Development of Reduced Order Model for Reacting Gas-Solids Flow using Proper Orthogonal Decomposition

HBCU/MI Award DE-FE0023114 Kick-off Meeting
Program Manager: Jessica Mullen

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Technical background

- Developers of gasifiers, combustors, chemical reactors, and owners of energy power plants are incorporating simulation in their design and evaluation processes to enhance process control and increase efficiency yield and selectivity.
- Several computational fluid dynamics (CFD) codes have been developed to simulate the hydrodynamics, heat transfer, and chemical reactions in fluidized bed reactors (MFIX[1], CFDLIB[2] , etc.).
- The numerical simulation of transient transport phenomena requires a large amount of computational time, in spite of the developments in computer hardware.
- While it is likely there will be another five generations of transistor scaling, ending at the 8 *nm* process technology node in ten to twelve years, the traditional models of general purpose computing are unlikely to provide more than a $\sim 8\times$ increase in performance despite a $32\times$ increase in transistor density.

[1] Syamlal, DOE/METC-95/1013, 1995

[2] Kashiwa and Lewis. Technical Report, 2002

Technical background

- Consequently, since the computational cost of high-fidelity computational fluid dynamics simulations is still a limiting factor, there is a need to continue the development of algorithms and numerical methods for efficiently modeling engineering/scientific relevant problems
- Numerical simulations of multiphase flows involving chemical reactions pose an additional challenge due to the need of accurate description of these reactions and their rates.
- Reduced chemical kinetics are commonly used because detailed chemical kinetics significantly increase the computational cost.

Technical background

- The proposed research includes utilization of a numerical approach based on the proper orthogonal decomposition to provide reduced order models for the reacting multiphase flows in gasifiers.
- The robustness of existing POD-based ROM for multiphase flows will be improved by avoiding non-physical solutions of the gas void fraction and ensuring the reduced kinetics models used for reactive flows in fluidized beds is thermodynamically consistent.
- Finally, the developed ROMs will be compared against the MFIX software for accuracy and computational efficiency.

Potential significance of the results of the work

- Supports the vision of the NETL 2006 Workshop on Multiphase Flow Research[9]:
  - *"To ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants."*
- *"Develop reduced order models from accurate computational results for use by design engineers" is listed as HIGH priority under Numerical Algorithm and Software Development category of the Roadmap.*
- *DE-FOA-0001041 requires that the proposed ROMs should:*
  - *"be at least 100 times faster than an equivalent multiphase CFD simulation."*
  - *"allow extrapolation within certain parameter ranges." (could be based on the results of several multiphase CFD simulations)*
  - *"be quantified for uncertainty, and the ROM must run without failure in the allowed parameter ranges."*
- *Computational advances will be provided to NETL's open-source CFD tool MFIX and validation cases will be provided.*

[9] Report on Workshop on Multiphase Flow Research, Morgantown, WV, Ed. M. Syamlal, DOE/NETL-2007/1259, 2006.

The project team

This proposed study is a collaborative effort between Florida International University (FIU) and Texas A&M University (TAMU).

- Dr. Seçkin Gökaltun, (PI, FIU):
  - technical supervision of project progress, maintaining the budget, overall project coordination and quality control (Task 1.0), supervision of the MFIX simulations (Subtasks 2.2, 3.2, 4.2), execution of ROM development (Subtasks 2.3, 3.3 and 4.3) and reporting to NETL-DOE.

- Prof. George S. Dulikravich, (Co-PI, FIU):
  - supervision of the data analysis for uncertainty quantification (Subasks 2.4, 3.4 and 4.4) and advising the graduate student dedicated to the project and course development at FIU, and dissemination of results.

- Prof. Paul Cizmas, (Co-PI, TAMU):
  - technical supervision of the ROM development and modification of the reduced kinetics model (Subtasks 4.3).

Statement of Project Objectives

Objectives:

The objectives of the proposed research are :

- to apply advanced computational techniques in order to develop reduced order models in the case of reacting multiphase flows, based on high fidelity numerical simulation of gas-solids flow structures in risers and vertical columns obtained by the MFIX software;
- generate numerical data, necessary for validation of the models for multiple fluidization regimes;
- expose minority students to scientific research in the field of fluid dynamics of gas-solids flow systems;
- and maintain and upgrade the educational, training and research capabilities of Florida International University.

Statement of Project Objectives - Scope of Work:

The proposed research project will be completed in three years. The following tasks will be completed during the project:

Task 1. Project management (36 months)

Subtask 1.1 **Project management and planning:**
Review and revise the project management plan (PMP) if necessary.

Subtask 1.2 **Project management and planning:**
Review, and if necessary revise the PMP following the annual review. Plan for second year deliverables and reporting.

Subtask 1.3 **Project management and planning:**
Review, and if necessary revise the PMP following the annual review. Plan for third year deliverables and reporting.

Statement of Project Objectives - Scope of Work:

Task 2. Develop ROM for Isothermal Gas-Solids Flow (12 months)

Subtask 2.1 **Prepare a detailed test matrix**
In this sub-task, a detailed plan for conducting the numerical simulations will be prepared. Specific conditions, flow rates and simulation data to be needed for ROM derivations will be specified.

Subtask 2.2 **Conduct MFIX simulations for isothermal flow in a bubbling bed**
The two-fluid CFD multiphase code, MFIX, will be used to produce simulation data necessary to reduce the governing equations of the hydrodynamics of fluidized systems and obtain a representative ROM derivation. Heat transfer and chemical reactions will be ignored within this subtask.

Subtask 2.3 **Derivation and implementation of a constrained POD model for isothermal, non-reacting gas-solids system**
The existing proper orthogonal decomposition (POD) method implemented in the ODEx code developed under NETL's auspices will be augmented by constraining the gas void fraction variable. The methodology for constraining the gas void fraction will be based on the Kuhn-Tucker conditions. This methodology will be implemented in the ODEx code.

Subtask 2.4 **Verification of the ROM for isothermal and non-reacting gas-solids systems**
The results obtained with the reduced model in Subtask 2.3 will be analyzed for uncertainty quantification by comparing against the MFIX simulations obtained in Subtask 2.2 for multiple flow regimes in a bubbling fluidized bed. The speed-up in computation time obtained using the ROMs will be calculated as compared to the MFIX simulation cases produced within Subtask 2.2.

Statement of Project Objectives - Scope of Work:

Task 3. Develop ROM for Gas-Solids Flow with Heat Transfer (12 mnt)

Subtask 3.1 **Prepare a detailed test matrix**
The outcome of the Task 2 will be used to update the test matrix for simulations with heat transfer.

Subtask 3.2 **Conduct MFIX simulations for gas-solids flow and heat transfer in the riser section of a fluidized bed**
The two-fluid CFD multiphase code, MFIX, will be used to produce simulation data necessary to reduce the governing equations of the coupled hydrodynamics and the temperature field of fluidized systems and obtain a representative ROM derivation. Chemical reactions will be ignored within this subtask.

Subtask 3.3 **Derivation and implementation of ROMs for non-reacting gas-solids systems including heat transfer**
The POD method developed at task 2.3 will be expanded to include heat transfer calculation.

Subtask 3.4 **Verification of the ROM for non-reacting gas-solids systems including heat transfer**
The results obtained with the reduced model in Subtask 3.3 will be analyzed for uncertainty quantification by comparing against the MFIX simulations obtained in Subtask 3.2 for multiple flow regimes and thermal loadings in the riser section of a circulating fluidized bed. The speed-up in computation time obtained using the ROMs will be calculated as compared to the MFIX simulation cases produced within this Subtask 3.2.

Statement of Project Objectives - Scope of Work:

Task 4. Develop ROM for Gas-Solids Flow with Heat Transfer and Chemical Reactions (12 months)

Subtask 4.1 **Prepare a detailed test matrix**
The outcomes of the Task 1 and Task 2 will be used to update the test matrix for simulations with heat transfer and chemical reactions.

Subtask 4.2 **Conduct MFIX simulations for reacting gas-solids flow and heat transfer in the riser section of a fluidized bed**
The two-fluid CFD multiphase code, MFIX, will be used to produce simulation data necessary to reduce the governing equations of the coupled hydrodynamics and the temperature field of fluidized systems and obtain a representative ROM derivation. Chemical reactions will also be included within this subtask.

Subtask 4.3 **Derivation and implementation of ROMs for reacting gas-solids systems including heat transfer**
The reduced kinetics mechanisms will be modified such that they will satisfy the second law of thermodynamics (or differential entropy inequality). The simulations will be compared with current reduced kinetics and the reduced kinetics we will derive against experimental data. The ROM model developed in Task 3.3 will be extended to reacting multiphase flow simulations.

Subtask 4.4 **Verification of the ROM for reacting gas-solids systems including heat transfer**
The results obtained with the reduced model in Subtask 4.3 will be analyzed for uncertainty quantification by comparing against the MFIX simulations obtained in Subtask 4.2 for multiple reacting flow cases in the riser section of a circulating fluidized bed. The speed-up in computation time obtained using the ROMs will be calculated as compared to the MFIX simulation cases produced within Subtask 4.2.

Project milestones, budget and schedule

Technical Milestones:

Milestone #	Description	Completion Date
1	Complete the ROM development and validation for isothermal non-reacting gas-solid flow	09/01/15
2	Complete the ROM development and validation for non-reacting gas-solid flow with heat transfer	09/01/16
3	Complete the ROM development and validation for reacting gas-solid flow	09/01/17

Project Budget:

Year	Student Salary	Tuition (Co-share)	PI (FIU)	Co-PI (FIU)	Travel	Materials Supplies	Subcontract (TAMU)	Total Cost
1	$19,330	$9,295.78	$8,386	$0	$4,500	$3,423	$25,433	$80,896
2	$19,414	$9,760.56	$8,638	$6,718	$3,000	$0	$26,13	$80,896
3	$19,853	$10,248.59	$8,897	$6,919	$1,500	$0	$26,849	$80,744

Project milestones, budget and schedule

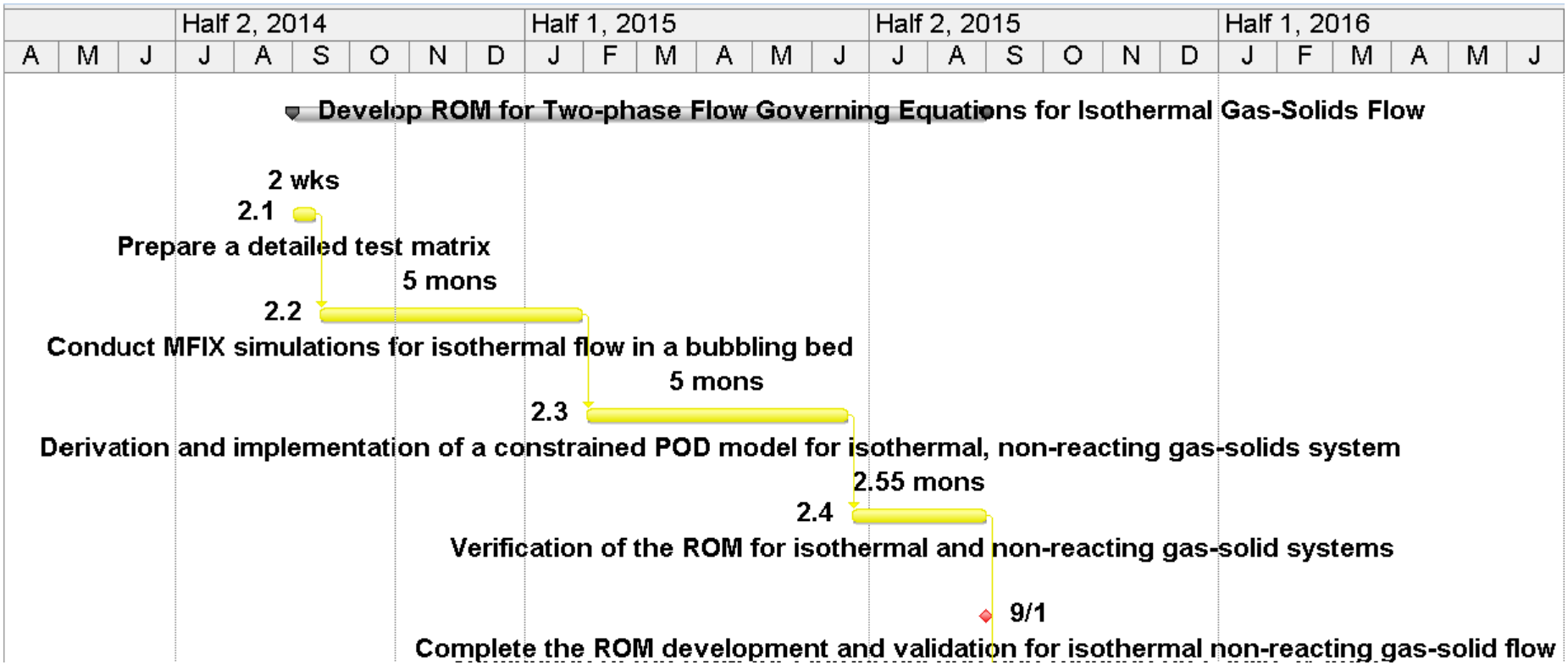


Figure: Project schedule for Year 1.

- Year 1: Non-reacting, isothermal, gas-solid flow (bubbling bed)
- Year 2: Non-reacting gas-solid flow + heat transfer (fluidized bed riser)
- Year 3: Reacting gas-solid flow + heat transfer (fluidized bed riser)

Project deliverables

- Quarterly reports describing the numerical simulations, actual status of and progress of the project, milestone status, any proposed changes in the project schedule, and recent results and findings in accordance with the "Federal Assistance Reporting Checklist" and the instructions accompanying the checklist.
- Intermediate reports shall provide more detailed updates on the progress of the project with respect to the four (3) technical Tasks and the Milestones specified in the Project Management Plan.

Project Technical Deliverables:

- A year-end report at the end of year 1, year 2 and a final report at the end of the performance period (year 3) with the description of the methodology and implementation of the reduced order model;
- Computer code for the POD-based reduced-order model with user manual
- Input and output data for code validation.
- Publication of results in refereed journals and presentation of results at technical conferences.

Project risks and risk management plan

Technical Issues:

Description of Potential Risk	**Consequences for this Project**	**Impact on project success**	Strategies to Minimize Impact.
Computational expense of MFIX simulations is more than anticipated	Delays or inability to complete some full-order model simulations to develop the ROMs	High	Use extrapolation procedures if possible. Reassign resources to get more computer time. The number of runs in each matrix will be reduced to compensate for the extra time. Perform fewer simulations and draw a limited set of conclusions
MFIX results do not match with reduced order model, and no plausible explanation is found for differences.	Delay in ROM validation.	High	Check the ROM code for errors. Explore sensitivity of results to simulation parameters.

Project risks and risk management plan

Resource Issues:

Description of Potential Risk	**Consequences for this Project**	**Impact on project success**	Strategies to Minimize Impact.
Long lead time in the procurement of materials and supplies	Delays in simulations	Low	Identify alternative sources for materials to be acquired. Look for local vendors or internal sources that can supply the items quicker.
Computer downtime or failure of components	Delay in performing simulations and data analysis	Medium	Try to obtain alternative computing resources through DOE INCITE competition. Repair or replace the failed components with in-house resources. Request extension for some milestones.

Management Issues:

Description of Potential Risk	**Consequences for this Project**	**Impact on project success**	Strategies to Minimize Impact.
Students do not perform as expected, or effective work performance is not achieved.	Slow progress on project.	High	Try alternative mentoring strategies for student. Provide additional training and educational resources for student.

Project status

FIU:

- Most of the funds are uploaded to financial management system (10/21/14).
- Graduate student at FIU hired.

TAMU:

- Subcontract initiated.

