DEVELOPMENT OF REDUCED ORDER MODEL FOR REACTING GAS-SOLID FLOW USING PROPER ORTHOGONAL DECOMPOSITION

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Outline

- Introduction
- Project Objectives
- Basic Concepts of Mathematical Modeling
- Validation of ROM for flows with heat transfer
- Constrained ROM for improved stability
- Development of ROM for Chemically Reacting Flows

Introduction

- Need for mathematical modelling of multiphase flow devices in fossil fuel processing plants
- Highly coupled nature of partial differential equations representing such flows
- Tremendous computational time requirements for the numerical simulation of transient transport phenomena
- Application of POD based ROM to reduce computational time in multiphase flows is a prominent approach

Statement of Project Objectives

- Supports the vision of the NETL 2006 Workshop on Multiphase Flow Research[1]:
  - ”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.

- Computational advances will be provided to NETL’s open-source CFD tool MFIX and validation cases will be provided.

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

Statement of Project Objectives

- 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.”
- 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
- Maintain and upgrade the educational, training and research capabilities of Florida International University

Current Focus

- Validation of ROM for multiphase flows with heat transfer
  - Development of a test case for non-isothermal fluidized bed flow
  - Development of constrained ROM to improve the stability
- Development and validation of ROM for chemically reacting multiphase flows with heat transfer
  - Reduced kinetics model for Methane combustion
  - Satisfying the Entropy Inequality Equation
  - Development of a test case for validation

Reduced Order Modeling (ROM)

- To reduce computational time by a factor of 100+
- To quantify accuracy of ROM with respect to FOM
- Several methods for model reduction
  - Transfer Function Interpolation
  - Krylov Subspace method
  - Proper Orthogonal Decomposition

Proper Orthogonal Decomposition (POD)

- Powerful method of data analysis aimed at obtaining low dimensional approximate descriptions of high-dimensional processes

- Provides optimal basis for modal decomposition of data set

- Extracts time-independent orthonormal basis function and time-dependent amplitude coefficients

$$u(x,t_i) = \sum_{k=1}^{M} \alpha_k(t_i)\,\varphi_k(x), \qquad i = 1,\dots,M$$

Modal Decomposition (Method of Snapshots)

- Reconstruction such as to minimize least square truncation error

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

- Equivalent to finding basis functions that maximizes the average normalized projection of the basis functions onto the snapshots

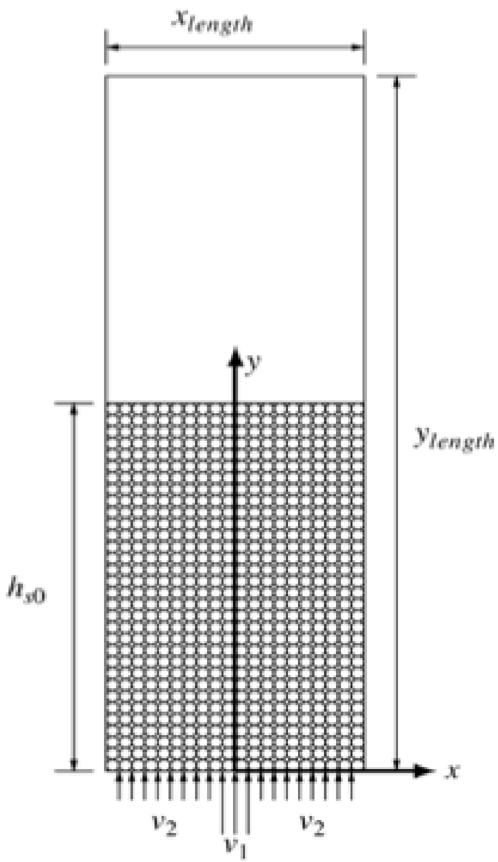
$$\max_{\phi \in L^2(\Omega)} \frac{\left\langle \left| (u,\phi) \right|^2 \right\rangle}{\|\phi\|^2}$$

- Condition reduces to: $\int_{\Omega} \langle u(x) u^*(y) \rangle \phi(y)\, dy = \lambda \phi(x)$

