Implementing General Framework in MFiX for Radiative Heat Transfer in Gas–Solid Reacting Flows

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V M K Kotteda
Postdoctoral Researcher
University of Wyoming

David Tobin
Master Student
University of Wyoming

Michael Stoellinger
Associate Professor of Mechanical Engineering
University of Wyoming

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UNIVERSITY OF WYOMING

NATIONAL ENERGY TECHNOLOGY LABORATORY

Outline

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1. Project Description and Objectives
2. Project Update
3. Preparing Project for Next Steps
4. Concluding Remarks

1. Project Description and Objectives

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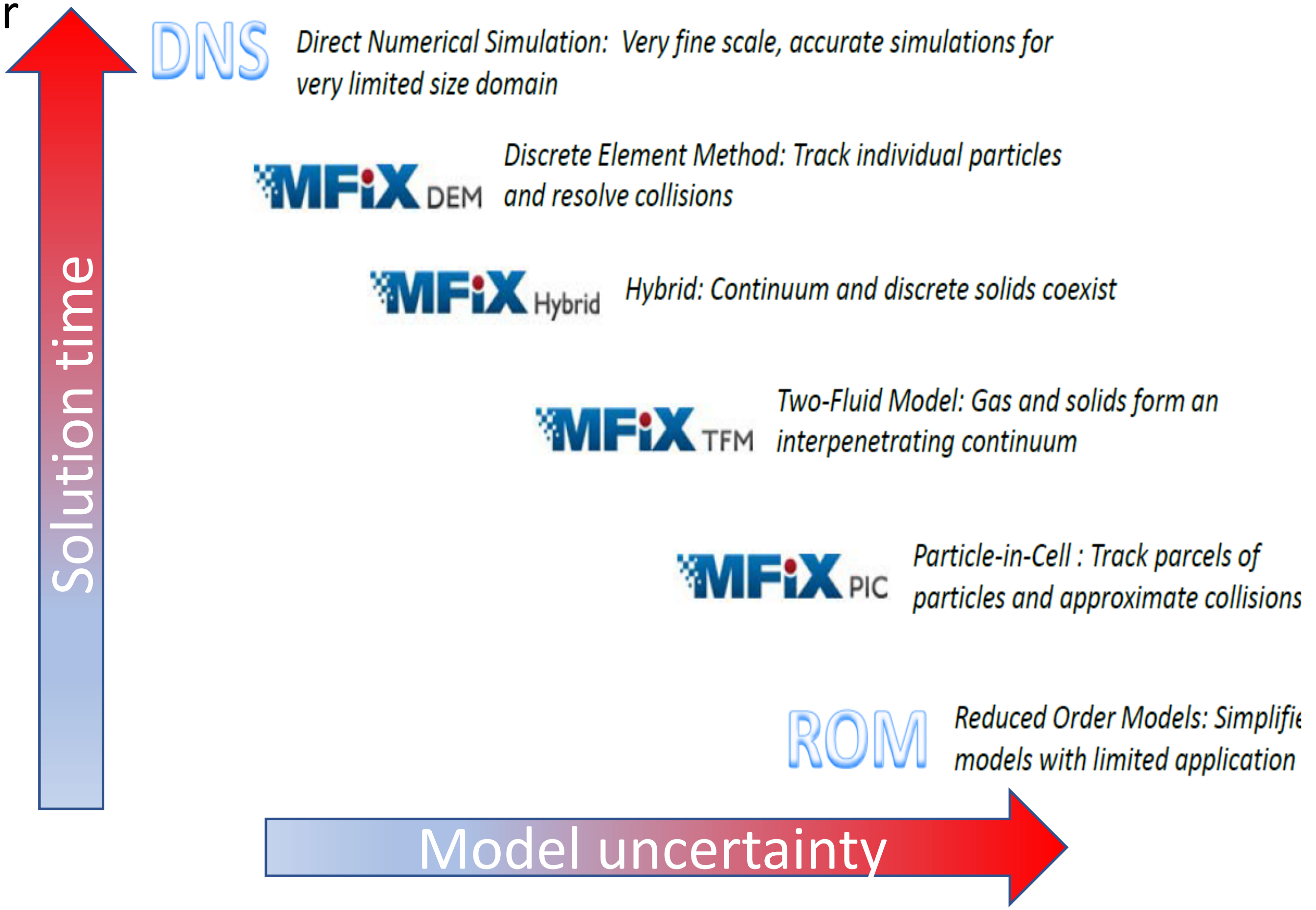
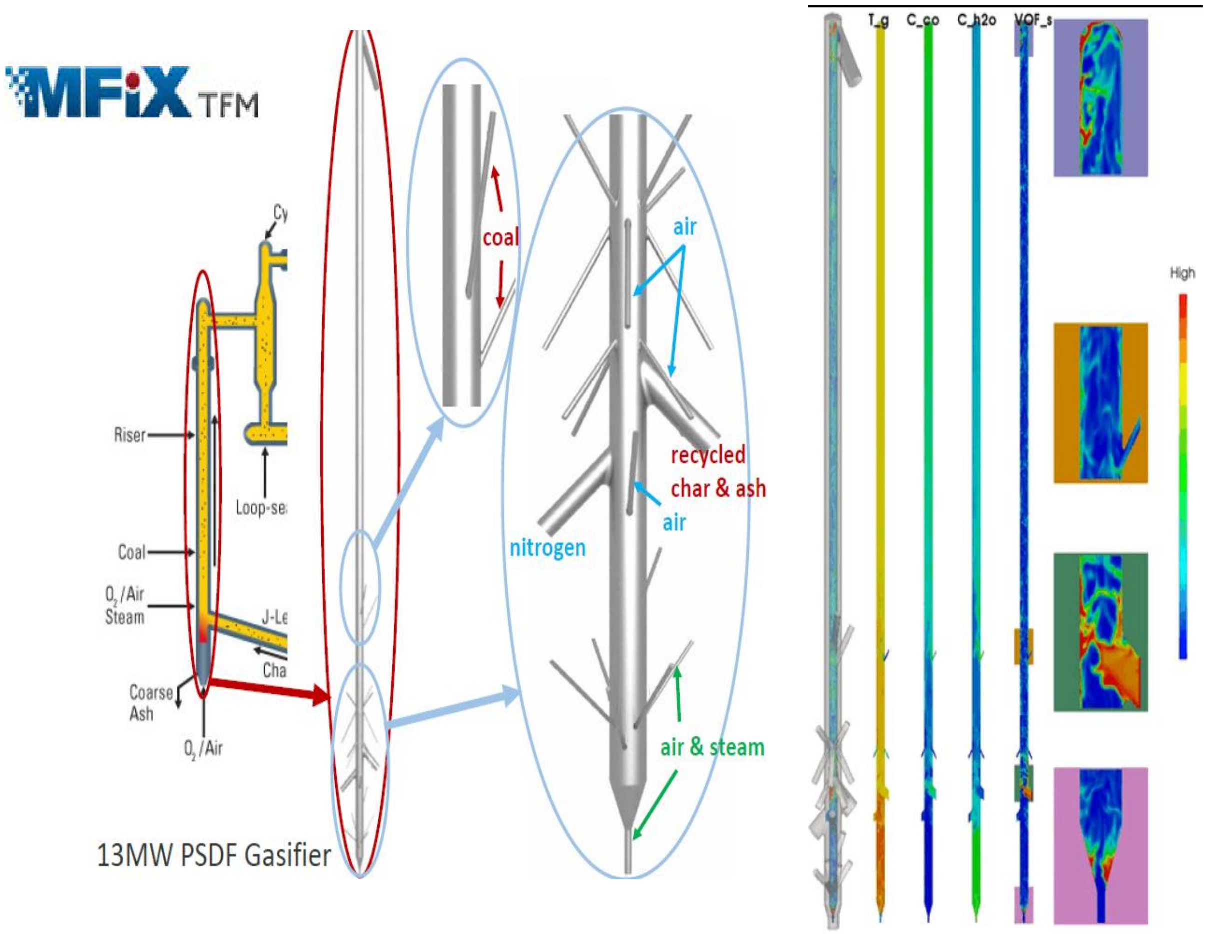
NETL's MFiX —Multiphase Flow with Interphase eXchange

