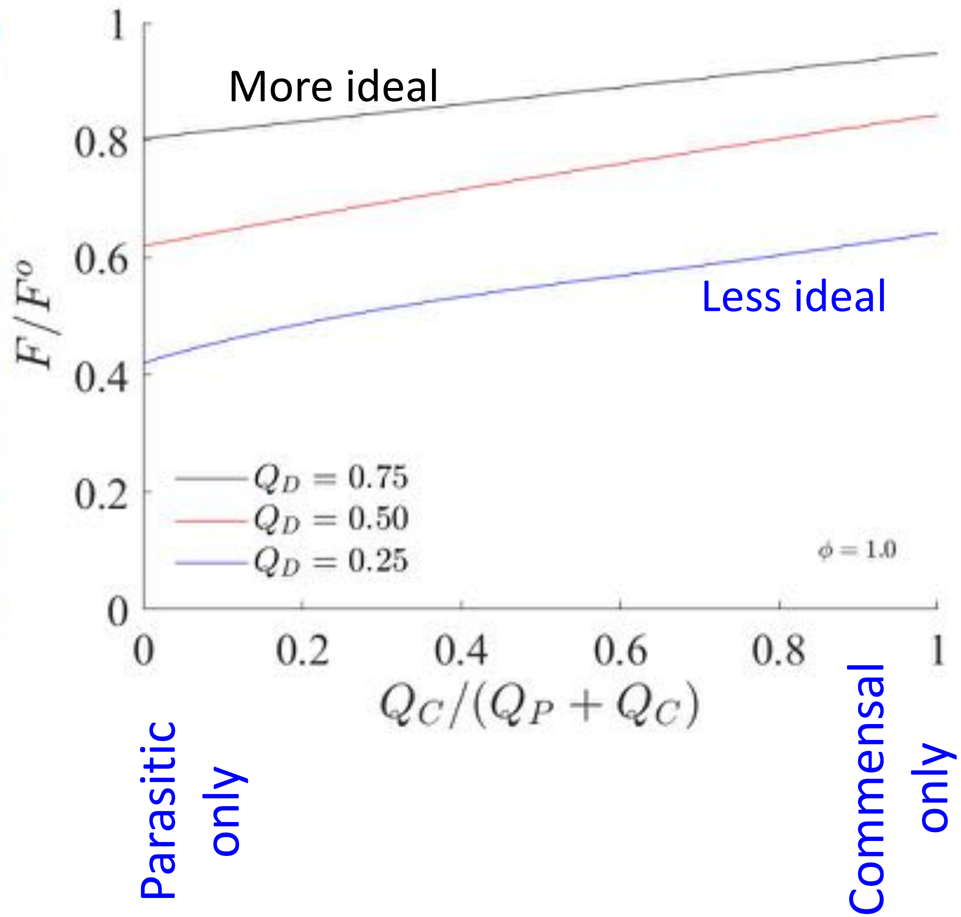
From the past: impact of secondary combustion

Apply a reduced RDE model (state-to-state thermodynamic model)

Post-detonation pressure and wave speed

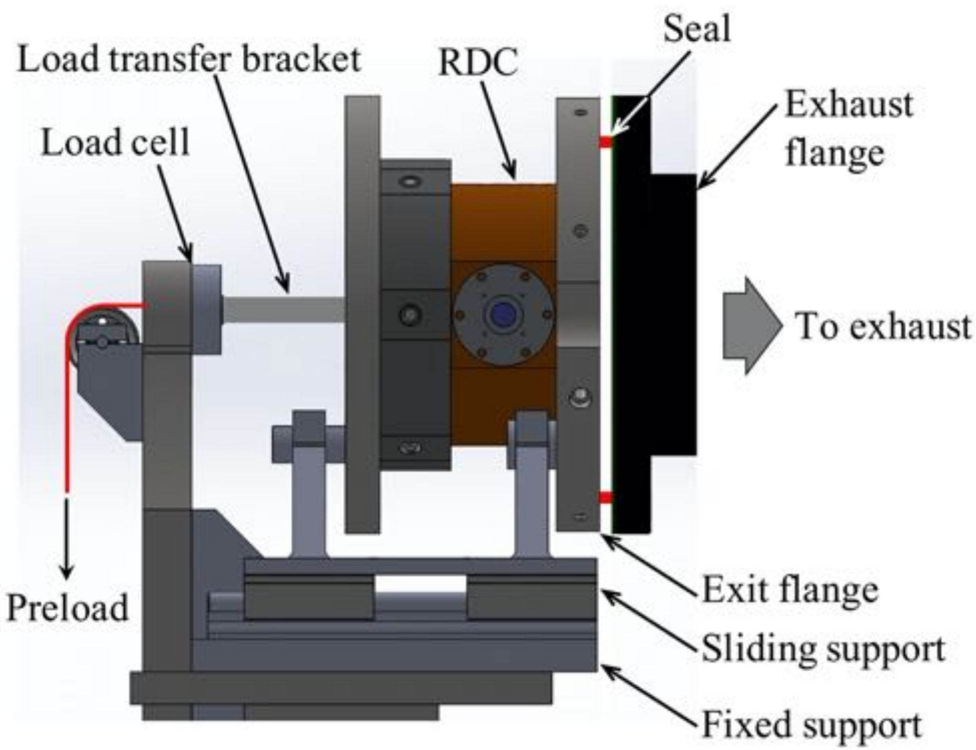
Thrust: $$\frac{F}{F^o} = \left(\frac{\Delta P_{CJ}}{\Delta P^o_{CJ}}\right)\left(\frac{D^o_{CJ}}{D_{CJ}}\right)\left(\frac{\rho^o_b}{\rho_b}\right)$$

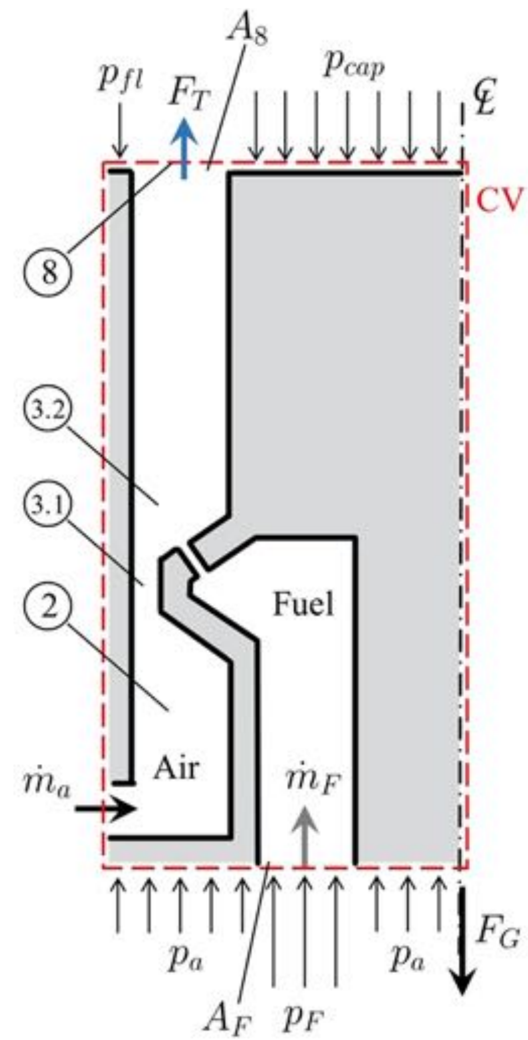




Improvements on our thrust measurements

- **Developed a second generation thrust measurement device**
  - Resolves some of the known uncertainties and systematic errors





$$F_T = F_G + A_F \Delta p_F + A_{fl} \Delta p_{fl} + A_{cap} \Delta p_{cap} - \frac{\dot{m}_F^2 R_F T_F}{A_F p_F}$$

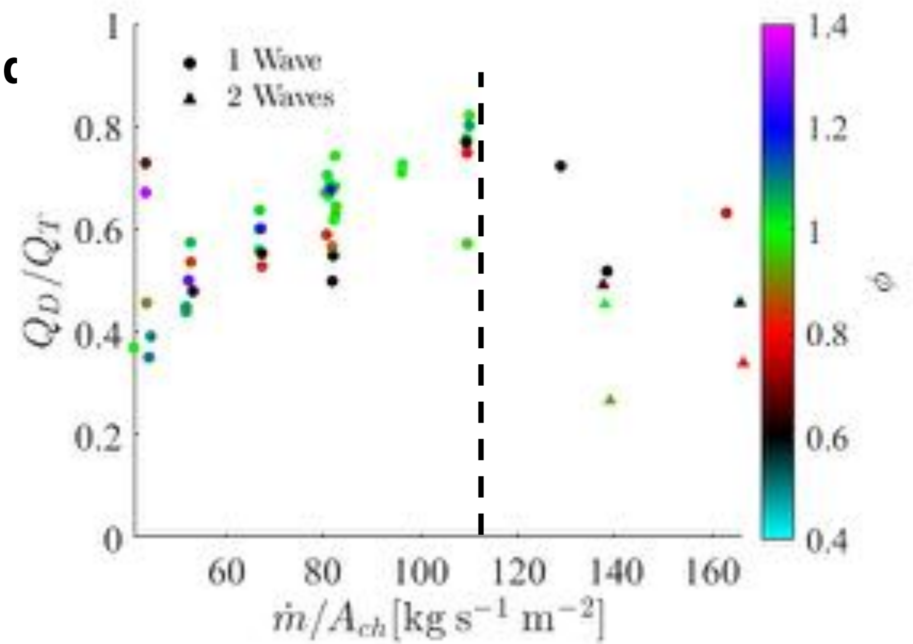
Pressure Gain and Heat Release

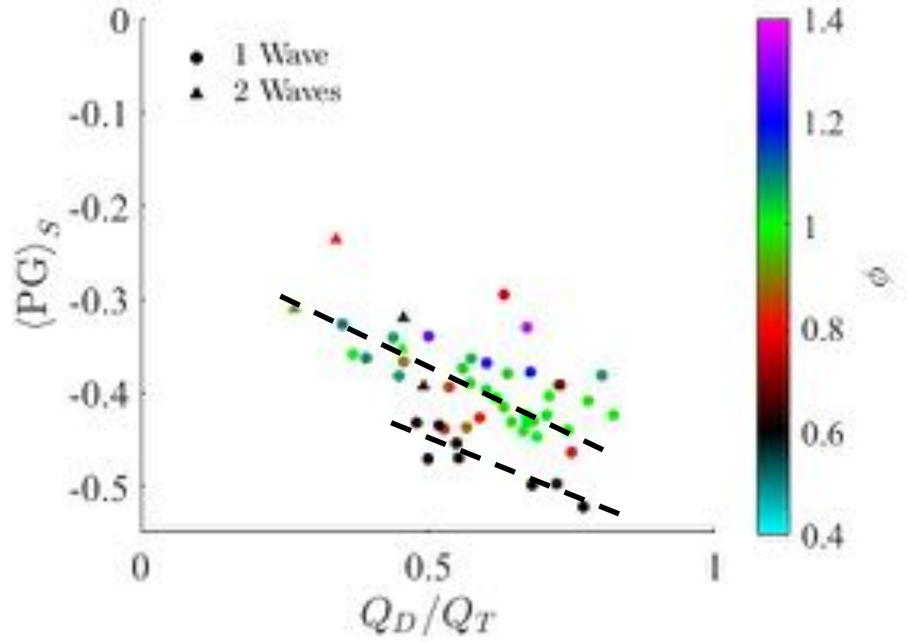
- **Relative amount of heat release associated with detonation (Q_D/Q_T)** **decreases after 110 kg s^{-1} m^{-2}**
- **Increasing observed Q_D/Q_T** **decreases PG**
  - Dependence on Φ
- **Detonation wave grows to be more ideal with larger Q_D/Q_T**
- **Might also indicate dependence on detonation structure**

$$\tilde{p}_8 = \frac{F_T + p_\infty A_8}{(1+\gamma M_8^2)A_8}$$

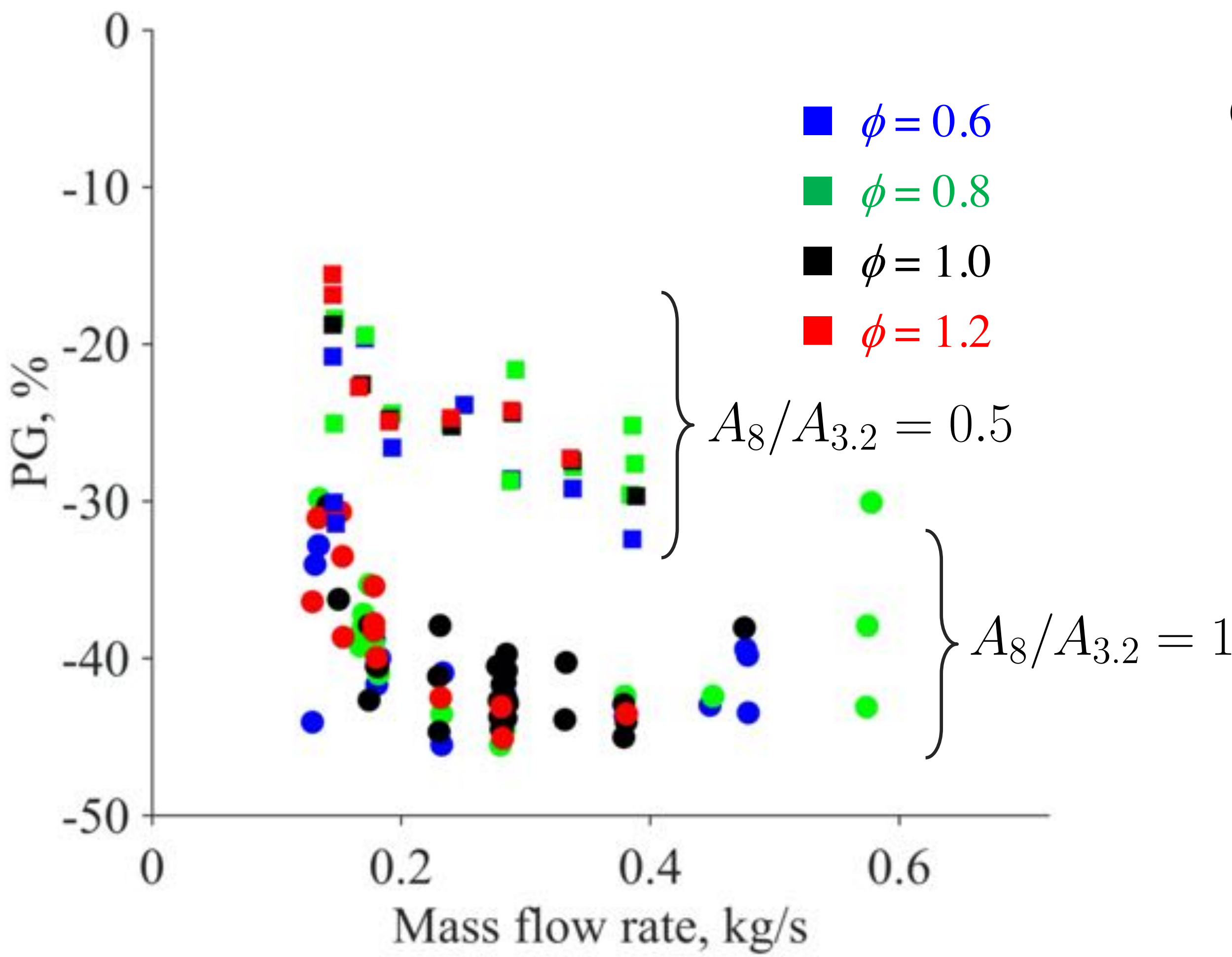
$$\text{EAP} = \tilde{p}_8 \left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}}$$

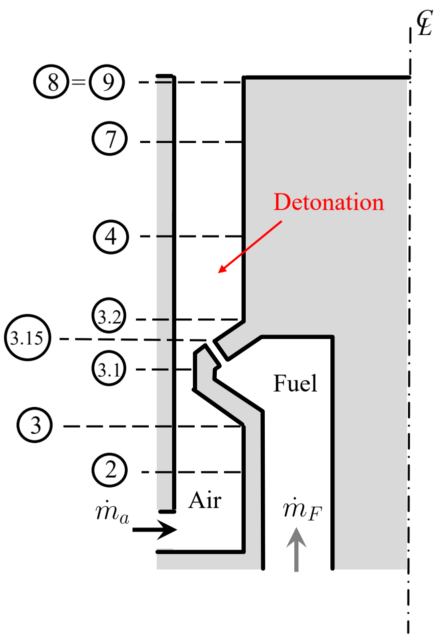
$$\text{PG} = \frac{\text{EAP}}{p_{T,2}} - 1$$





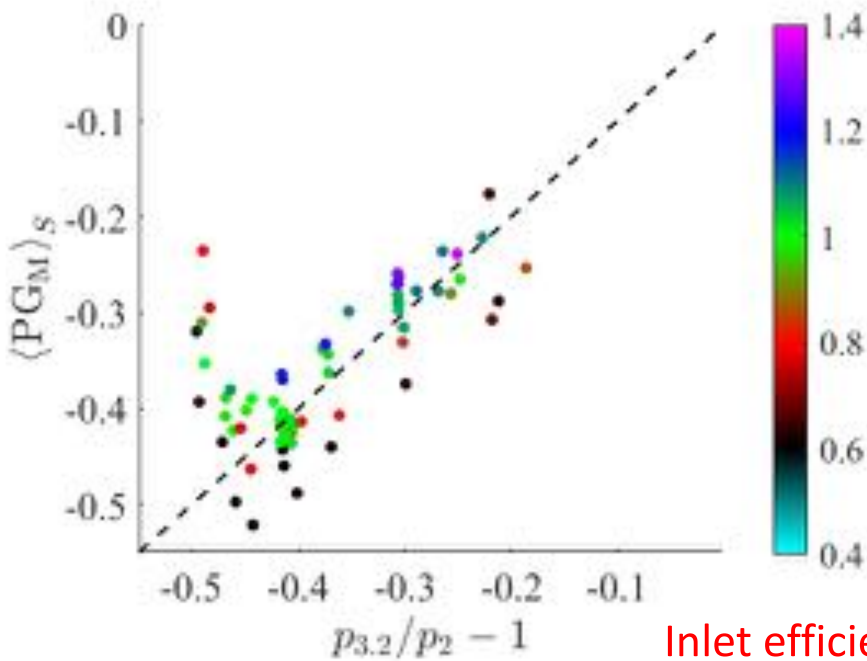
Effects of exit nozzle restriction

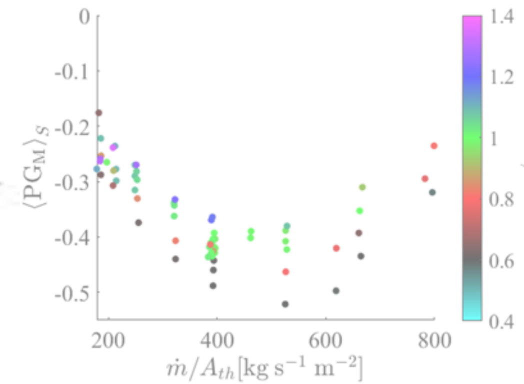




Link between pressure gain and inlet pressure loss

Measured gain:





Inlet efficiency (loss)

Gain:

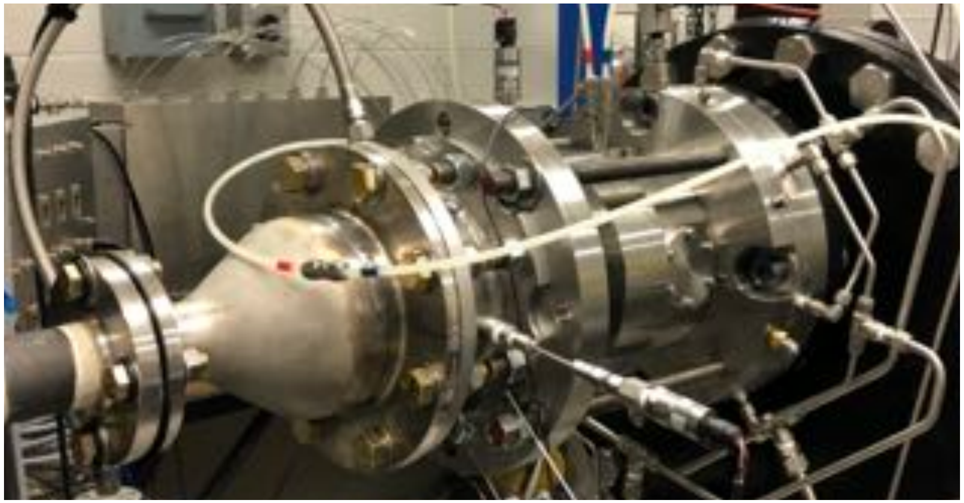
$$G = \frac{p_{o,n}}{p_{o,i}} - 1$$
$$= \frac{p_{o,n}}{p_{o,d}}\frac{p_{o,d}}{p_{o,u}}\frac{p_{o,u}}{p_{o,i}} - 1$$
$$= \eta_e (G_{CJ} + 1)\eta_i - 1$$

Inlet efficiency (loss)

Gain at detonation wave (includes losses)

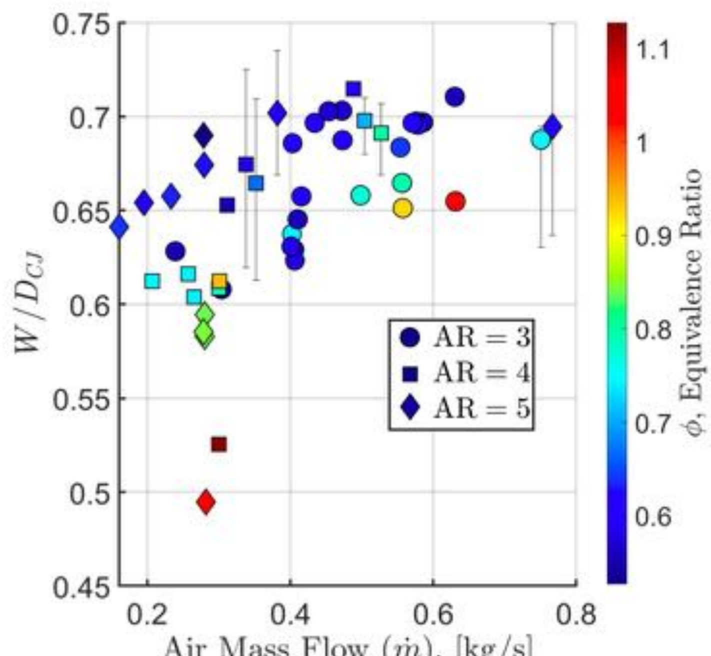
Expansion efficiency (loss)

