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

DE-FE0030485

2021 FE R&D PROJECT REVIEW MEETING, May 24, 2021

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NATIONAL ENERGY TECHNOLOGY LABORATORY

Outline

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

1. Project Description and Objectives

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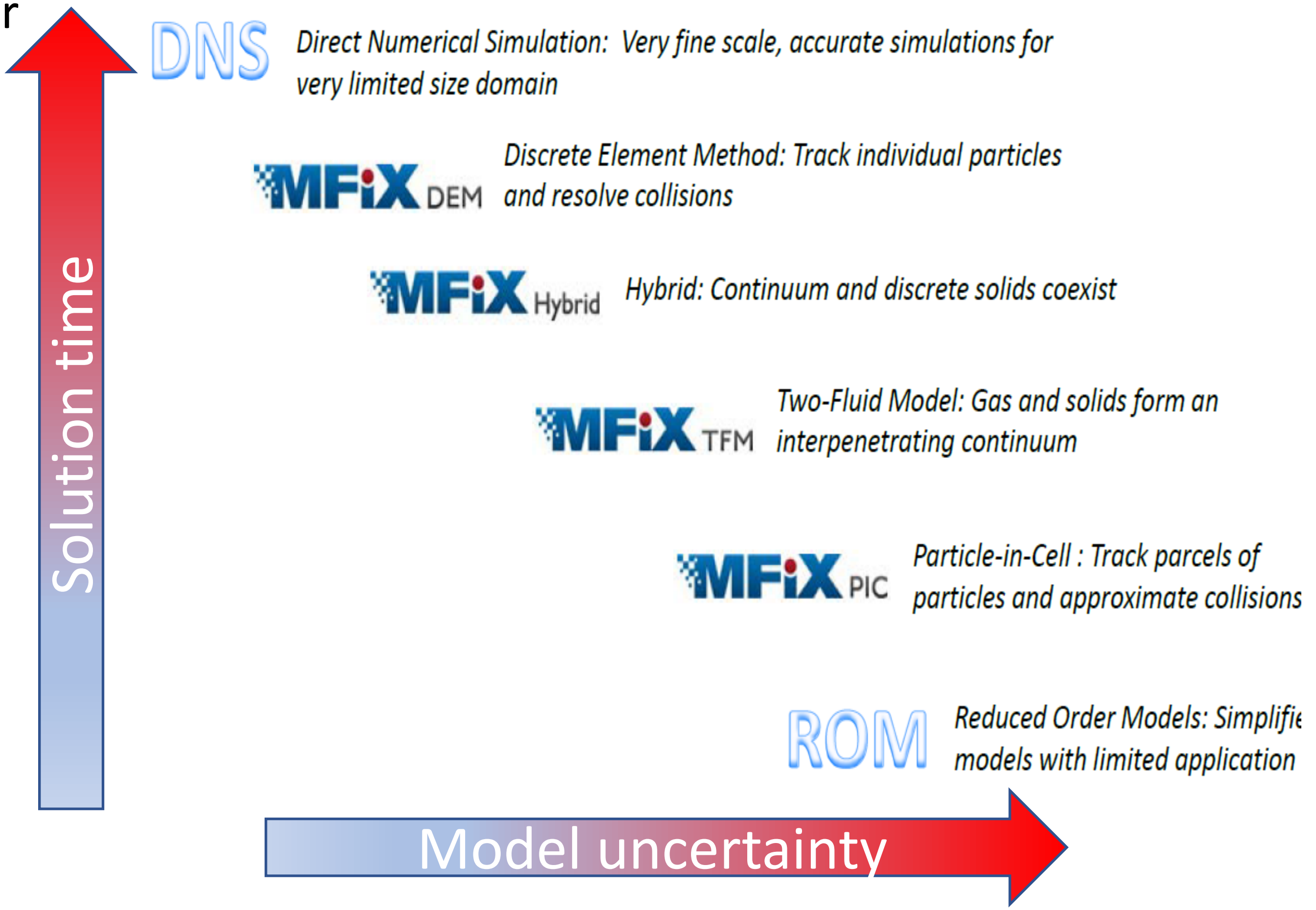
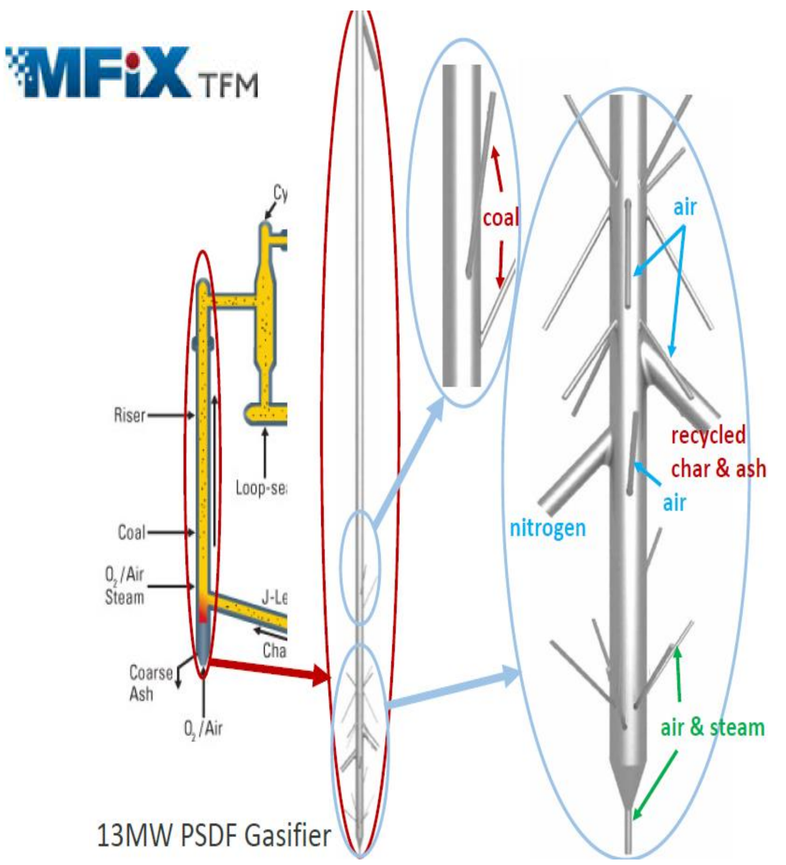
NETL's MFiX —Multiphase Flow with Interphase eXchange