- Simplifies to eigenvalue problem: $R(x,y)\Phi(x) = \lambda \Phi(y)$

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

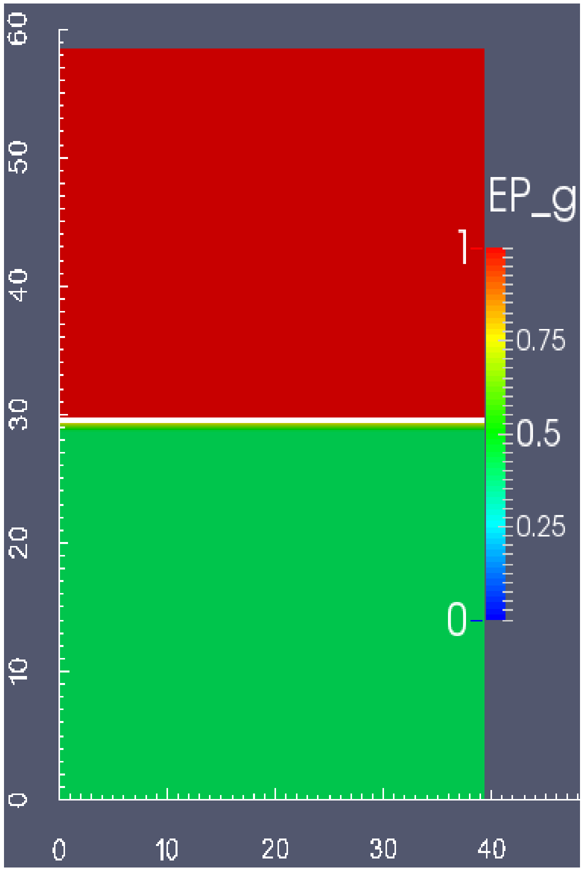
Non Isothermal Fluidized Bed

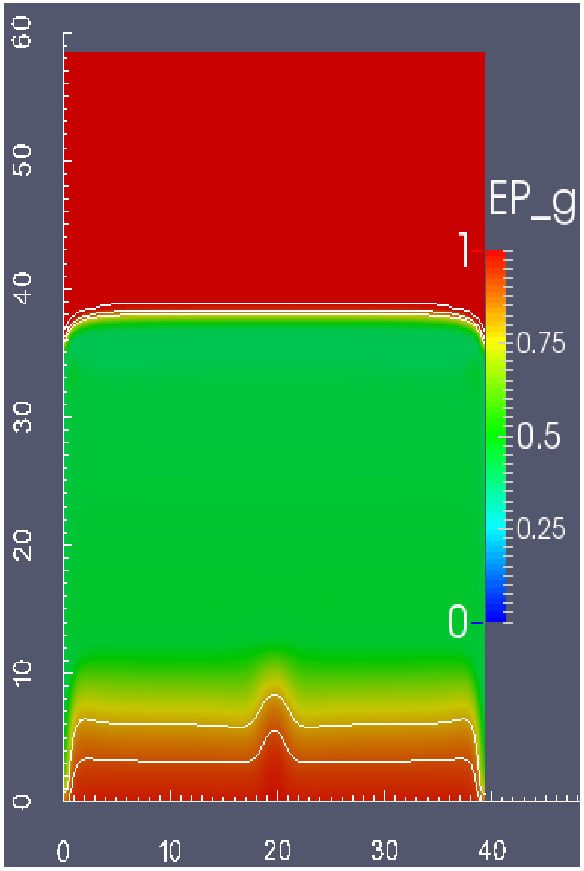


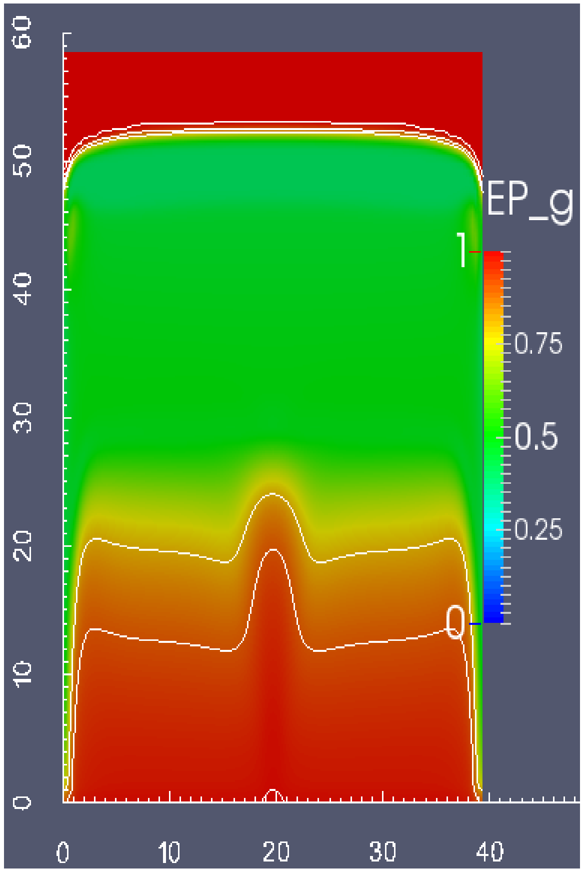
Gas: Air
Solid: Ottawa Sand

Parameter	Description	Units	Value
Xlength	Domain length X direction	cm	39.37
Ylength	Domain length Y direction	cm	58.44
Imax	# of cells in X direction	-	124
Jmax	# of cells in Y direction	-	108
V1	Vertical Jet Velocity	cm/sec	577
V2	Vertical Co-flow Velocity	cm/sec	284
Pg	Static Pressure at Outlet	$g/cm/s^2$	$1.01e^6$
Tg	Gas Temperature	K	450
Ts	Solids Temperature	K	297
μ_g	Gas Viscosity	g/cm/s	$1.8e^{-4}$
ρ_s	Particle Density	g/cm^3	2.61
D_p	Particle Diameter	cm	0.05
h_{so}	Packed Bed Height	cm	29.22