Outline

- Constrained POD
- Simulation of Chemical Reactions with Reduced Kinetics Models

Constrained POD

POD Method

Extracts:

- time-independent orthonormal basis functions $\Phi_k(x)$
- time-dependent orthonormal amplitude coefficients $a_k(t_i)$

such that the reconstruction

$$u(\mathbf{x}, t_i) = \sum_{k=1}^{M} a_k(t_i)\, \Phi_k(\mathbf{x}), \quad i = 1, \ldots, M$$

is optimal in the sense that the average least square truncation error

$$\varepsilon_m = \left\langle \left\| u(\mathbf{x}, t_i) - \sum_{k=1}^{m} a_k(t_i)\, \Phi_k(\mathbf{x}) \right\|^2 \right\rangle$$

is a minimum for any given number $m \leq M$ of basis functions over all possible sets of orthogonal functions

POD Method

Optimal property (1) reduces to (2)

$$\int_D < u(x)u^*(y) > \Phi(y)dy = \lambda\Phi(x)$$

$\{\Phi_k\}$ are eigenfunctions of integral equation (2), whose kernel is the averaged autocorrelation function

$$< u(x)u^*(y) > \equiv R(x,y) \tag{3}$$

For a finite-dimensional case, (3) replaced by tensor product matrix

$$R(\mathbf{x},\mathbf{y}) = \frac{1}{M}\sum_{i=1}^{M} u(\mathbf{x},\, t_i)\, u^T(\mathbf{y}, t_i)$$

POD Method

Features

- Provides optimal basis for modal decomposition of a data set
- Extracts key *spatial* features from physical systems with spatial and temporal characteristics
- Reduces a large set of governing PDEs to a much smaller of ODEs

Steps

- Database generation
- Modal decomposition
- Galerkin projection
- Time coefficients computation

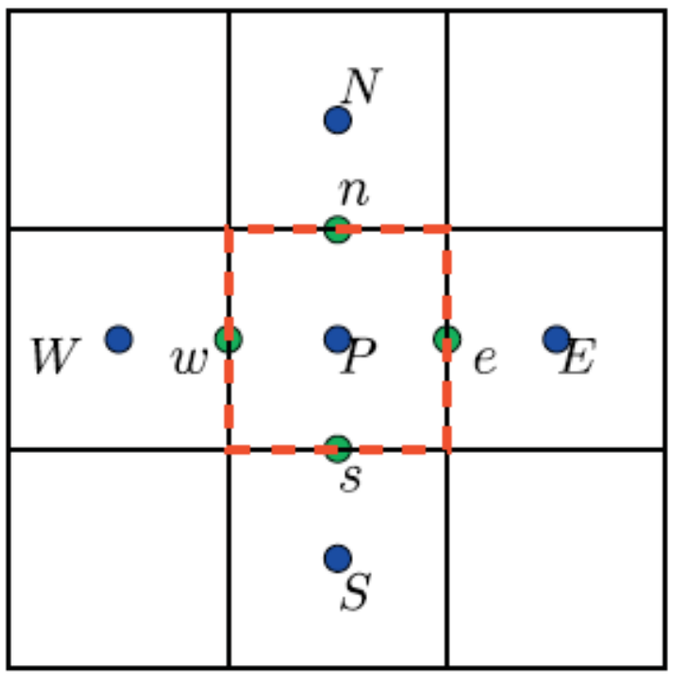
POD Method

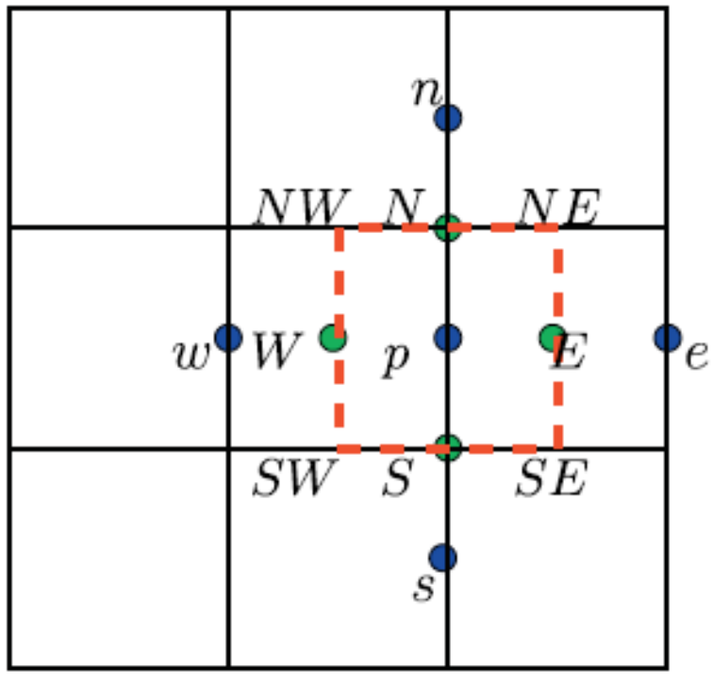
Full-order model governing equations

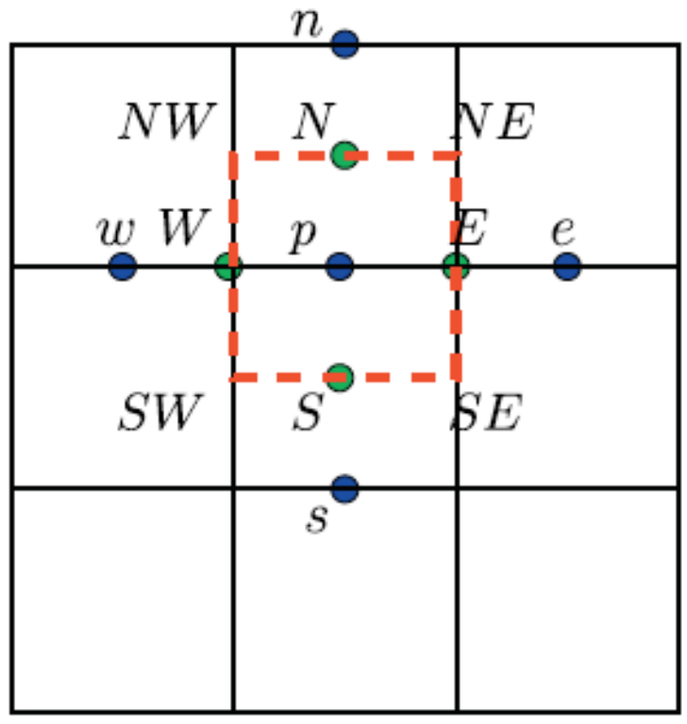
$$\frac{\partial}{\partial t}(\epsilon_m \rho_m) + \nabla \cdot (\epsilon_m \rho_m \vec{v}_m) = 0$$

$$\frac{\partial}{\partial t}(\epsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\epsilon_m \rho_m \vec{v}_m \vec{v}_m) = -\epsilon_m \nabla p_g + \nabla \cdot \overline{\overline{S}}_m + F_{gs}(\vec{v}_s - \vec{v}_g) + \epsilon_m \rho_m \vec{g}$$

$$\epsilon_m \rho_m C_{p_m} \left(\frac{\partial T_m}{\partial t} + \vec{v}_m \nabla T_m \right) = -\nabla \vec{q}_m - \gamma_m (T_m - T_\ell) - \Delta H_{rm} + \gamma_{Rm} (T_{Rm}^4 - T_m^4)$$







POD Method

$$(a_m^v)_p(v_m)_p = \sum_{nb}(a_m^v)_{nb}(v_m)_{nb} + (b_m^v)_p$$

$$v(x,t) = \sum_{k=1}^{m^v} \alpha_k^v(t)\varphi_k^v(x)$$

$$\sum_{k=1}^{m} \alpha_k \left(a_i\varphi_k(x_i) - \sum_{i_{nb}=1}^{NB} a_{i_{nb}}\varphi_k(x_{i_{nb}}) \right) = b_i, \qquad i = 1, \ldots, N$$

$$\sum_{k=1}^{m} \alpha_k \left([A]\{\varphi_k\} - \sum_{nb=1}^{NB} [A_{nb}]\{\varphi_{k_{nb}}\} \right) = \{b\}$$

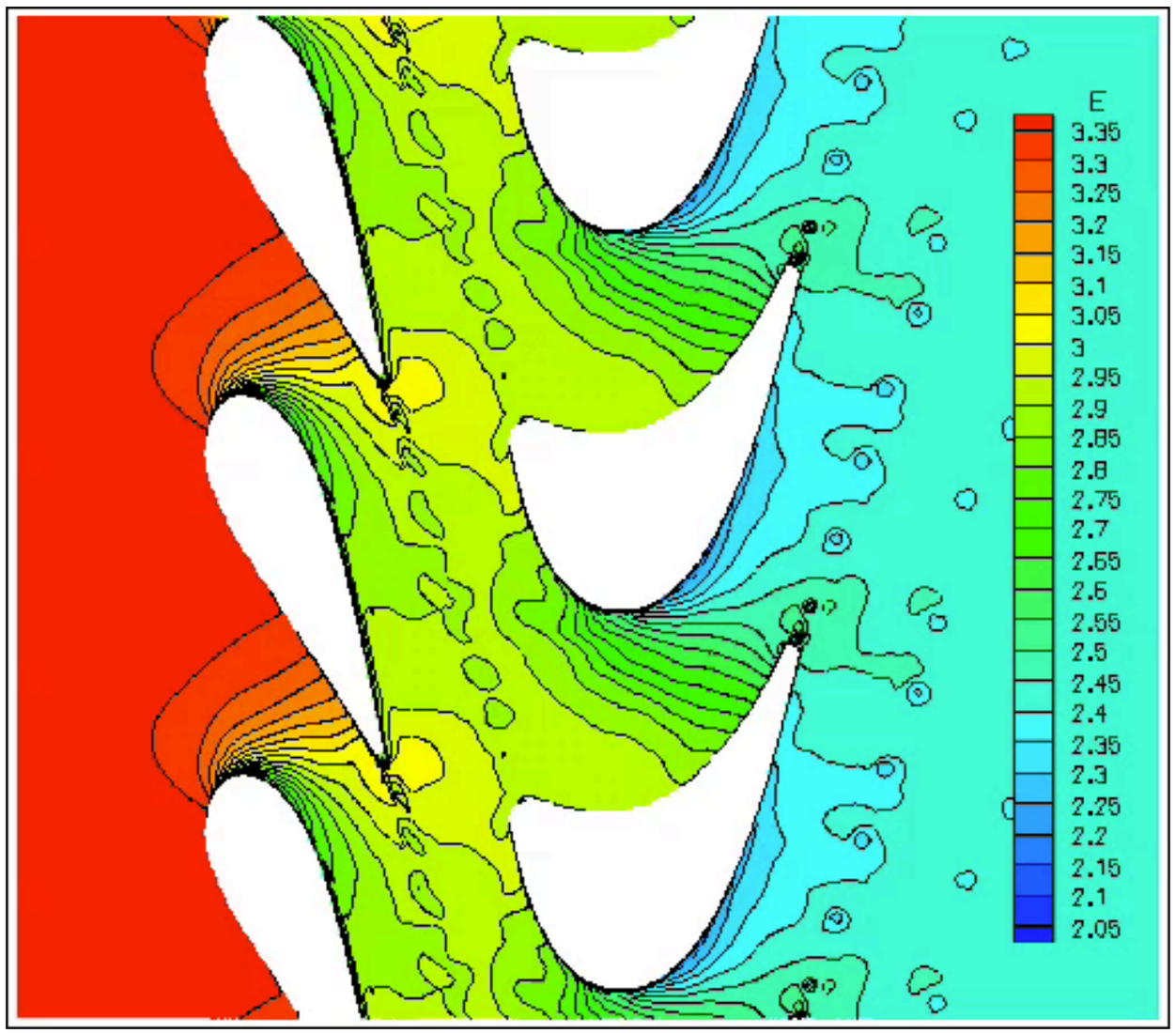
$$\{\varphi_\ell\}^T \sum_{k=1}^{m} \alpha_k \left([A]\{\varphi_k\} - \sum_{nb=1}^{NB} [A_{nb}]\{\varphi_{k_{nb}}\} \right) = \{\varphi_\ell\}^T\{b\}, \qquad \ell = 1, \ldots, m$$

$$\left[\tilde{\mathcal{A}}^v\right]\{\alpha^v\} = \left\{\tilde{\mathcal{B}}^v\right\}$$

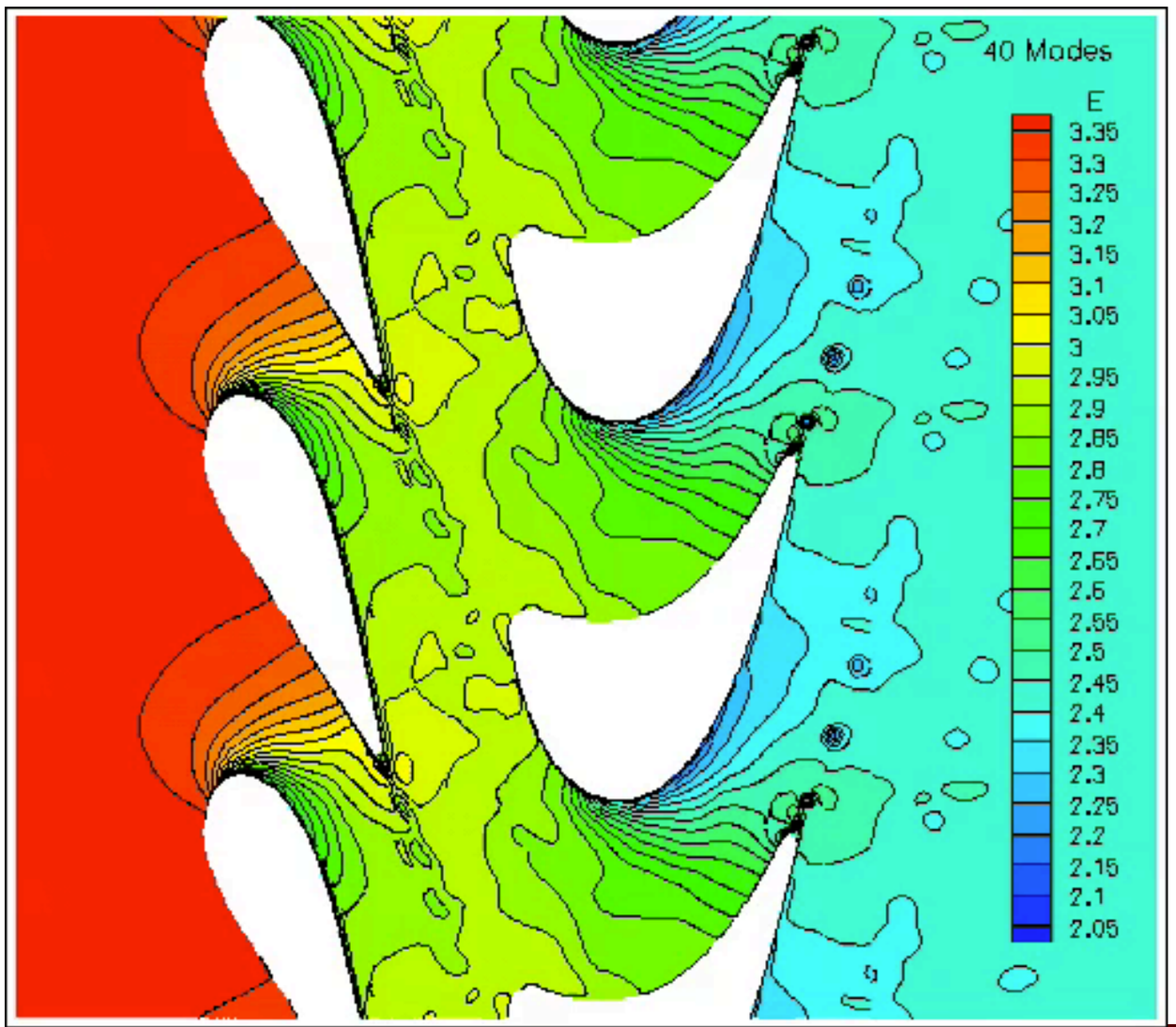
POD for Turbomachinery Aeroelastic Analysis

A reduced-order model is not necessarily a low-fidelity solution!