Characterization of new configuration

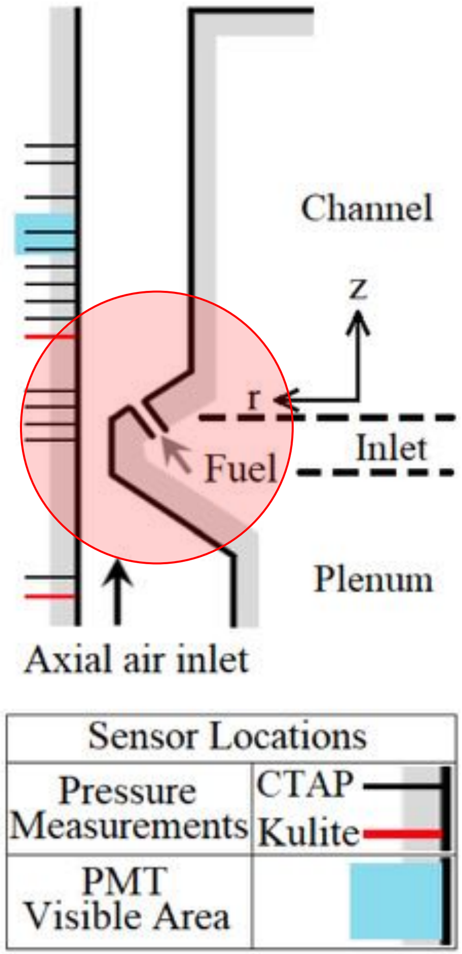


Different geometric configurations:

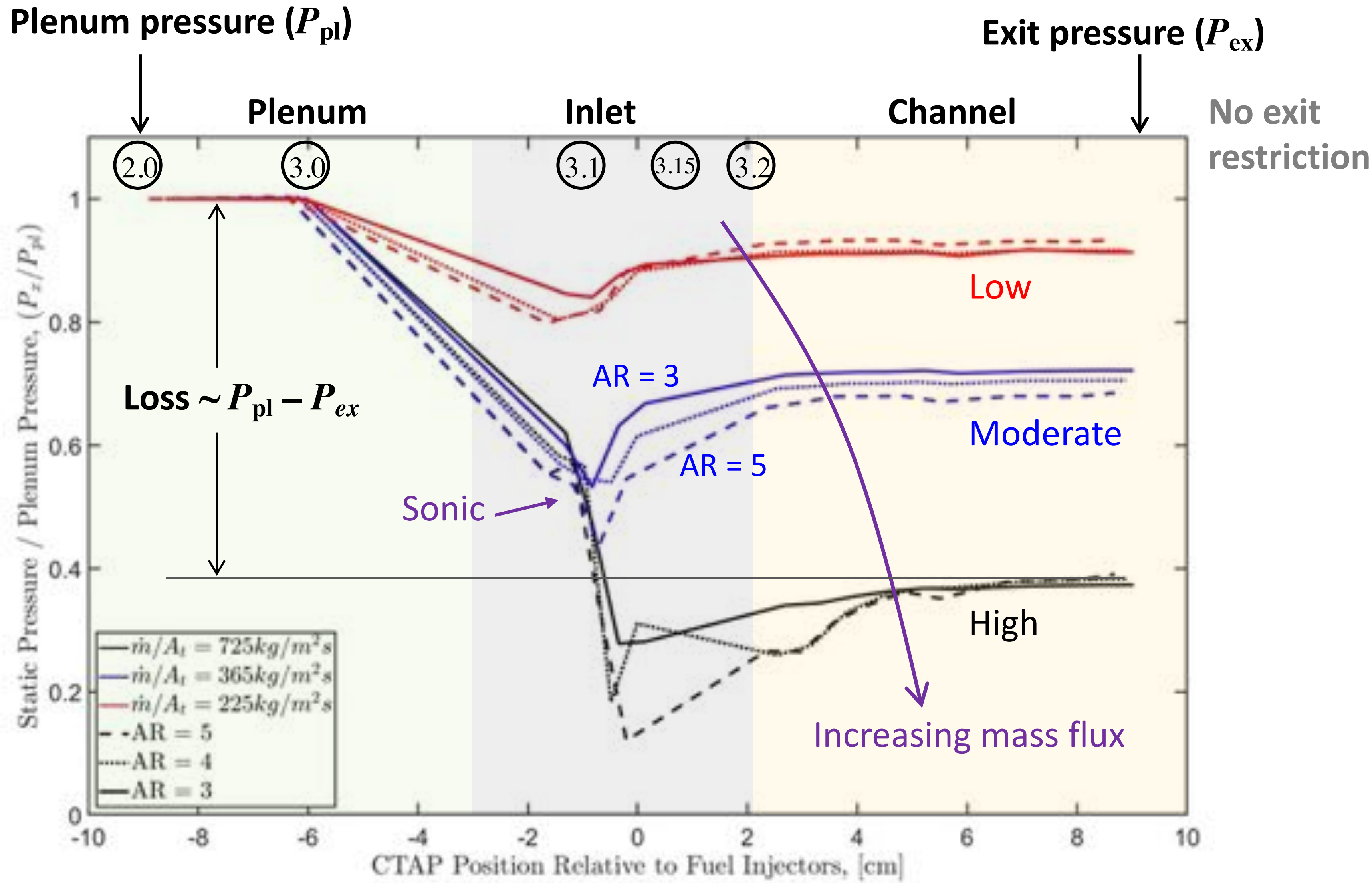
- Inlet area
- Channel profile
- Exit restriction



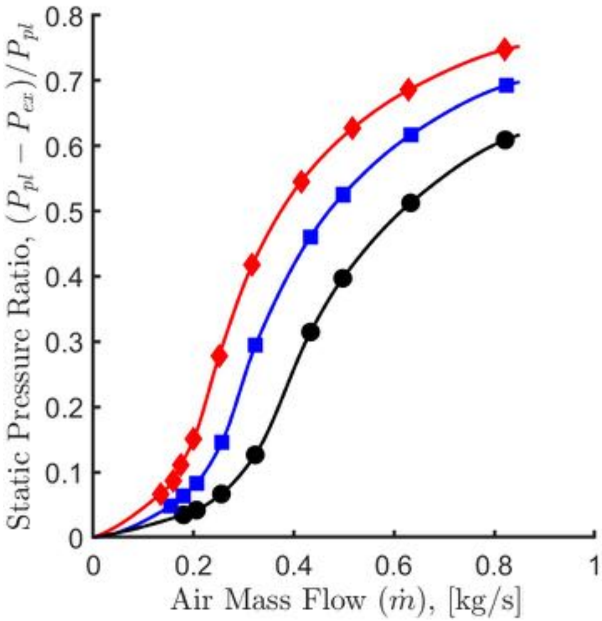
Our current focus

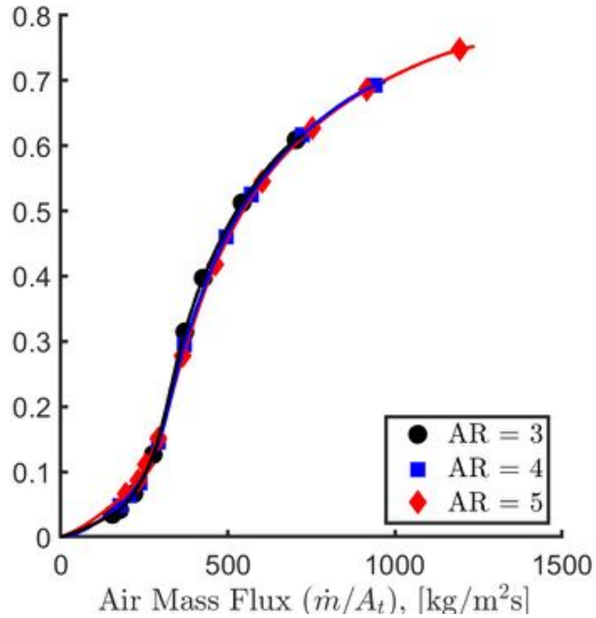


From steady no-fuel flow (cold flow)

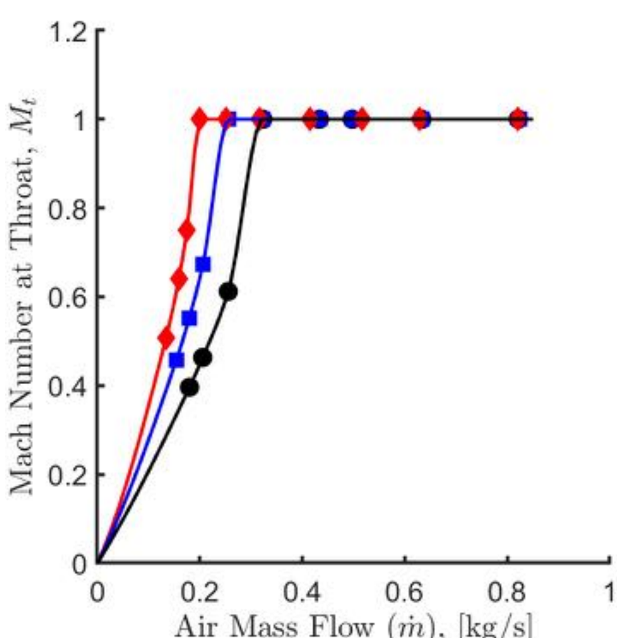


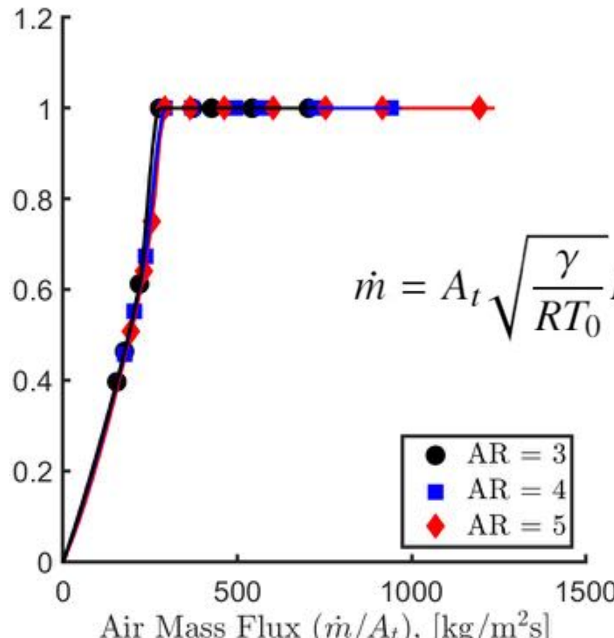
Characteristics of Inlet in Non-Reacting Flow





Static pressure ratio is used as an indicator of static pressure loss from plenum to channel exit

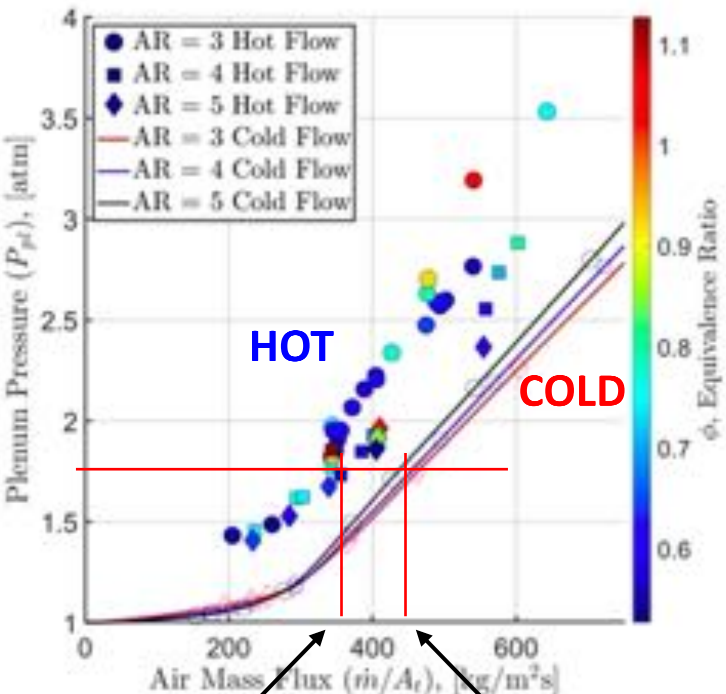




$$\dot{m} = A_t \sqrt{\frac{\gamma}{RT_0}} M P_{pl} \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-\frac{\gamma+1}{2(\gamma-1)}}$$

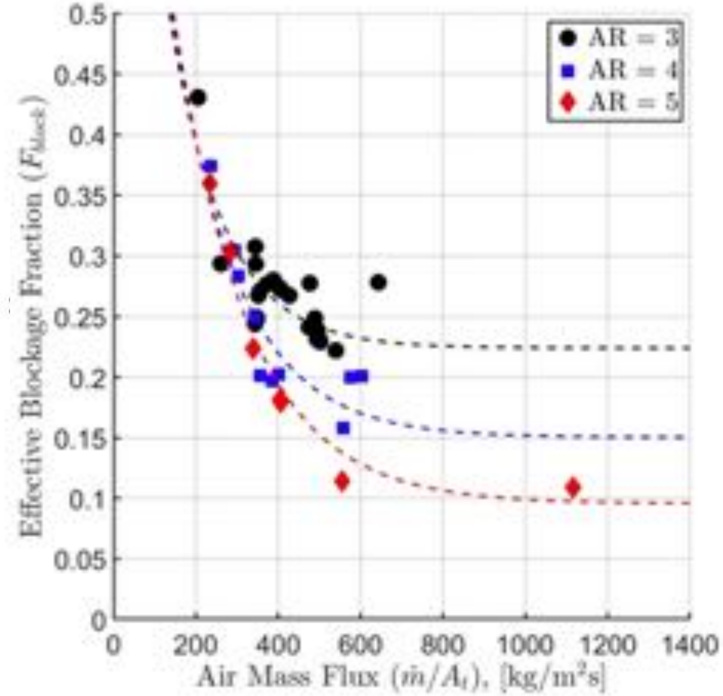
Estimation of air inlet blockage

$p_{t,3}$



$(\dot{m}/A_t)_{\text{Hot}}$ $(\dot{m}/A_t)_{\text{Cold}|P_{\text{pl}}}$

F_{block}



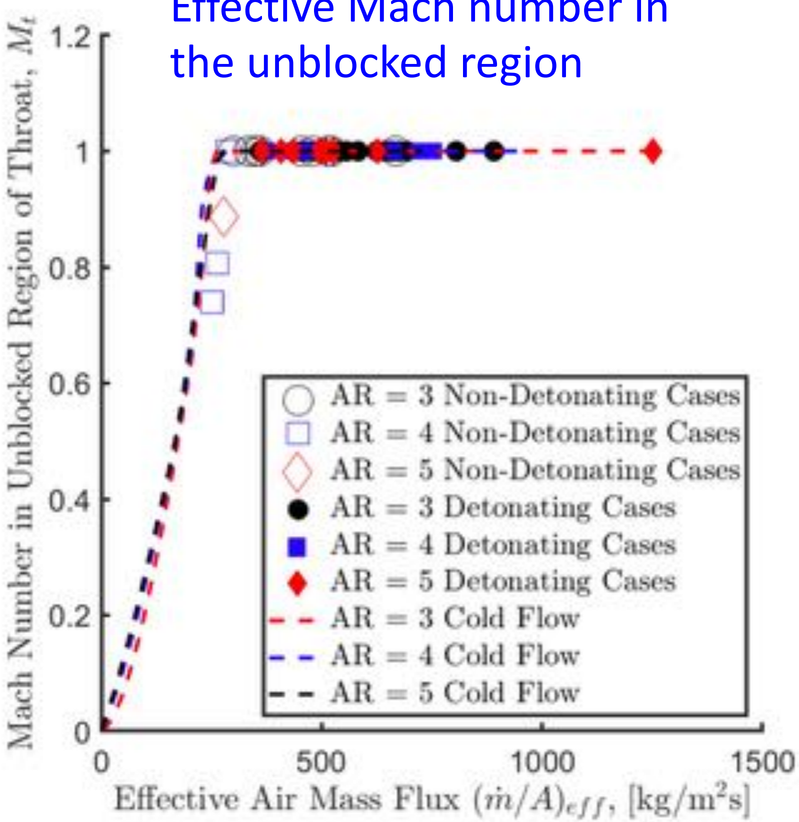
$$F_{\text{block}} = 1 - \frac{(\dot{m}/A_t)_{\text{Hot}}}{(\dot{m}/A_t)_{\text{Cold}|P_{pl}}}$$

Mass flow rate for hot flow at a given plenum pressure

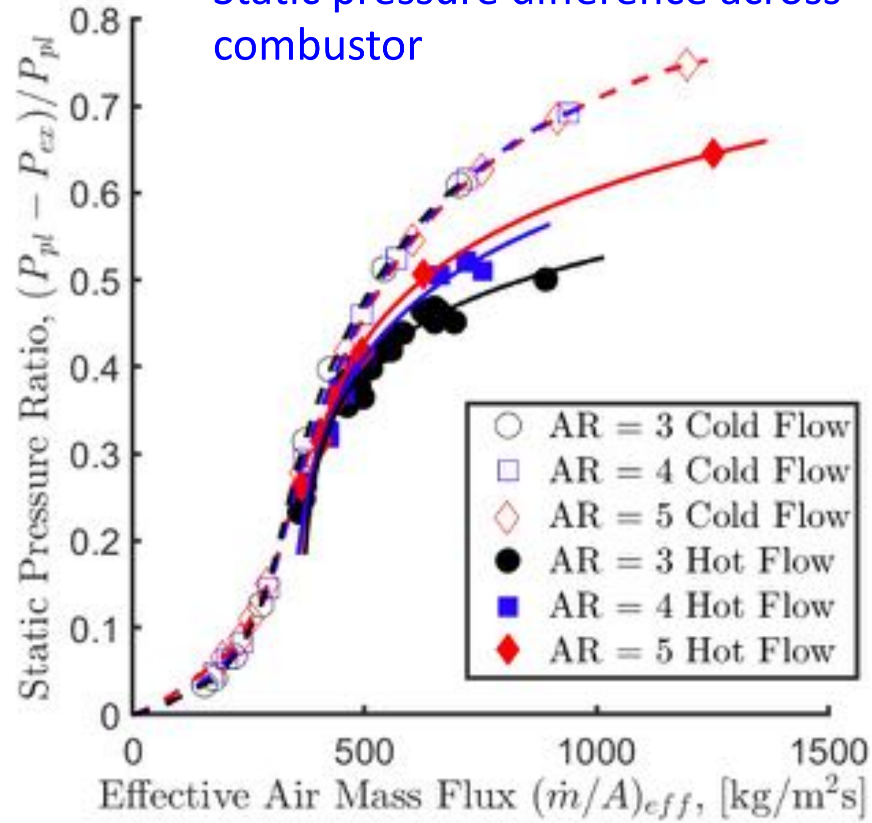
Mass flow rate for a cold flow at the same plenum pressure of that of the hot flow

Operable conditions all have $M_t = 1$

Effective Mach number in the unblocked region



Static pressure difference across combustor



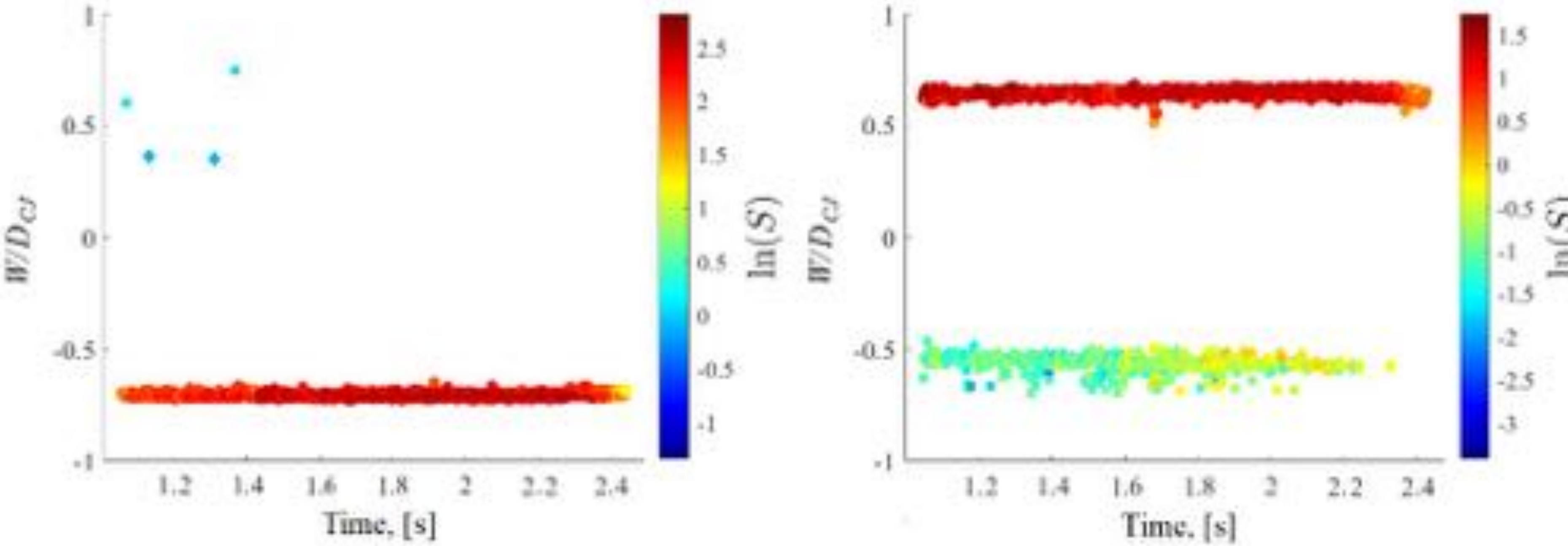
Effective mass flux through inlet:

$$\left(\frac{\dot{m}}{A}\right)_{eff} = \frac{\dot{m}}{A_t(1 - F_{\text{block}})}$$