- Central to the laboratory's multiphase flow reactor modeling efforts
- Provides support to achieve DOE's goals
  1. Cost of Energy and Carbon Dioxide (CO2) Capture from Advanced Power Systems
  2. Power Plant Efficiency Improvements
- Built with varying levels of fidelity/computational cost
  - Lower fidelity models for large scale reactor design
  - High fidelity models to support the development of lower fidelity models



1. Project Description and Objectives
Status of the beginning of the project



Results from : "Fluidized Beds – recent applications", W. Rogers, 215 IWTU Fluidization Workshop

High-end validation study:

- Fine grid with 1.3M cells
- Two solid phases (coal and recycled ash)
- Detailed gasification chemical kinetic (17 gas species, 4 solid species)

What was missing the in the model?

No real radiative heat transfer modeling available in MFiX!

Driving Question/Motivation

Enhance MFiX capabilities by including models for radiative heat transfer following MFiX's multi-fidelity approach

1. Project Description and Objectives

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MFIX-RAD development plan

Research Models (used for benchmarking)

PMC + Line-by-line model (full spectral resolution ~10 million lines) -> model error free

PMC + Weighted Sum of Gray Gases (WSGG) model

Industrial Model (main application)

P1 + WSGG model (gas & particles)

P1 + WSGG model & gray particles

Usable in MFIX-TFM and MFIX-DEM!

P1 + Gray gas & particle model (neglect all spectral variations)

P1 + gray constant (neglect all spectral and spatial variations)

"Basic Model"

Solution time

Model uncertainty

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2. Project Update

We have received a 1 year, no cost extension

	Year 1				Year 2				Year 3				Year 4			
Tasks	10/17	01/18	04/18	07/18	10/18	01/19	04/19	07/19	10/19	01/20	04/20	07/20	10/20	01/21	04/21	07/21
T-1: Project Management and Planning																
T-2: Testing of the previously developed MFIX-RAD Radiation Model Plug-In				1												
T-3: Implementing basic radiation model within MFIX-DEM							2									
T-4: Implementation and Verification of Industrial Models								3								
T-5: Industrial Model Application and Analysis										4						
T-6: Development of High-End Research Models													5			
T-7: Comprehensive Validation and Benchmark																6

Done!

Near completion!

2. Project Update

Modeling approach

Energy equations for MFiX-TFM

Gas $$\varepsilon_g \rho_g c_{pg}\left(\frac{\partial T_g}{\partial t} + u_g . \Delta T_g\right) = \nabla q_g + \sum_{m=1}^{M} H_{gsm} - \Delta H_{rg} + H_{wall}(T_{wall} - T_g) - \nabla . \vec{q}_{rg}$$

Solids $$\varepsilon_{s_m} \rho_{s_m} c_{ps_m}\left(\frac{\partial T_{s_m}}{\partial t} + u_{s_m} . \Delta T_{s_m}\right) = \nabla q_{s_m} + \sum_{m=1}^{M} H_{gsm} - \Delta H_{rs_m} - \nabla . \vec{q}_{rs_m}$$

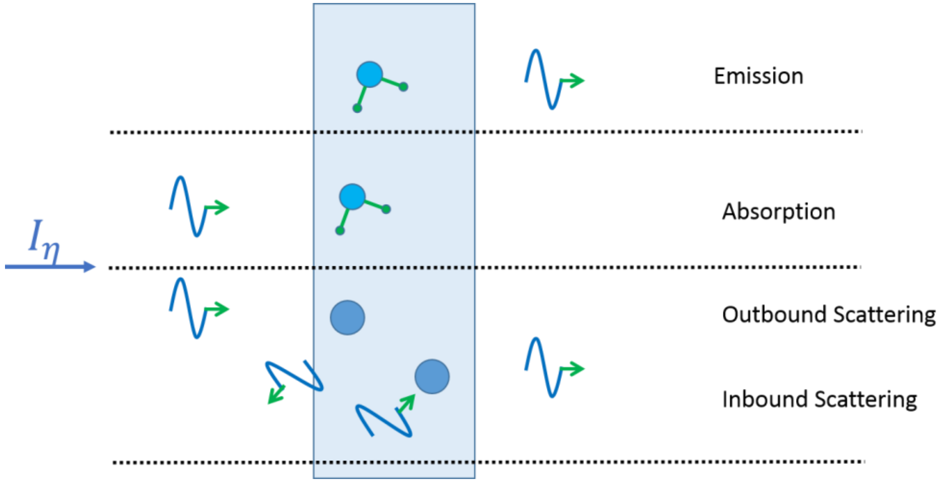
Single particle/parcel Energy equation for MFiX-DEM or MFIX-PIC

$$m_i c_{p,i} \frac{dT_i}{dt} = \sum_{n=1}^{N_i} q_{i,j} + q_{i,f} + q_{i,rad} + q_{i,wall}$$

Source/Sink Terms are obtained from the thermal radiation model!

2. Project Update

Modeling approach



$$\frac{dI_\eta}{ds} = \vec{s} \cdot \nabla I_\eta = a_\eta I_{b\eta}$$

$$-a_\eta I_\eta$$

$$-\sigma_{s\eta} I_\eta + \frac{\sigma_{s\eta}}{4\pi} \int I_\eta(\vec{s}\,')\Phi_\eta(\vec{s}, \vec{s}\,')d\Omega$$

The RTE is an integro-differental equation for the spectral intensity $I_\eta(x, y, z, \phi, \psi, \eta)$
(a function of 6 variables!)

Source term in the energy equation:

$$S_{rad} = \nabla \cdot \vec{q}_{rad} = \int_0^\infty a_\eta \left(4\pi I_{b\eta} - \int_{4\pi} I_\eta d\Omega\right) d\eta$$

G_η spectral incident radiation

Solution approach:

- 3 spatial dimensions $\vec{r}(x, y, z)$: CFD discretization
- 2 directional dimensions $\vec{s}(\phi, \psi)$: RTE solvers
- 1 spectral dimension (η): spectral models

2. Project Update

Modeling approach

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Gray P1 model assumptions

1) Gray participating medium (gas and solids) -> no dependence on wavenumber η

2) Use a "Fourier series" ansatz $I(\vec{r},\vec{s}) = \sum_{l=0}^{\infty} \sum_{-l}^{l} I_l(\vec{r}) \cdot Y_l(\vec{s})$ ← Spherical harmonics