Full-Order Model

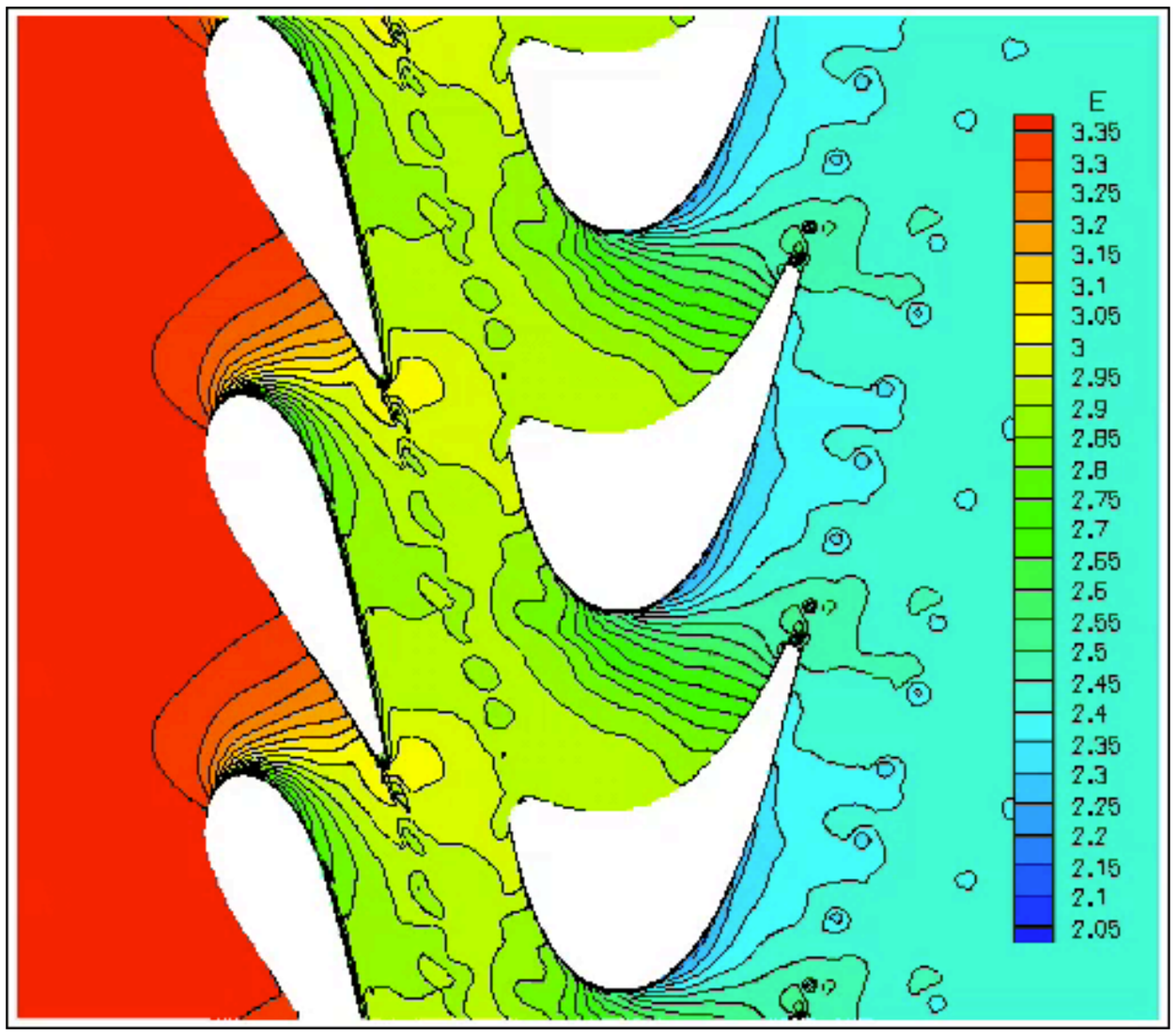


Reduced-Order Model, POD 40 modes

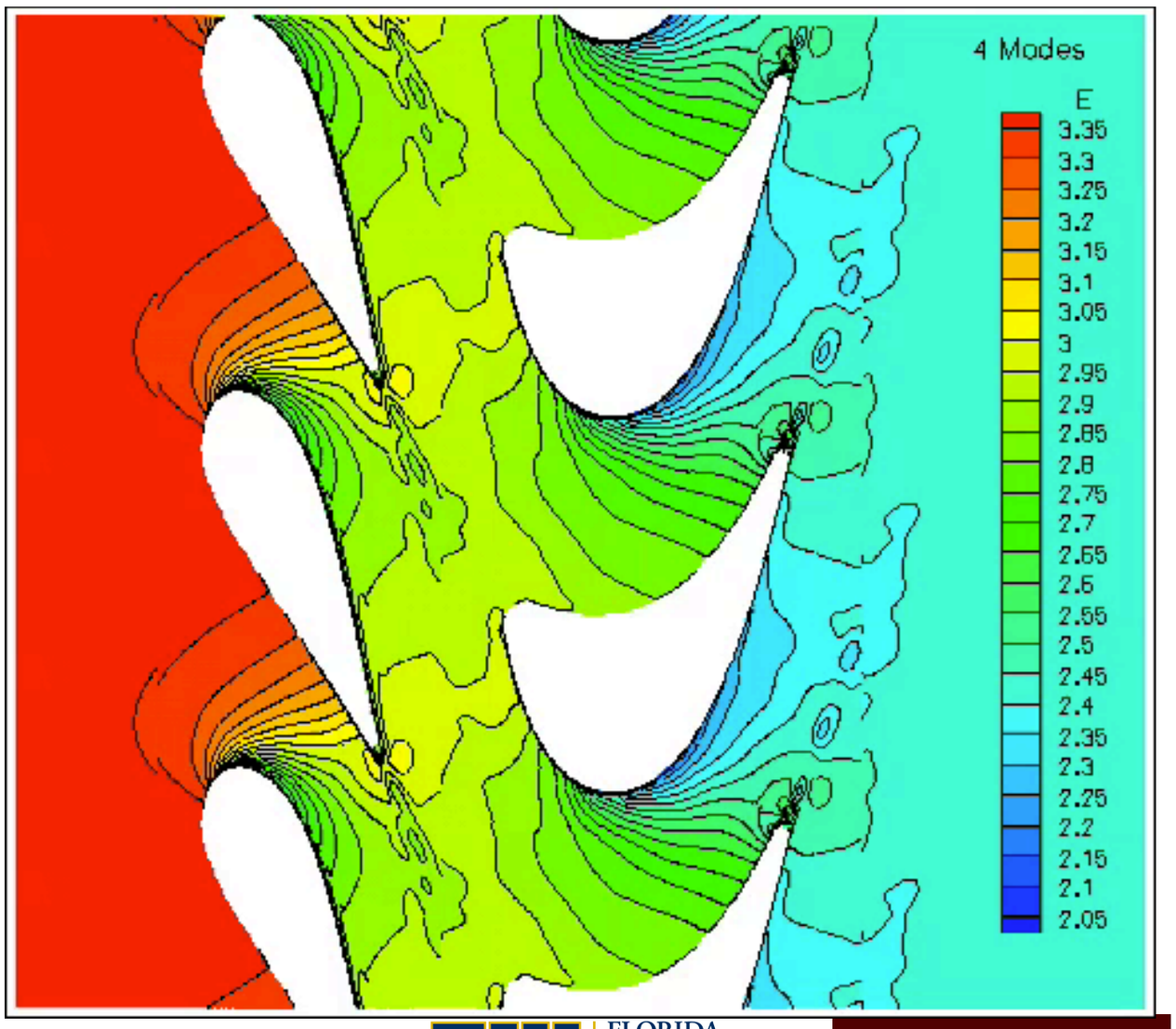


POD for Turbomachinery Aeroelastic Analysis

Full-Order Model



Reduced-Order Model, POD 4 modes



POD Research Trends

- Improving prediction of off-reference conditions
- Improving efficiency (further reduce computational time)
- Modeling moving/deforming meshes

POD Research Trends (2)

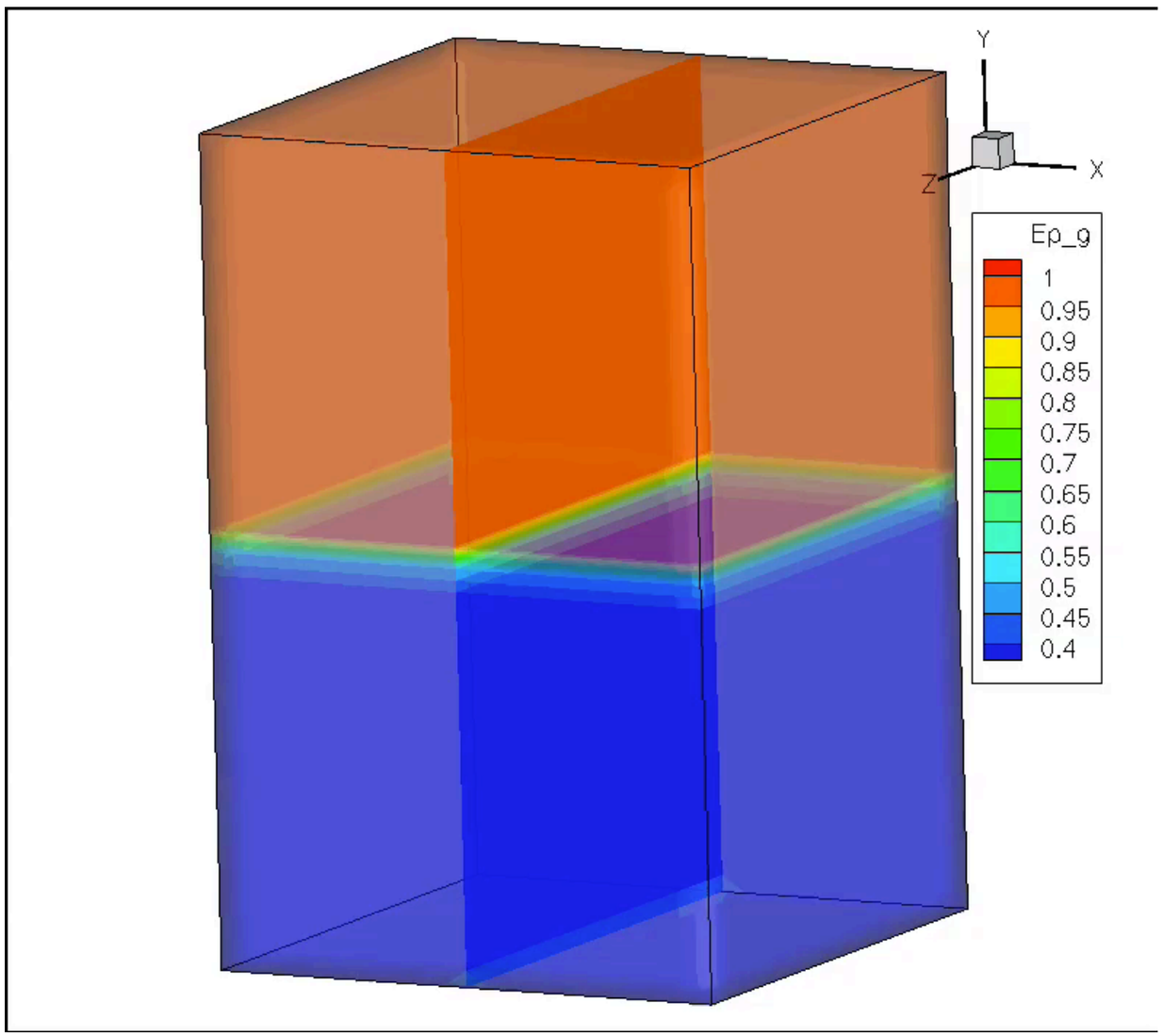
- Improving prediction of off-reference conditions
  - Direct interpolation
  - Enrich snapshot database
  - Sensitivity analysis using parametric derivatives
  - Actuation modes
  - Tangent space to Grassmann manifold

POD Research Trends (3)

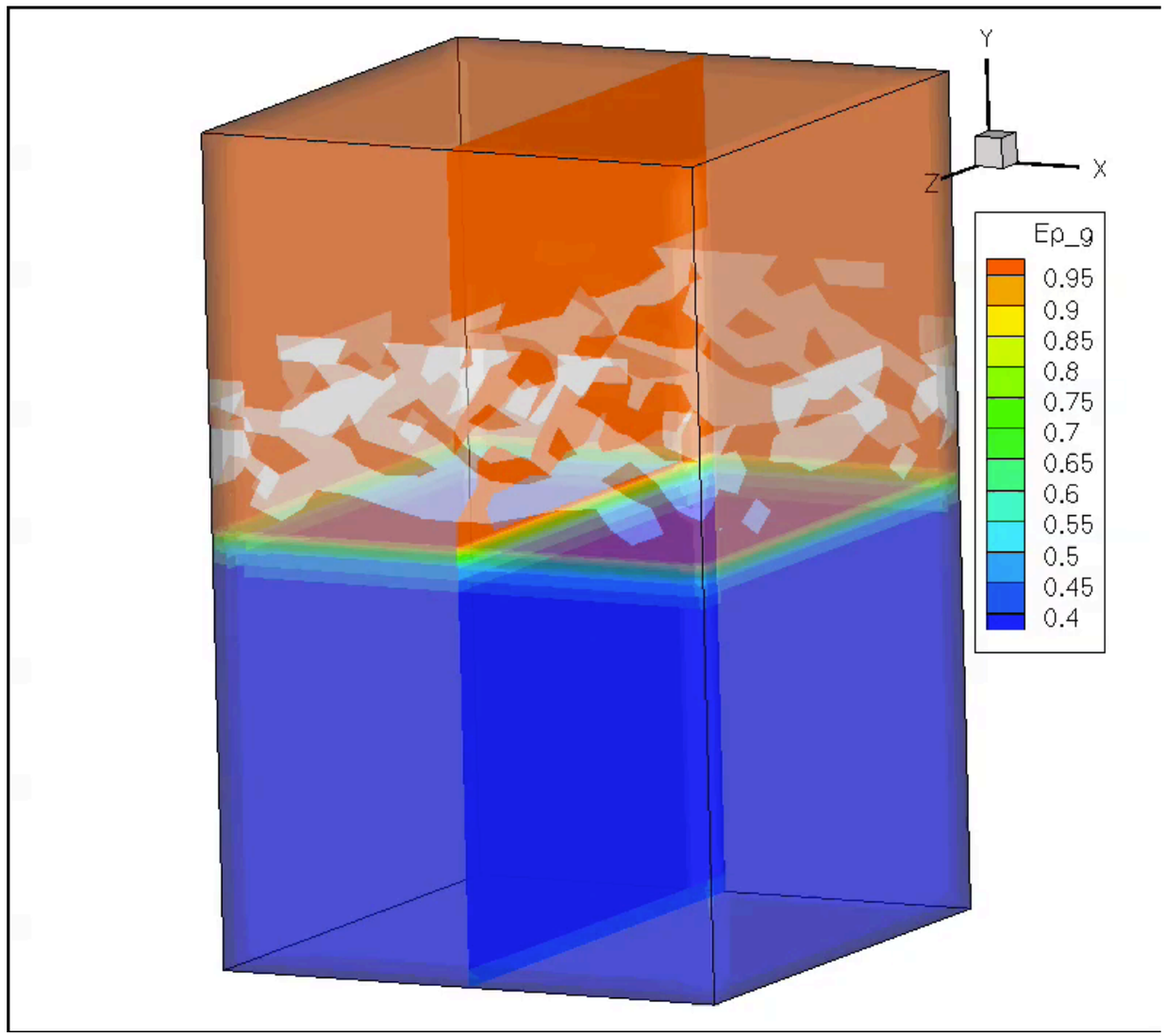
- Modeling moving/deforming meshes (motivated by aeroelastic applications)
  - Sets of index-based functions associated with deformations
  - Interpolation: fluid-structure as multiphase flow (interpolation, modified BCs)
  - Dynamic basis functions