Void Fraction for the Non-Isothermal Fluidized Bed Flow

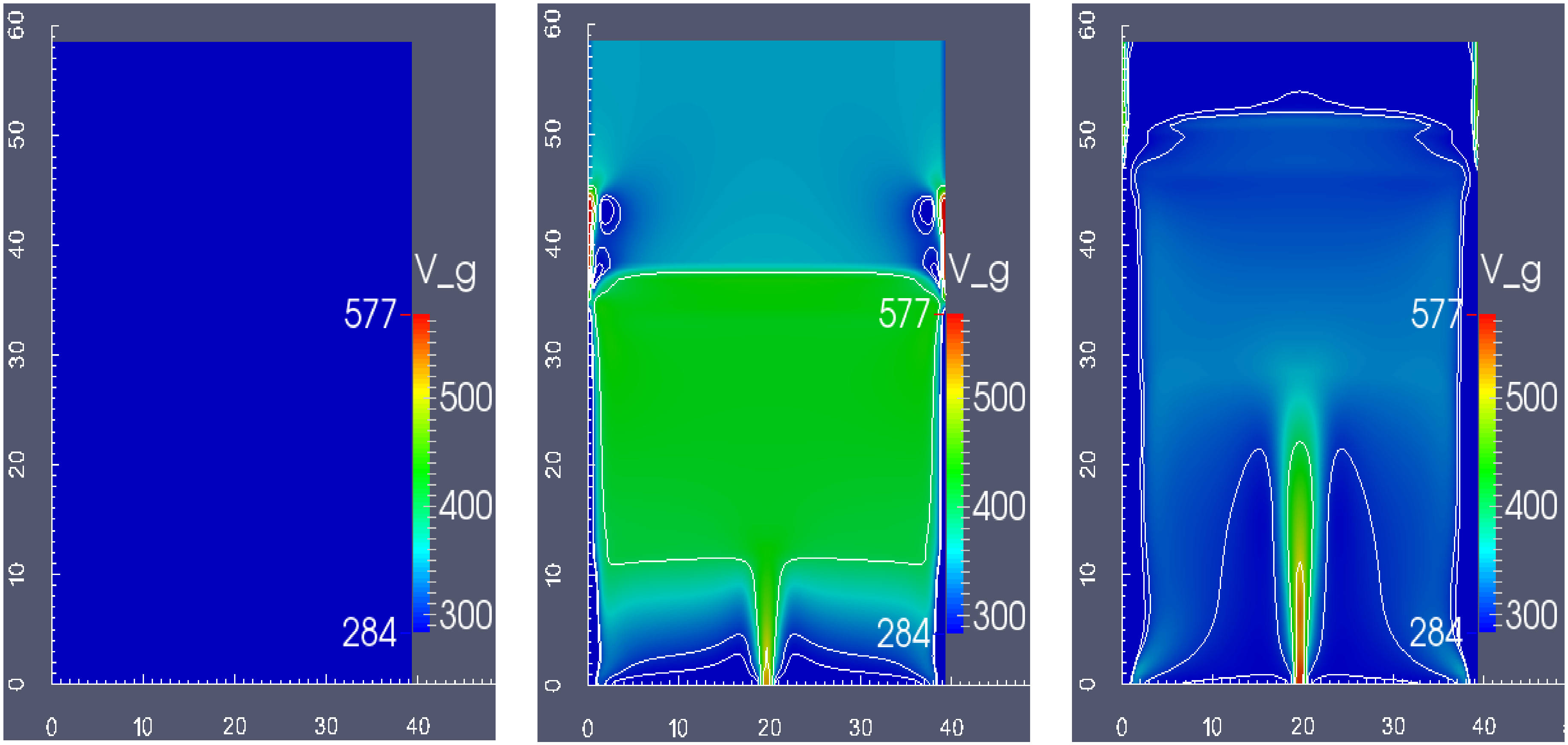






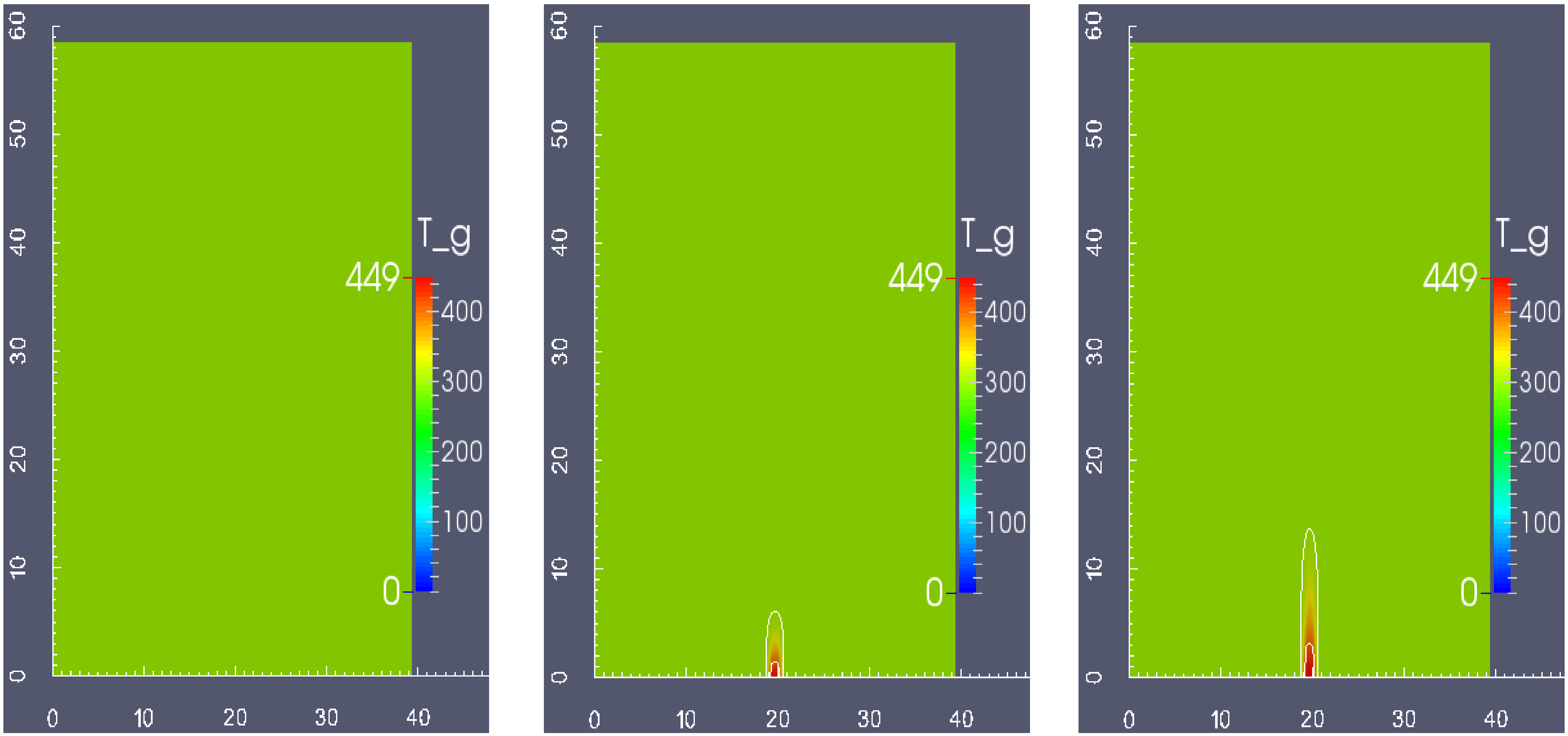
0 Sec	0.05 Sec	0.1 Sec

Vertical Gas Velocity for the Non-Isothermal Fluidized Bed Flow



0 Sec	0.05 Sec	0.1 Sec

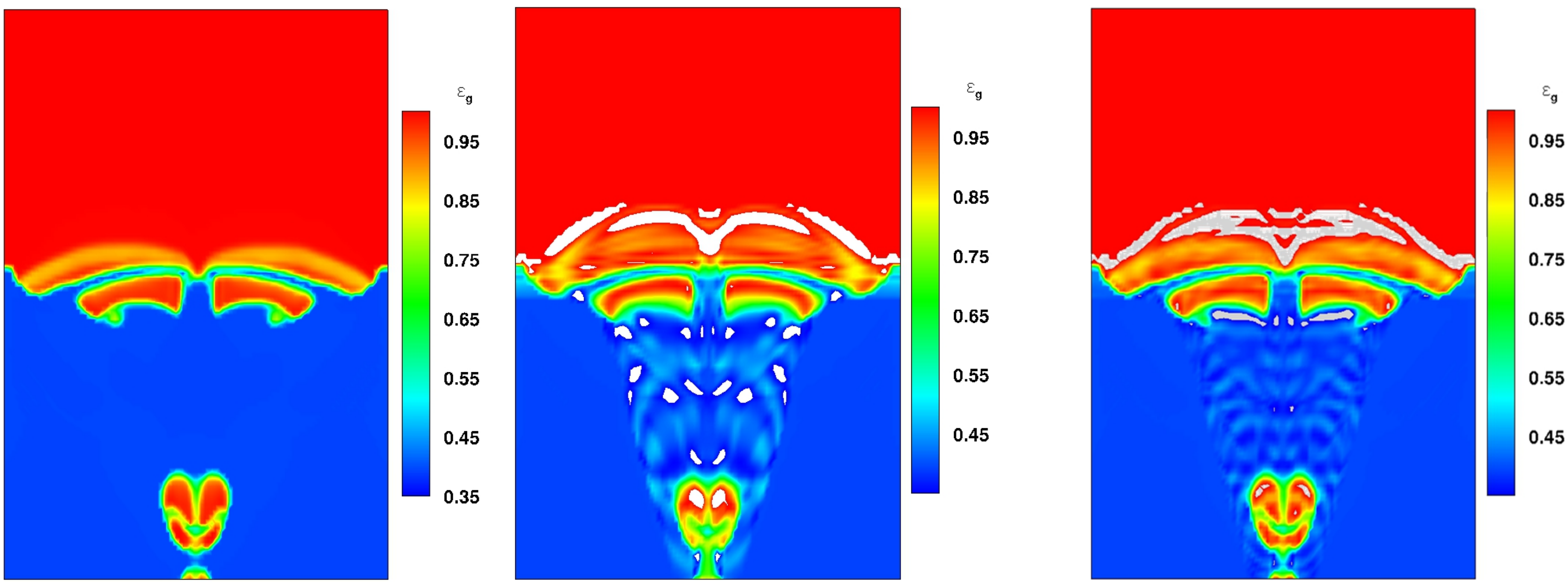
Gas Temperature for the Non-Isothermal Fluidized Bed Flow



0 Sec	0.05 Sec	0.1 Sec

Isothermal Fluidized Bed

- Reconstruction of a void fraction when bubbles (discontinuities) are present leads to infeasible results



FOM　　ROM (16 modes)　　ROM (32 modes)

Karush-Kuhn Tucker (KKT) Conditions

- Heavily used in mathematical optimization for satisfying equality and inequality constraints

- First Order Conditions

  - Minimize f subjected to $g_i \leq 0$
  - Stationary Condition $\nabla f + \sum_{i=1}^{m} \lambda_i \nabla g_i = 0$
  - Complementary Slackness $\lambda_i g_i = 0$
  - Non-Negative Lagrange Multipliers $\lambda_i \geq 0$

Application of KKT Conditions to Gas Void Fraction

- Function to minimize $J = \left\| \tilde{A}^{\varepsilon_g} \alpha^{\varepsilon_g^{'}} - \tilde{B}^{\varepsilon_g} \right\|^2$