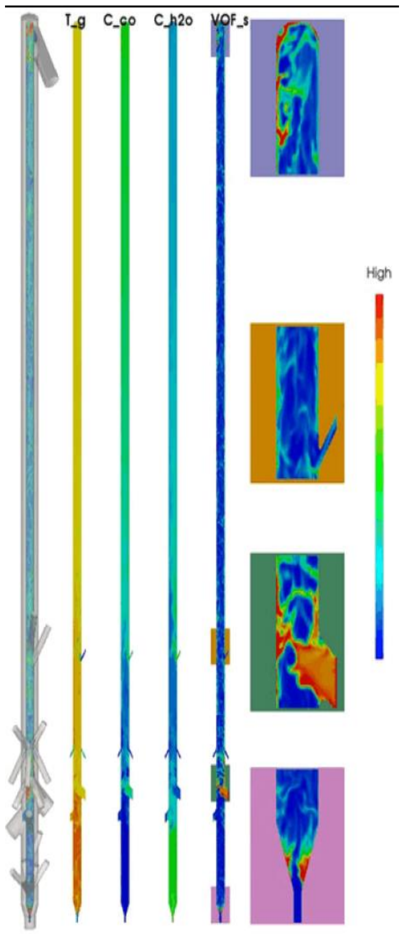
- Central to the laboratory's multiphase flow reactor modeling efforts
- Provides support to achieve DOE's goals
  1. Cost of Energy and Carbon Dioxide (CO2) Capture from Advanced Power Systems
  2. Power Plant Efficiency Improvements
- Built with varying levels of fidelity/computational cost
  - Lower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



13MW PSDF Gasifier



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 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

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!