Void Fraction, ϵ_G

Full-order model



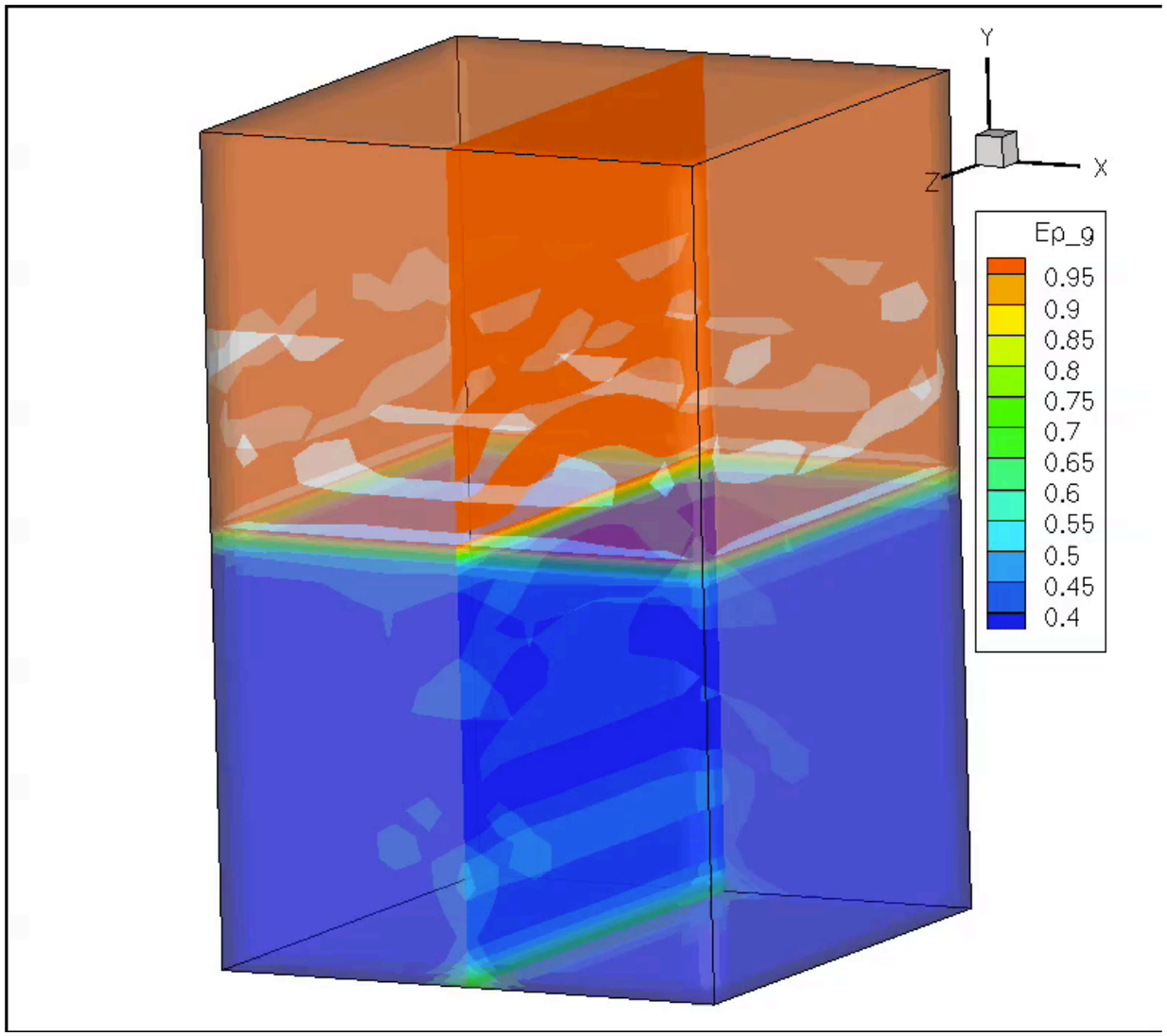
Reduced-order model



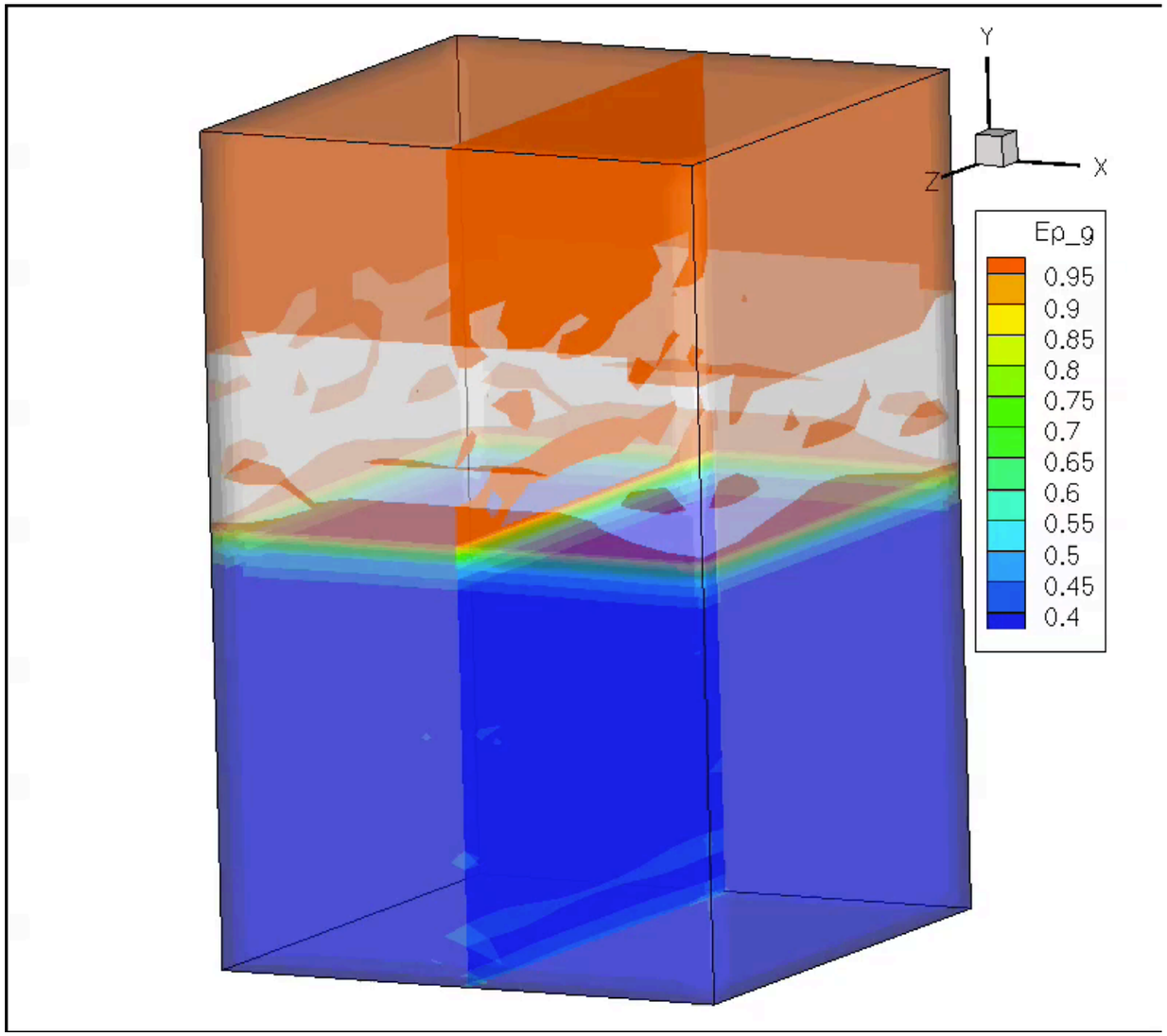
Reduced-Order Model

Void Fraction, ϵ_G

20 modes

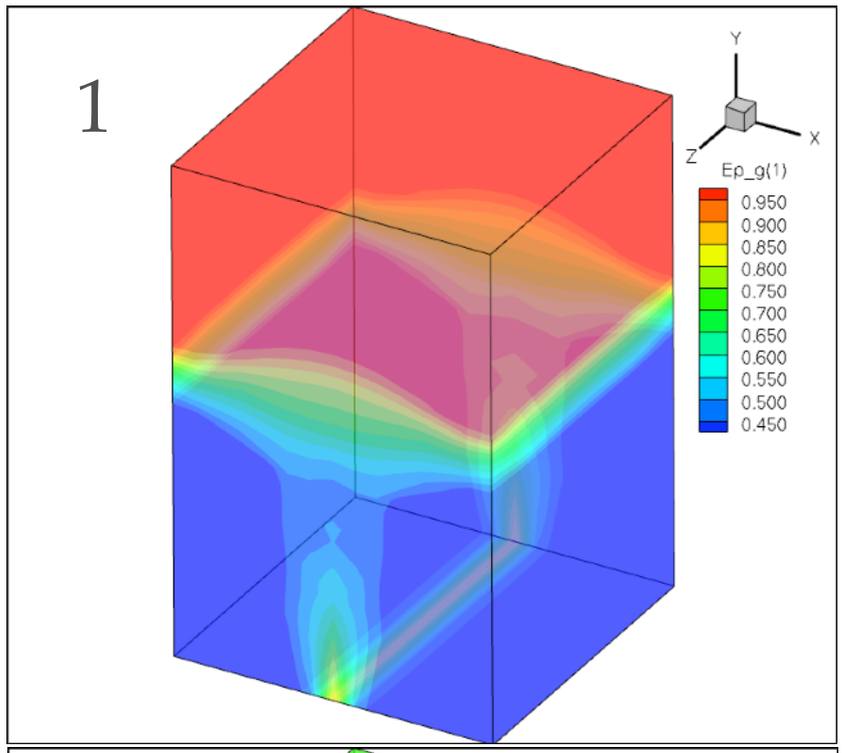


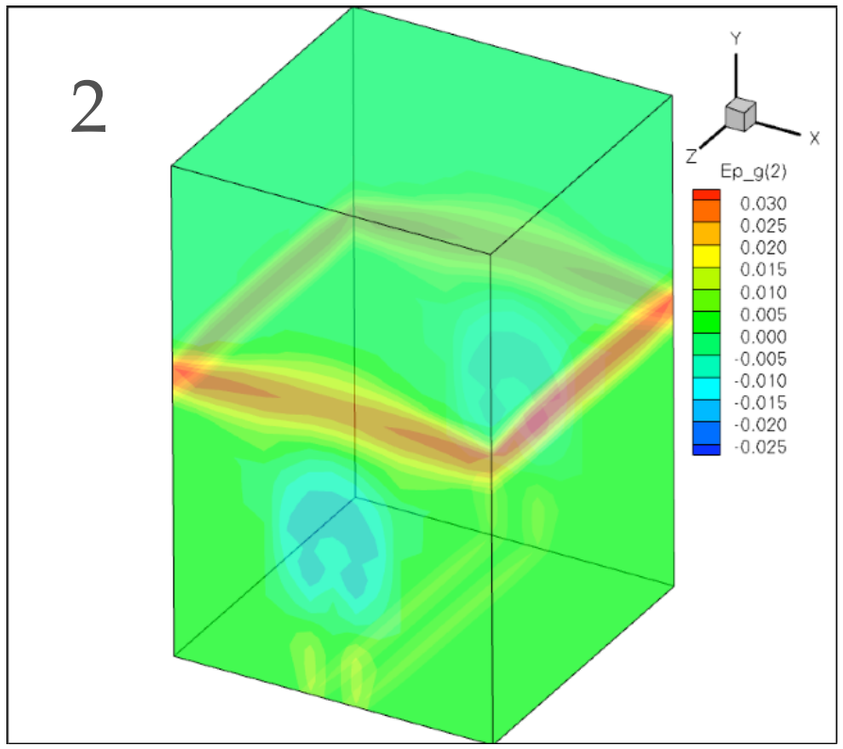
40 modes

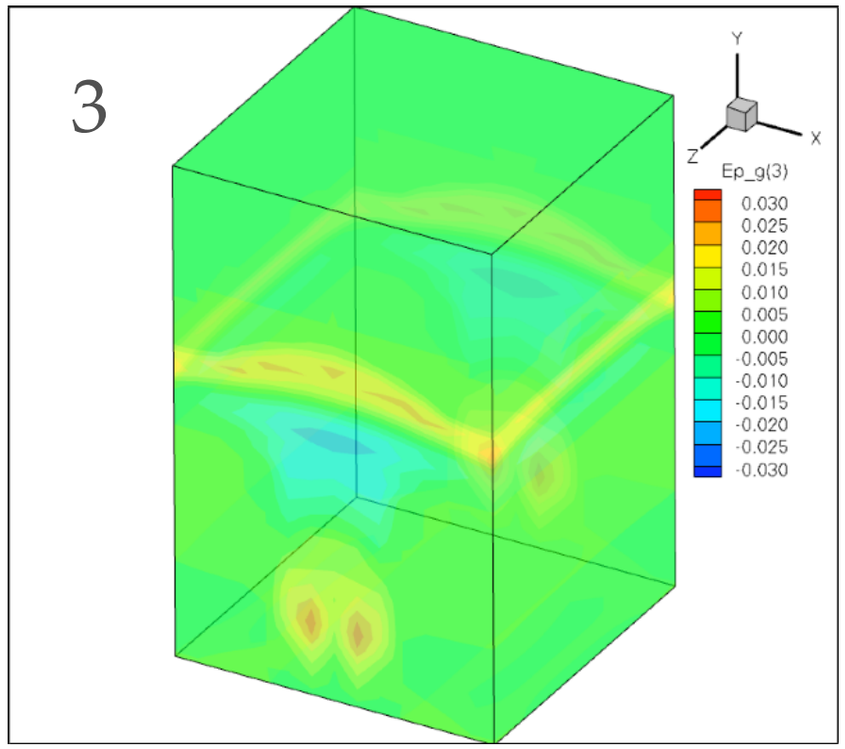


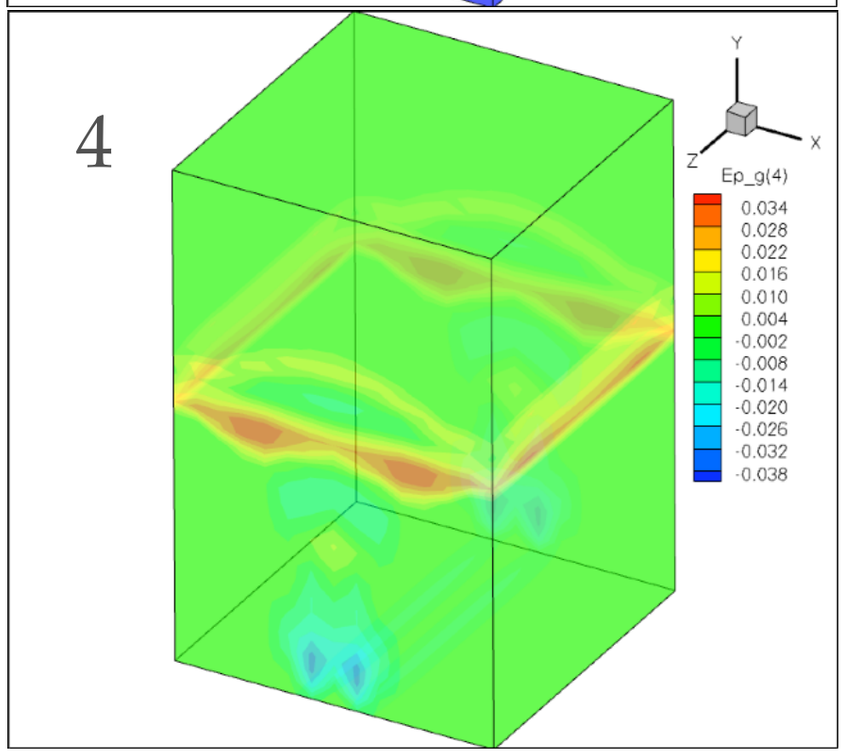
POD Modes

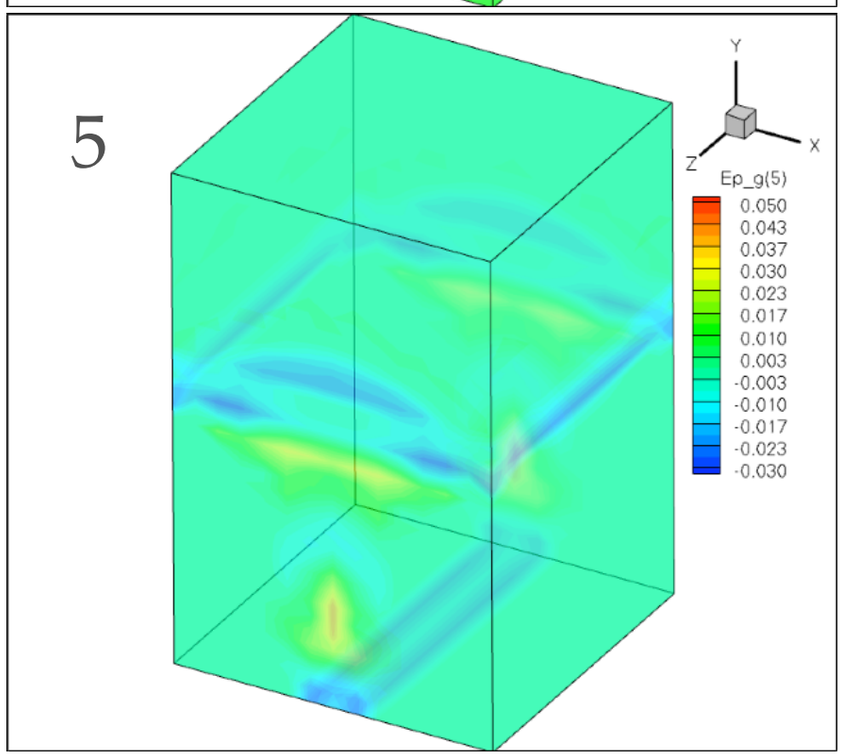
Void Fraction, ϵ_G

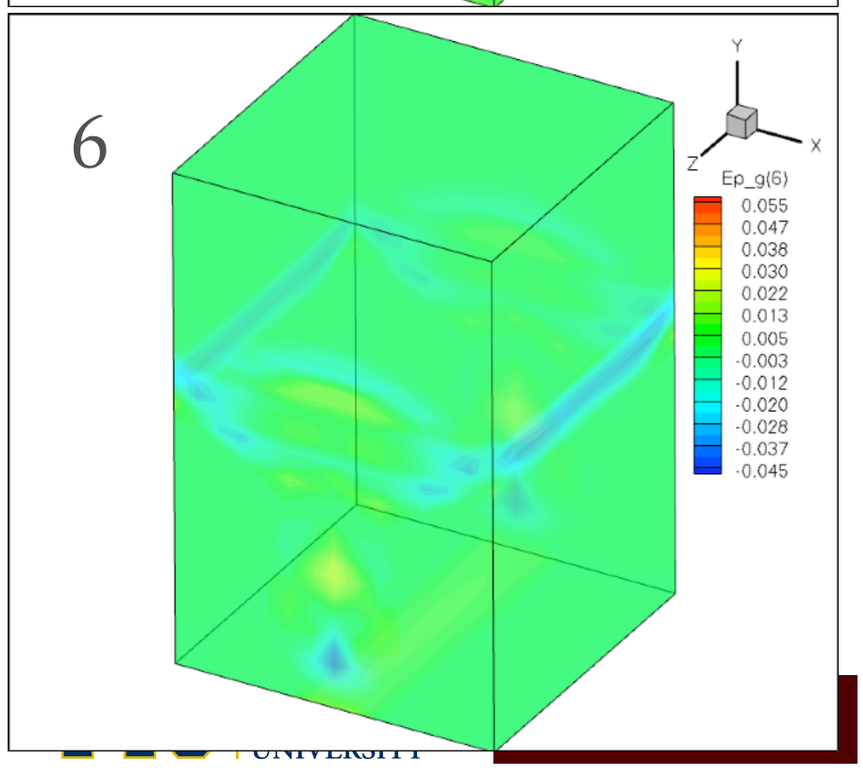




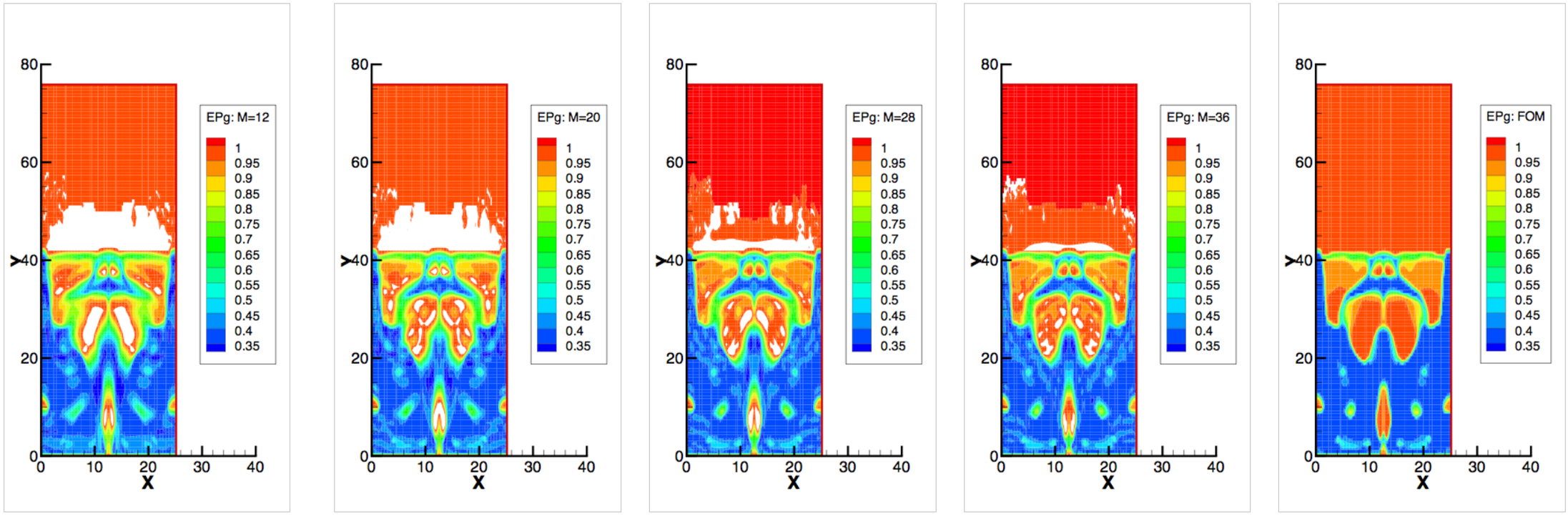








Gas void fraction



12 20 28 36 Full-order model

modes

Constrained POD

- Approach
  - Use Kuhn-Tucker (or Karush-Kuhn-Tucker) conditions to constrain time coefficients such that gas void fraction is in (0.38,1) interval

Example of Constrained POD

- First-order wave equation

$$u_t + cu_x = 0, \quad x \in [0,1], \quad c > 0$$

with initial condition

$$u(x,0) = f(x) \geq 0$$

$$u(x,t) \approx \sum_{i=1}^{m} a_i(t)\phi_i(x)$$

Constrained POD
Wave Equation

$$\dot{a}_i \phi_i + c a_i \phi_i' = 0$$

- Galerkin projection

$$\int_0^1 \dot{a}_i \phi_i \phi_j dx + \int_0^1 c a_i \phi_i' \phi_j dx = 0$$

$$\dot{a}_j + c \left(\int_0^1 \phi_i' \phi_j dx \right) a_i = 0$$

$$\underline{\dot{a}} + \boldsymbol{B} \underline{a} = \underline{0}$$

$$B_{ij} = c \left(\int_0^1 \phi_i' \phi_j dx \right)$$

Constrained POD
Wave Equation (cont'd)

$$(\boldsymbol{I} + \Delta t\ \boldsymbol{B})\,\underline{a}^{n+1} - \underline{a}^{n} = \underline{0}, \quad \underline{a}^{n} := \underline{a}(t^{n})$$