  subject to: $\varepsilon_g \leq 1.0 \longrightarrow \varepsilon_g = \varepsilon_g^* + \Phi \alpha'$

- Stationary Condition: $J_{\alpha'} = 2\tilde{A}^T \tilde{A} \alpha' - 2\tilde{A}^T \tilde{B} + \Phi^T \lambda = 0$
- Constraint: $g_1 : \varepsilon_g^* + \Phi \alpha' - 1.0 \leq 0$

$$\begin{bmatrix} 2\tilde{A}^T \tilde{A} & \Phi^T \\ \Phi & 0 \end{bmatrix} \begin{Bmatrix} \alpha' \\ \lambda \end{Bmatrix} = \begin{Bmatrix} 2\tilde{A}^T \tilde{B} \\ 1.0 - \varepsilon_g^* \end{Bmatrix}$$

Chemically Reacting Flows

- Accurate representation of reaction mechanism and rate

- Reduced kinetics model for a chemical reaction
  - Motivation
    - Model Complexity
    - Increased Computational Time

- Importance of satisfying entropy inequality equation

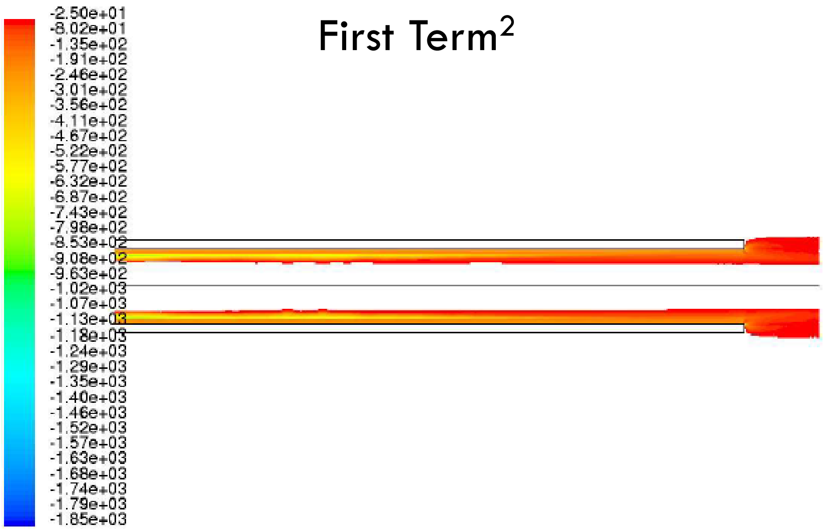
Entropy Inequality Equation (EIE)

$$-tr[(\boldsymbol{T} + PI).D] + \frac{1}{\mathrm{T}}\boldsymbol{\epsilon}.\nabla T +$$
$$cRT\sum_{B=1}^{N} j_{(B)}\cdot\frac{d_{(B)}}{\rho_{(B)}} + \sum_{j=1}^{K}\sum_{B=1}^{N}\mu(B)r(B,j) \leq 0$$