Mass flow rate through the unblocked portion of the inlet

Used to get the effective Mach number in the unblocked region

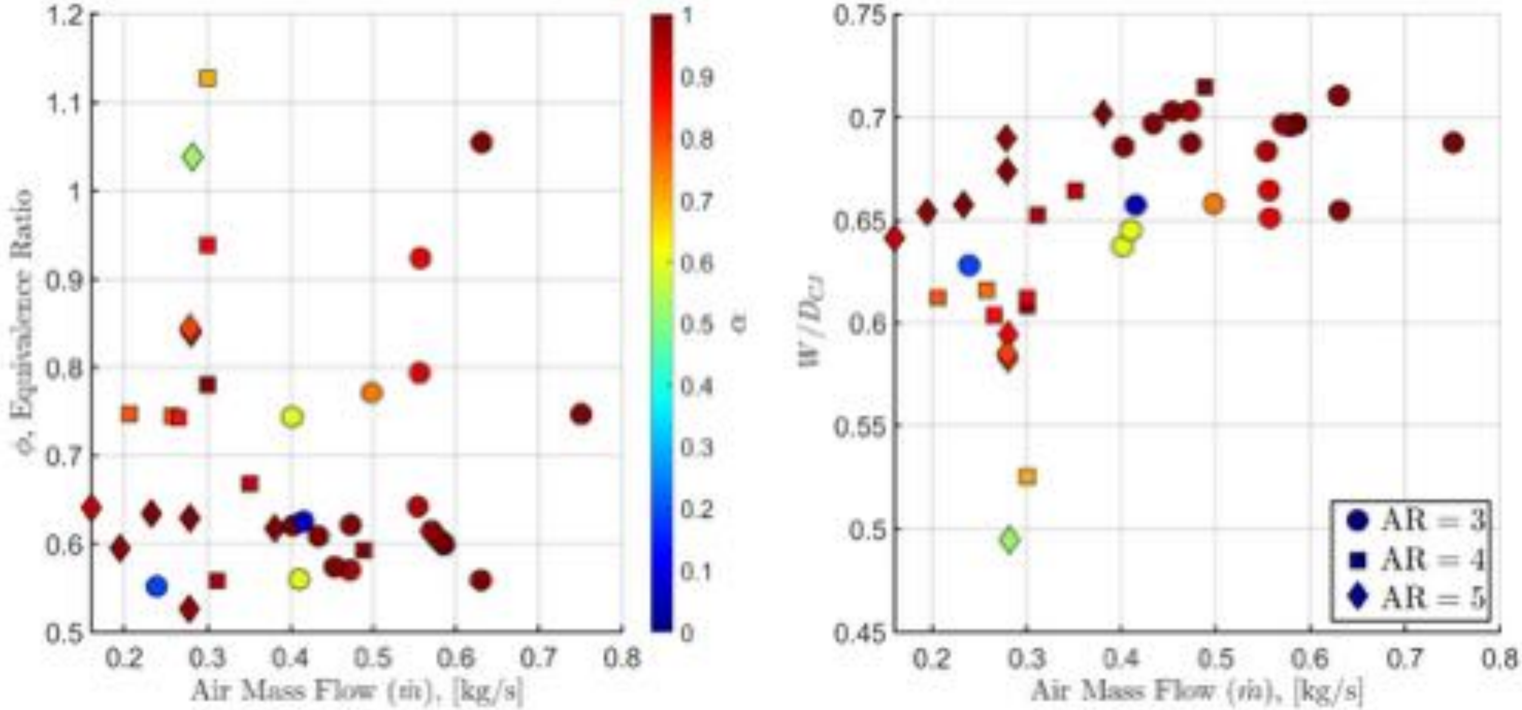
Working on developing a measure of *Relative Wave Quality*



- Based on Circuit Wave Analysis from high-speed video
  - Used to classify and quantify primary and secondary wave systems
- Relative Wave Quality metric was devised to condense CWA data to single quantity

$$\alpha = \underbrace{\left(\frac{K_{0.5*CJ}}{K_{total}}\right)}_{\alpha_1} \underbrace{\left(1 - \frac{K_{sec}}{K_{total}} \frac{\overline{S}_{sec}}{\overline{\overline{S}}_{prim}}\right)}_{\alpha_2} \underbrace{\left(1 - \frac{K_{cr}}{K_{total}} \frac{\overline{S}_{cr}}{\overline{\overline{S}}_{prim}}\right)}_{\alpha_3}$$

Working on developing a measure of *Relative Wave Quality*

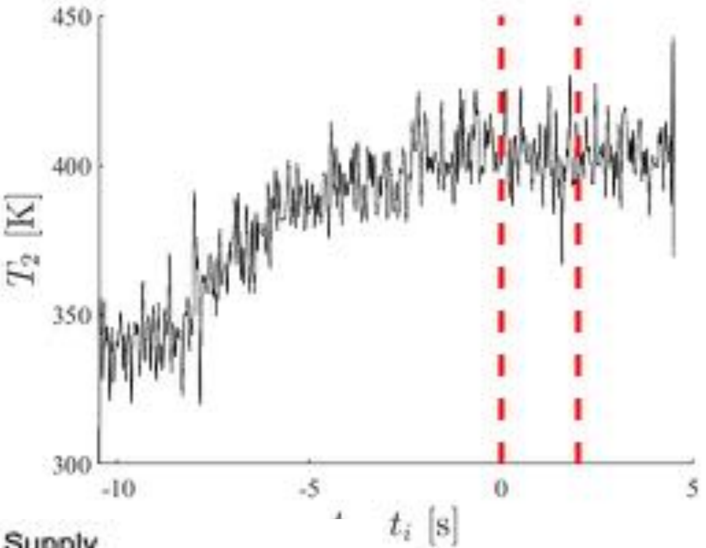


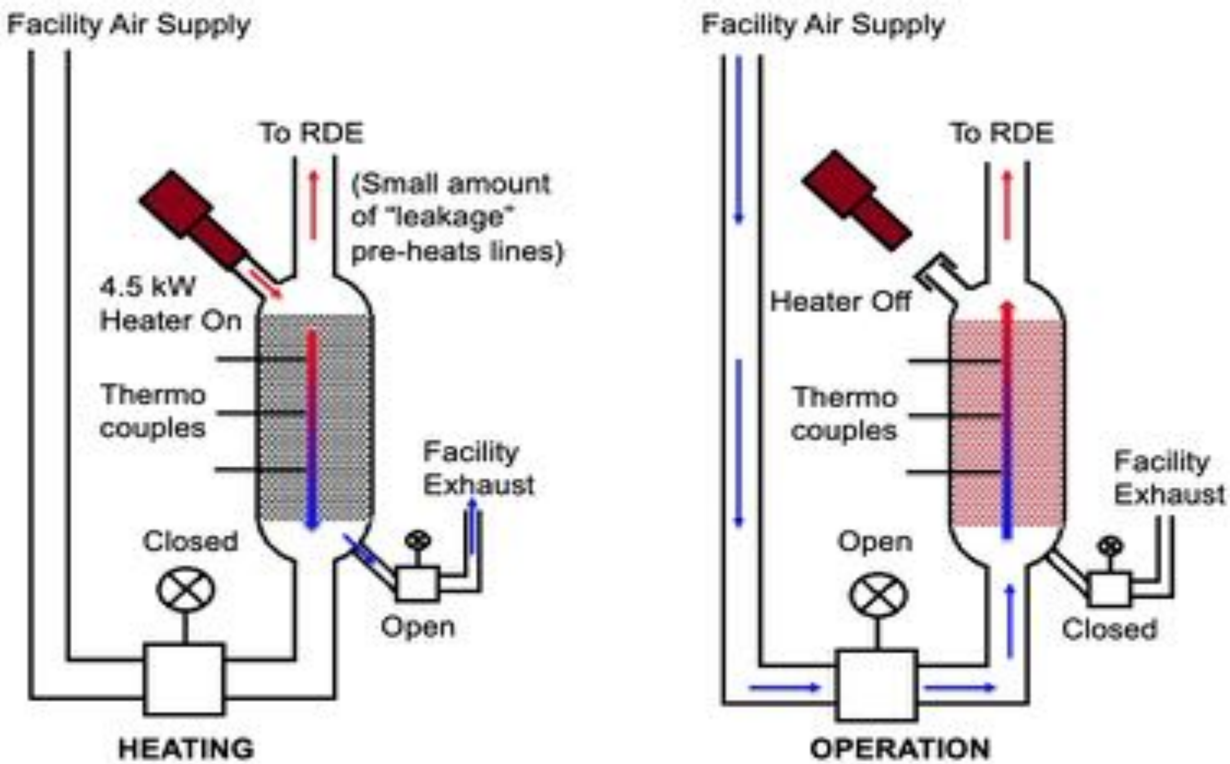
- Based on Circuit Wave Analysis from high-speed video
  - Used to classify and quantify primary and secondary wave systems
- Relative Wave Quality metric was devised to condense CWA data to single quantity

$$\alpha = \underbrace{\left(\frac{K_{0.5*CJ}}{K_{total}}\right)}_{\alpha_1} \underbrace{\left(1 - \frac{K_{sec}}{K_{total}} \frac{\overline{S}_{sec}}{\overline{\overline{S}}_{prim}}\right)}_{\alpha_2} \underbrace{\left(1 - \frac{K_{cr}}{K_{total}} \frac{\overline{S}_{cr}}{\overline{\overline{S}}_{prim}}\right)}_{\alpha_3}$$

Assessing inlet temperature effects

- In-line pebble-bed used to achieve higher inlet temperature (T_2)
- Air scavenges heat prior to fuel introduction to achieve quasi-steady temperature
  - Max tested $T_2 = 480K$



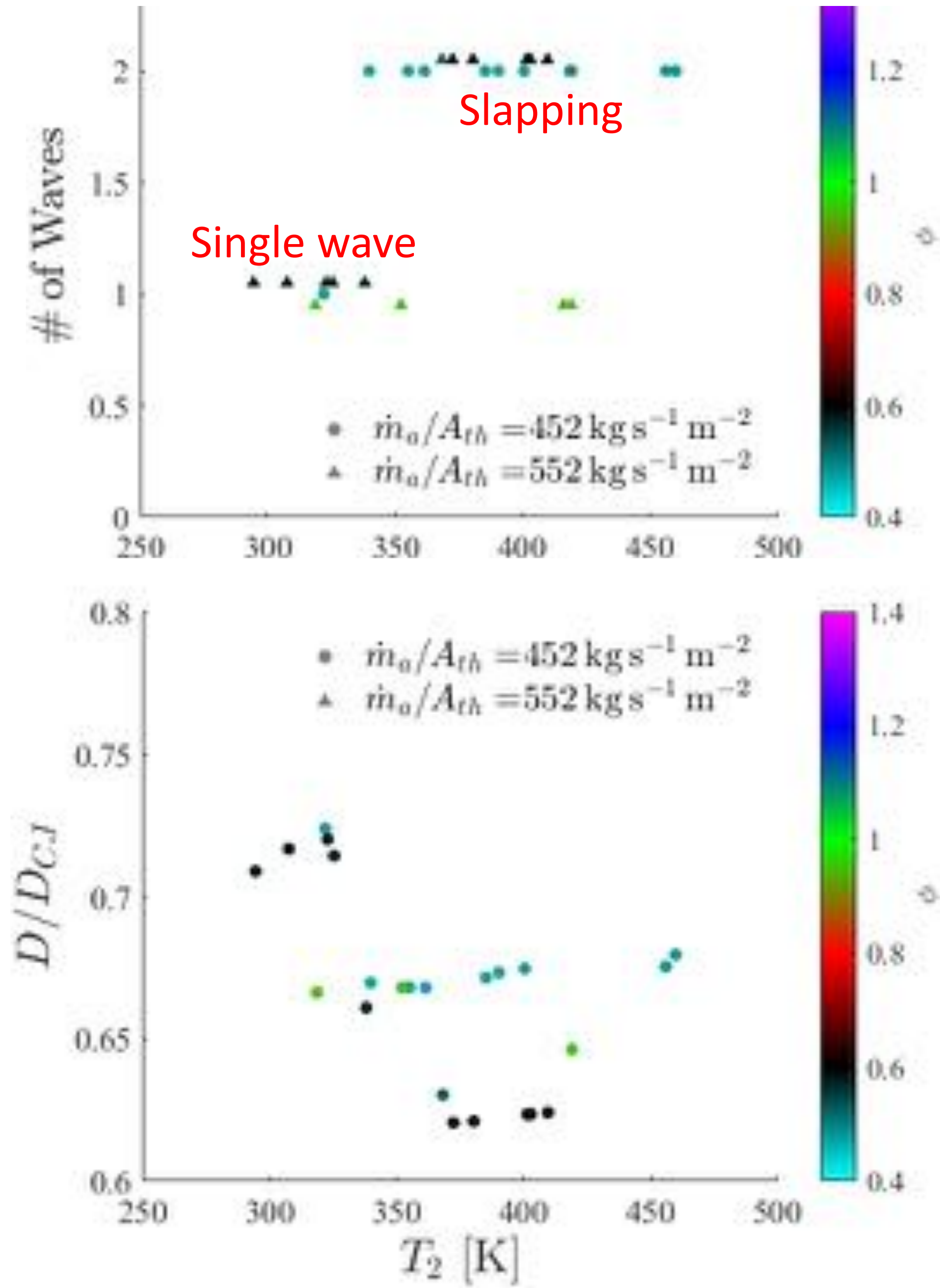


Operation mode changes at higher inlet temperature

- **H_2/air operation**
  - Area ratio of 4 and no nozzle

$\frac{\dot{m}_a}{A_{th}}$ $[\mathrm{kg\,s^{-1}\,m^{-2}}]$	ϕ	T_2 [K]
452	0.5	320 – 467
552	0.6	295 – 410
552	1	319 – 420

- **Observations**
  - Transition to slapping mode
  - Wave speed drops at transition to slapping mode
  - Pressure ratio increases with inlet temperature

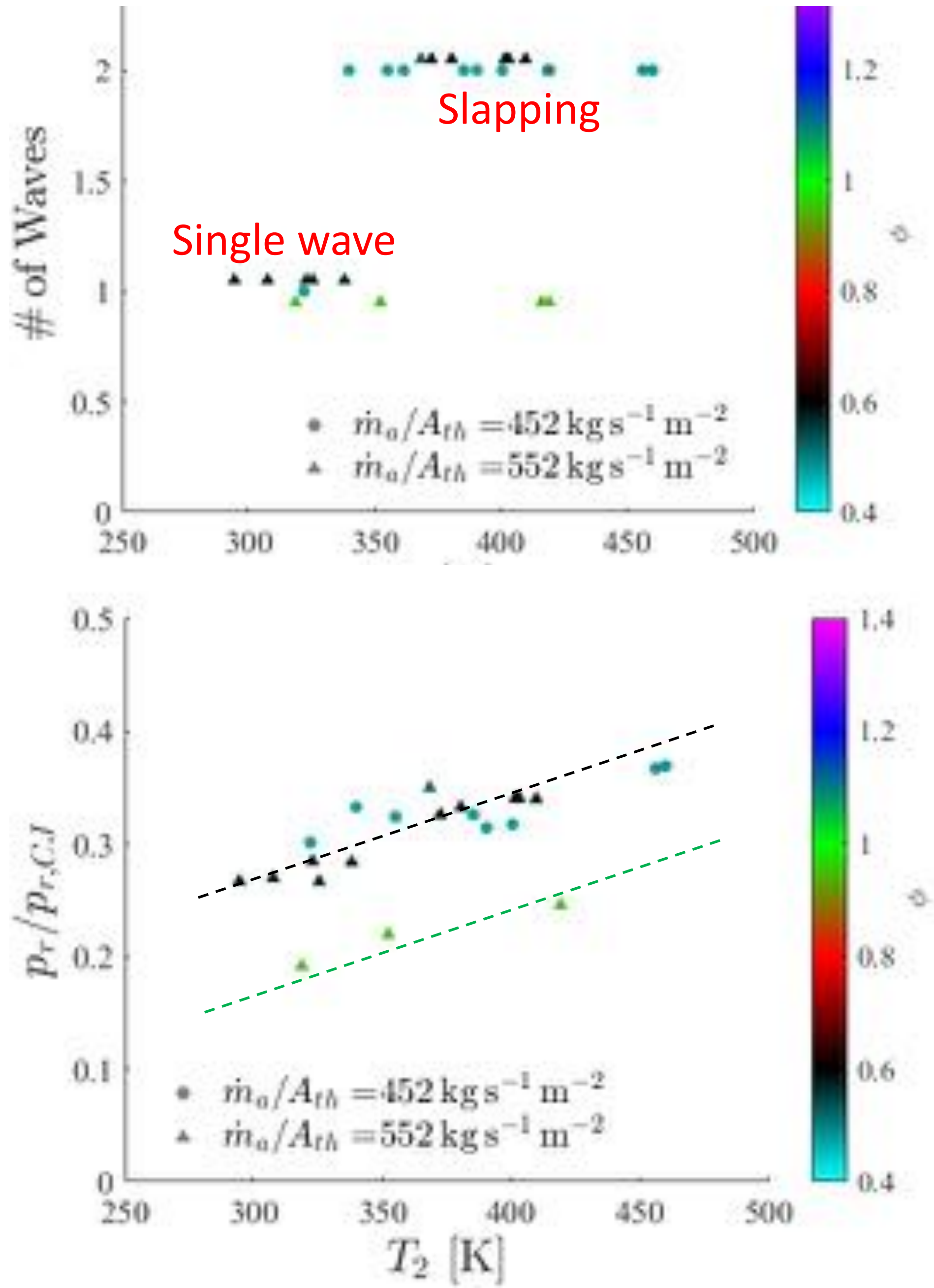


Operation mode changes at higher inlet temperature

- **H_2/air operation**
  - Area ratio of 4 and no nozzle

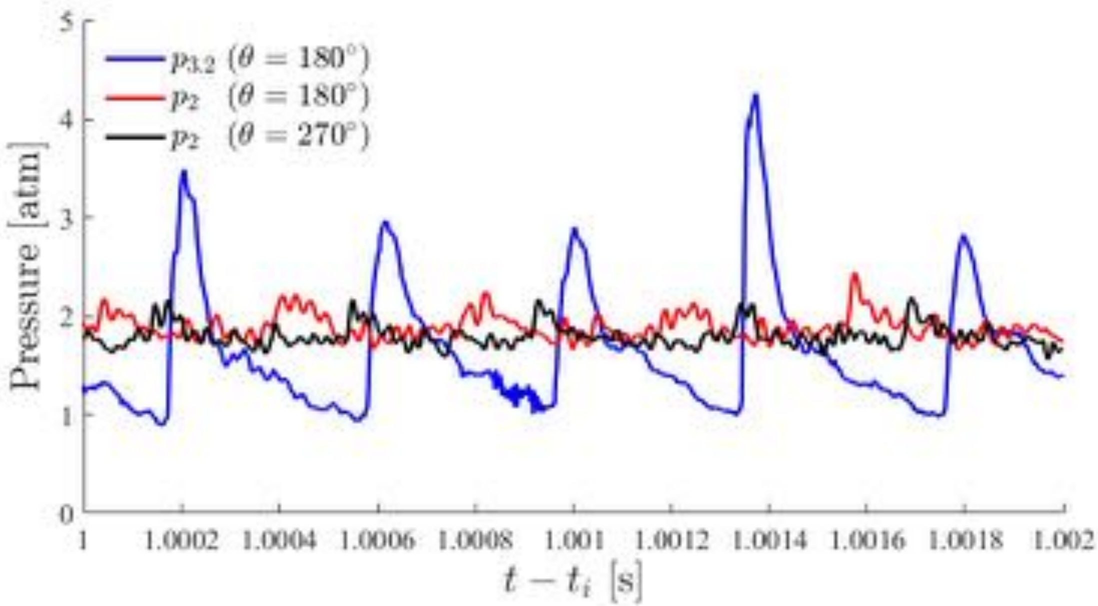
$\frac{\dot{m}_a}{A_{th}}$ $[\mathrm{kg\ s^{-1}\ m^{-2}}]$	ϕ	T_2 [K]
452	0.5	320 – 467
552	0.6	295 – 410
552	1	319 – 420

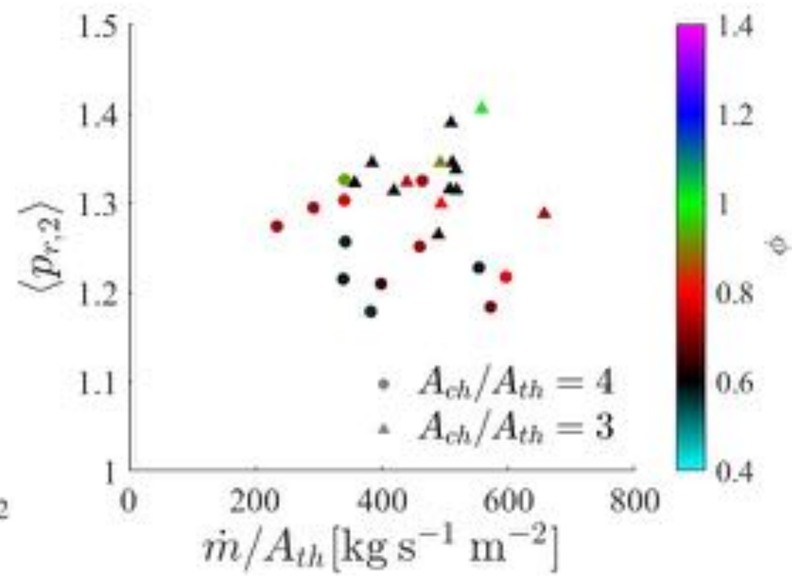
- **Observations**
  - Transition to slapping mode
  - Wave speed drops at transition to slapping mode
  - Pressure ratio increases with inlet temperature