Spatially varying coefficients

3) Keeping only the first term $l = 0$ leads to the P1 approximation

4) Solve a "combined" (including all phases) P1 equation for G (Helmholtz type)

$$\nabla.(\Gamma\, \nabla G) + 4\,\pi \left(a_g \frac{\sigma\, T^4}{\pi} + E_s \right) - (a_g + a_s) G = 0$$

$$\Gamma = \frac{1}{3(a_g + a_s + \sigma_s) - C\sigma_s}$$

Gas phase absorption

Solid phase absorption

Gas phase emission

Solid phases emission

2. Project Update
Modeling approach

Distributing the source terms with P1

$$\nabla.(\Gamma\,\nabla G) + 4\,\pi\left(a_g\,\frac{\sigma\,T^4}{\pi} + E_s\right) - (a_g + a_s)G = 0$$

Continuous phase

$$-\boldsymbol{\nabla}.\boldsymbol{q_{rg}} = \boldsymbol{a_g}\ \boldsymbol{G}\ -\ \boldsymbol{4a_g\sigma\,T_g^4}$$

Spectral models for a_g

- "gray constant" $a_g = const$ (user input)
- "gray" => Planck mean absorption using CO_2 and H_2O
- "gray and non-gray" WSGG based on CO_2 and H_2O

Dispersed phase m (M total)

in TFM or parcels in DEM and PIC

$$-\boldsymbol{\nabla}\cdot\boldsymbol{q_{rs,m}} = \boldsymbol{a_{s,m}}(\boldsymbol{G} - \boldsymbol{4\sigma\,T_{s,m}^4})$$

Spectral models for $a_{s,m}$

- "gray constant" based on constant emissivity and diameter of particles
- "gray" based on Buckius-Hawang correlation (depends on refractive index, mean particle size, void fraction and temperature)
- "gray and non-gray" WSGG

2. Project Update

Modeling approach

Weighted Sum of Gray Gas (WSGG) model

$$\nabla.(\Gamma\,\nabla G) + 4\,\pi\left(a_g\,\frac{\sigma\,T^4}{\pi} + E_s\right) - (a_g + a_s)G = 0$$

- Derived by fitting model coefficients such that total emissivity in a 1-d slab of gas matches full spectral result
- Typically 4-5 gray gases are sufficient

Gray WSGG model

The mean absorption coefficient is

$$a_g = \frac{ln(1-\varepsilon)}{L}$$

The total emissivity of a H_2O/CO_2 mixture is

$$\varepsilon = \sum_{i=0}^{N_g} k_i\left(1 - e^{-a_i\,P\,(X_{H2O}+X_{CO2})L}\right)$$

N_g = number of gray gases
L = path length
k_i = weighting factor
$b_{i,j}$ = constants
a_i = i-th gray gas absorption coefficient

Path length either defined as $L = \frac{3.6V}{A}$ (mean beam length) or as $L = V_{cell}^{1/3}$ (results are mesh dependent!)

Non-gray WSGG model

Solve N_g “gray-gas” equations i.e. for the ith gray gas

$$\nabla.\left(\frac{1}{3a_i}\nabla G_i\right) + 4\mathrm{a_i}\,\mathrm{k_i}\,\sigma\,T^4 - a_i G_i = 0$$

The weighting factors are given by

$$k_i = \sum_{j=0}^{N_k} b_{i,j} T^{\,j}$$

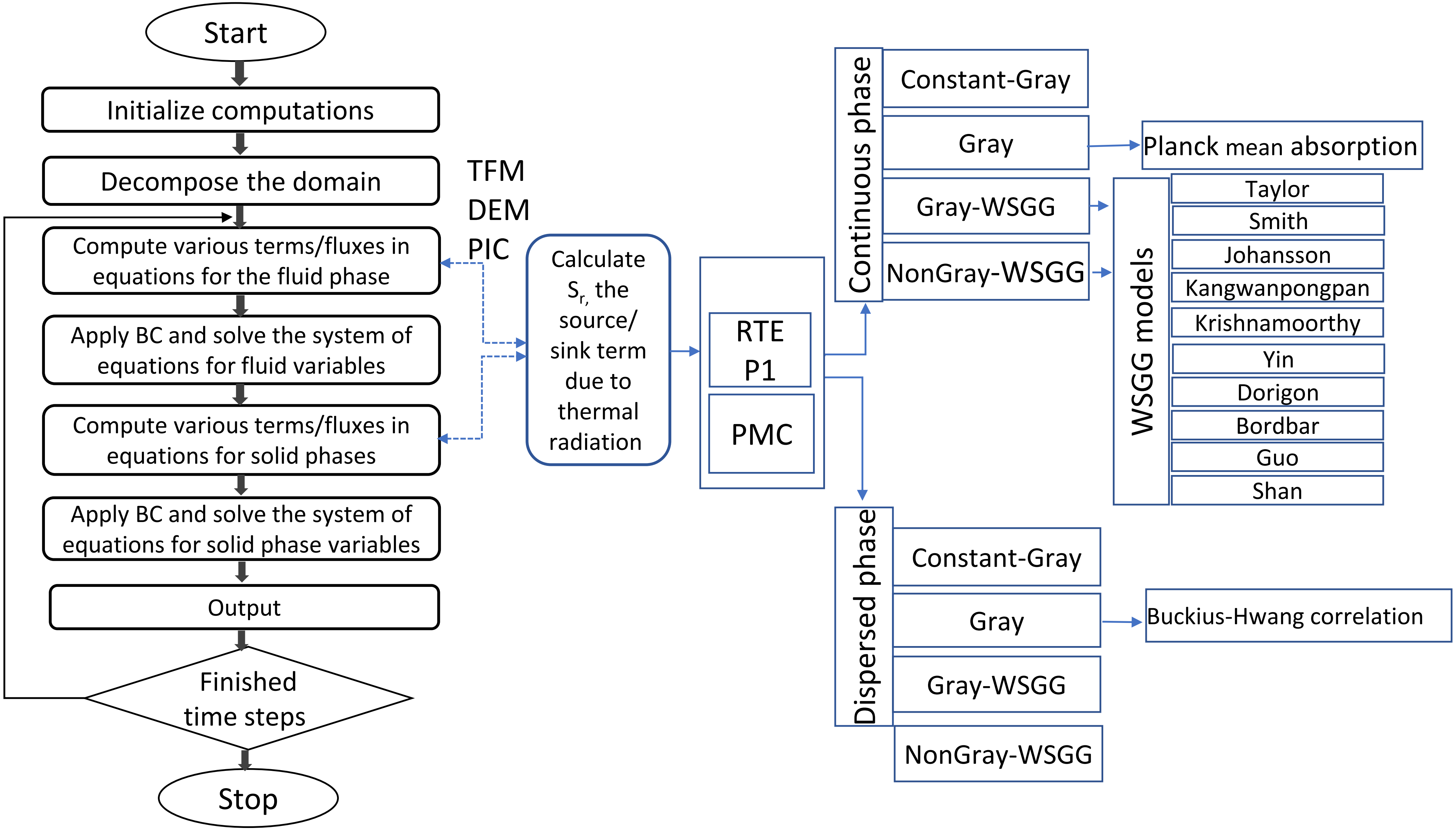
The source terms are then given by

$$-\nabla.\,q_{rg} = \sum_{i=0}^{N_g} a_i\,G_i - 4a_i k_i \sigma\,T_g^4$$

L is not needed!!!