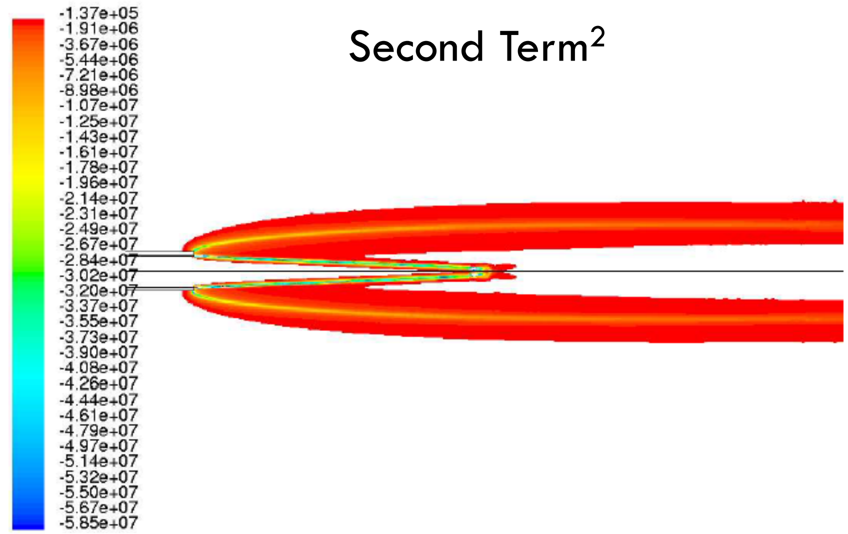
- T -Stress Tensor
- P -Thermodynamic Pressure
- I – Identity Matrix
- D-Rate of Deformation Tensor
- c- Total Molar Density
- R- The Gas Law Constant
- T- Temperature
- N- Number of Species
- J(B)- Mass flux of Species B relative to v
- ρ(B) – Mass density of Species B
- K- Number of Reactions
- $\mu(B)$-Chemical Potential of Species B
- $r(B,j)$- Rate of Production of moles of species B per unit volume by homogeneous chemical reaction j

EIE for Methane Combustion

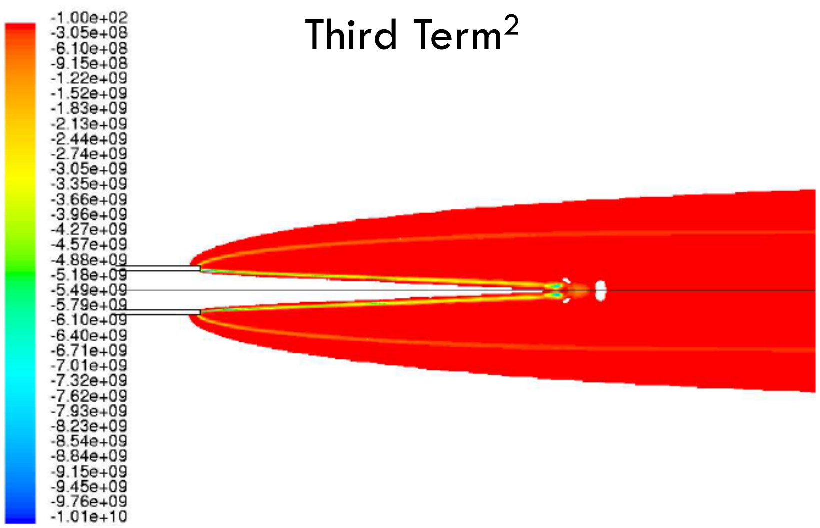
First Term[2]



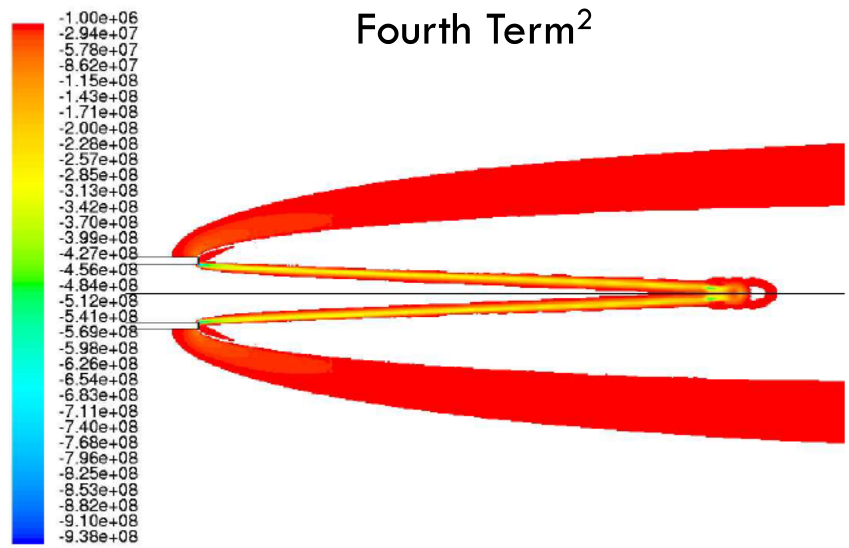
Second Term[2]



Third Term[2]



Fourth Term[2]



[2]Chambers,S.B. (2005). Investigation of combustive flows and dynamic meshing in computational fluid dynamics (M.Sc Thesis, Texas A&M University).

Reduced Kinetics Model for Methane Combustion

- Basic Reaction Equations

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O \qquad \text{------}1$$

$$CO + 0.5O_2 \leftrightarrow CO_2 \qquad \text{------}2$$

- Calculation of Rate of Reaction

$k_1 = A_1 e^{\frac{(\frac{E1}{R})}{T}} [CH_4]^{0.7} [O_2]^{0.8}$ Where $A_1 = 5.012 * 10^{11} s^{-1}$, $\frac{E_1}{R} = 24054\,^{\circ}K$

$k_{2f} = A_{2f} e^{\frac{(\frac{E2f}{R})}{T}} [CO_2]^1 [O_2]^0 0.25 [H_2O]^0 * 0.5$

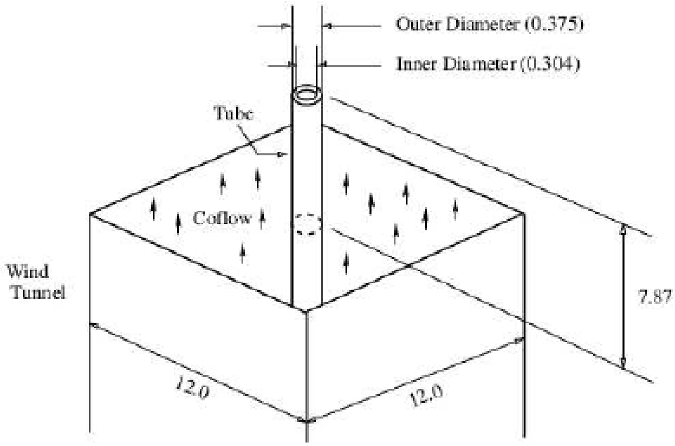
Where $A_{2f} = 2.239 * 10^{12} (m^3/Kmol)^{0.75} s^{-1}$, $\frac{E_{2f}}{R} = 20807\,^{\circ}K$