Toward predicting upstream propagating disturbances (plenum)

- Pressure rise observed in plenum of axial air inlet RDC
  - Occurs despite believed local choking of inlet
- Disturbance rotates at same speed as detonation



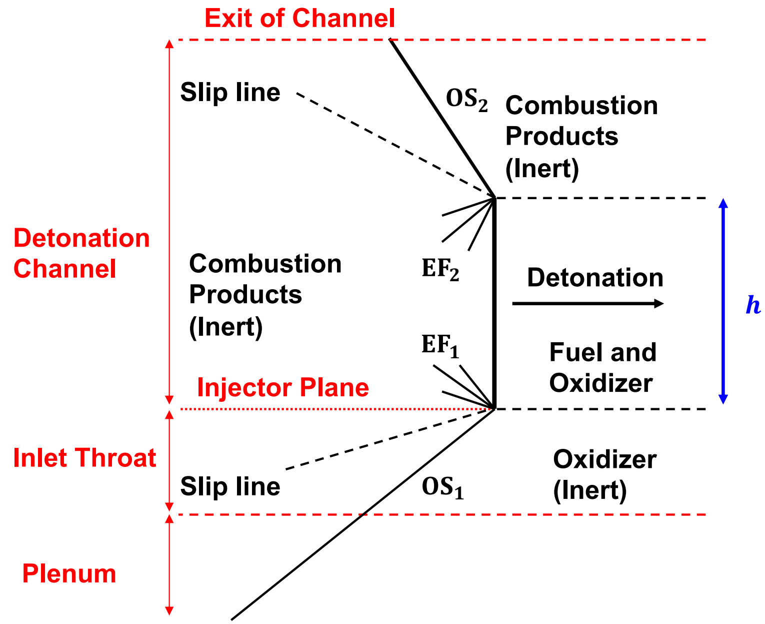


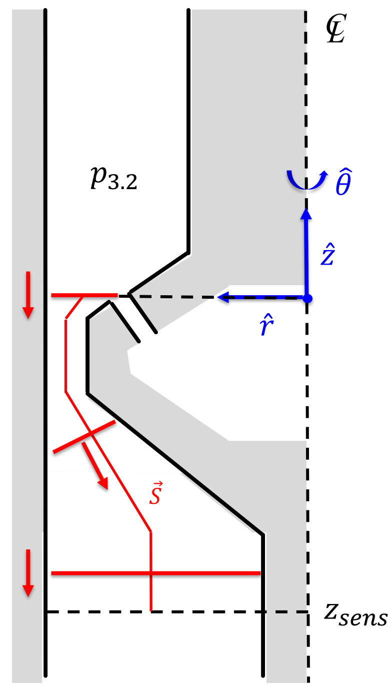
Quasi-1D model

- Shock strength changes with area in shock tube problem
  - Chisnell and Whitham's formulation

$$\frac{dA}{A(S)} = -\left[\frac{2M_S}{K(M_S)(M_S^2-1)} + \frac{\eta\left(M_S, A(S)\right)}{M_S}\right] dM_S$$

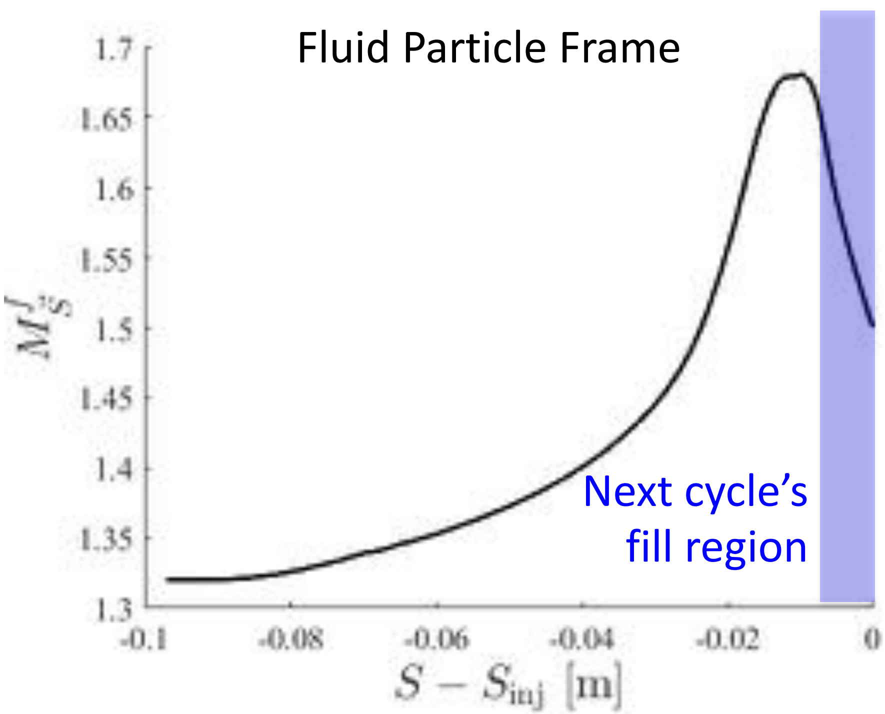
- Parametrize along "streamline" $\vec{S}$
- Incoming oxidizer flow impacts perceived velocity of wave
  - Need distribution along $\vec{S}$
- Assume pressure downstream of wave is constant

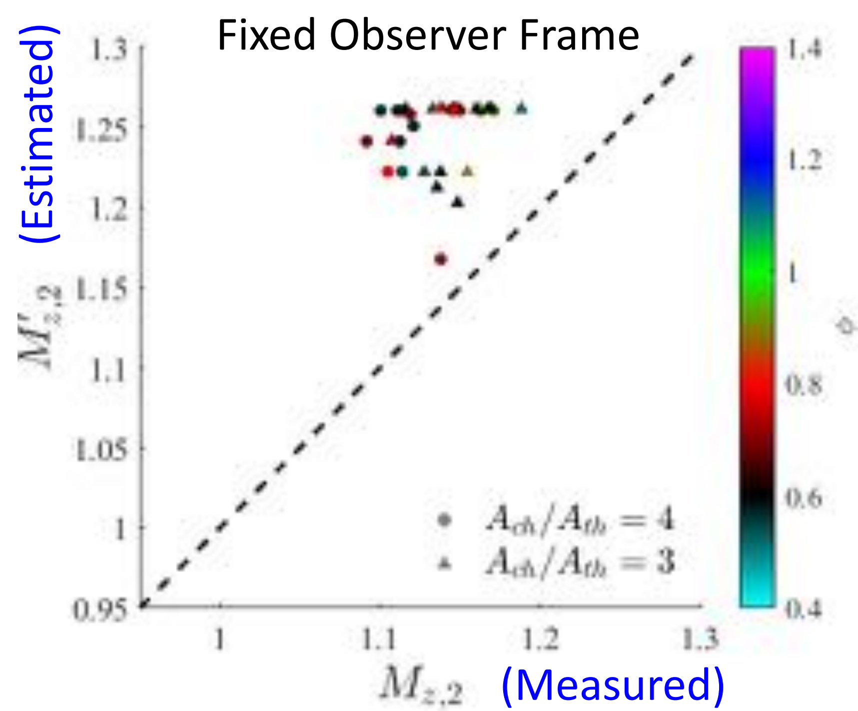




Results from model and comparison with data

- Different fluid particles would experience shocks of differing strength
- Model predicts higher Mach number than the one from observed pressure ratio
  - May be the result of constant downstream pressure
- We are now refining the model to overcome present limitation





Next steps in the experimental studies

- **Continue to relate operational details to performance (e.g., thrust/gain)**
  - Global operational conditions (e.g., mass fluxes, …)
  - Geometric effects
  - Component responses (e.g., time scales), with focus on inlet and plenum/combustor coupling
- **Continue development of gain/loss model to identify contribution of losses**
  - Experimental characterization
  - Reduced order models
  - This will inform our next designs
- **Transient investigations**
  - Ignition transient and establishment of steady state
  - Transient operation (load changes)
  - Response to perturbations (resilience of operation)

Our contribution for the year

- **Continued the investigation of H_2/CO_2 and H_2/CH_4 mixtures**
  - We have built from last year’s work
  - Focus on secondary wave suppression, and modification of secondary combustion
- **Investigated inlet temperature effects on H_2/air operation**
  - Identified changes in stability properties
  - Mode of operation changes as inlet temperature increases
    - From stable single wave to slapping wave
  - We need to refine some of the analysis tools for slapping wave modes
- **Continued the investigation of pressure gain and losses in RDCs**
  - Some improvements on thrust measurements made, more in preparation
- **Characterized and investigate new axial air inlet RDC configuration at different inlet area ratios**
  - Investigation of inlet characteristics
  - Dependence of operation on inlet characteristics
- **Investigated the response properties of the air inlet**
  - Developed a one-dimensional model to describe the propagation of disturbances into the air plenum

Outline

- **Programmatic overview**
- **Experimental activities**
- **Computational activities**

Towards Computational Design of RDEs

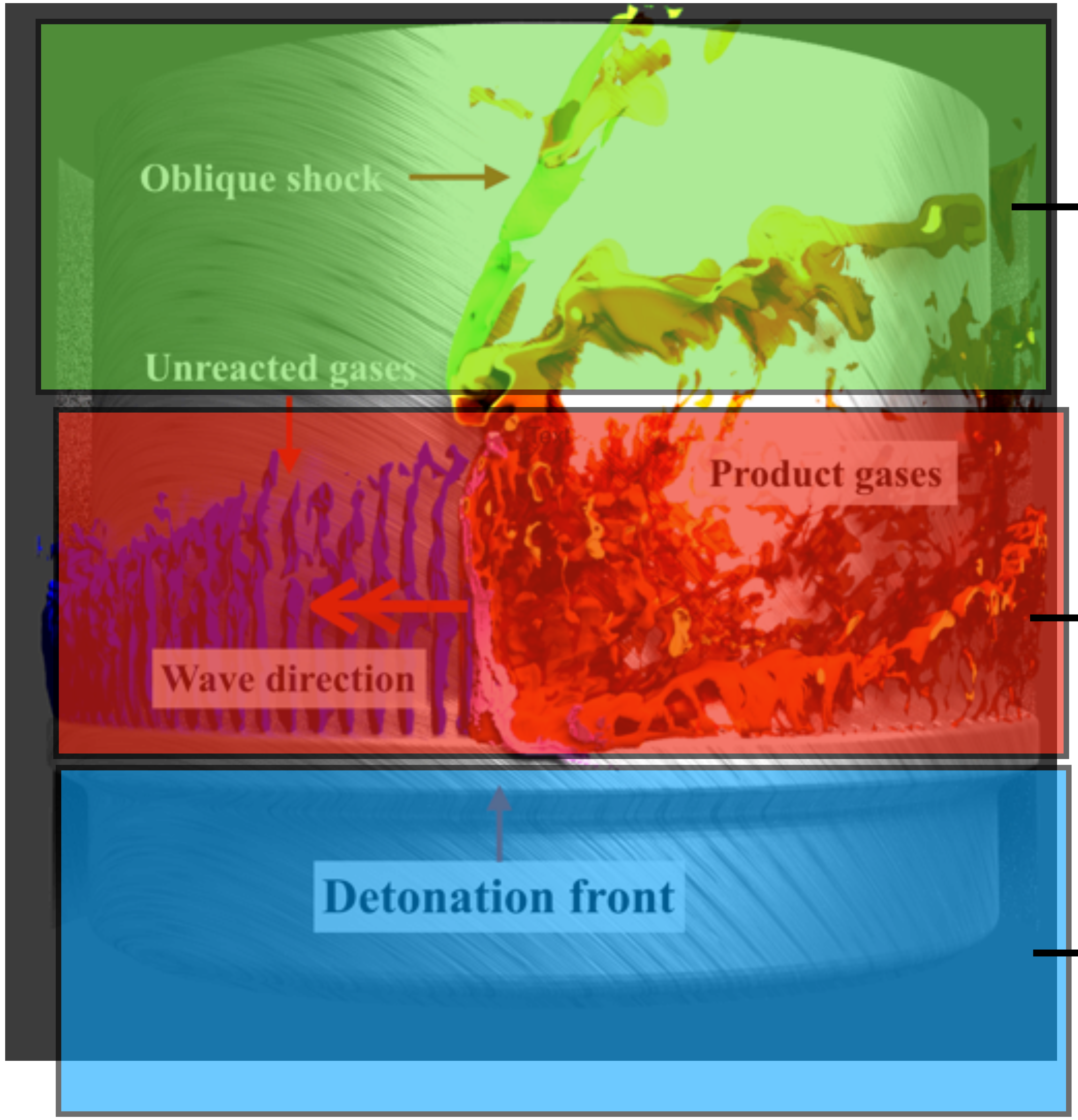
Contributors

University of Michigan, Ann Arbor
Department of Aerospace Engineering

Objectives

- **Develop multi-fidelity computational models**
  - ➡ Fast execution of full scale simulations
  - ➡ Reduced-fidelity models
  - ➡ Multi-fidelity design tool
- **Year 1**
  - ➡ Development of highly efficient CFD solver
    - Use machine learning for acceleration
- **Year 2**
  - ➡ Develop reduced-fidelity model
- **Year 3**
  - ➡ Multi-fidelity design

Key Modeling Challenges



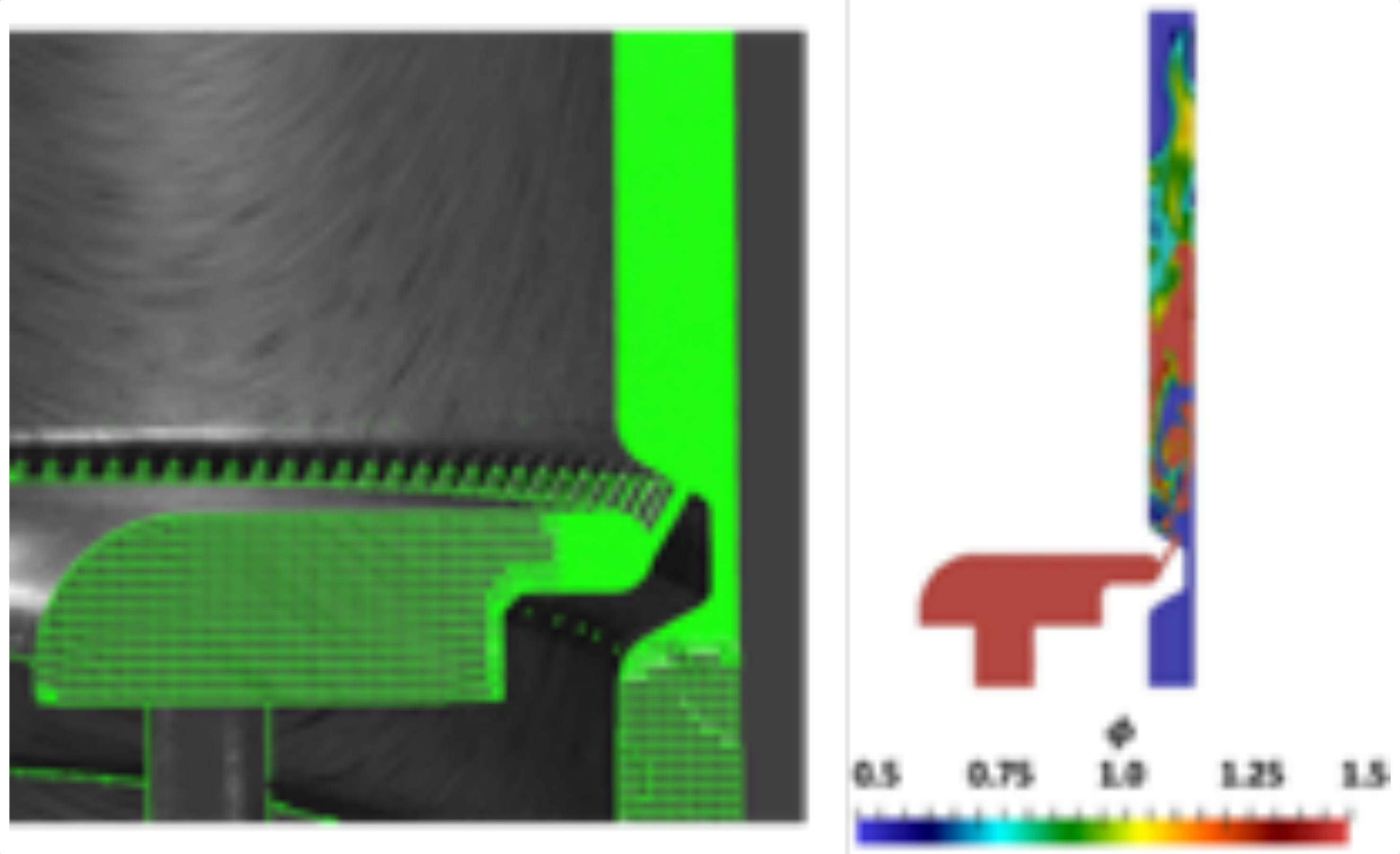
- **Expansion region**
  - ➡ Subsonic/supersonic flow
  - ➡ Thrust estimation depends on mesh resolution
  - ➡ Need to handle reflections from downstream components
- **Turbulent mixing, multiscale interactions**
  - ➡ Mesh/time-step estimations based on turbulence theory
  - ➡ $\mathcal{O}(10\ \mu\mathrm{m})/1-10$ ns
- **Upstream plenum**
  - ➡ Runtime pressurization
  - ➡ Acoustic speed pressure wave propagation

AI For Improving Detonation-Driven Gas Turbine Technology

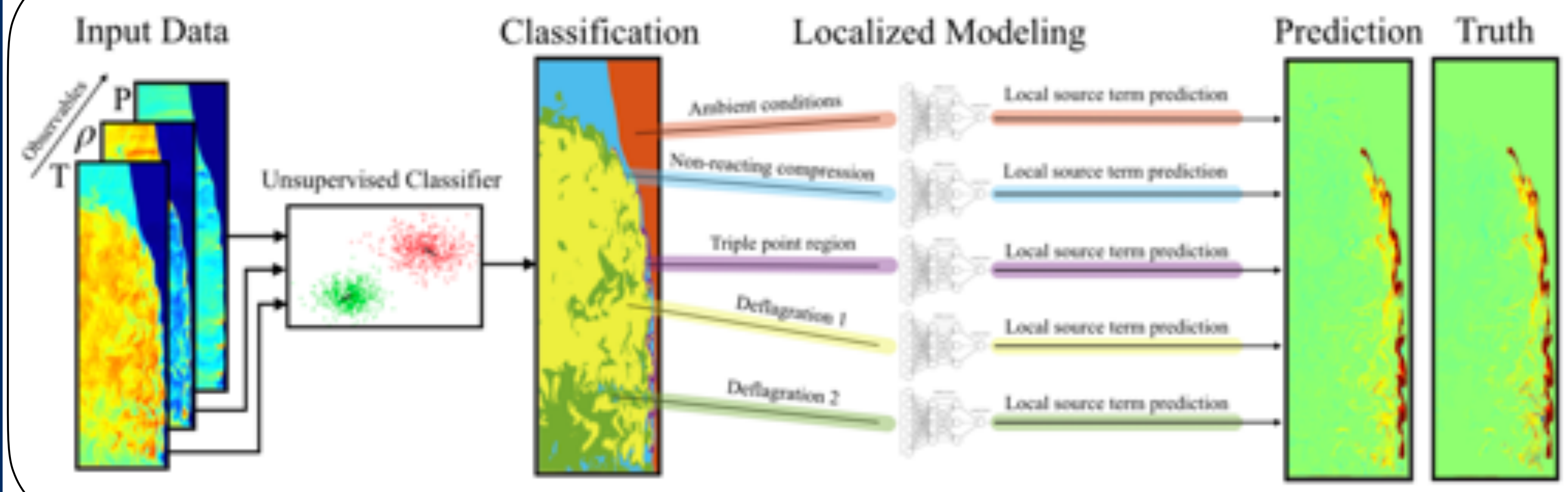
DOE Summit — 200 PetaFLOP Machine

UM-GE-NETL Collaboration

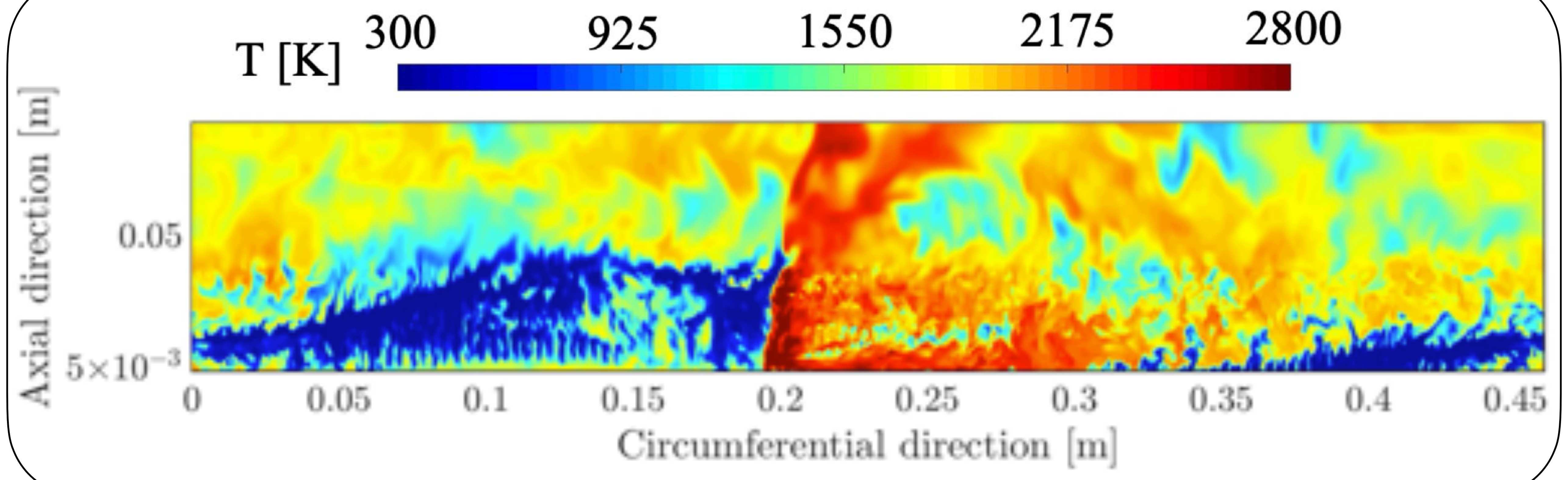
UTSR Funded Detonation Engine



Machine Learning Applied to Combustion Modeling (1000X Speed up Potential)