2. Project Update

Modeling overview

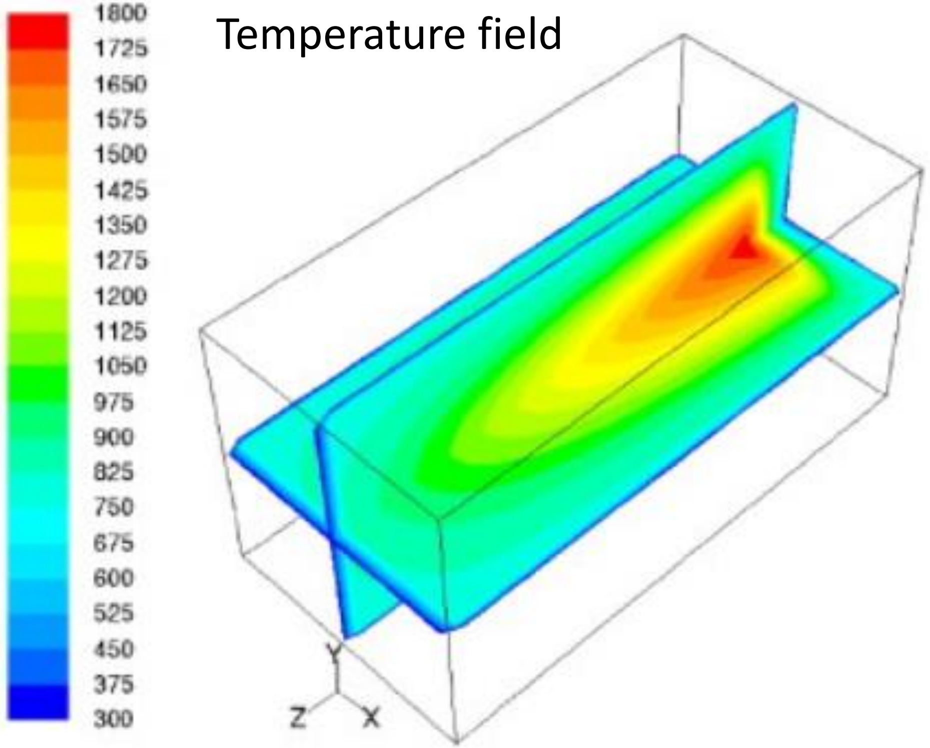


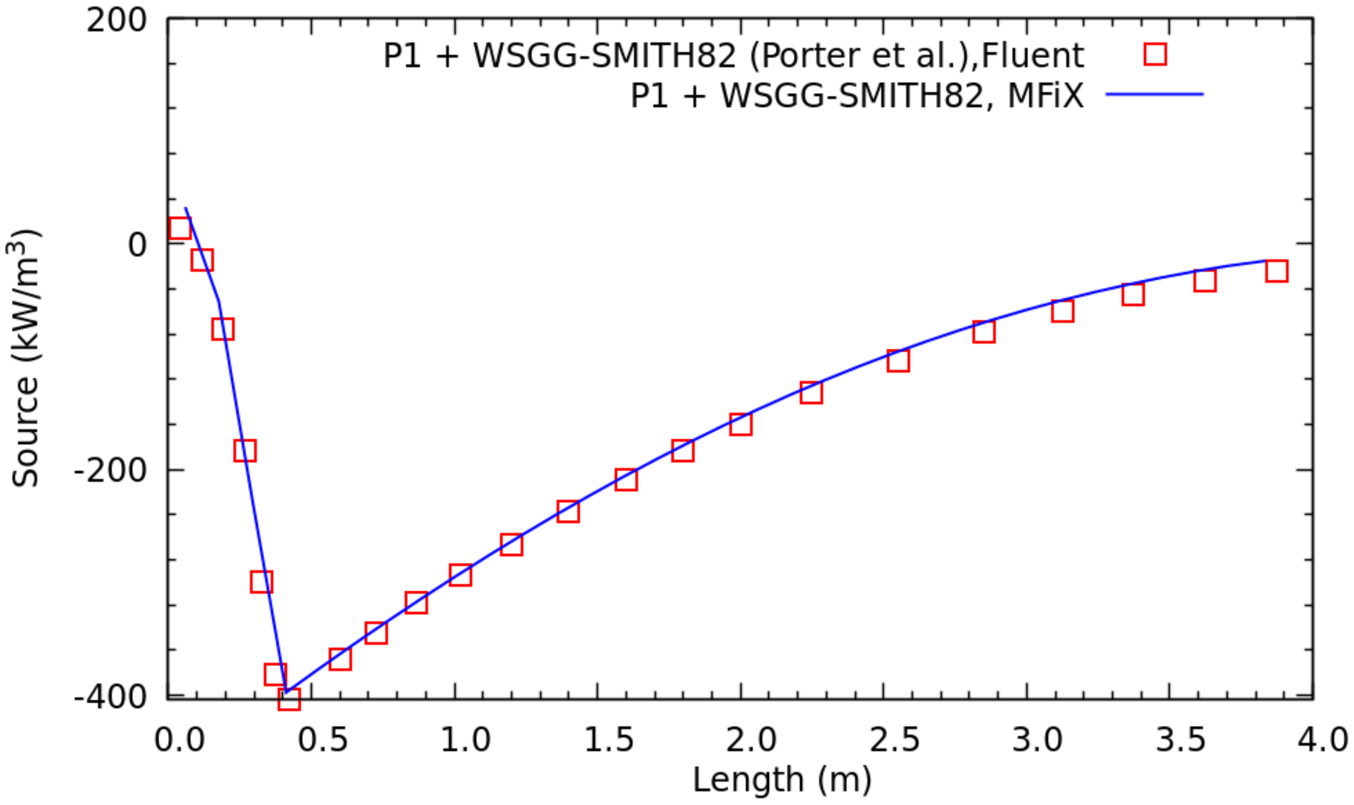
2. Project Update

T4: Implementation and Verification of Industrial Models

- 3D Steady, single phase, **gray**
- Radiation model- P1, WSGG – SMITH82
- L = 1.44 (3.6 V/A, based on domain) optical thickness = 0.49
- X_{H20} = 0.2; X_{CO2}= 0.1; p = 1.0 atm
- Mesh: 17x17x34

Verification of gray-WSGG implementation by comparison with ANSYUS-FLUENT results





Porter, R., et al. "Evaluation of solution methods for radiative heat transfer in gaseous oxy-fuel combustion environments." Journal of Quantitative Spectroscopy and Radiative Transfer 111.14 (2010): 2084-2094.