$$\boldsymbol{C}\underline{a}^{n+1} - \underline{a}^{n} = \underline{0}, \quad \boldsymbol{C} = \boldsymbol{I} + \Delta t\ \boldsymbol{B}$$

- Karush-Kuhn-Tucker condition

$$\underline{\lambda}^{T}\boldsymbol{\Phi}\underline{a}^{n+1} \geq 0, \quad \boldsymbol{\Phi} = [\underline{\phi}_1 \ldots \underline{\phi}_m], \quad \boldsymbol{\Phi} \in \mathbb{R}^{N\times m}$$

$$\underline{\lambda} \in \mathbb{R}^{N}, \quad N \text{ number of spatial points}$$

- Minimize functional

$$J = ||\boldsymbol{C}\underline{a}^{n+1} - \underline{a}^{n}||^2 + \underline{\lambda}^{T}\boldsymbol{\Phi}\underline{a}^{n+1}$$

$$J_{\underline{a}^{n+1}} = 2\boldsymbol{C}\underline{a}^{n+1} - 2\underline{a}^{n} + \boldsymbol{\Phi}^{T}\underline{\lambda} = 0$$

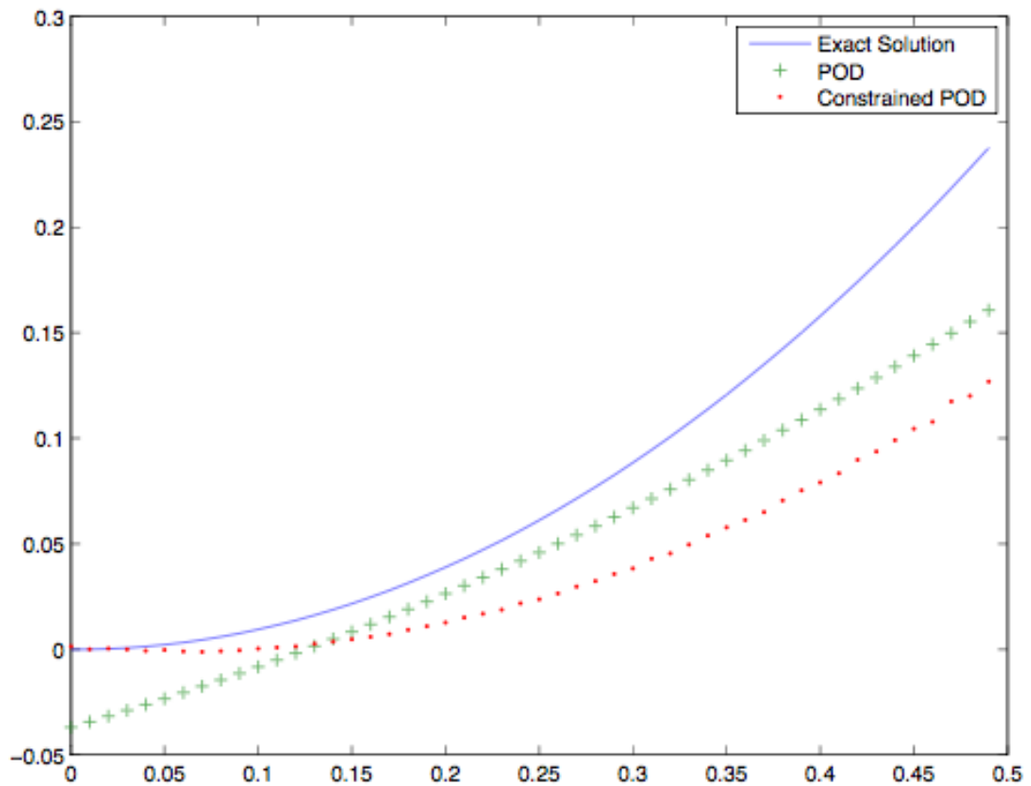
$$J_{\underline{\lambda}} = \boldsymbol{\Phi}\underline{a}^{n+1} = 0$$

Constrained POD Wave Equation (cont'd)

$$\begin{bmatrix} 2C & \Phi^T \\ \Phi & \underline{0} \end{bmatrix} \begin{Bmatrix} \underline{a}^{n+1} \\ \underline{\lambda} \end{Bmatrix} = \begin{Bmatrix} 2\underline{a}^{n} \\ \underline{0} \end{Bmatrix}$$

- Numerical implementation

$$f(x) = x^2 - 10^{-4} \qquad m = 4, \Delta x = 0.01 \ (N = 100)$$



Constrained POD Burgers Equation

$$u_t + uu_x = 0, \quad x \in [0,1]$$

$$\dot{a}_k + a_i a_j G_{ijk} = 0, \quad i,j,k = 1,m$$

$$G_{ijk} = \int_0^1 \phi_j \phi_i' \phi_k dx$$

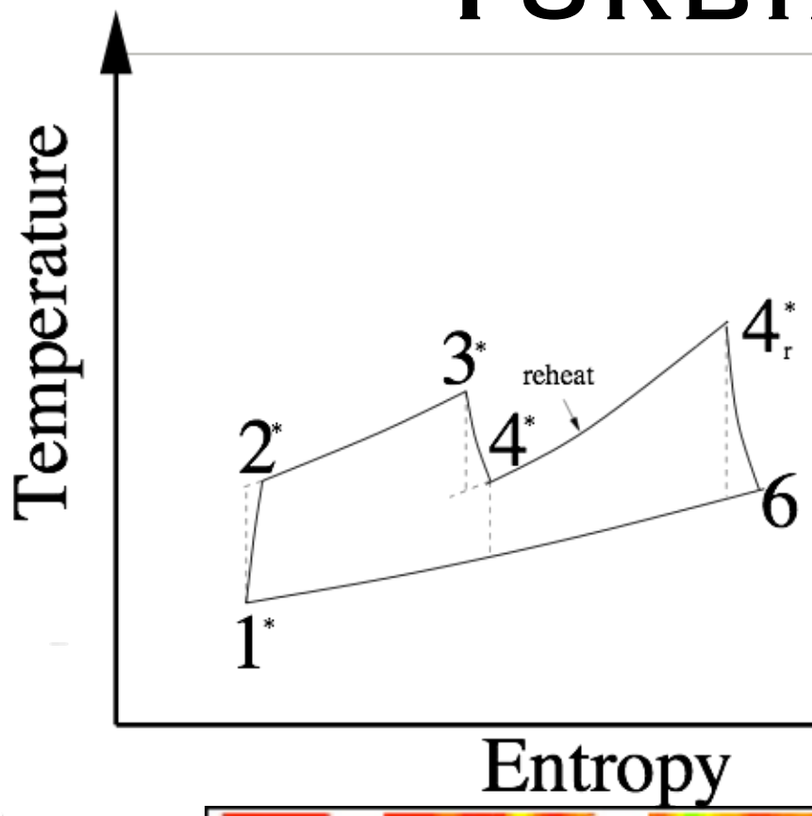
$$\boldsymbol{C_{n\ell}}\, \underline{a}^{n+1} - \underline{a}^n = \underline{0}$$