$k_{2b} = A_{2b} e^{\frac{(\frac{E2b}{R})}{T}} [CO_2]^1$

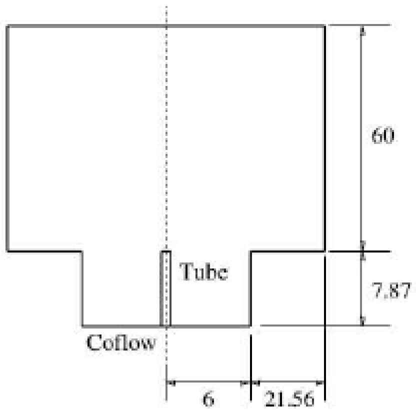
Where $A_{2b} = 5 * 10^8 (m^3/Kmol)^{0.75} s^{-1}$, $\frac{E_{2b}}{R} = 20807\,^{\circ}K$

Methane Combustion Test Case

- Methane is injected through central tube at 285 cm/sec
- Co-flow consists of air at 40 cm/sec



Species Mass Fraction at boundaries		
Species	Central Tube	Co-Flow
CH_4	0.1527	0
O_2	0.1944	0.2295
CO_2	0.0004	0.0005
H_2O	0.0066	0.0078
N_2	0.6459	0.7491



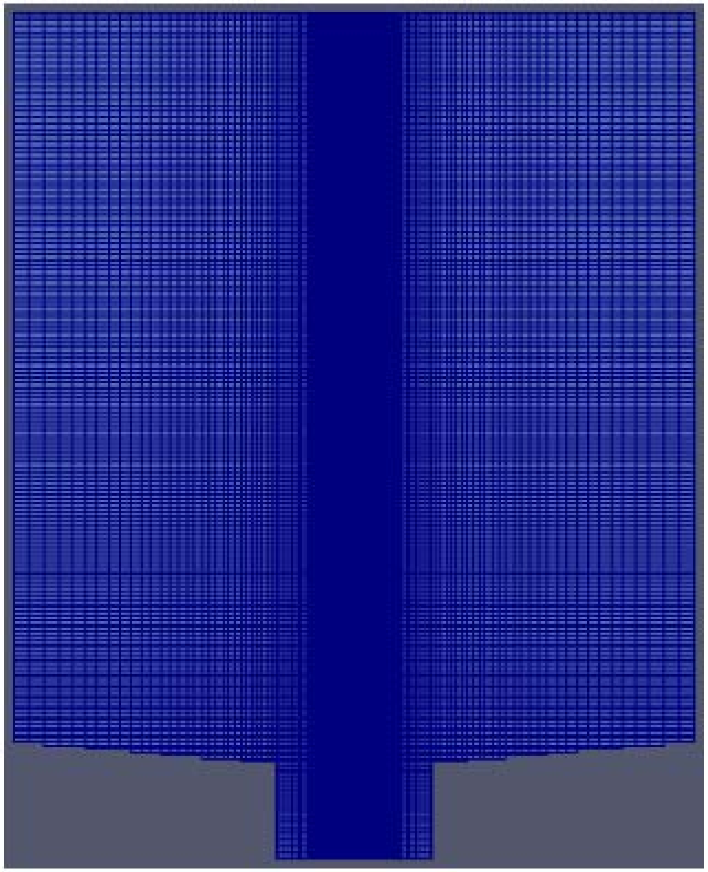
All dimensions are in inches
Drawing is not to the scale

Methane Combustion Case in MFIX

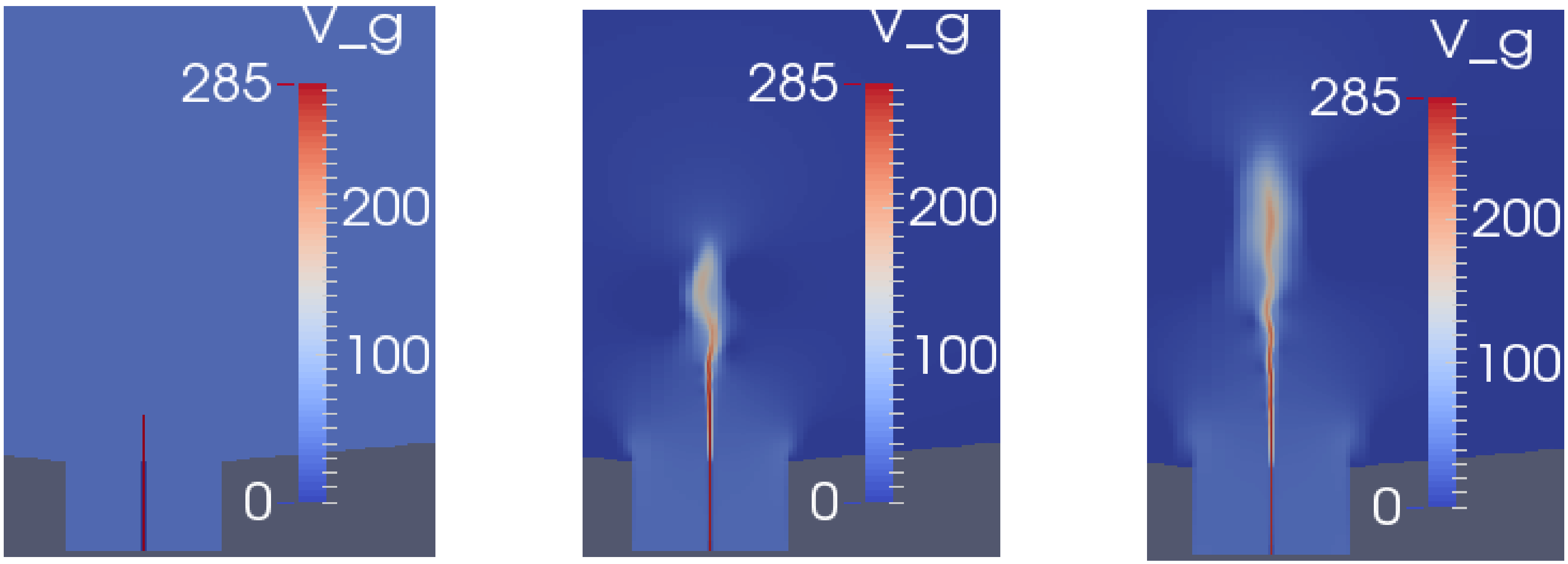
- Converging-Diverging Grid using Cut Cell Technique