2. Project Update

T4: Implementation and Verification of Industrial Models

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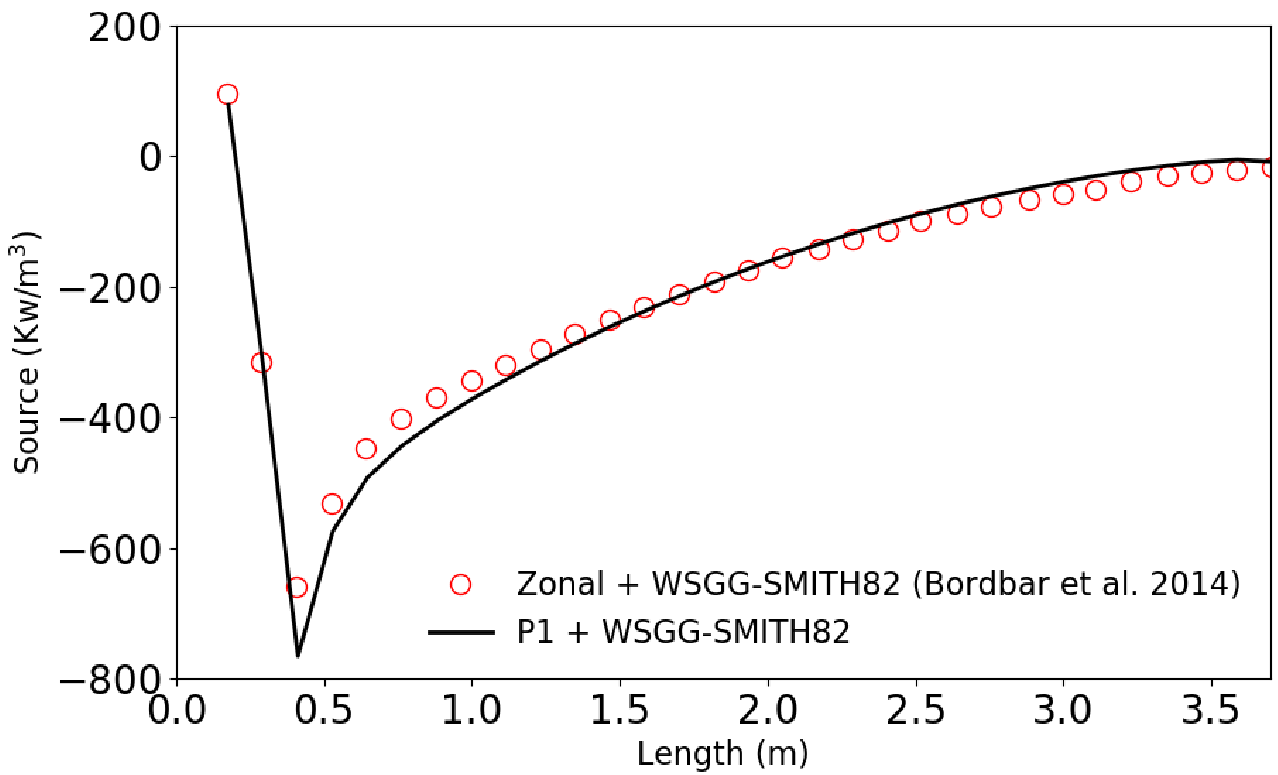
Verification of non-gray WSGG implementation by comparison with results reported in Literature



2. Project Update

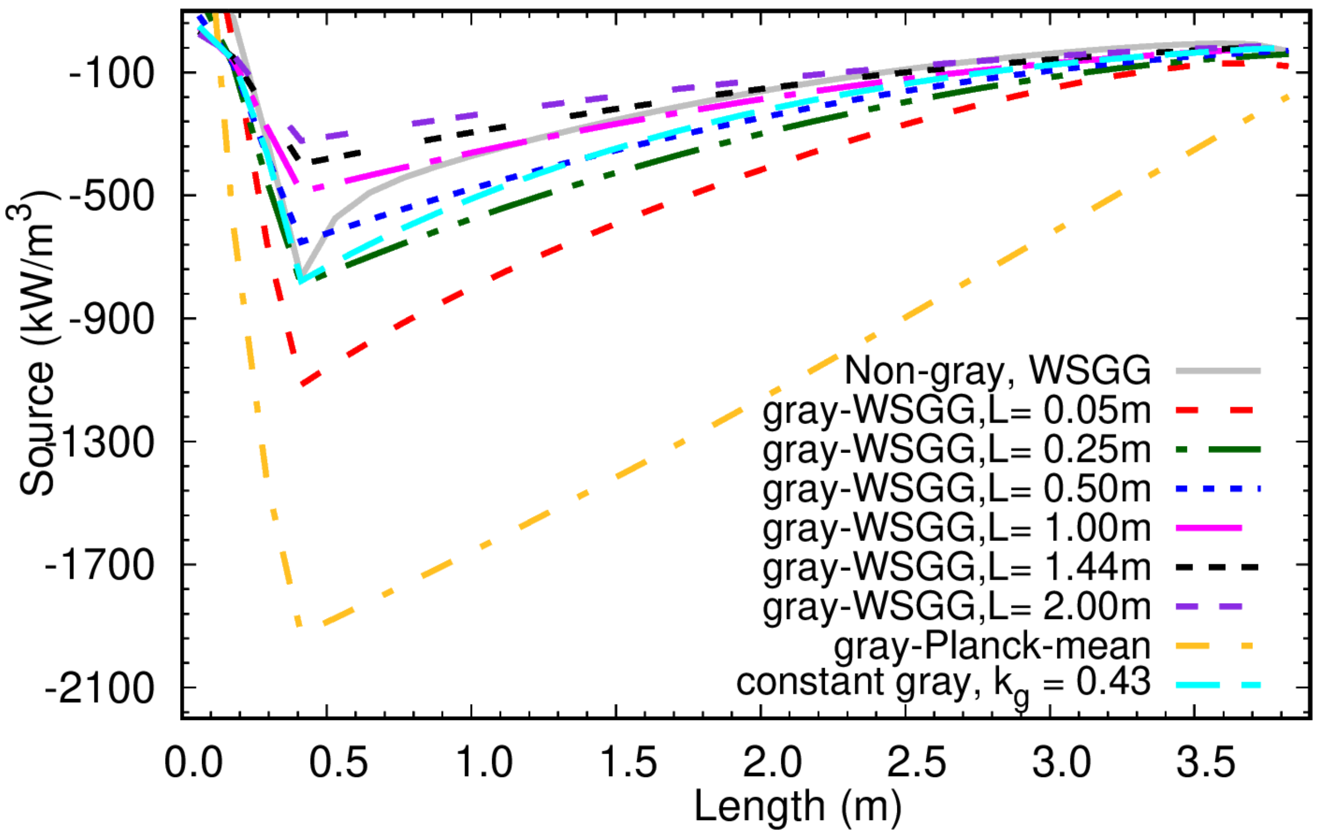
T4: Implementation and Verification of Industrial Models

Gray and non-gray WSGG models implemented correctly, which one should we use as "Industrial Model"?

Problems with the gray-WSGG

- Results strongly depend on the choice for L
- Results differ from non-gray result

We prefer the non-gray version as our "Industrial Model" since it does not require arbitrary choice for L!

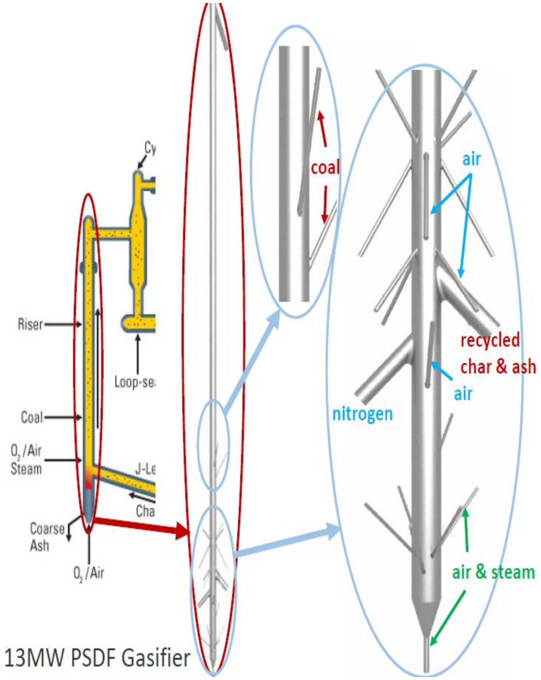


Further analysis of this choice will be provided in Task 7!