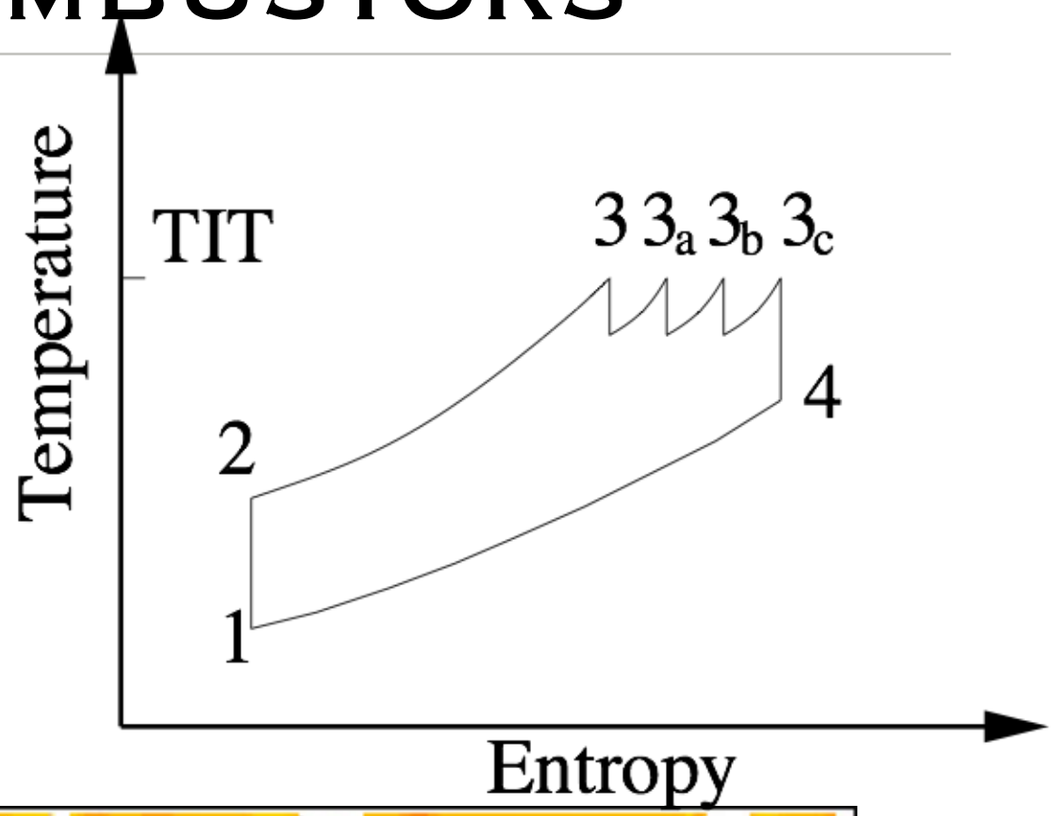
$$\boldsymbol{C_{n\ell}} = \begin{bmatrix} 1 + a_i^n G_{i11}\Delta t & a_i^n G_{i21}\Delta t \\ a_i^n G_{i12}\Delta t & 1 + a_i^n G_{i22}\Delta t \end{bmatrix}$$

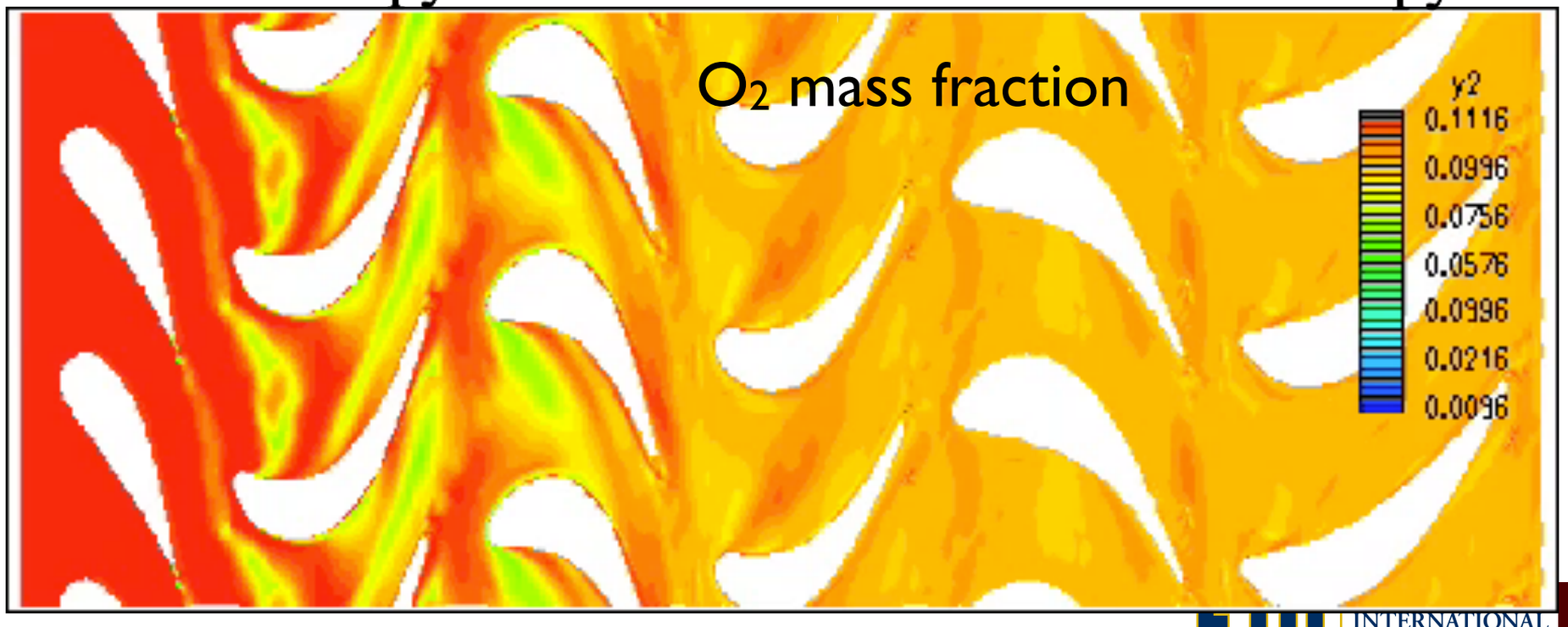
Simulation of Chemical Reaction with Reduced Kinetics Models & Second Law of Thermodynamics†

†In collaboration with John Slattery

In-Situ Reheat and Turbine-Combustors







Westbrook & Dryer Methane Combustion Model

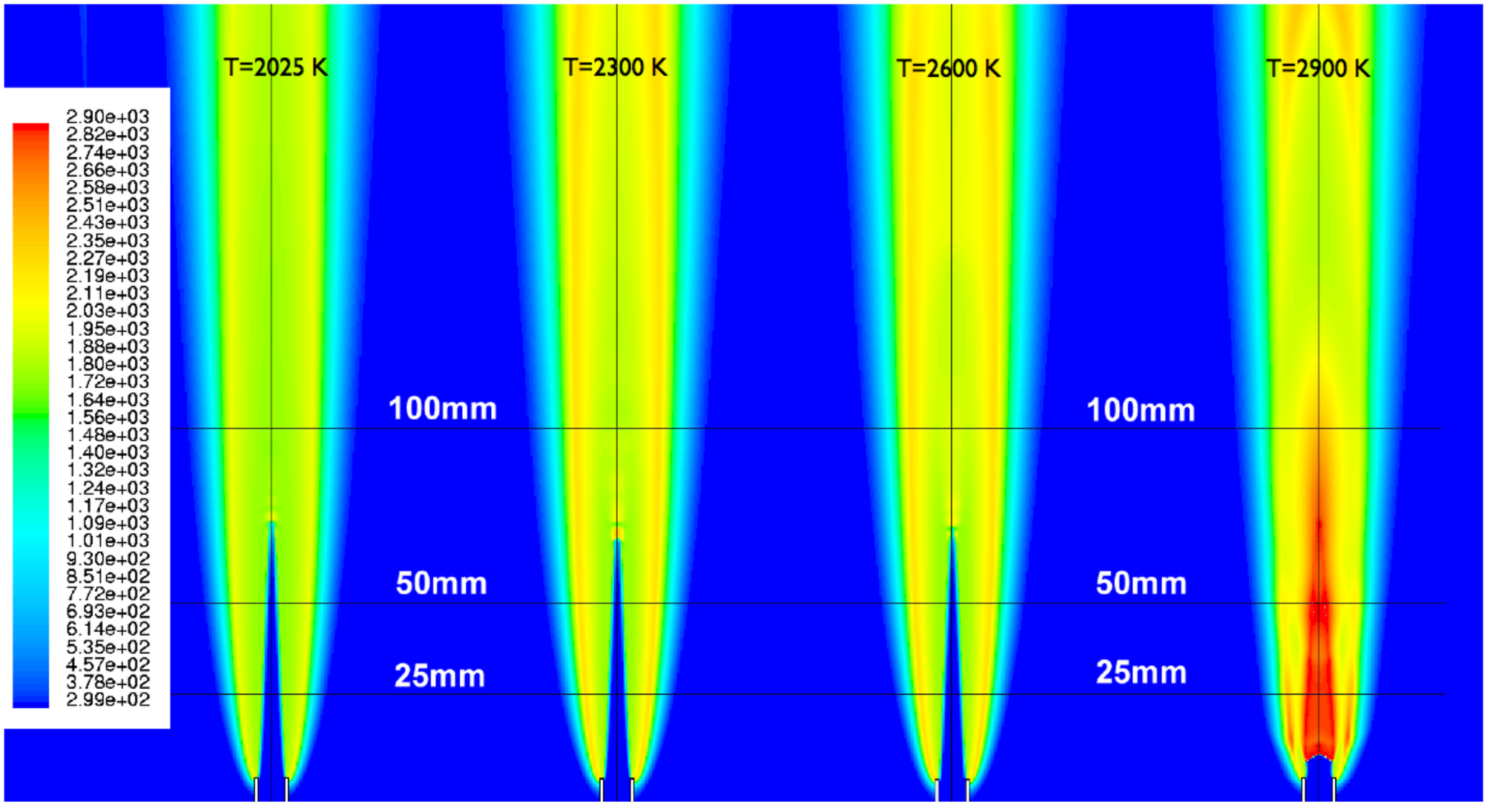
reaction 1: $\mathrm{CH_4} + 1.5\ \mathrm{O_2} \rightarrow \mathrm{CO} + 2\ \mathrm{H_2O}$

reaction 2: $\mathrm{CO} + 0.5\ \mathrm{O_2} \rightleftharpoons \mathrm{CO_2}$

$$\omega_1 = A_1 \exp\left(-E_1/\mathcal{R}/T\right)\ c_{(CH_4)}^{0.7}\ c_{(O_2)}^{0.8}$$

$$\omega_2 = A_{2f} \exp\left(-E_{2f}/\mathcal{R}T\right)\ c_{(CO)}\ c_{(O_2)}^{0.25}\ c_{(H_2O)}^{0.5} - A_{2b} \exp\left(-E_{2b}/\mathcal{R}T\right)\ c_{(CO_2)}$$

Sandia Flame A
Temperature Limiter Effect



Differential Entropy Inequality

$$-\mathrm{tr}[(\mathbf{T}+P\mathbf{I})\cdot\mathbf{D}]+\frac{1}{T}\epsilon\cdot\nabla T+cRT\sum_{B=1}^{N}\mathbf{j}_{(B)}\cdot\frac{\mathbf{d}_{(B)}}{\rho_{(B)}}+\sum_{j=1}^{K}\sum_{B=1}^{N}\mu_{(B)}r_{(B,j)}\leq 0$$

- $\mathbf{T}$ - stress tension
- $\mathbf{D}$ - rate of deformation
- ϵ - energy flux (corr. mass)
- c - total molar density
- $\mathbf{j}_{(B)}$ - mass flux of species B relative to v
- $\mathbf{d}_{(B)}$ - driving force for mass transfer (corr. T, P)
- $\mu_{(B)}$ - chemical potential
- $r_{(B\ \ j)}$ - rate of production

Terms of Entropy Inequality

- Compressible Newtonian fluid

$$-tr[(\mathbf{T}+P\mathbf{I})\cdot\mathbf{D}]\leq 0$$

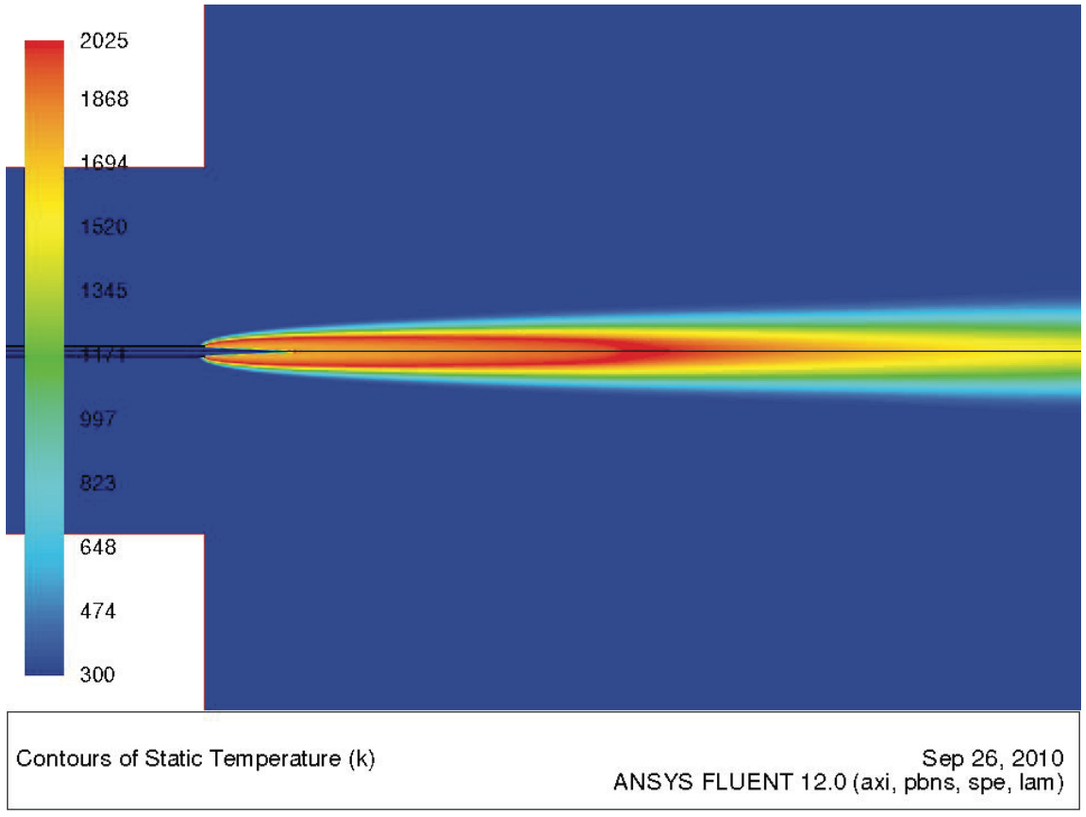
- Fourier's law of heat conduction

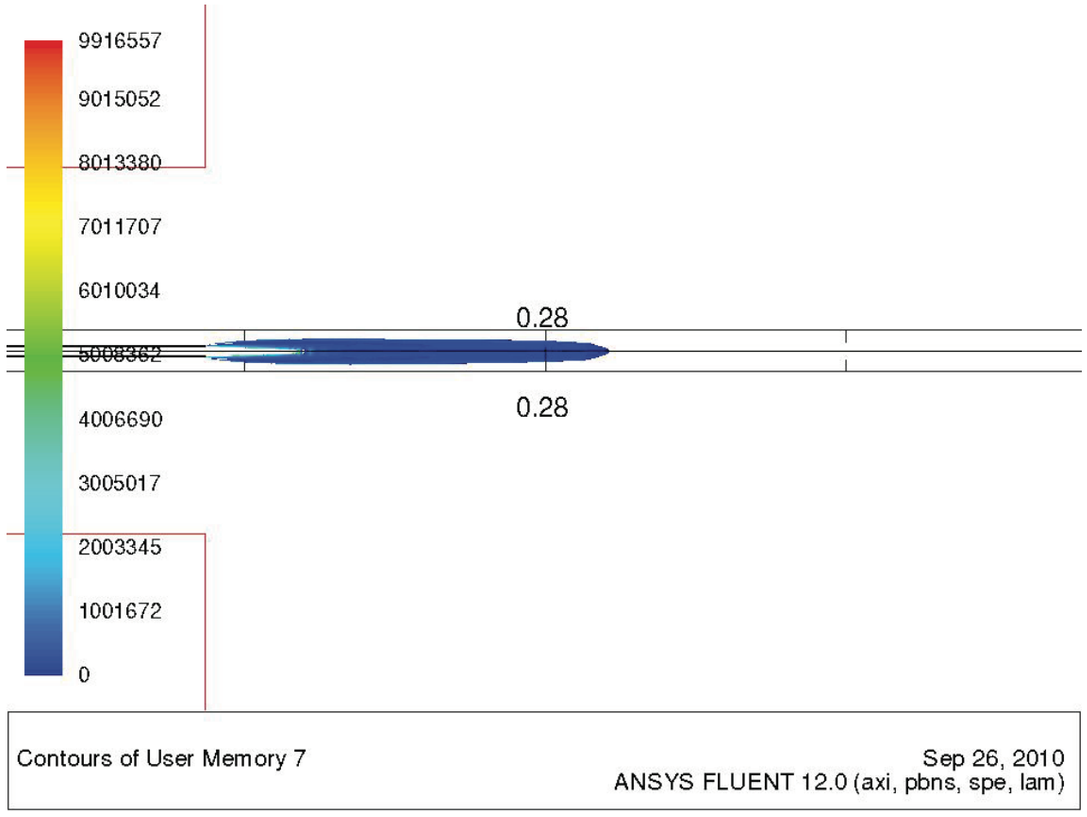
$$\frac{1}{T}\boldsymbol{\epsilon}\cdot\nabla T\leq 0$$