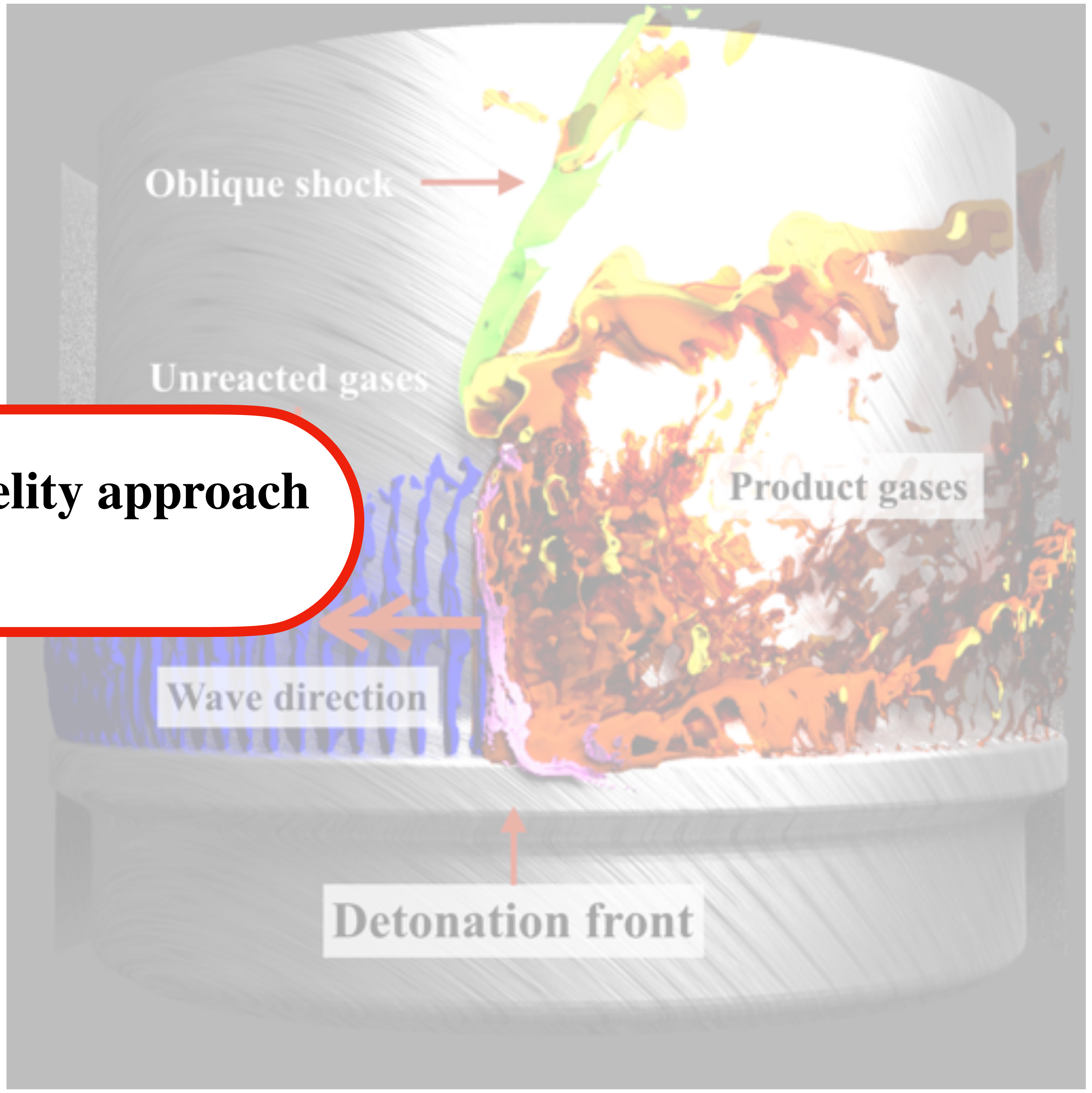
- First Full Scale Simulation of RDEs with Axial Injection
- Capable of simulating 100-1000 cycles in 1 day



UMdetFOAM-GPU solver

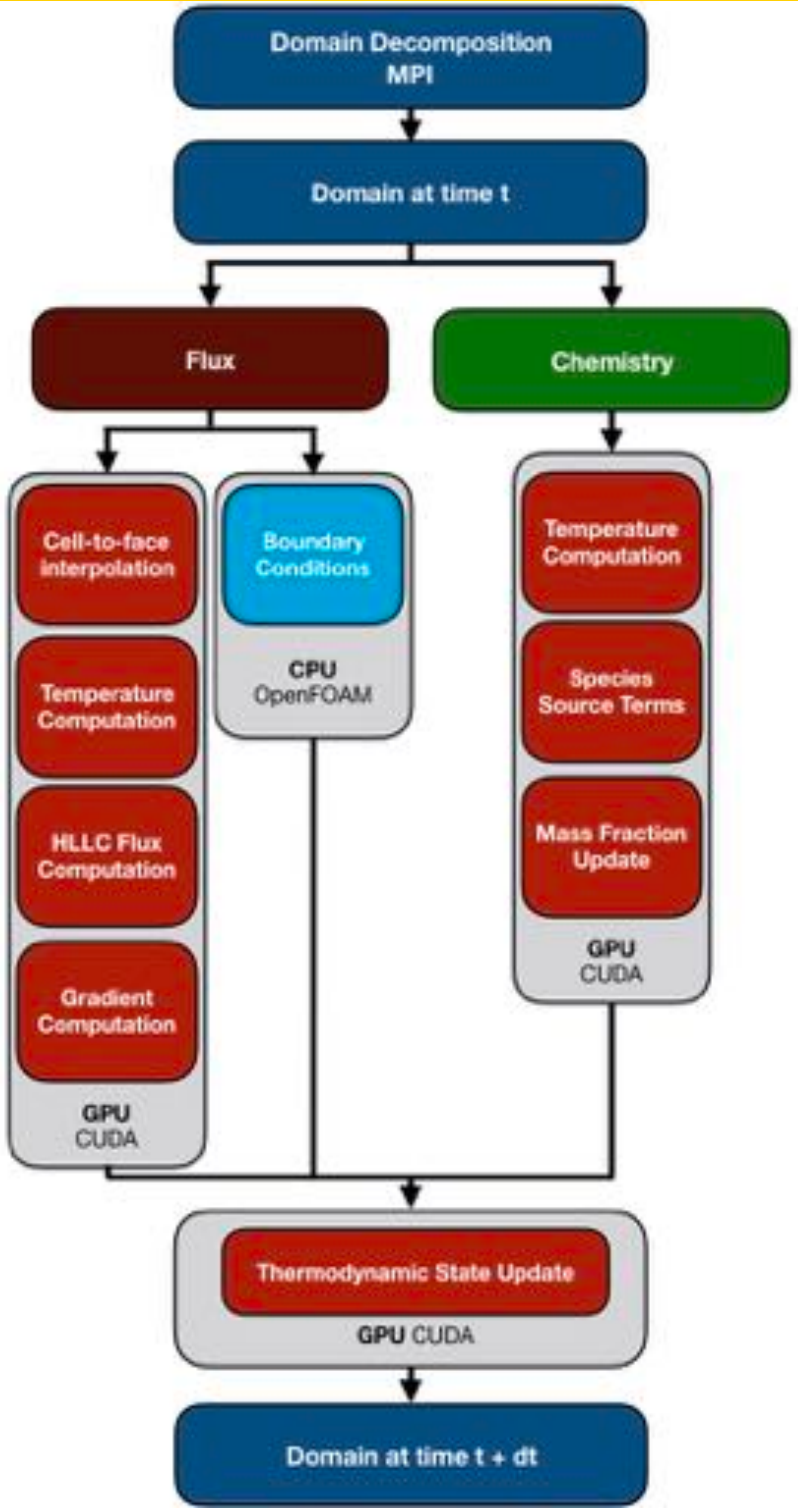
- **OpenFOAM + Cantera = UMdetFOAM**
  - ➡ Compressible flow solver for *full* Navier-Stokes equations
  - ➡ Finite Volume Method (FVM)
    - Unstructured grid for complex geometries
    - HLLC + MUSCL (2^{nd} order) spatial scheme
    - KNP diffusion scheme
    - 2^{nd} order Runge Kutta fo
  - ➡ CUDA-based GPU offloading
  - ➡ Detailed/skeletal chemical kinetics through user-specified model
    - GPU-based chemistry library (Barwey *et al*. 2021)

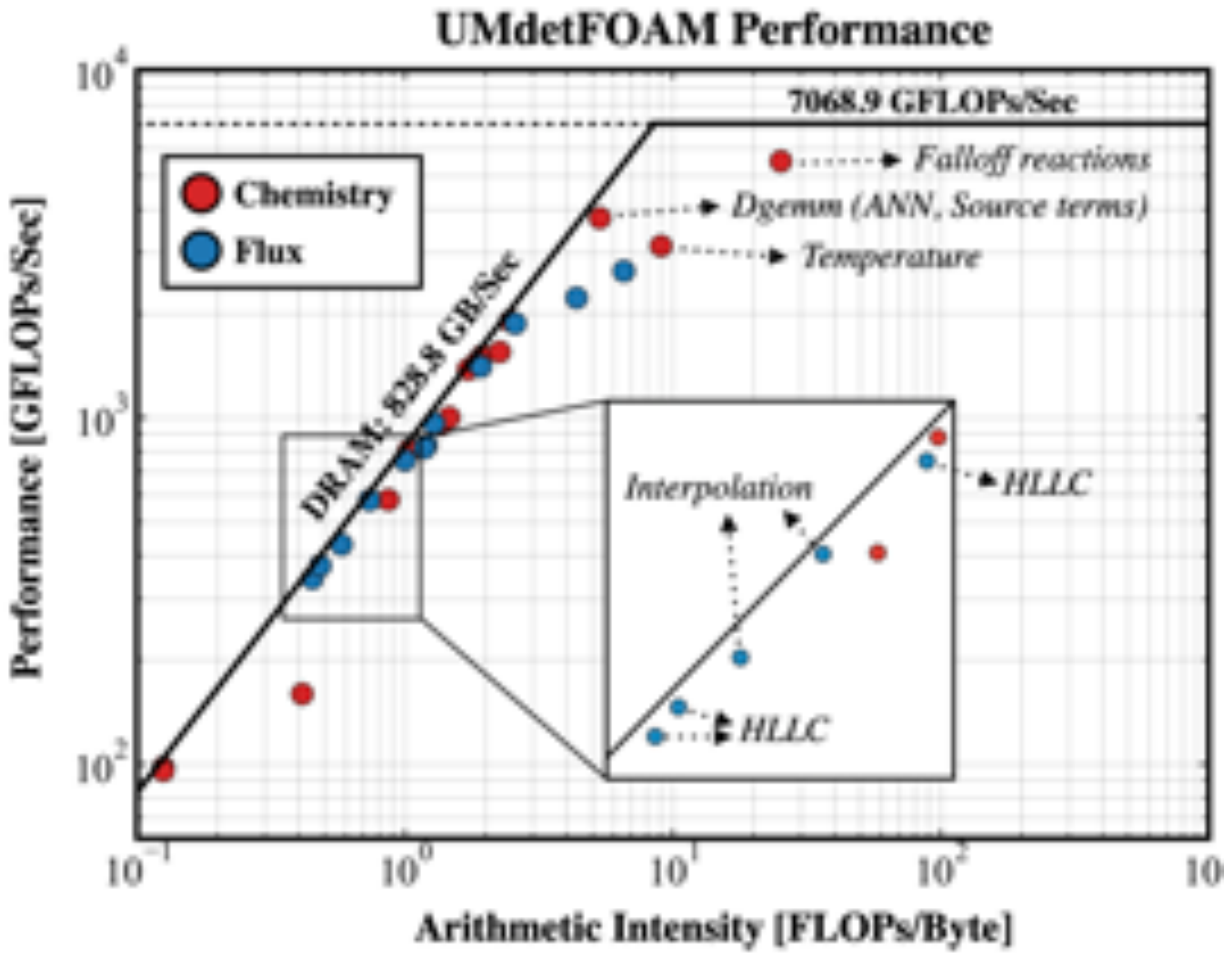
Instantaneous snapshot of UM AAI geometry using UMdetFOAM



Solve N-S + Energy + Species equations via high-fidelity approach
No turbulence models

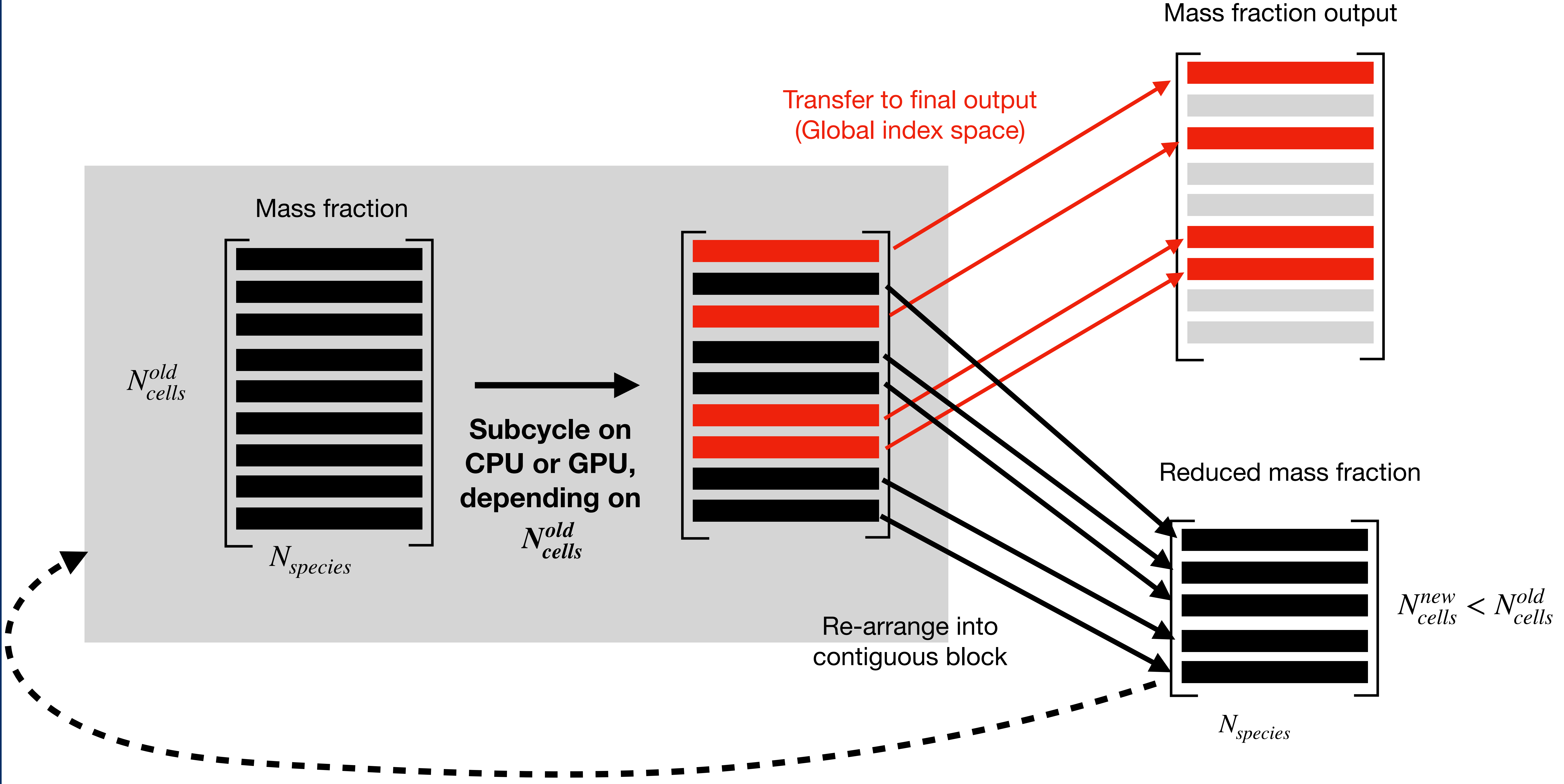
Solver overview

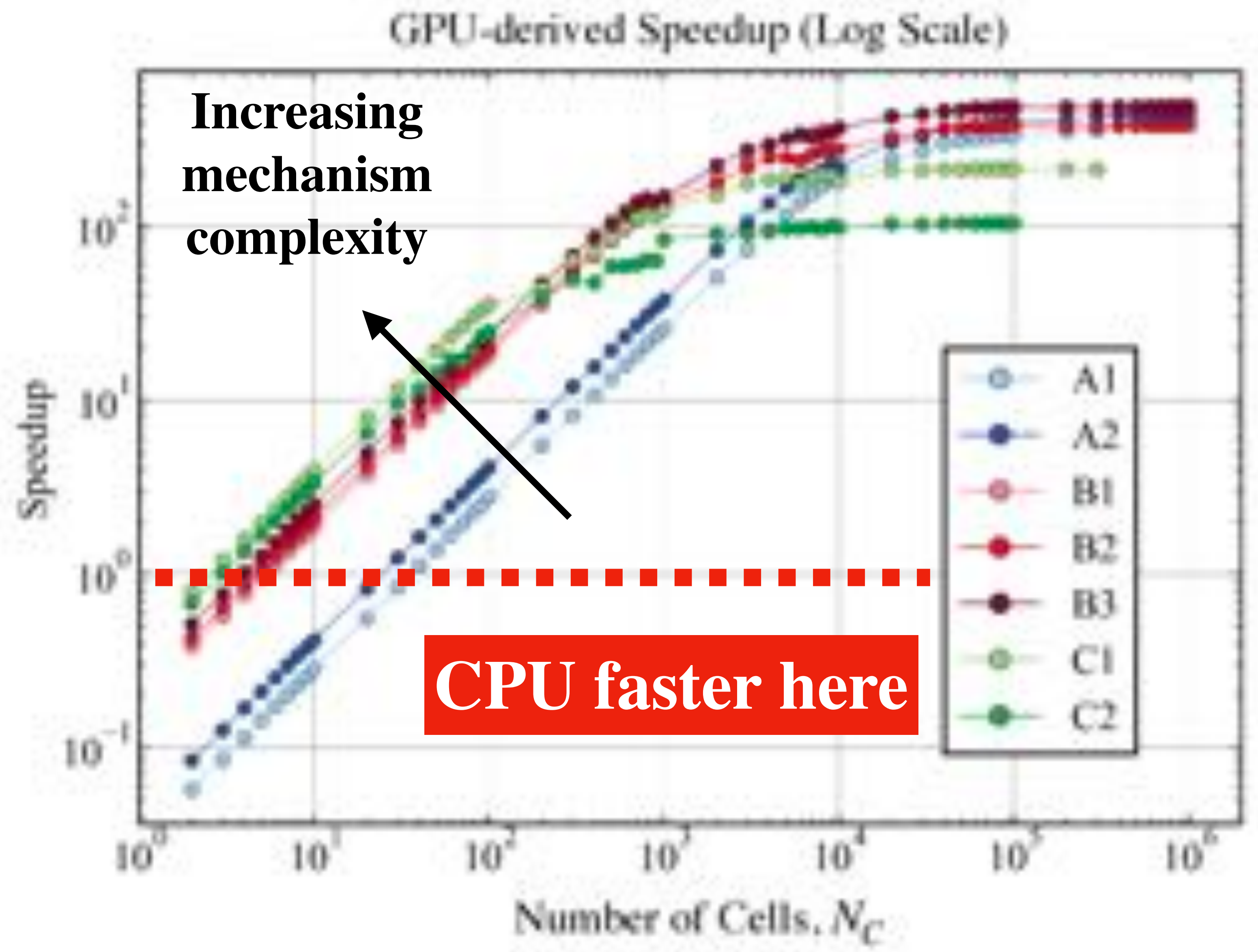




- **Near theoretical limit for computational efficiency**
- ***Order of magnitude* reduction in solver time to solution**