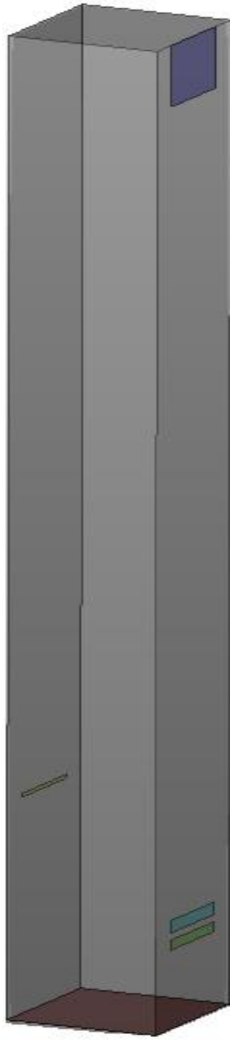
2. Project Update

T-5: Industrial Model Application and Analysis

13MW Power Systems Development Facility (PSDF) gasifier



Geometric simplification



Outlet
x= 0.5, y=[7.5,8.0], z= [0.1,0.4]
155683.6Pa, 1227 K

x=0.5, y=[0.88,0.895],z=[0.1,0.4]
Coal: 0.3522 kg/s, 300K (Char, volatiles, Moisture, ash)
Gas : 0.18157 kg/s, 300K (N2)
234225.0 Pa

x=0.5, y=[0.39,0.44],z=[0.1,0.4]
Char & ash : 3.746 kg/s, 1190K
Gas : 0.2935 kg/s, 1190K
(CO, CO_2, CH_4, H_2, H_20, N_2),
234225.0 Pa

x=0,y=[0.32,0.36],z=[0,0.5]
Gas : 0.035 kg/s, 300K (N2)
234225.0 Pa

Inlet
234225.0 Pa, 482 K (N_2, O_2, H_2O), 0.342 kg/s

- Mesh with 4M cells
- Chemistry based on 17 gas species, 4 solid species

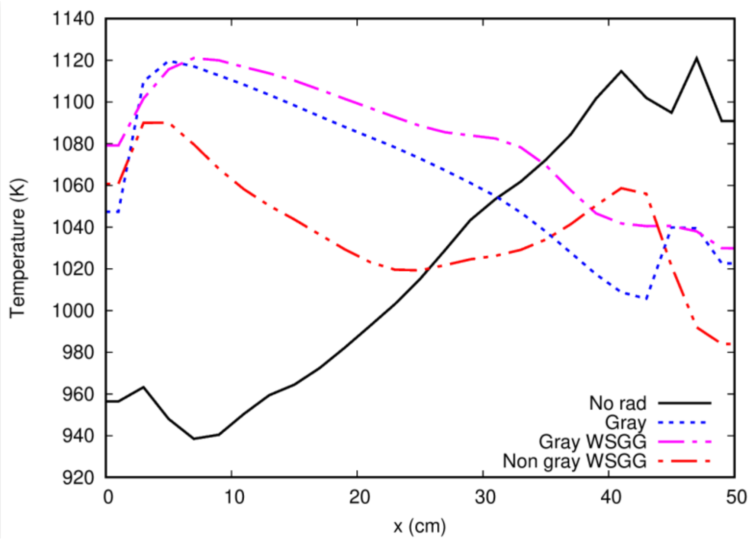
2. Project Update

T-5: Industrial Model Application and Analysis

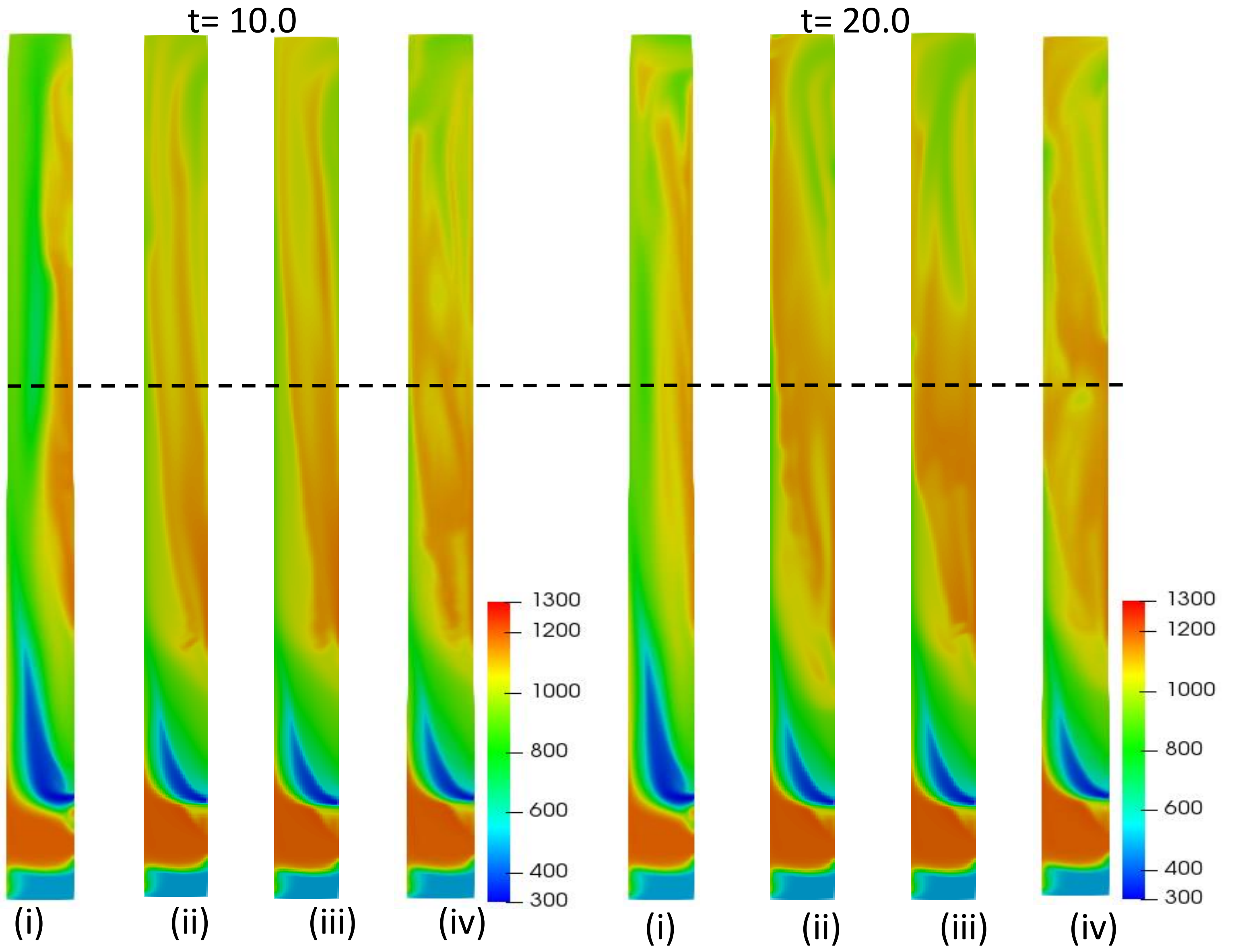
(i) No radiation (ii) Gray

(iii) Gray-wsgg (iv) Nongray-wsgg

y = 6m, z = 0.25m, t = 20s



Significant difference $\Delta T > 120K$ observed!