- Fick's first law for dilute gases

$$cRT\sum_{B=1}^{N}\mathbf{j}_{(B)}\cdot\frac{\mathbf{d}_{(B)}}{\rho_{(B)}}\leq 0$$

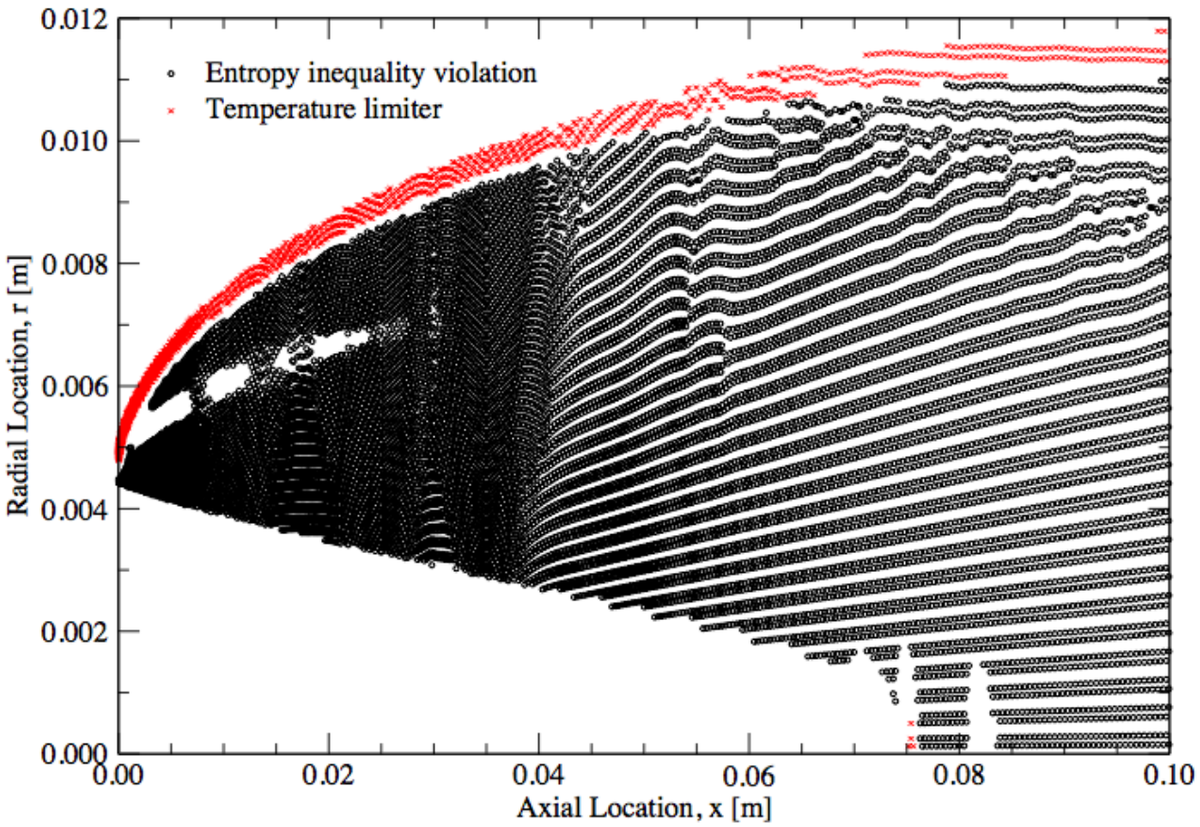
Sandia Flame A
Entropy Inequality Violations

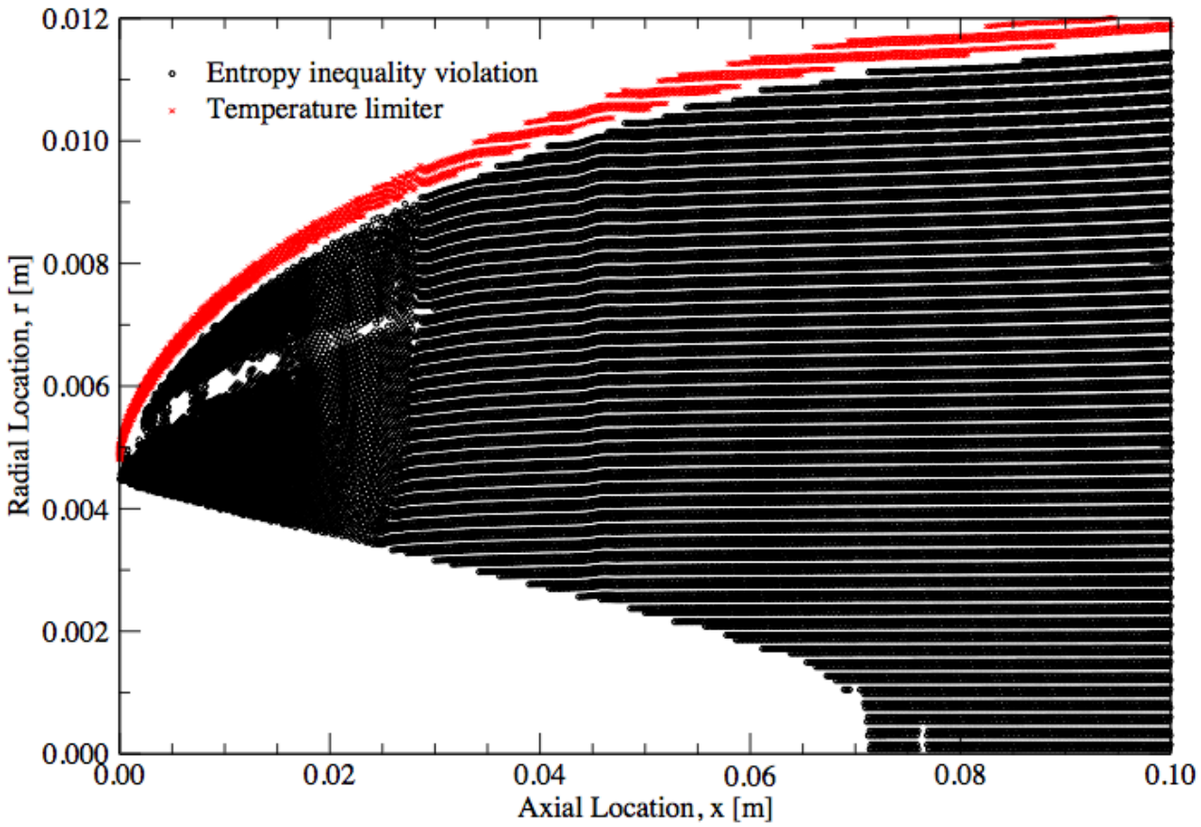




$$-\mathrm{tr}[(\mathbf{T}+P\mathbf{I})\cdot\mathbf{D}]+\frac{1}{T}\boldsymbol{\epsilon}\cdot\nabla T+cRT\sum_{B=1}^{N}\mathbf{j}_{(B)}\cdot\frac{\mathbf{d}_{(B)}}{\rho_{(B)}}+\sum_{j=1}^{K}\sum_{B=1}^{N}\mu_{(B)}r_{(B,j)}\leq 0$$

Cells that Violate Entropy Inequality†





†Creating reduced kinetics models that satisfy the entropy inequality, ASME Journal of Engineering for Gas Turbine and Power, 2015

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Fourth Term

1. Dilute solution or ideal gas
2. For each species B and each reaction j

$$r_{(B,j)} = \left(\nu''_{(B,j)} - \nu'_{(B,j)}\right)\left(k_{(f,j)}\prod_B {c_{(B)}}^{\nu'_{(B,j)}} - k_{(b,j)}\prod_B {c_{(B)}}^{\nu''_{(B,j)}}\right)$$

3. All reactions are reversible
4. All reactions conform to the law of mass action

$$\sum_{B=1}^{N}\mu_{(B)}r_{(B,j)} = XRT\left[\left(\frac{\prod_B y_{(B)}}{\prod_B y^\star_{(B)}}\right)^{\nu'_{(B,j)}} - \left(\frac{\prod_B y_{(B)}}{\prod_B y^\star_{(B)}}\right)^{\nu''_{(B,j)}}\right]\ln\left\{\frac{\prod_B \left(y_{(B)}/y^\star_{(B)}\right)^{\nu''_{(B,j)}}}{\prod_B \left(y_{(B)}/y^\star_{(B)}\right)^{\nu'_{(B,j)}}}\right\}$$

$$X \equiv k_{(f,j)}\prod_B {c^\star_{(B)}}^{\nu'_{(B,j)}} = k_{(b,j)}\prod_B {c^\star_{(B)}}^{\nu''_{(B,j)}}$$

Theorem†

- The differential entropy inequality (1) is automatically satisfied for dilute gases, if all the reactions are both reversible and conform to the law of mass action, that is, the exponents of the molar concentrations used to calculated the progress of reaction variables are the stoichiometric coefficients.

† Role of differential entropy inequality in chemically reacting flows, Chemical Engineering Science **66**, 5636-43, 2011

Arrhenius Coefficients

Table 1: Arrhenius parameters and molar concentration exponents for methane combustion mechanism.

Reaction	A [–]	E [J/kmol]	a	b	A [–]	E [J/kmol]	a	b
	Westbrook & Dryer 1981				Fluent			
1	2.8×10^9	2.025×10^8	-0.3	1.3	5.012×10^{11}	2×10^8	0.7	0.8
2_f	2.8×10^9	2.025×10^8			2.239×10^{12}	1.7×10^8		
2_b	5.0×10^8	1.673×10^8			5.0×10^8	1.7×10^8		

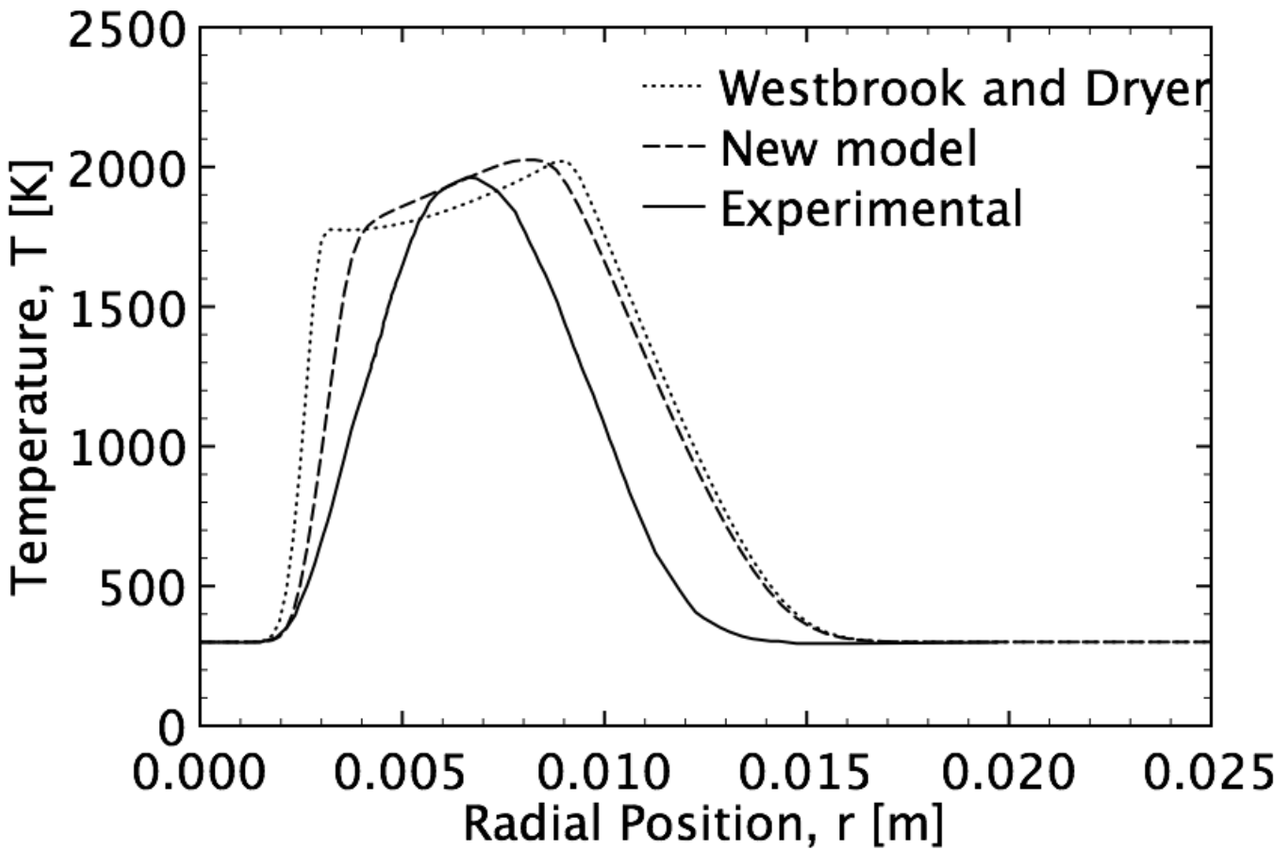
Table 2: New Arrhenius parameters for methane combustion mechanism.

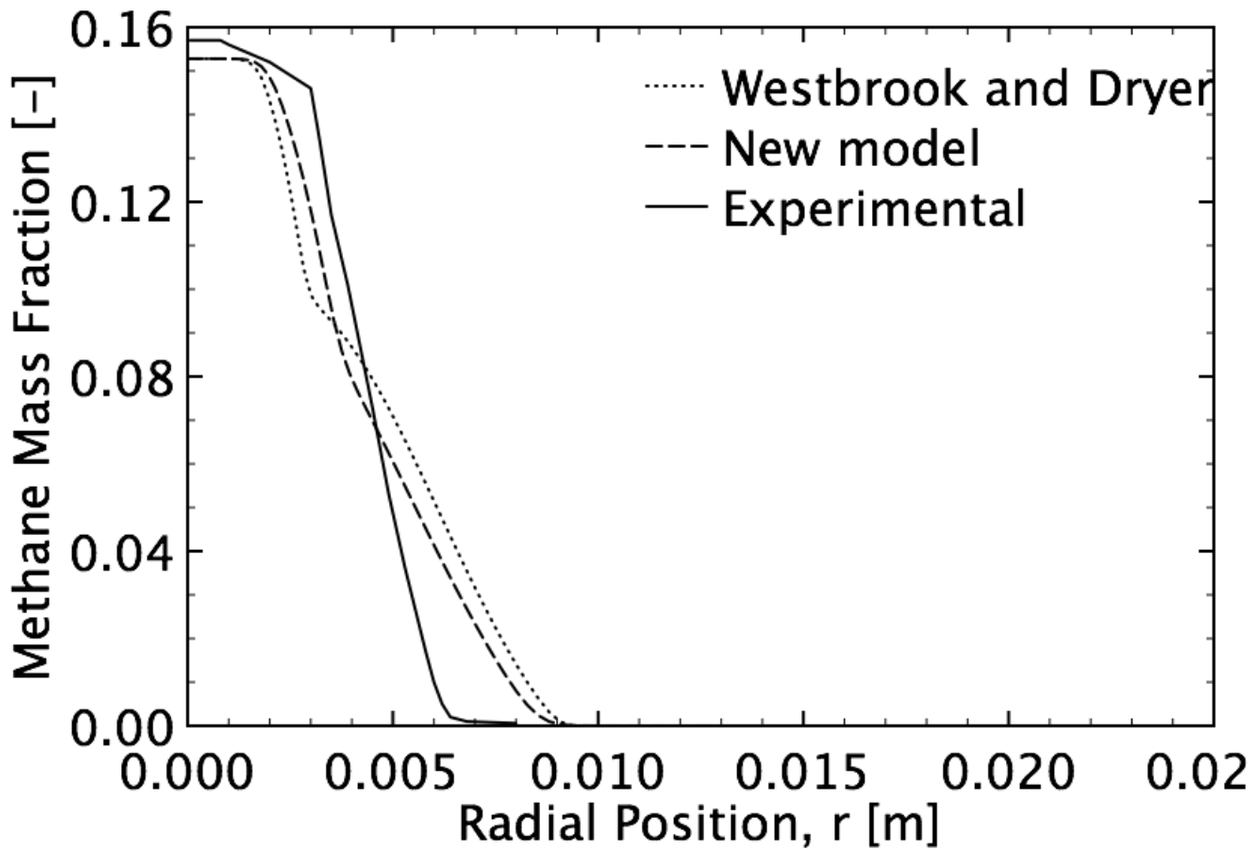
Reaction	A [–]	β [–]	E [J/kmol]
1	3.2926×10^8	2.2414	2.2888×10^8
2_f	6.8573×10^6	-0.6022	-9.0211×10^4
2_b	1.4286×10^9	2.8571	7.1429×10^8