Sr #	X_West	X_East	Length (cm)	# of cells	ERX
1	0	69.524	69.524	70	0.045
2	69.524	69.614	0.09	2	1
3	69.614	70.386	0.772	4	1
4	70.386	70.476	0.09	2	1
5	79.476	140	69.524	70	22.071

Sr #	Y_ North	Y_ South	Length (cm)	# of cells	ERY
1	0	20	20	20	0.5
2	20	193	173	173	2

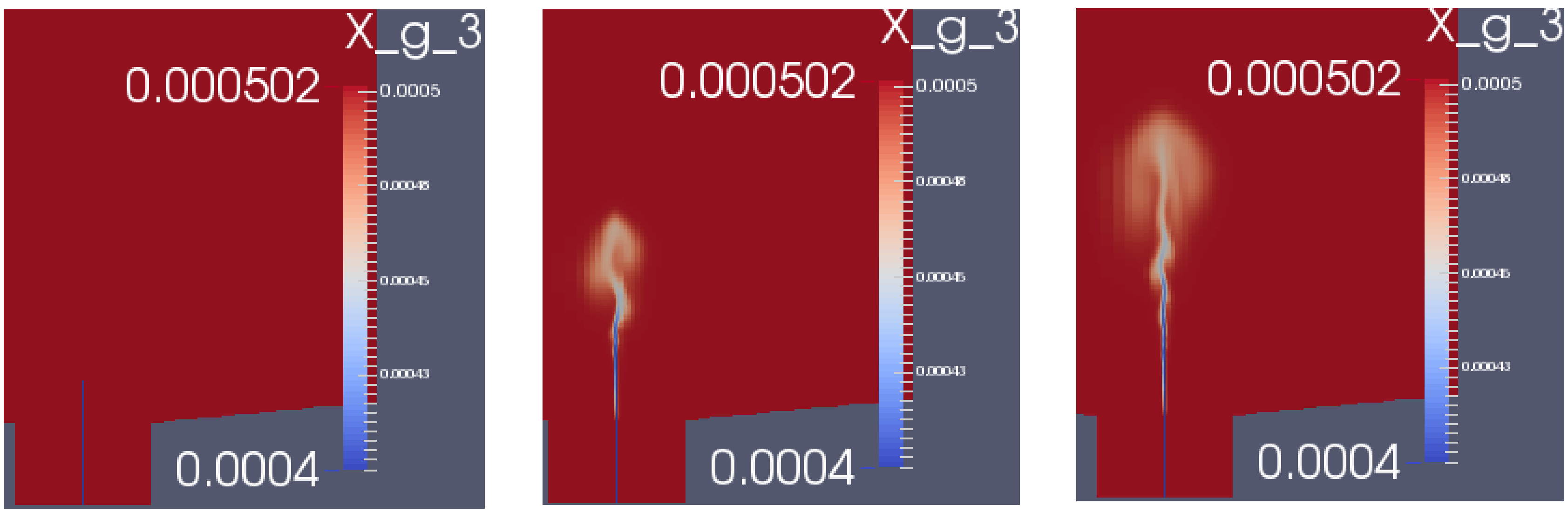


Vertical Gas Velocity in FOM



0 Sec	0.4 Sec	0.8 Sec

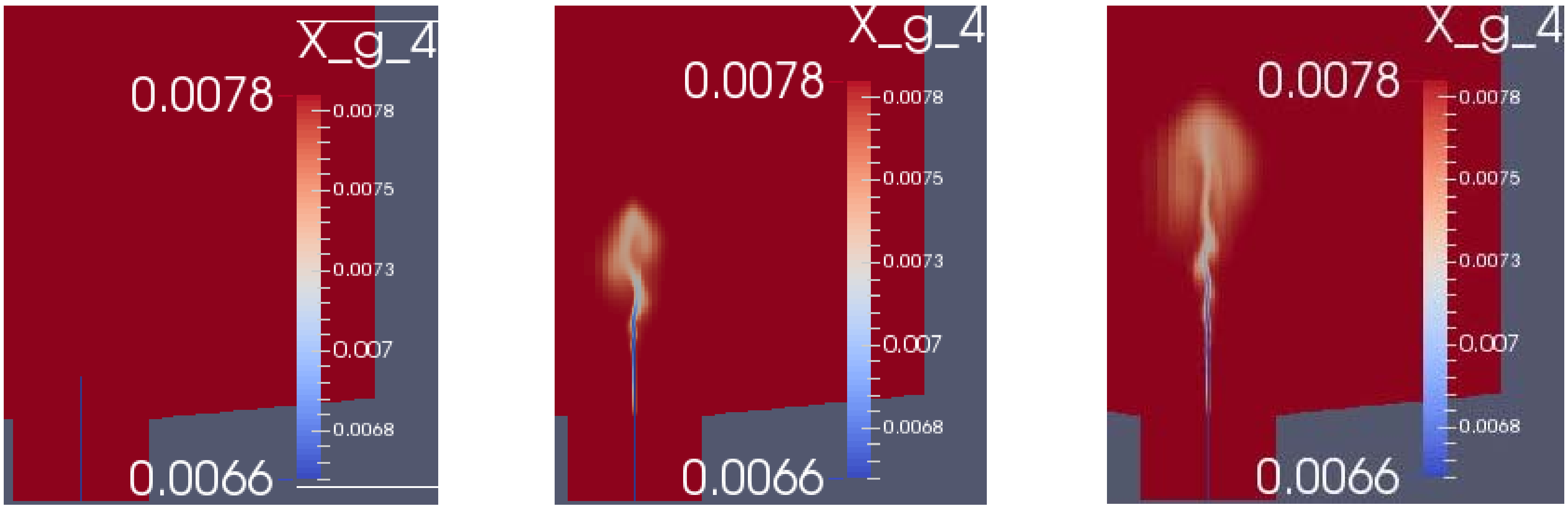
Product Species Mass Fraction in FOM



0 Sec	0.4 Sec	0.8 Sec

- The above graphs show mass fraction of CO_2 in the domain at 0, 0.4 and 0.8 sec