2. Project Update

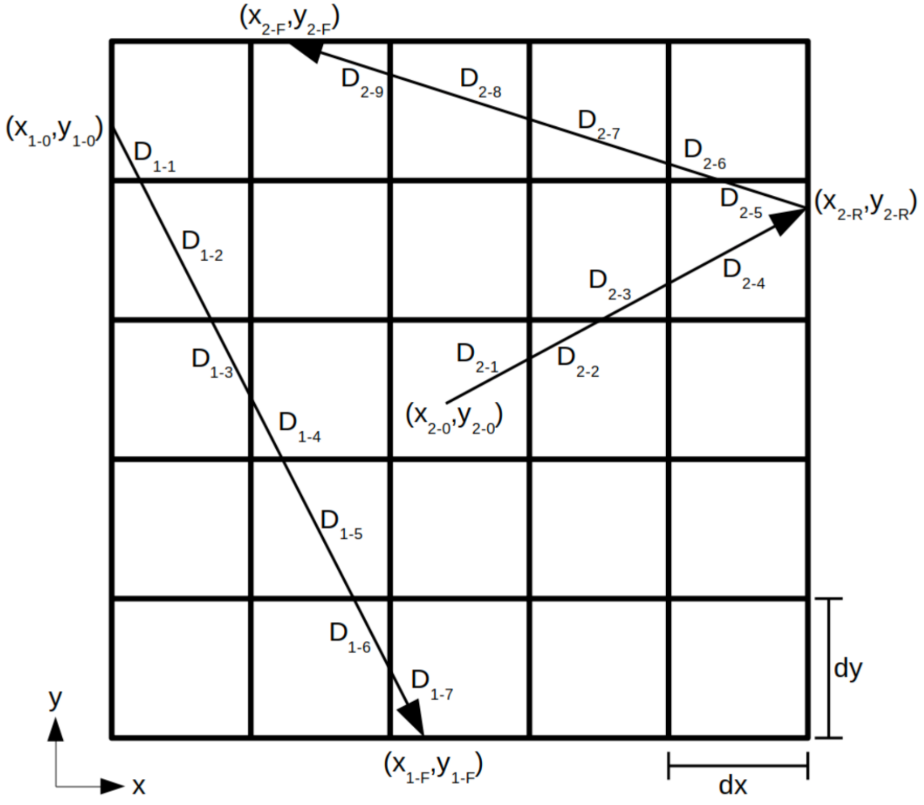
T6: Development of High-End Research Models

Photon Monte-Carlo Method (PMC)

- PMC is essentially a Monte Carlo Integration of the RTE
- If it is coupled with a spectral database, this leads to a “model error free” solution of the RTE (numerical errors still present though)
- Work mostly done by MS student David Tobin (graduated in August)

Development approach

- Defined a basic interface to MFIX
- David coded the serial PMC method as a stand-alone Fortran program using data structures following “MFIX”
- After testing, the PMC solver was fully integrated into MFIX-RAD with the help od Dr. Kotteda
- Dr. Kotteda finished the parallel implementation of the PMC solver



Integrate RTE along a given path length (Beer’s Law)

$$I_\lambda(S) = I_\lambda(0)e^{-\int_0^S \alpha_\lambda S^* dS^*} \approx I_\lambda(0)e^{-\alpha_\lambda S}$$

Fraction of ray’s energy absorbed in the cell

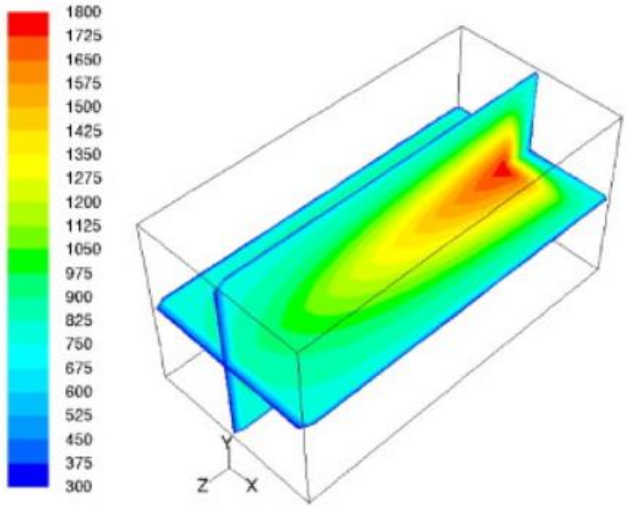
$$F_{absorb} = 1 - e^{\alpha D_{cell}}$$

2. Project Update

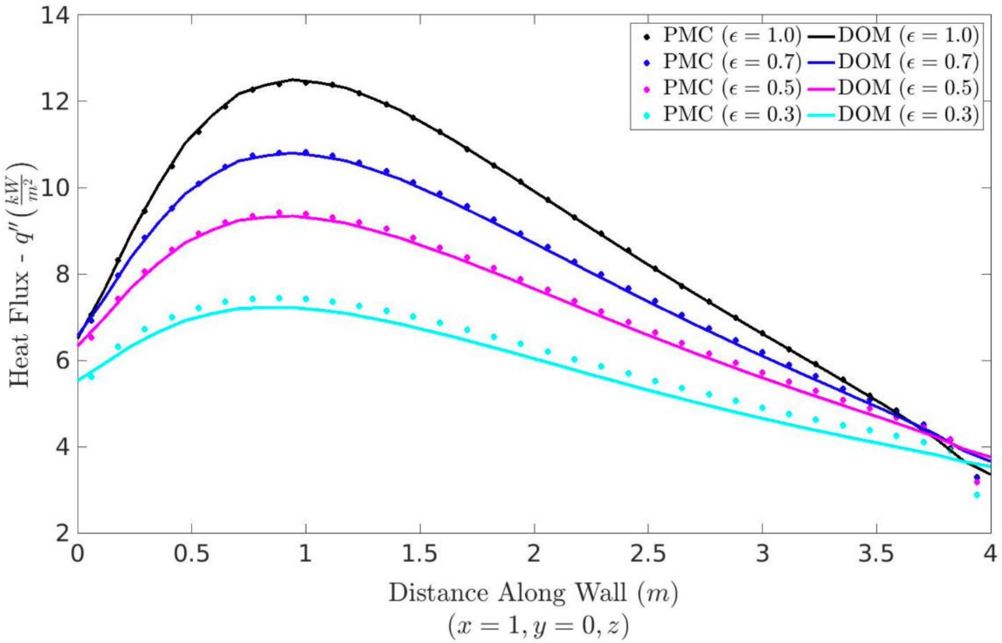
T6: Development of High-End Research Models

Verification of stand-alone PMC solver by comparison with highly resolved DOM (32x16 rays)

- 3D Steady, single phase, **constant gray**
- Constant absorption coefficient = 0.1, no-scattering
- Varying wall emissivity
- Mesh: 17x17x34, tracked $N = 10^9$ rays



Wall heat flux along front wall (more sensitive than source term!)



Check conservation of energy with divergence theorem:

$$\int_{\Omega} \nabla \cdot \vec{q}_{rad} dV = \int_{d\Omega} \vec{q}_{rad} \cdot \hat{n} \, dS$$

Average Relative Error of PMC Results: 0.00%

Average Relative Error of DOM Results: 4.94%

PMC inherently conserves energy!