In progress

2. Project Update

Modeling approach

Energy equations for MFiX-TFM

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

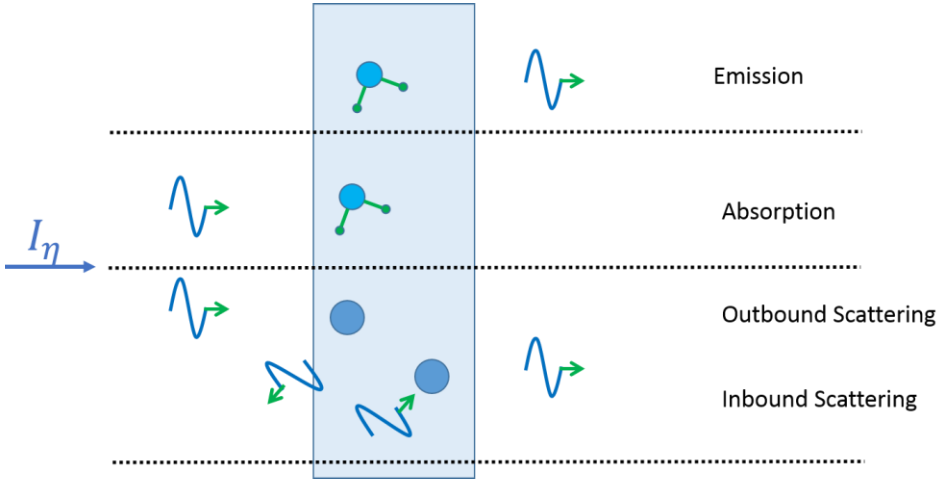
Solids $$\varepsilon_{s_m} \rho_{s_m} c_{ps_m}\left(\frac{\partial T_{s_m}}{\partial t} + u_{s_m} \, . \Delta T_{s_m}\right) = \nabla q_{s_m} + \sum_{m=1}^{M} H_{gsm} - \Delta H_{rs_m} - \nabla . \vec{q}_{rs_m}$$

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



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

$$-\kappa_\eta I_\eta$$

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

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:

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

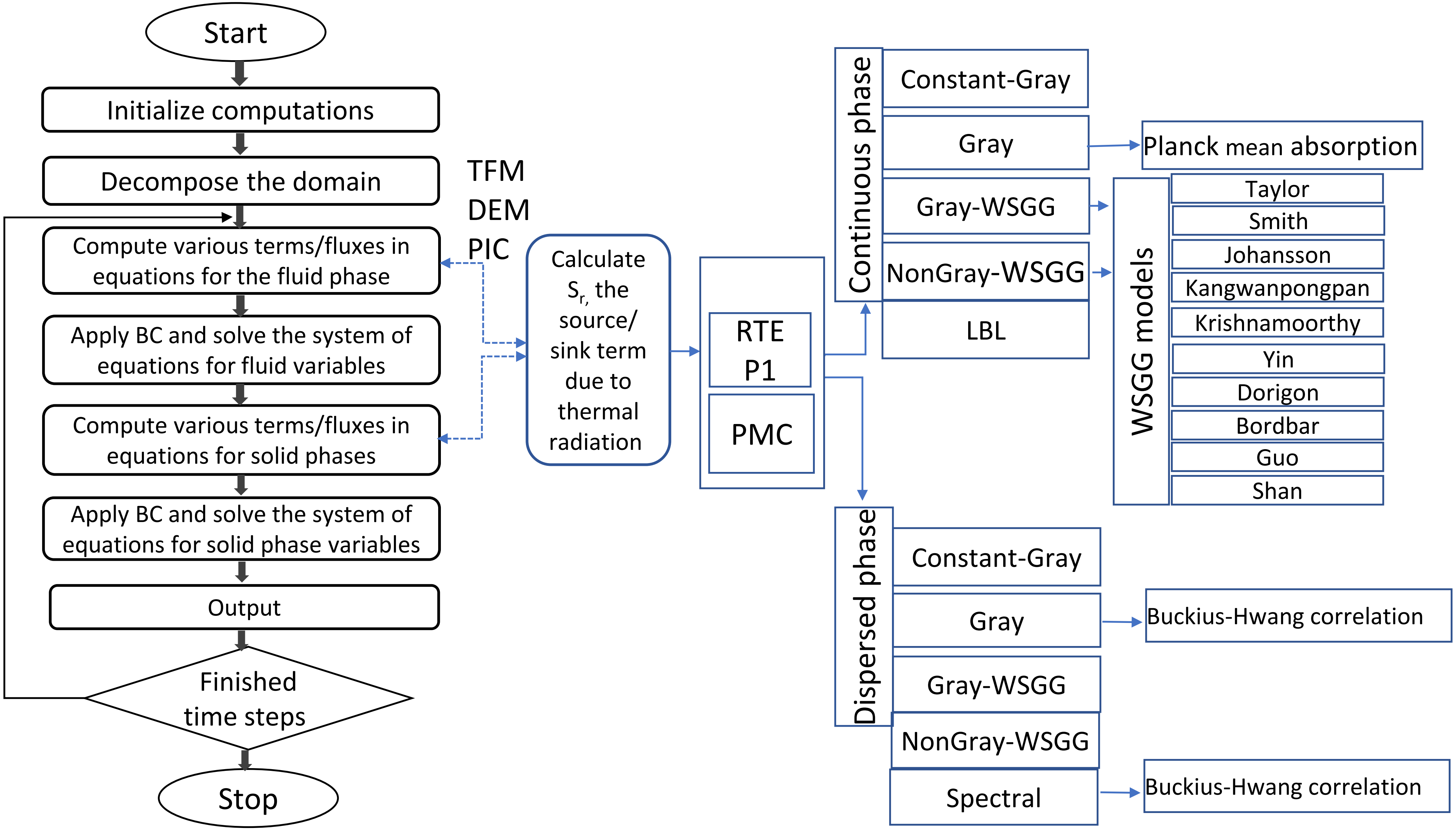
G_η spectral incident radiation

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 overview



2. Project Update

T6: Development of High-End Research Models

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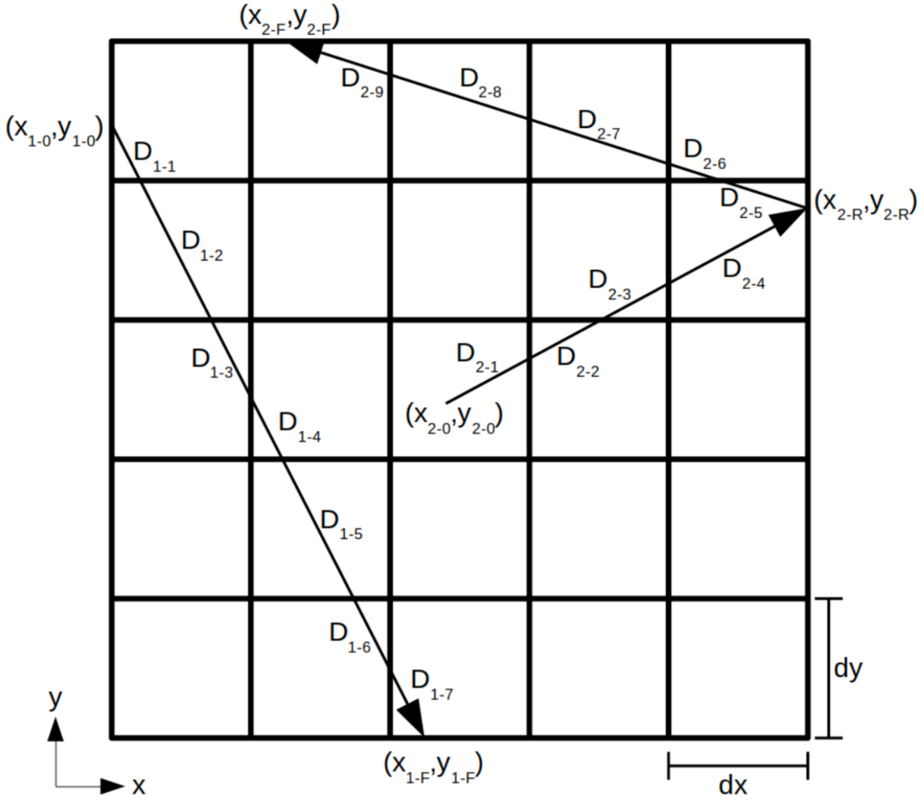
Photon Monte-Carlo Method (PMC)