Improved GPU Time Integration



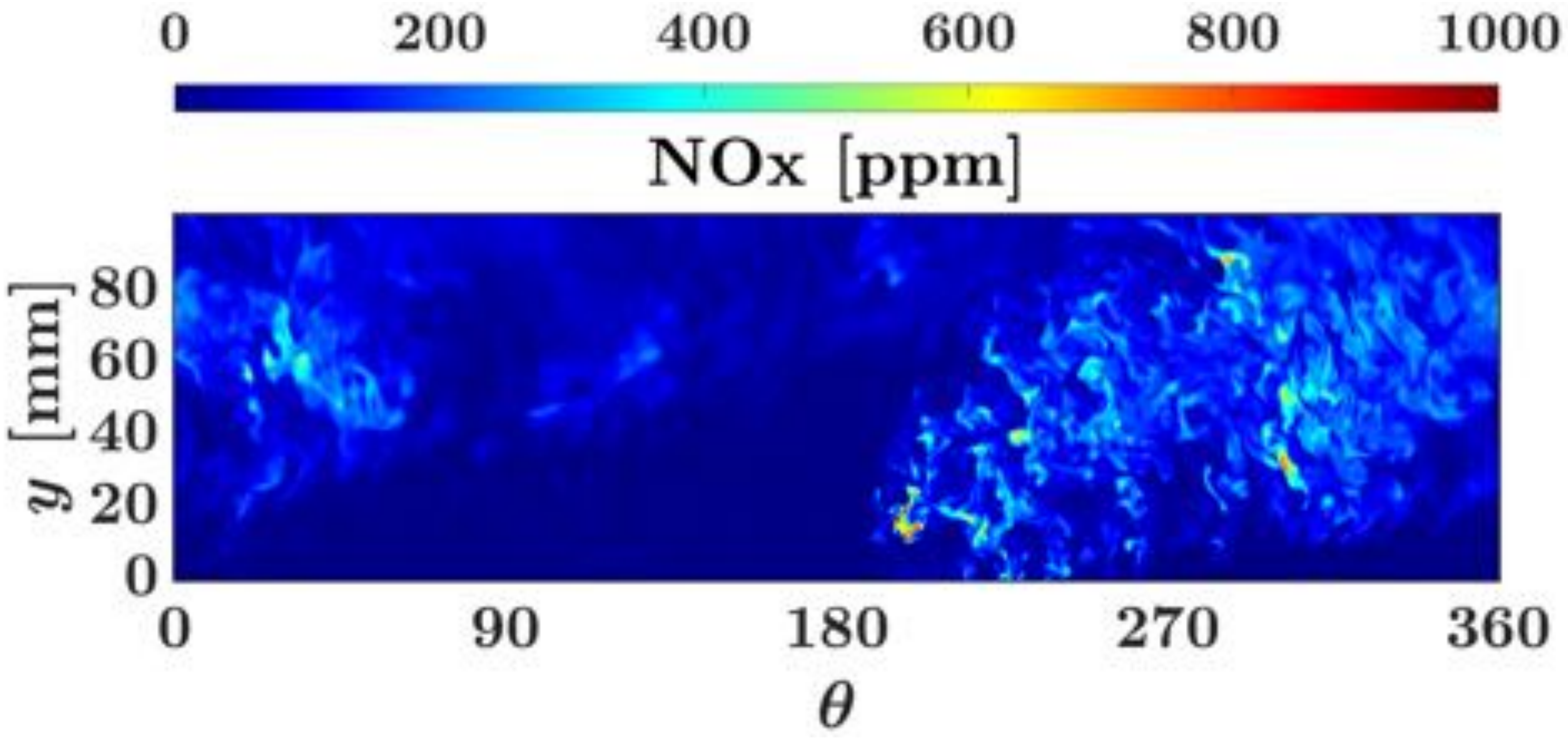


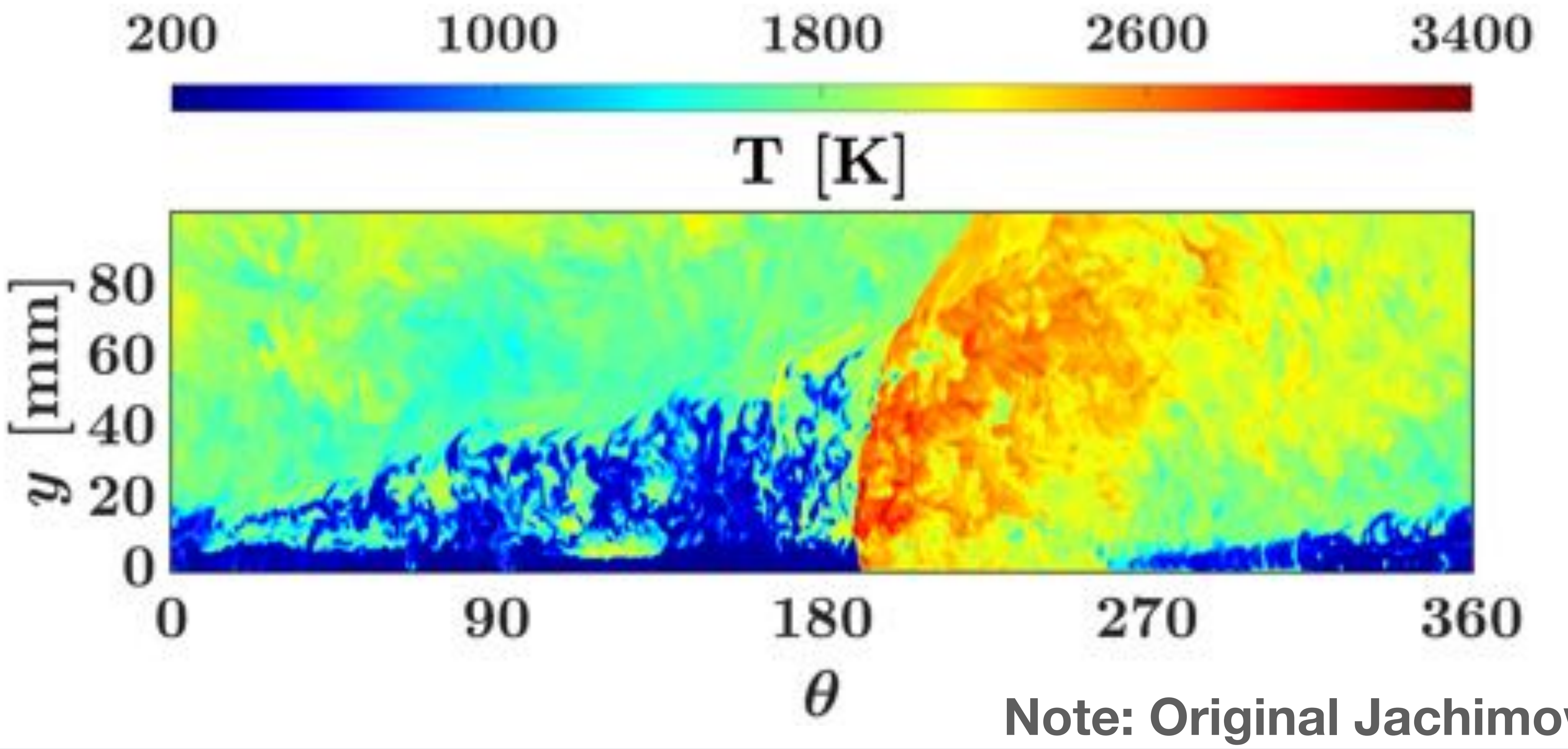
- **Reaction source term computed on the GPU for all active cells.**
- **Cells are periodically checked to determine if they require further time integration, and marked as inactive if complete.**
- **Results in a 4*x* reduction in chemistry cost for large hydrocarbon fuels**

- **GPUs operate best on large arrays**
- **If number of active cells drops below 10-100 computation is performed on the CPU**

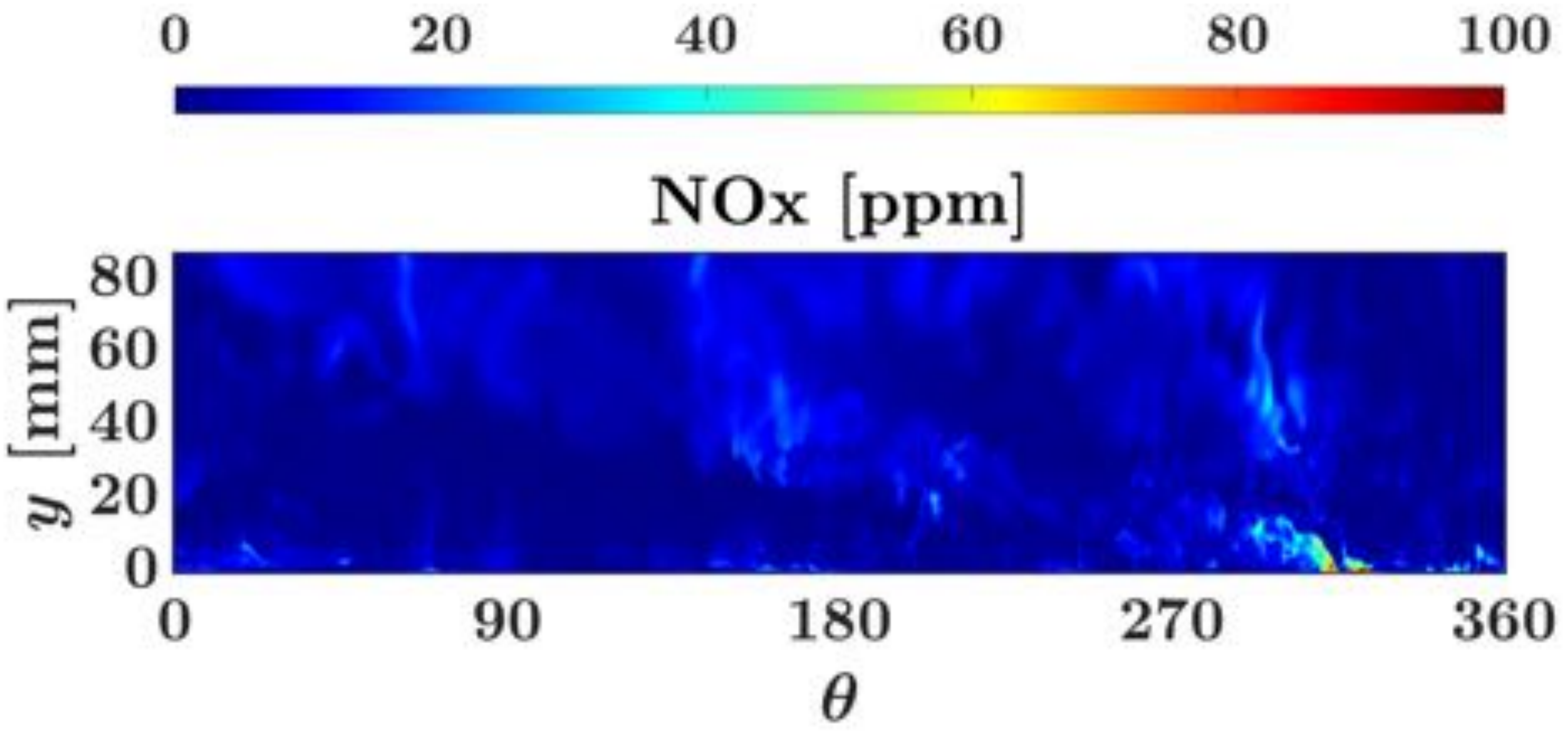
3D Unwrapped NOx Formation Plots (PPM)

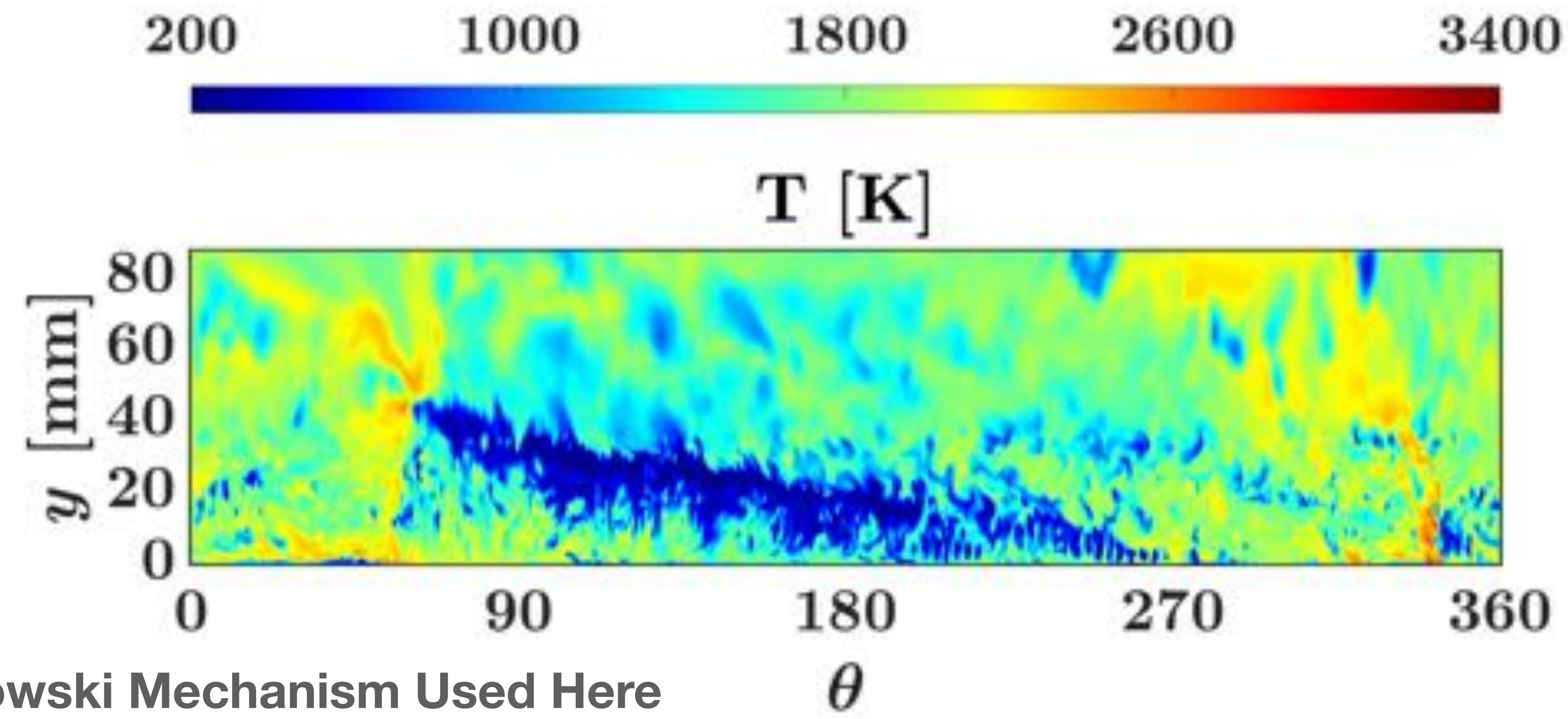
AFRL Radial Air Inlet Geometry @ 1.92 ms:





UM Axial Air Inlet Geometry @ 2.5 ms:

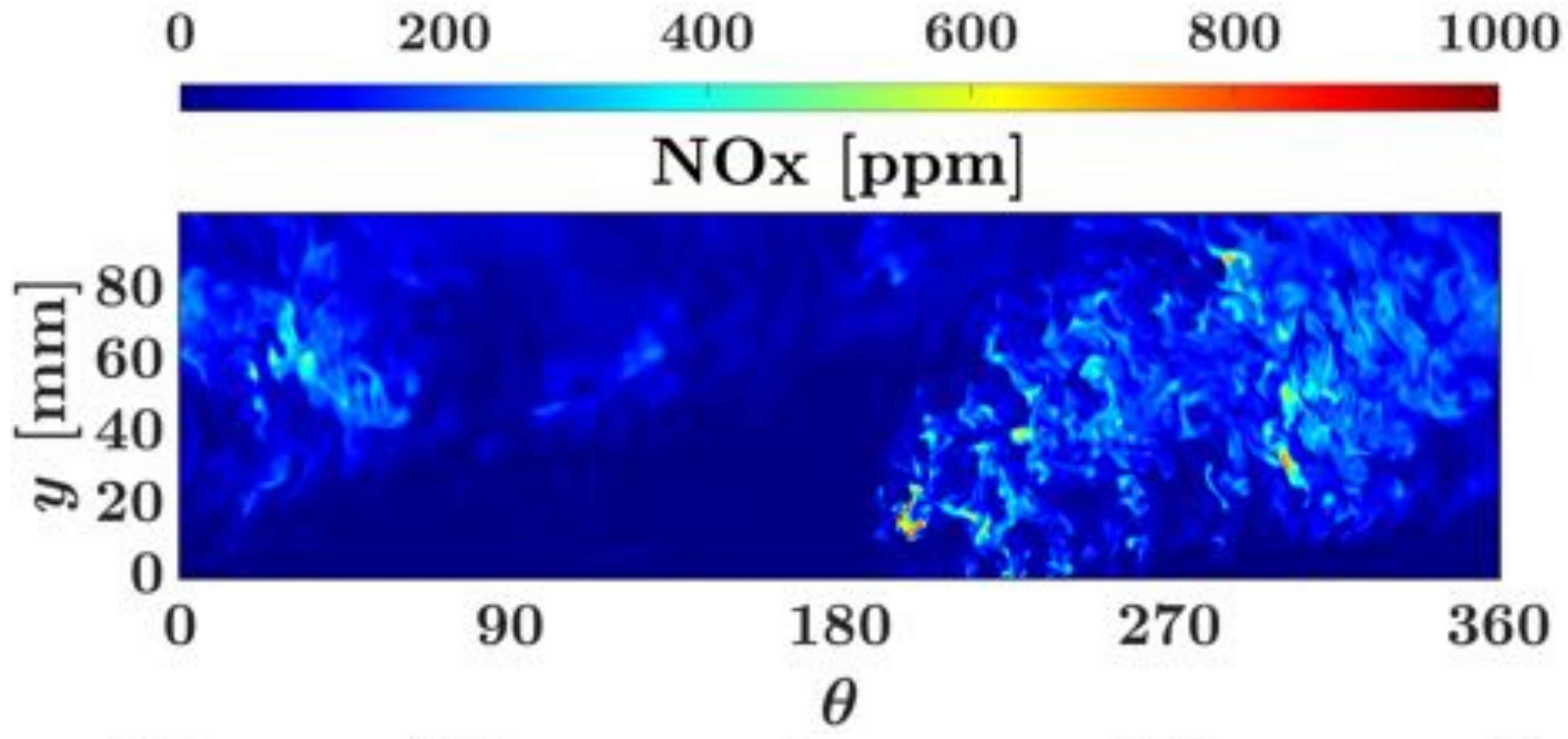


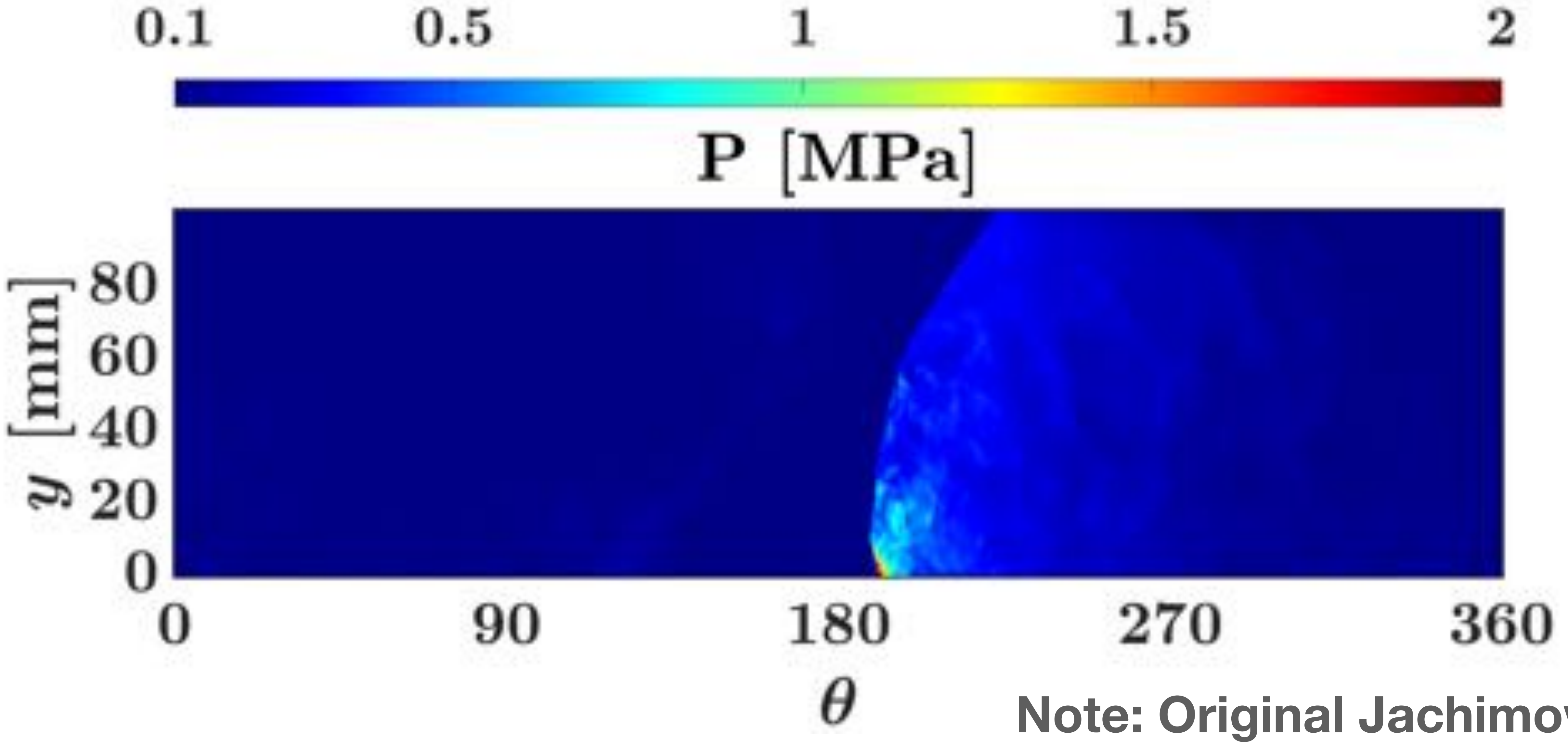


Note: Original Jachimowski Mechanism Used Here

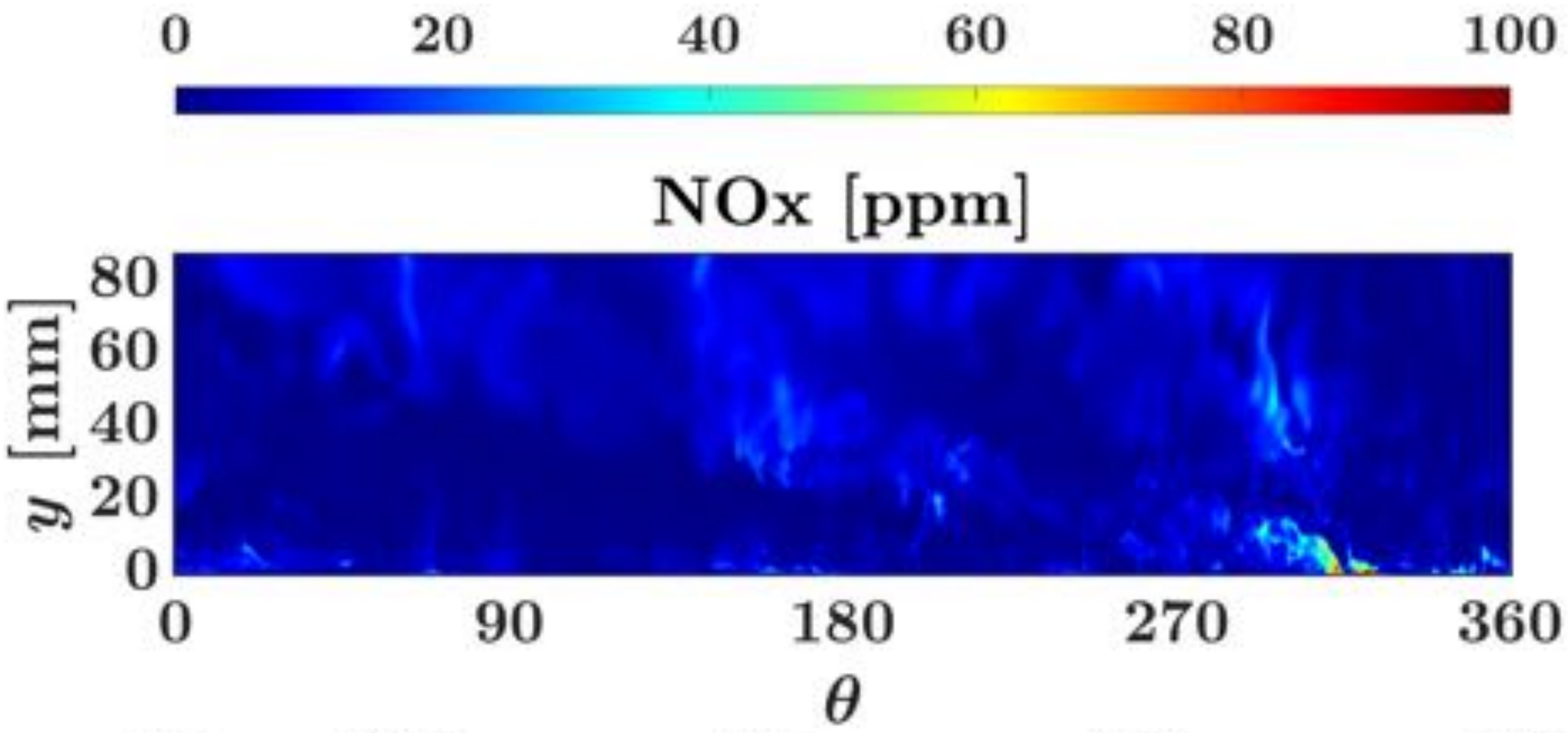
3D Unwrapped NOx Formation Plots (PPM)