2. Project Update

T6: Development of High-End Research Models

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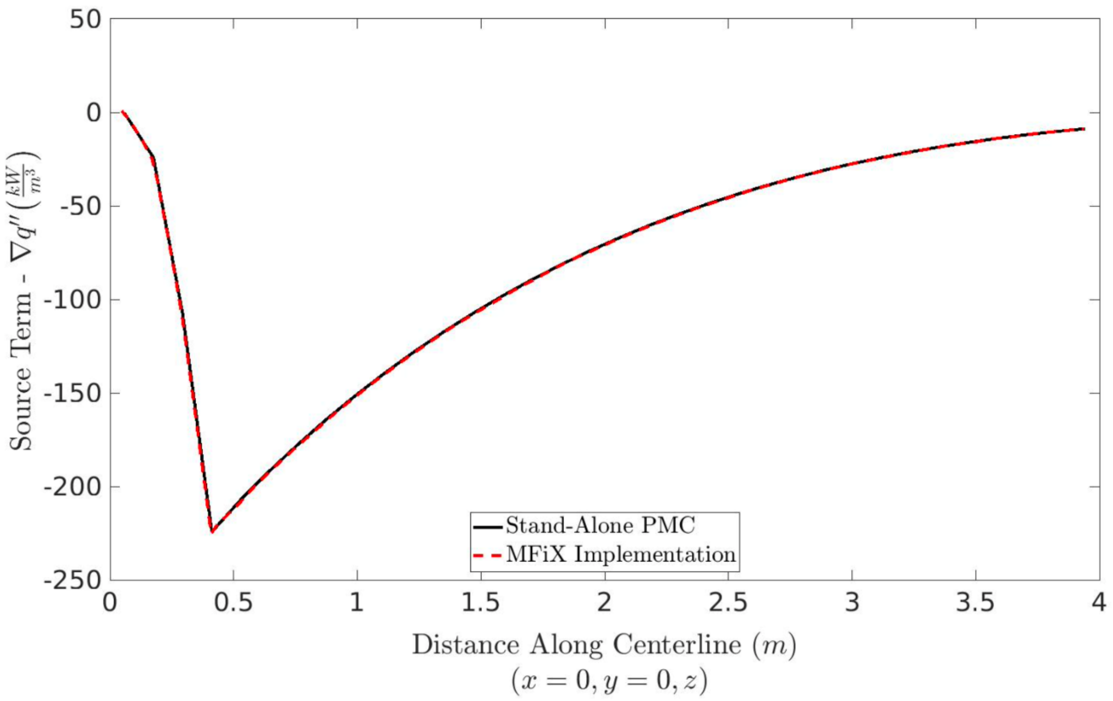
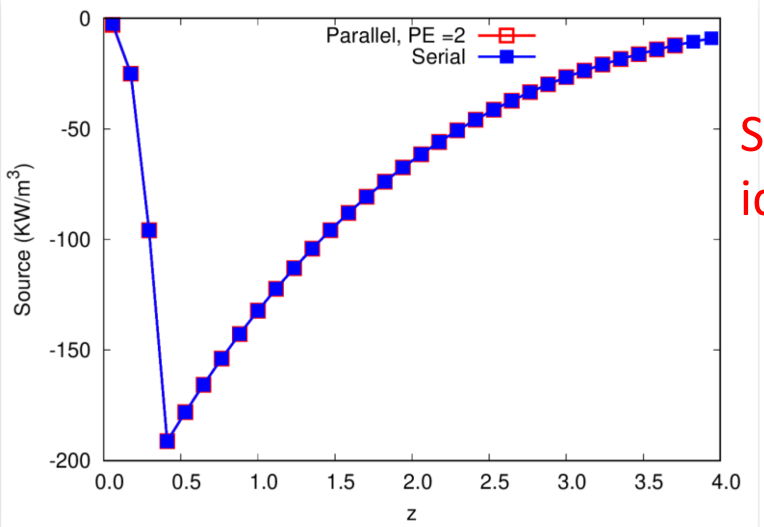
Verification of serial and parallel MFIX-RAD implementation

MFIX serial run-time ~4min

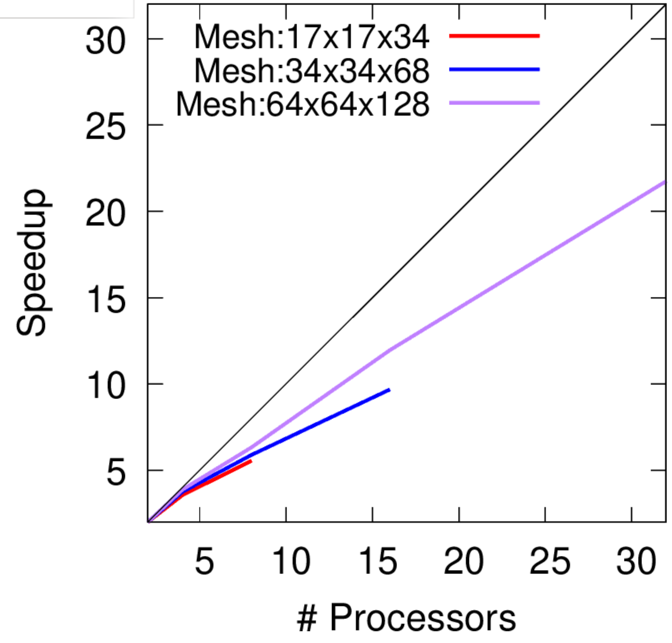




Serial & parallel results identical!

Initial result for parallel scaling are encouraging!

Scaling will improve greatly for non-gray applications



3. Preparing Project for Next Steps

Market Benefits/Assessment

- MFiX is widely used as CFD tool for modeling/optimization of reacting multiphase flow
- MFiX currently has only minimal radiative heat transfer modeling capability
- MFIX-RAD development adds
  - P1 + non-gray WSGG as the appropriate model for industrial applications (not available in either commercial (ANSYS-Fluent) or other open source (OpenFOAM) CFD codes
  - Model error free PMC solver to produce case specific benchmark data for RTE solver and Spectral Model accuracy assessment (not available in any other CFD codes)

Technology-to-Market Path

- MFiX-RAD Plug-In at current development state is available at GitLab => every MFiX user can download and use it their process modeling!
- We are seeking industry collaborators who want to use MFiX-RAD in their applications
- The MFiX-RAD Plug-In will be replaced by a full integration into the mainstream MFIX release towards the end of the project

4. Concluding Remarks

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Remaining tasks

- Non-gray MFIX PMC solver
  - ➢ Stand alone version for Statistical Narrow Band Model (Elsasser SNB) already implemented (see MS thesis of David Tobin)
  - ➢ Line-by-line (LBL) Spectral Database (HiTran) for benchmarking (Task 6)
  - ➢ Non-Gray WSGG PMC
- Task-7 “Comprehensive Validation and Benchmark”
  - Use non-Gray WSGG PMC to analyze model errors of P1 RTE solver (industrial model) for the large gasifier => P1 sufficiently accurate or not?
  - Comparison of PMC-LBL and PMC-ngWSGG results will reveal WSGG model errors
  - Such an analysis is only possible with PMC!
- Based on Task 7 make recommendations on next development steps
  - ➢ Is P1-ngWSGG “sufficiently” accurate?
  - ➢ If not, do we need a better RTE solver (i.e. P4, P6, or DOM)
  - ➢ If not, do we need a better spectral model (k-distribution model?)