- 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



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 of Dr. Kotteda
- Dr. Kotteda finished the parallel implementation of the PMC solver
- Implementing spectral line-byline (LBL) model

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

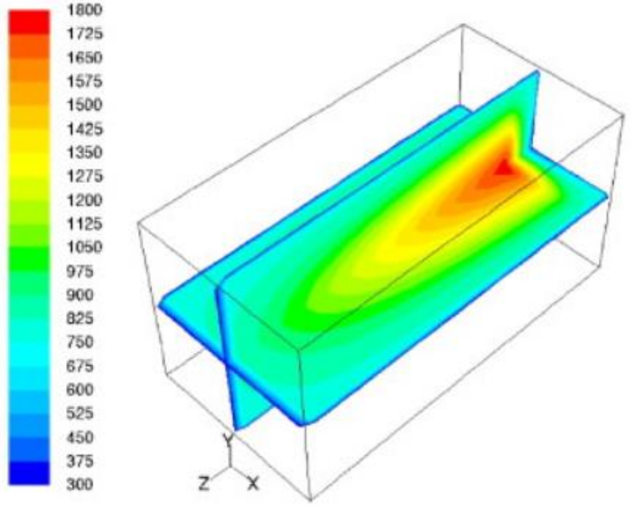
$$I_\lambda(S) = I_\lambda(0)e^{-\int_0^S \kappa_\lambda S^* dS^*} \approx I_\lambda(0)e^{-\kappa_\lambda S}$$

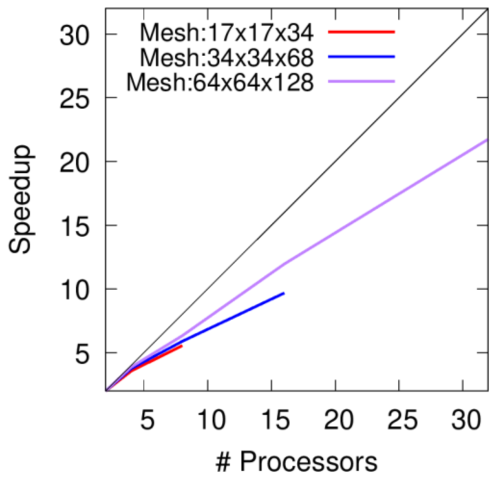
Fraction of ray’s energy absorbed in the cell

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

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

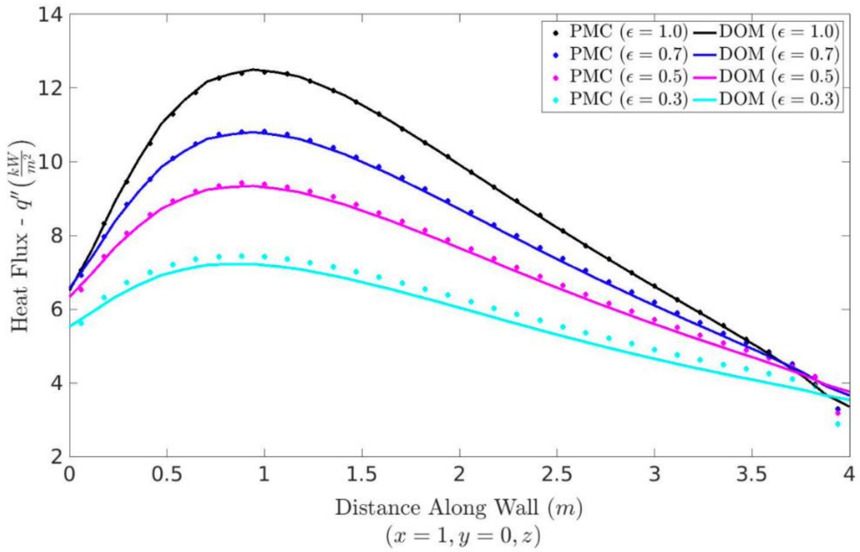
- 3D Steady, single phase, **constant gray**
- Constant absorption coefficient = 0.1, no-scattering
- Varying wall emissivity
- Mesh: 17x17x34, tracked $N = 10^9$ rays, serial run time about 10min