Zero violations of entropy inequality
No need for temperature limiter

Temperature & Methane Mass Fraction

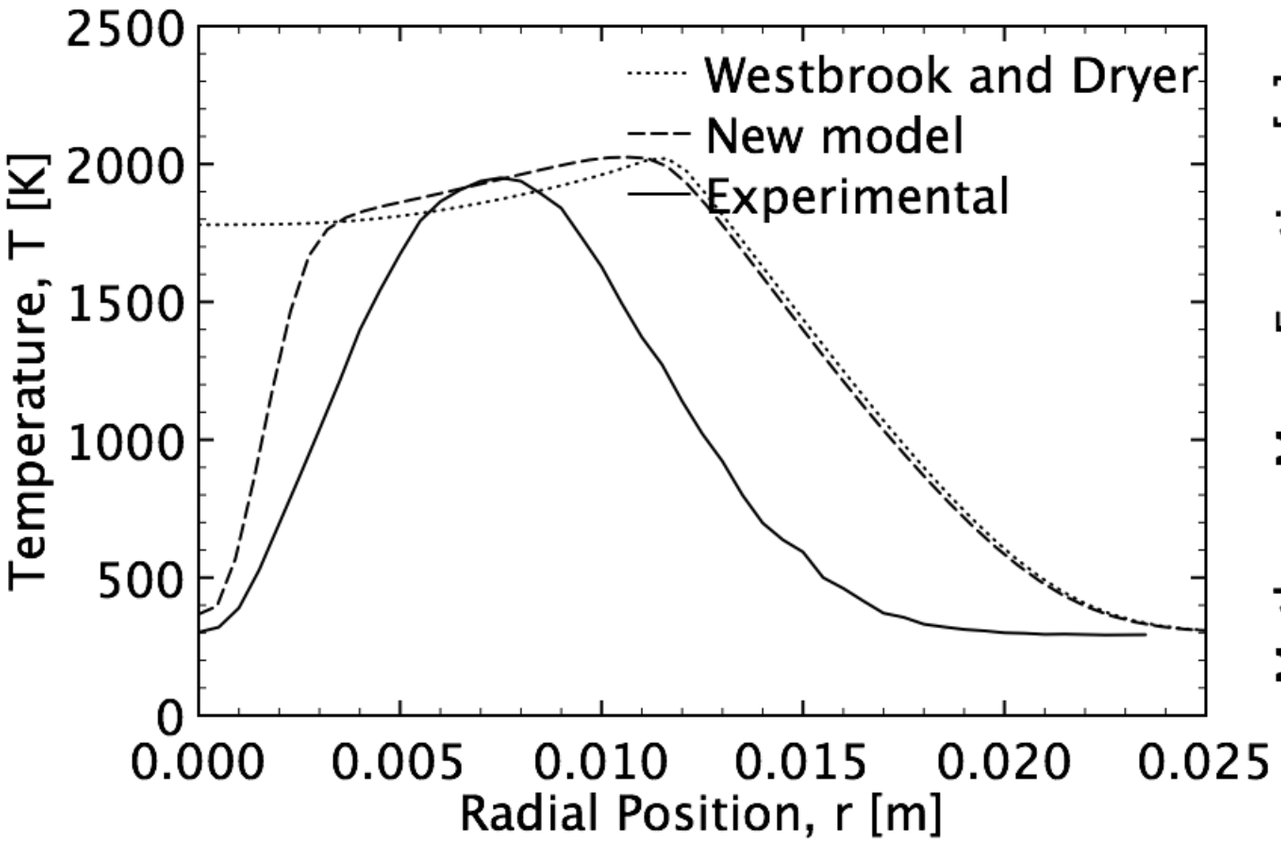
25 mm

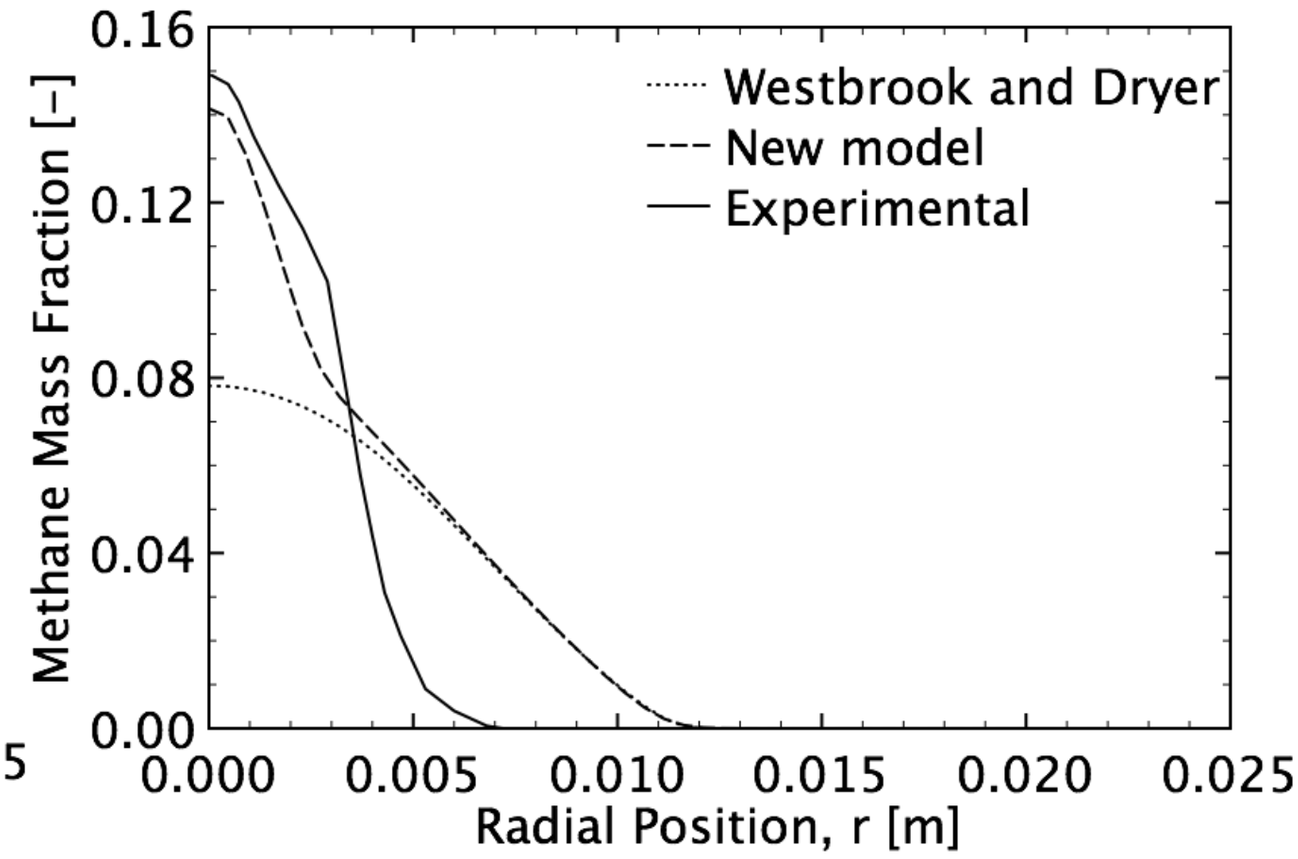




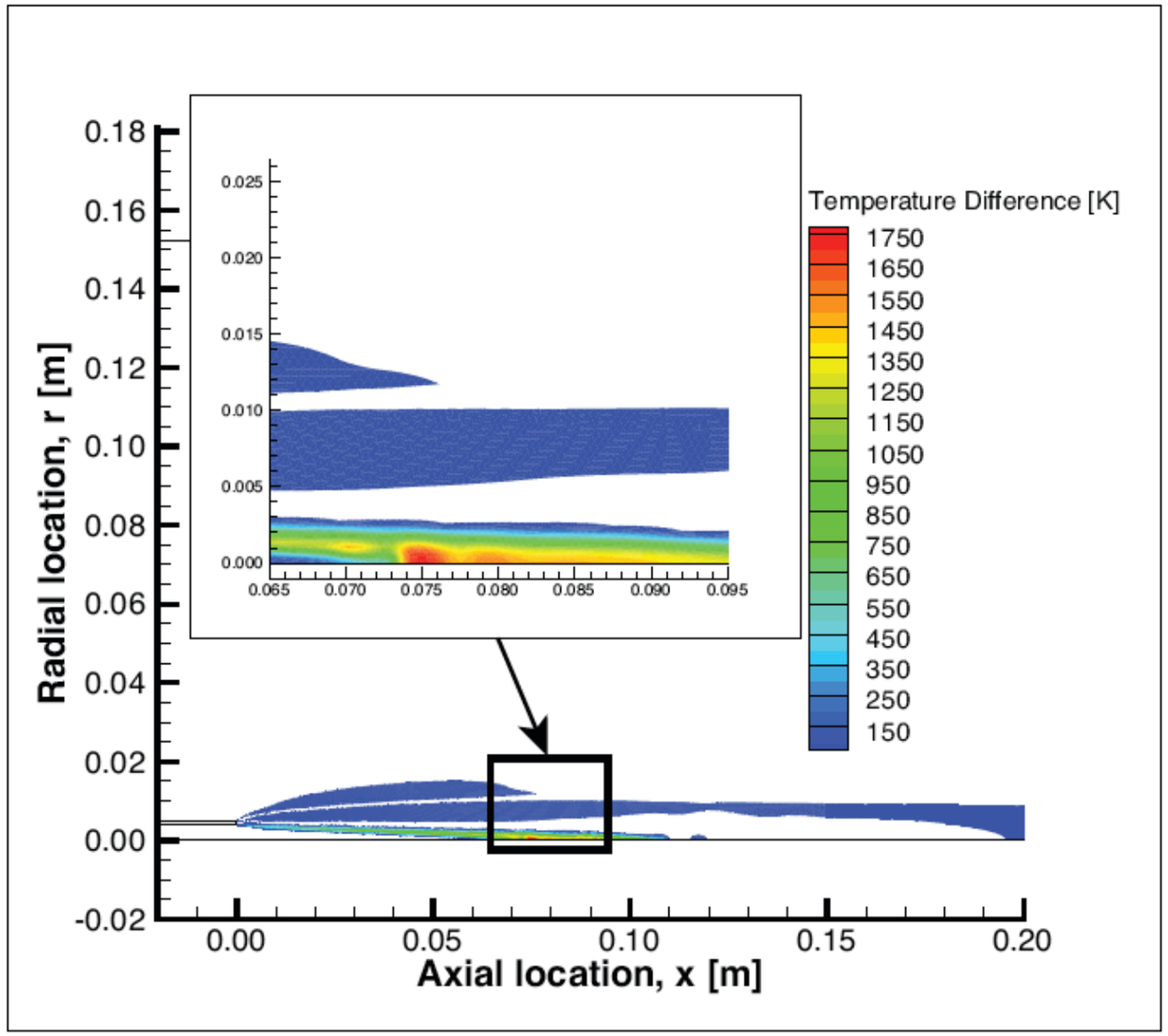
Temperature & Methane Mass Fraction

100 mm

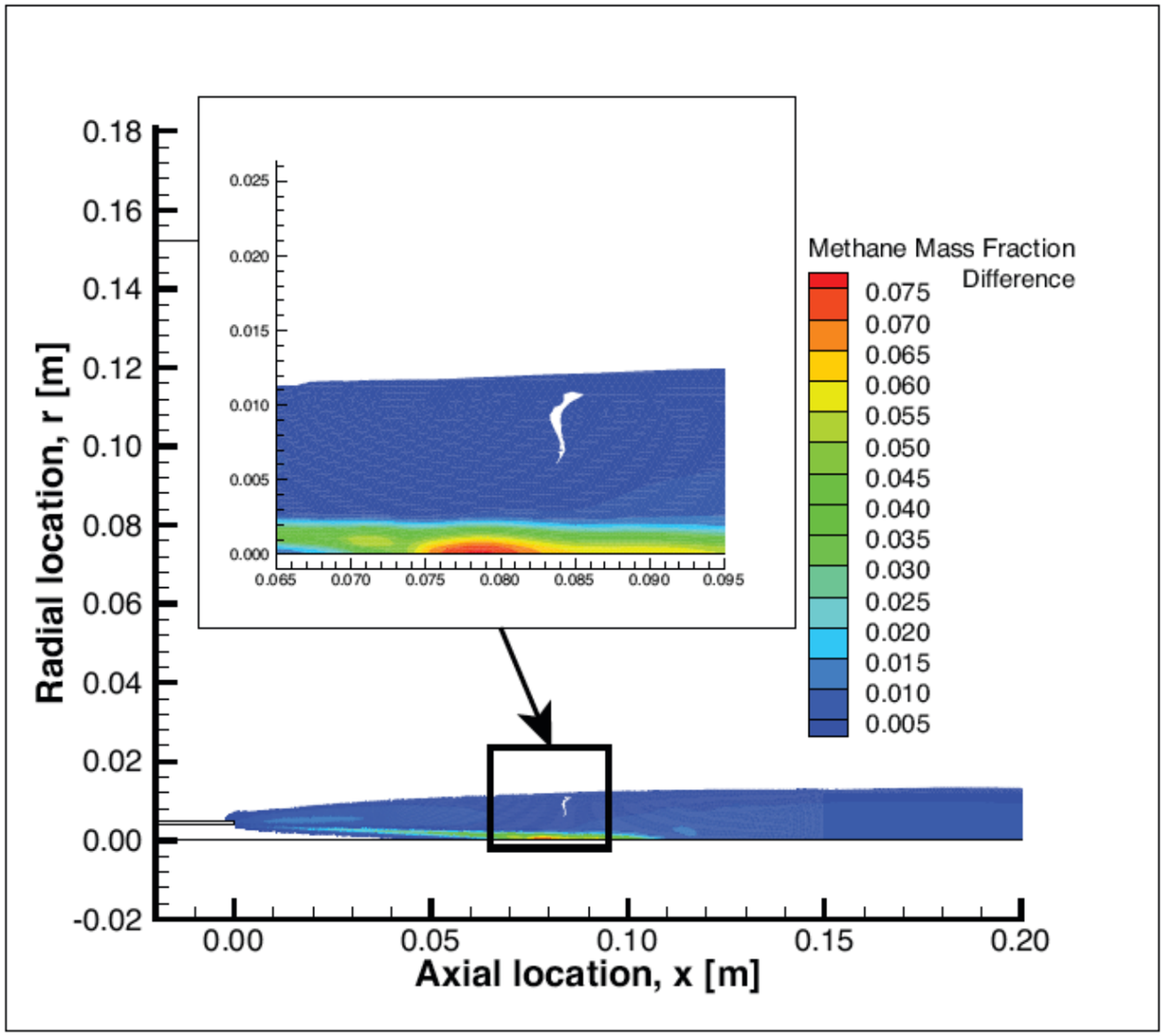




Temperature and Methane Mass Fraction Differences



(a)



(b)