Product Species Mass Fraction in FOM



0 Sec	0.4 Sec	0.8 Sec

- The above graphs show mass fraction of H_2O in the domain at 0, 0.4 and 0.8 sec

Conclusion

- Successfully developed test case for validation of ROM for flows with heat transfer
- Application of KKT conditions to improve model stability is in process
- Developed test case for validation of ROM for flows with reacting flows

Acknowledgements

U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

Thank You

Governing Equations

- **Continuity Equation**

$$\frac{\delta}{\delta t}\left(\varepsilon_g \rho_g\right) + \nabla . \left(\varepsilon_g \rho_{g \underset{vg}{\rightarrow}}\right) = \sum_{n=1}^{N_g} R_{gn}$$

- **Gas phase Temperature Equation**

$$\varepsilon_g \rho_g C_{pg} \left(\frac{\partial T_g}{\partial t} + \vec{v}_g . \nabla T_g\right) = -\nabla . \overrightarrow{q_g} - H_{g1} - H_{g2} - \Delta H_{rg} + H_{wall}\left(T_{wall} - T_g\right)$$

Governing Equations

- **Gas phase momentum Equation:**

$$\frac{\delta}{\delta t}\left(\varepsilon_g \rho_g \underset{v_g}{\rightarrow}\right) + \nabla . \left(\varepsilon_g \rho_g \underset{v_g}{\rightarrow} \underset{v_g}{\rightarrow}\right) = \nabla . \overline{\overline{S}}_{g+} \varepsilon_g \rho_g \vec{g} \sum_{l=1}^{M} \overrightarrow{I_{gm}}$$

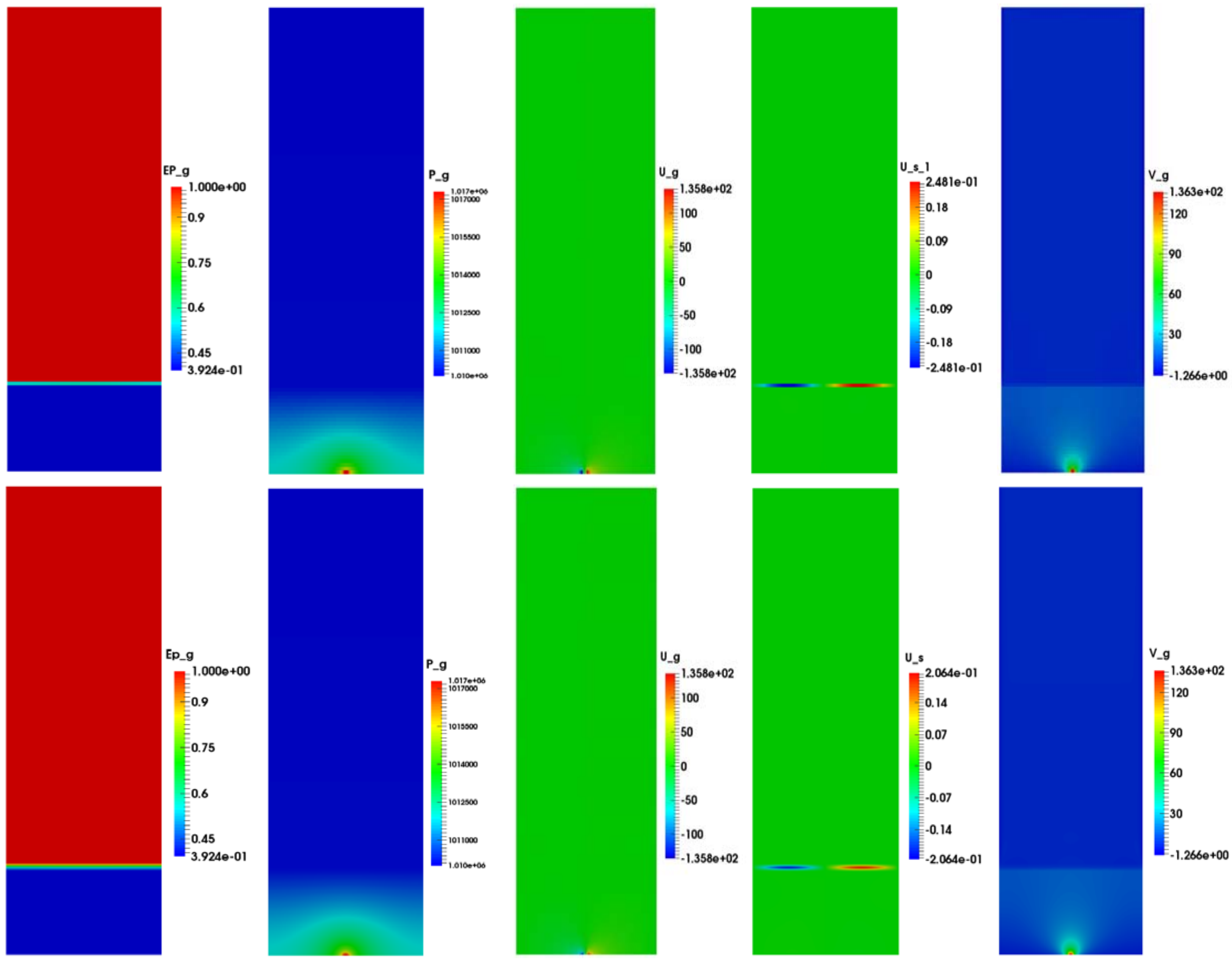
- **Species Mass Balance Equation:**

$$\frac{\delta}{\delta t}\left(\varepsilon_g \rho_g X_{gn}\right) + \nabla . \left(\varepsilon_g \rho_g X_{gn_{\vec{vg}}}\right) = \sum_{n=1}^{N_g} R_{gn}$$

Validation of ROM for Isothermal Fluidized Bed

Full Order Model (FOM)

Reduced Order Model (ROM)



Validation of ROM with KKT conditions