Serial and basic parallel implementation!

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!

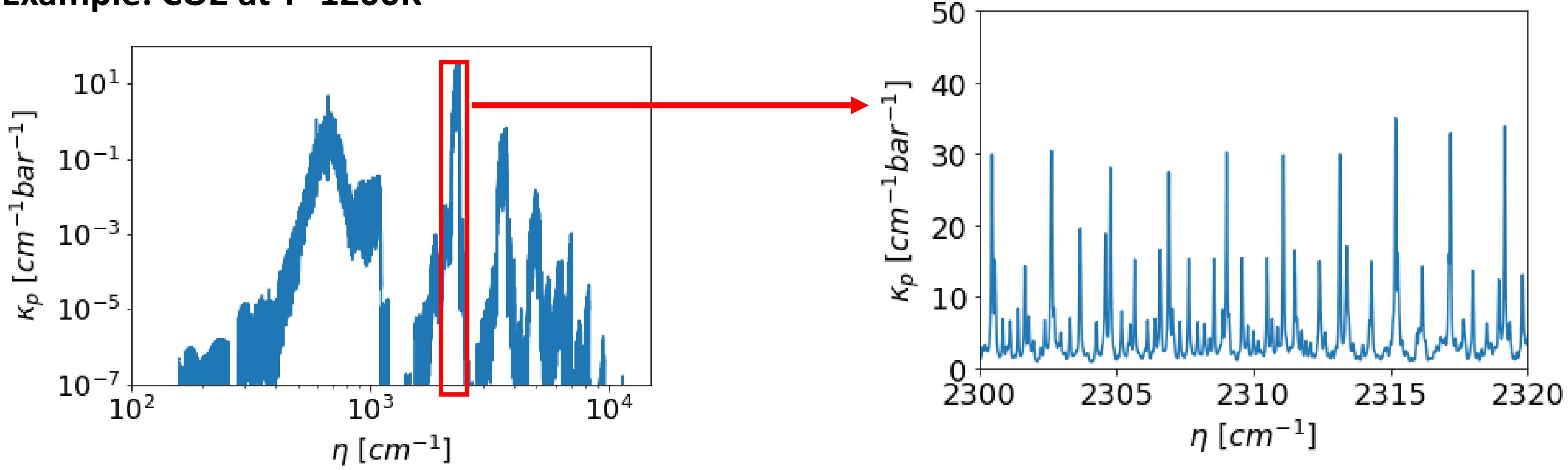
2. Project Update

T6: Development of High-End Research Models

PMC-LBL development

- Use the most up to date version of the HITRAN database https://hitran.org/
- Access through “HITRAN Application Programming Interface (HAPI)”
- HAPI is a set of routines in Python to download LBL spectral data and calculate absorption coefficient spectra (and many other functions)
- We developed several python scripts to generate the required database (1-2GB) using about 1.2 million lines

Example: CO2 at T=1200K



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T6: Development of High-End Research Models