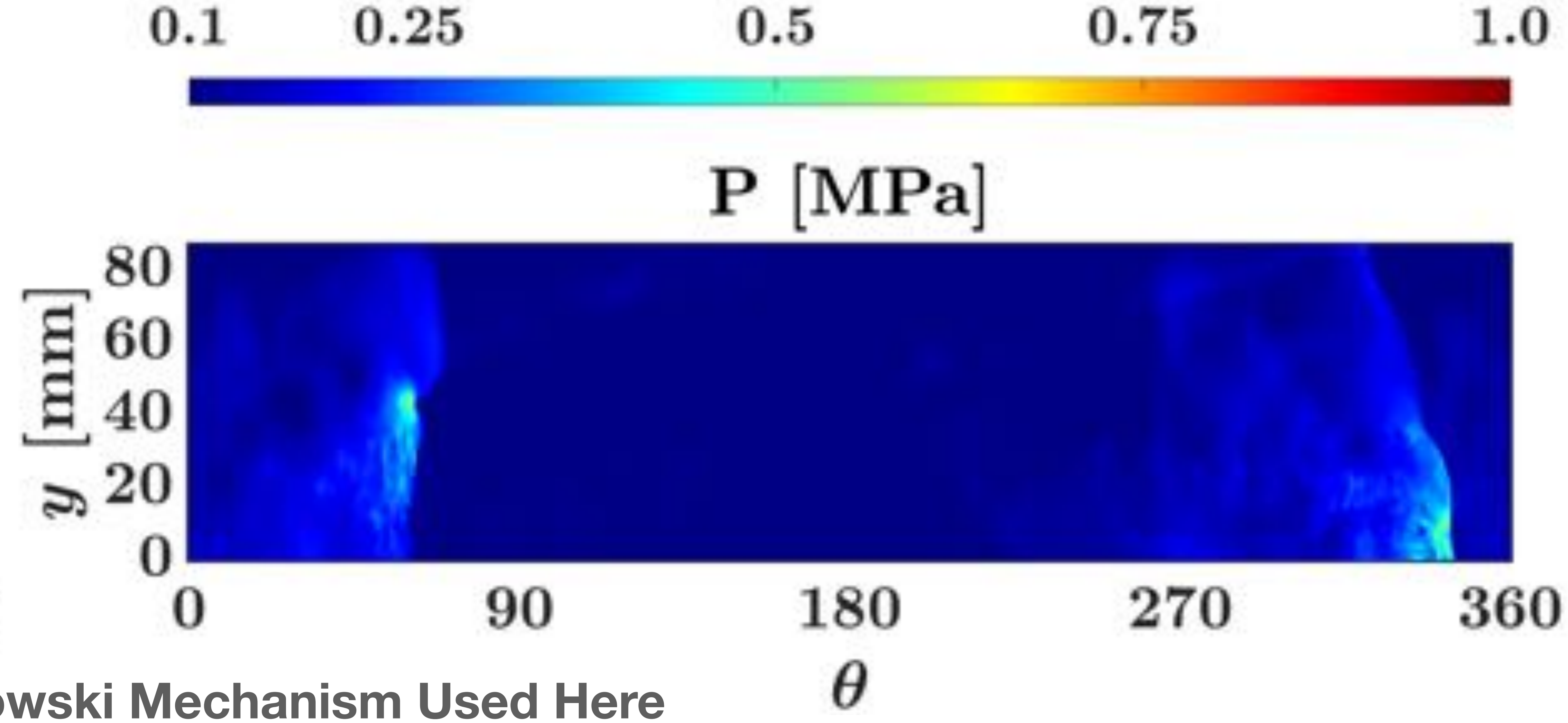
AFRL Radial Air Inlet Geometry @ 1.92 ms:





UM Axial Air Inlet Geometry @ 2.5 ms:

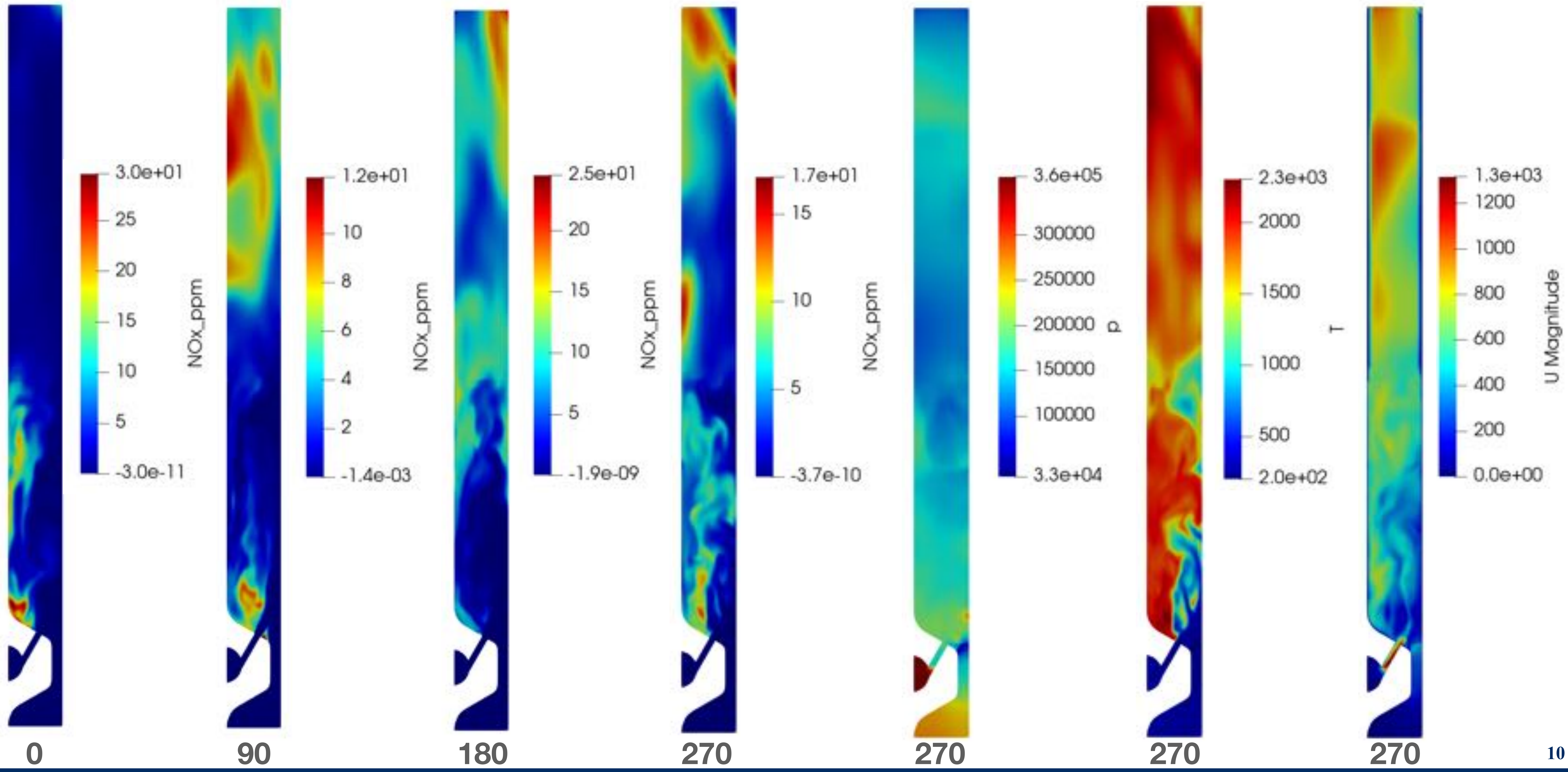




Note: Original Jachimowski Mechanism Used Here

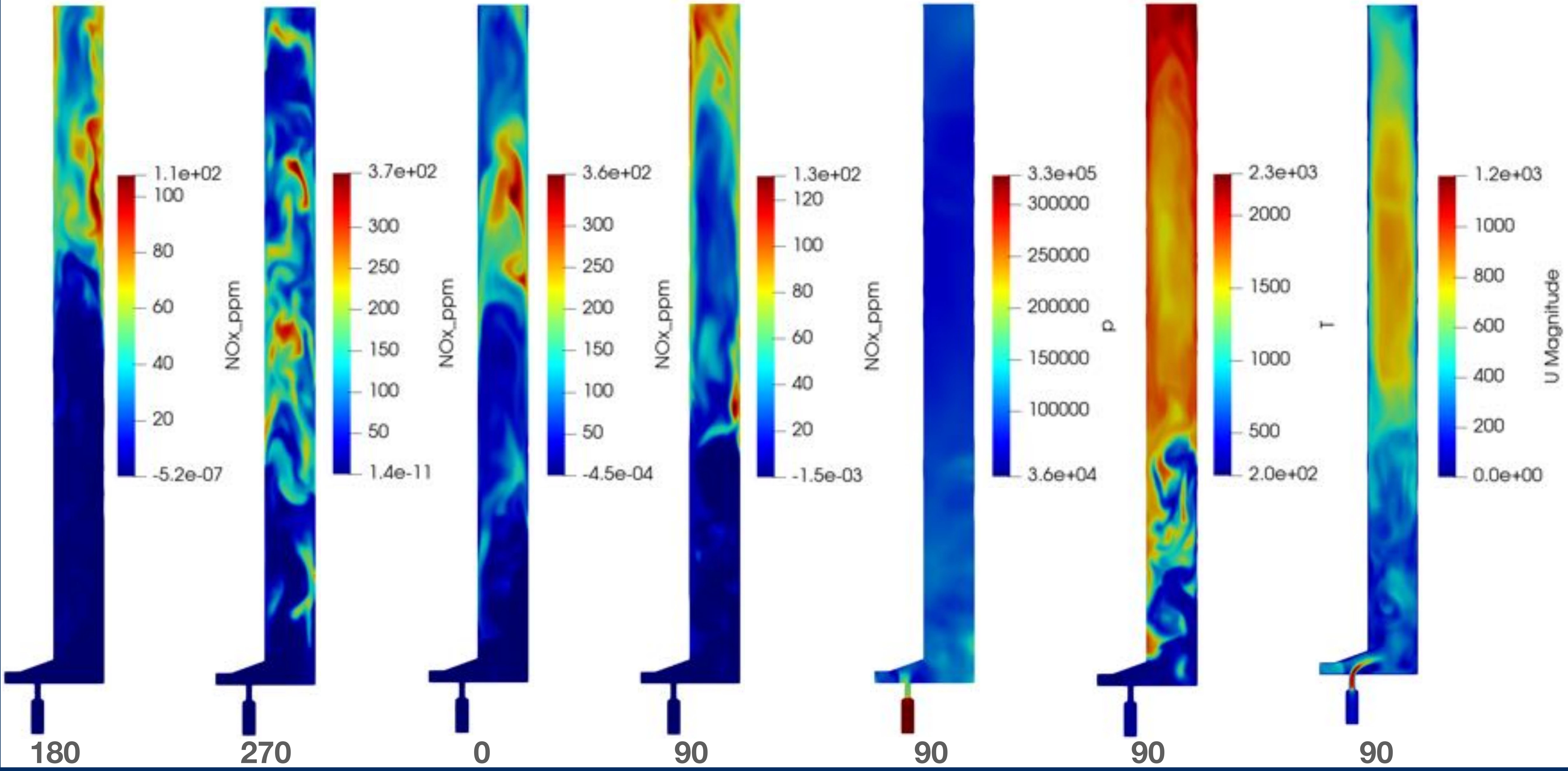
3D Detonation Chamber Cross Section Plots (UM Geometry @ 2.5 ms)

Coordinates in Direct Reference to Previous Unwrapped Map



3D Detonation Chamber Cross Section Plots (AFRL Geometry @ 1.92 ms)

Coordinates in Direct Reference to Previous Unwrapped Map

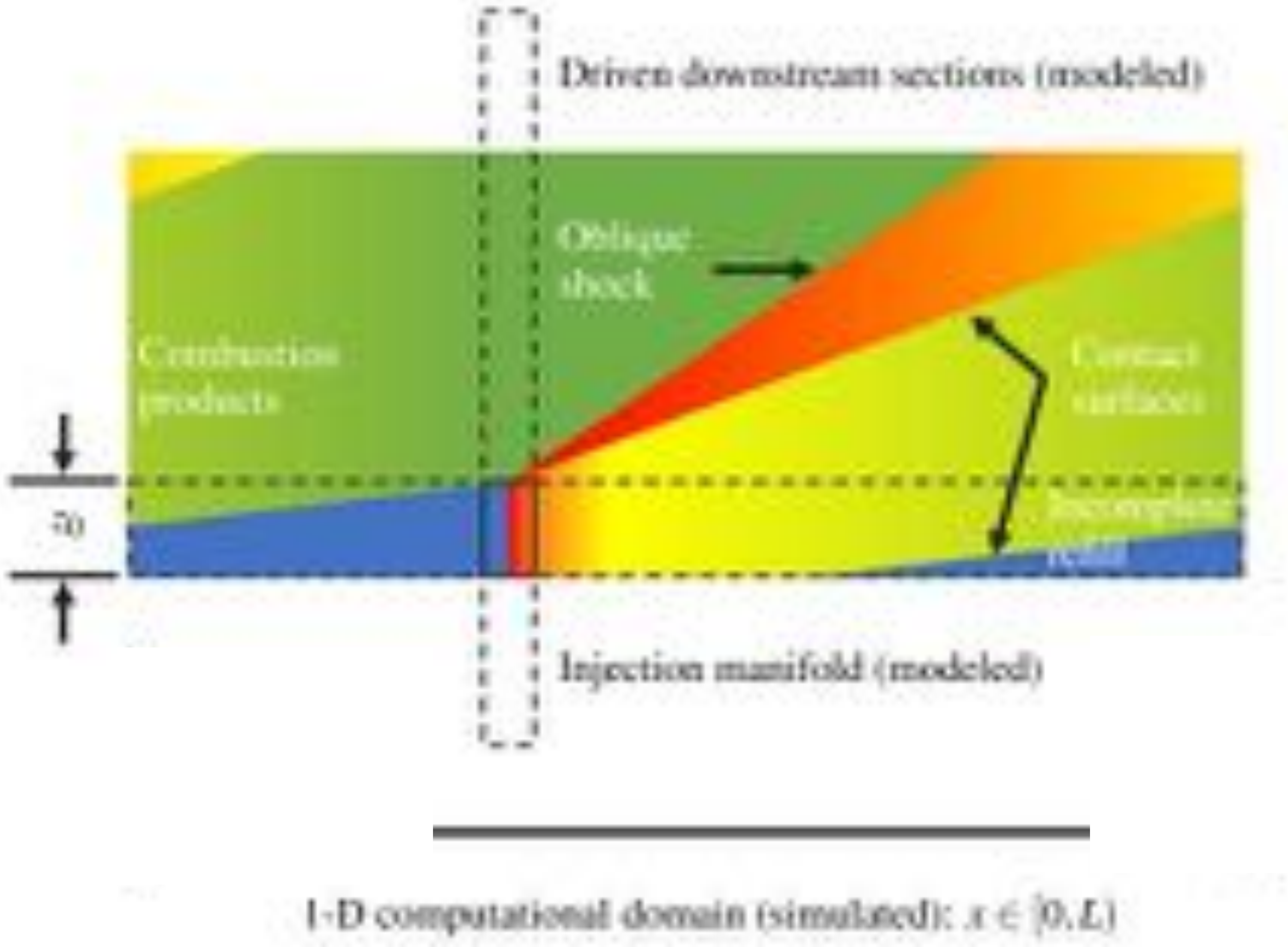


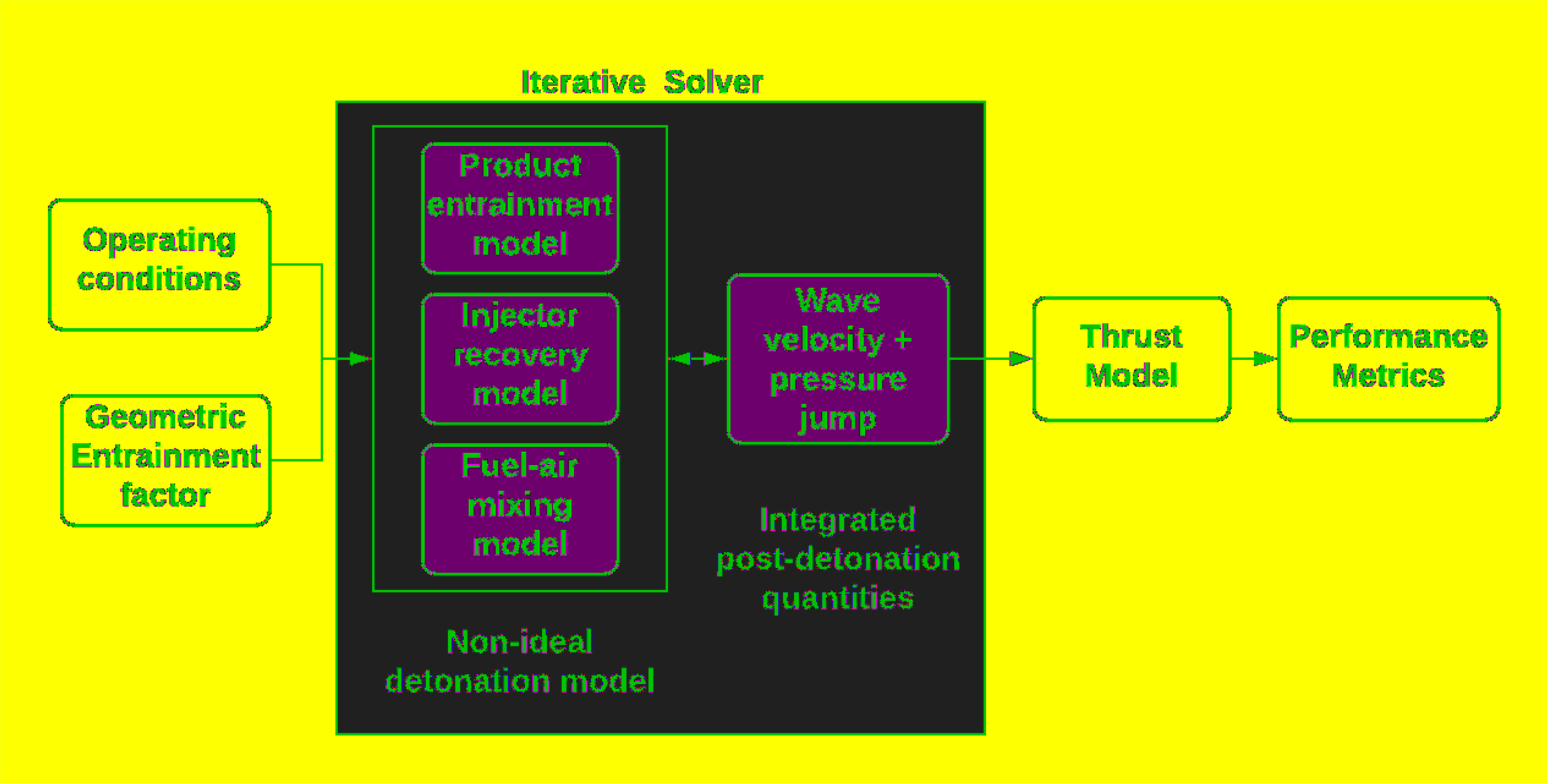
Notes on 3D Results

- **AFRL RAI produces significantly more NOx than UM AAI**
  - ➡ Stronger, single wave mode of operation in AFRL case (and thus higher temperature at this wave) provides good explanation for this behavior
- **AFRL RAI also shows a more well-defined trail of NOx production behind the detonation wave in the axial direction**
  - ➡ NOx production is concentrated lower in the detonation chamber right behind the wave and eventually move higher away from the wave as the gases are pushed out the chamber.
- **UM AAI shows a similar pattern to AFRL RAI in the form of NOx intensity levels in relation to azimuthal distance to detonation wave**
  - ➡ Larger amounts of NOx are produced right behind the wave, with smaller amounts produced further away from the wave (as expected)
- **Cross section images of both AFRL RAI and UM AAI also highlight Thermal NOx as the main mode of NOx production in these simulations**
  - ➡ Highest intensity NOx levels correspond to highest temperature regions within detonation chamber