PMC-LBL development

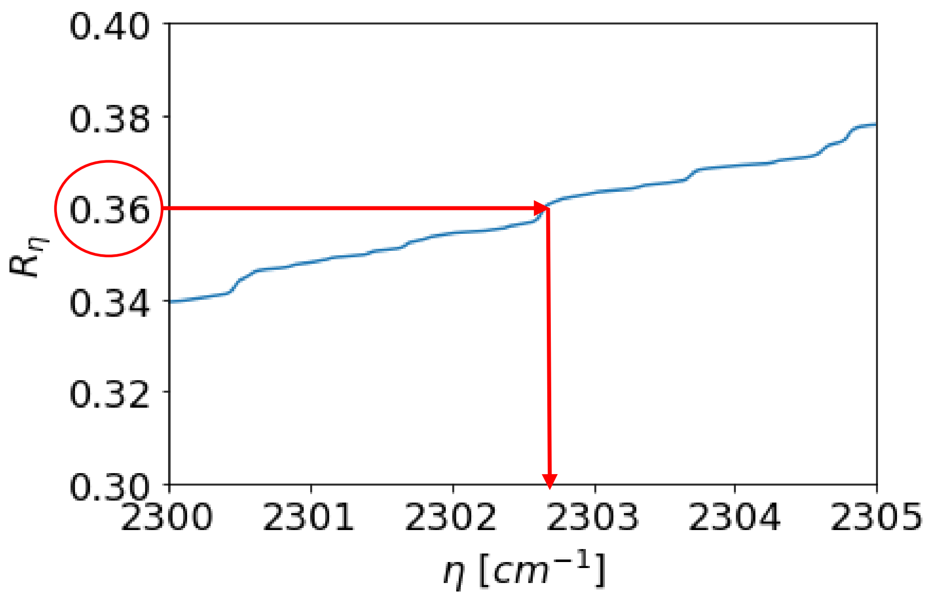
Probability of the number of Photons emitted in $[\eta - d\eta, \eta + d\eta]$ is proportional to $\kappa_\eta I_{b\eta} d\eta$

Random number relation for emission wavenumber:
$R_{\eta,i}$ is a uniform random number in [0,1)

$$R_{\eta,i} = \frac{\int_0^\eta \kappa_{p\eta,i} I_{b\eta} d\eta}{\int_0^\infty \kappa_{p\eta,i} I_{b\eta} d\eta} = \frac{\pi}{\kappa_{p,i}\sigma T^4} \int_0^\eta \kappa_{p\eta,i} I_{b\eta} d\eta$$

We don't want to calculate these integrals for every PMC step so we generate a database (look-up table) as a pre-processing step

- For every photon ray that is emitted in a cell, draw a uniform random number R_η and then find the corresponding wavenumber from the look-up table



2. Project Update

T6: Development of High-End Research Models

PMC-LBL development

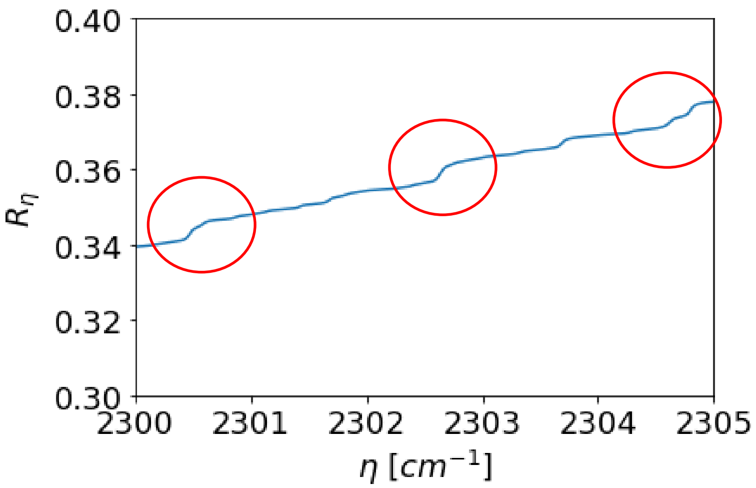
For a gas mixture with molar fractions x_i, things are a bit more tricky (following the algorithm of Wang and Modest IJHMT 50 (2007):

R_η denotes the uniform random number drawn for the mixture and we need to find the corresponding wavenumber of the photon ray!