Reduced-order performance model

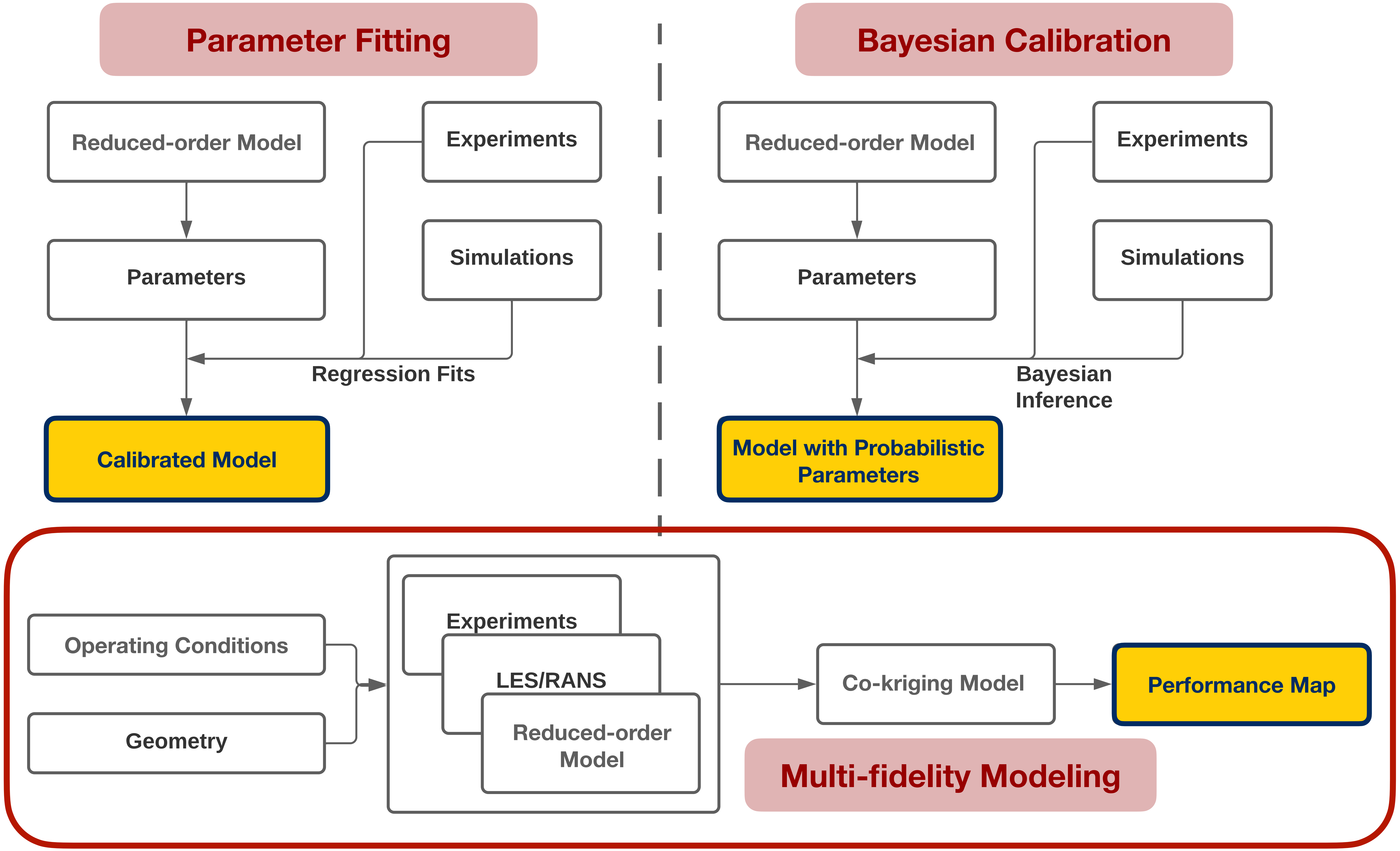
- **Developed from Euler equations**
  - ➡ Extract parameters (fill height z_0, shock angle, wave speed etc.) directly from CFD
  - ➡ Incorporates injector blockage
- **Model can be calibrated from full-scale simulations and experiments**





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



Co-kriging for model development

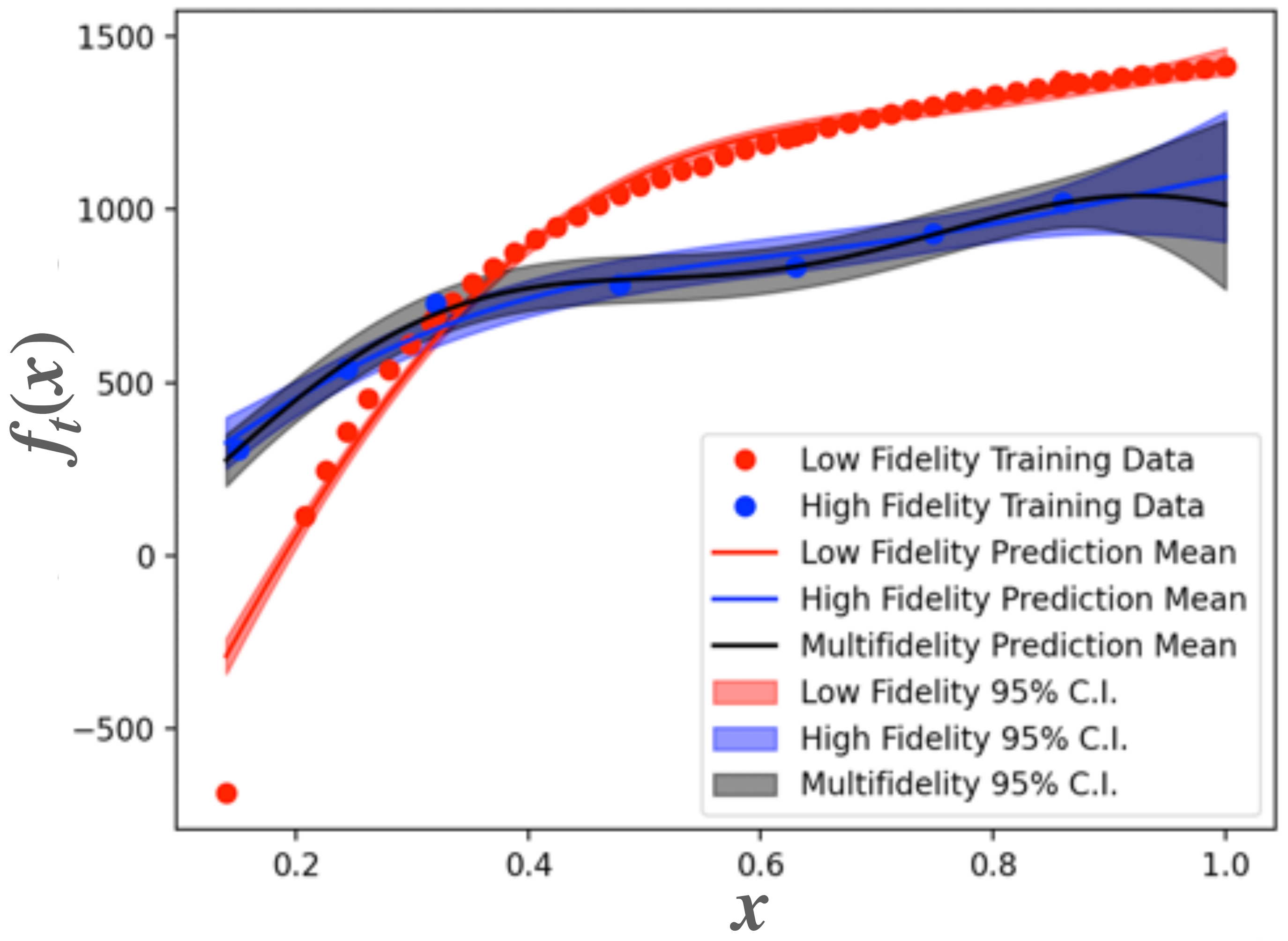
- **Co-kriging provides a way to create better fits of high fidelity data by incorporating low fidelity information**
  - ➡ Given low-fidelity data, can produce a fit trained on this data $f_{t-1}(x)$
  - ➡ Can produce additional fit trained only on high fidelity data $\delta_t(x)$
  - ➡ High-fidelity data is generally sparse compared to low-fidelity data
- **Co-kriging: Want to find fit at fidelity level t using fidelity level $t-1$ information such that $f_t(x) = \rho f_{t-1}(x) + \delta_t(x)$ where ρ is a constant**
- **Calibrate correlation between different levels of fidelity to *estimate performance with associated uncertainty***

Outcome: surrogate model for high-dimensional relationship

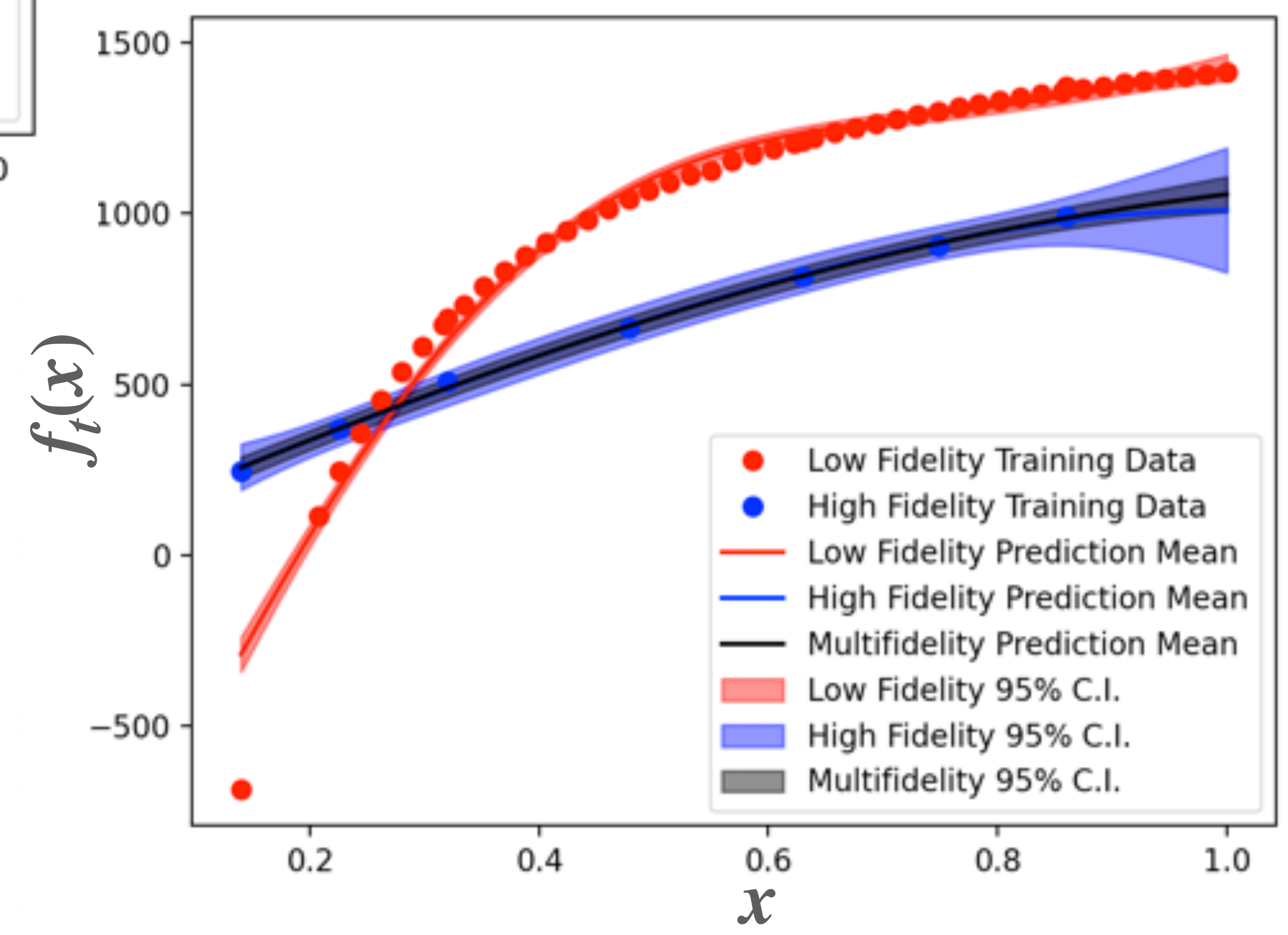
Performance estimation

- **Low fidelity: performance model**
- **High fidelity: experimental data and numerical simulations**

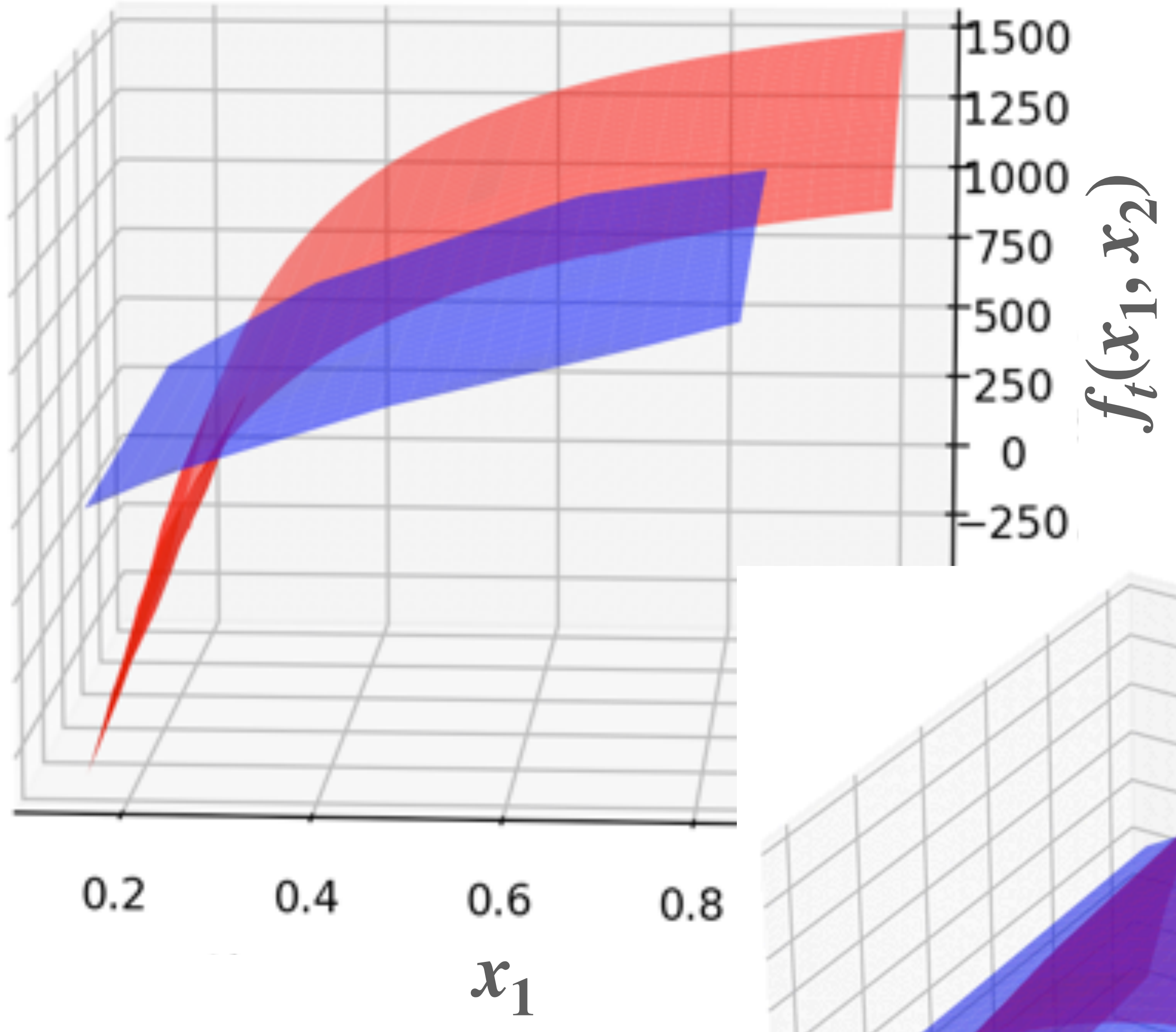
1D Co-kriging



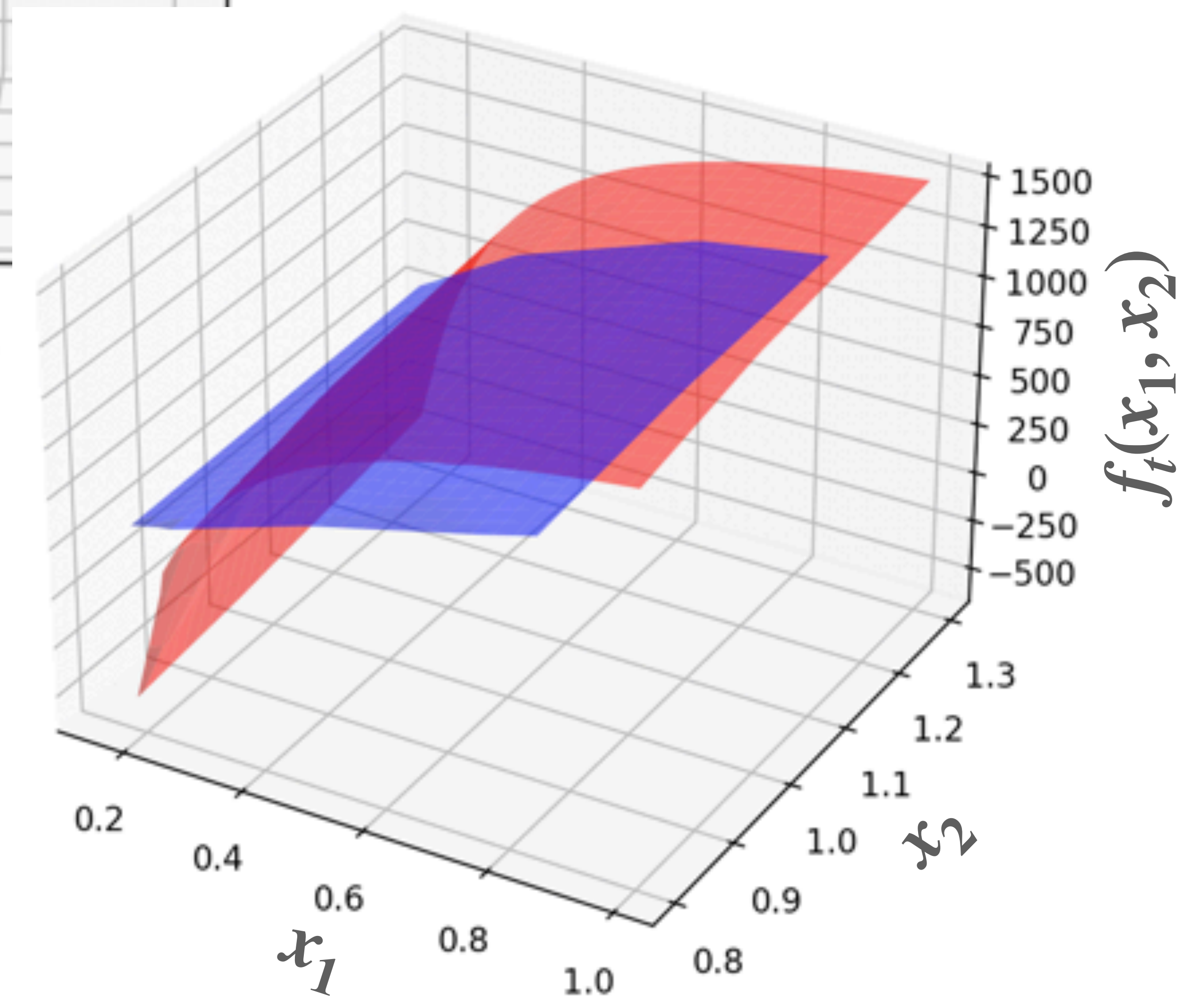
Additional data points at high-fidelity level: *narrower MF fit*



2D Co-kriging



Multivariate Co-kriging



Next Steps

- Collect statistics for NOx simulations
- Validation lower-order model
  - ➡ Macroscopic measurements (thrust, plenum pressure)
  - ➡ Detailed measurements (wave speed, pressure jump across wave)
- Demonstrate design loop
  - ➡ Use performance model to relate geometry variations to quantities of interest
  - ➡ Optimize for geometry
  - ➡ Use high-fidelity simulations to demonstrate increase in performance