Implicit relation

$$R_\eta = \frac{\sum_i x_i \kappa_{p,i} R_{\eta,i}}{\sum_i x_i \kappa_{p,i}}$$

Direct inversion from R_η to η not possible => solve numerically using bisection method (Newton method not possible due to strongly varying gradients!)



Using a hybrid root finding method such as Brent's method reduced cost by 33% compared to simple bisection!

Store the database

For all species, $i = 1,2, \ldots, N_{spec}$

$$R_{\eta,i} = f_{R,i}(\eta, T) \qquad \kappa_{p\eta,i} = f_{\kappa,i}(\eta, T)$$

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PMC-LBL development

Algorithm

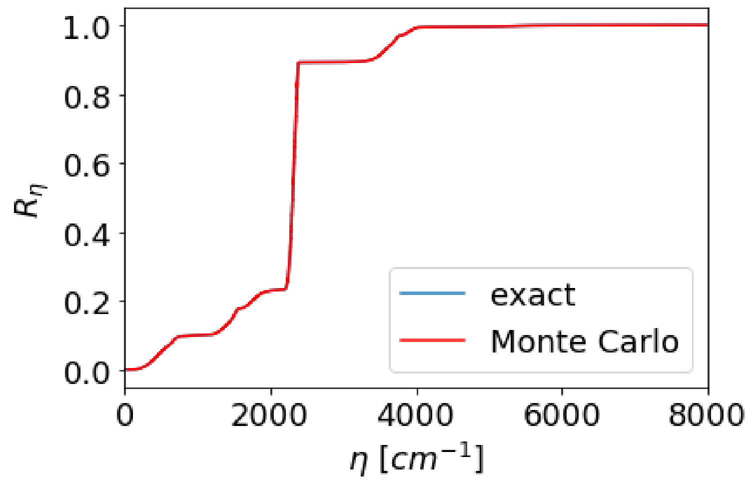
- Draw a uniform random number U
- Set bracketing guesses for bisection method e.g. $a = \eta_{min}, b = \eta_{max}$
- Use bisection method to find η such that

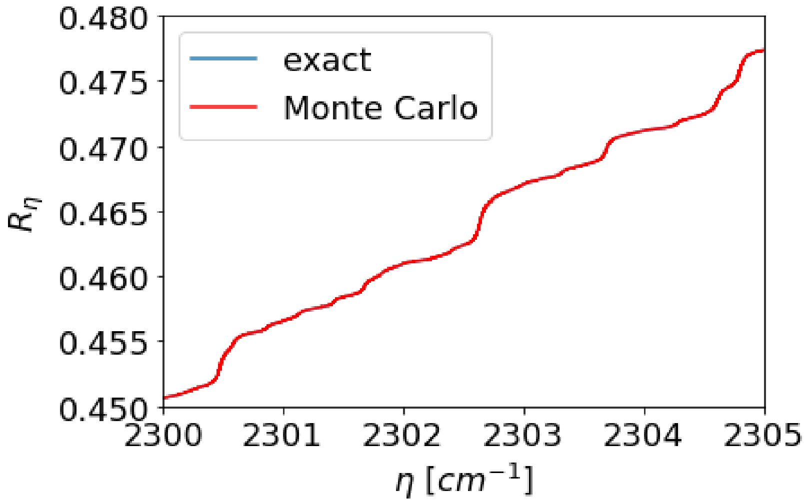
$$U - R_\eta = U - \frac{\sum_i x_i \kappa_{p,i} R_{\eta,i}}{\sum_i x_i \kappa_{p,i}} = 0$$

Test

- Choose a gas mixture: $T = 1200K, x_{CO_2} = 0.1, x_{H_2O} = 0.2$
- Calculate the exact mixture random number relation using $R_\eta = \frac{\pi}{\kappa_p \sigma T^4} \int_0^\eta \kappa_{p\eta} I_{b\eta} d\eta$
- Draw 1 million uniform random numbers
- Use the random number database and the mixture random number algorithm and then find the η values

Result

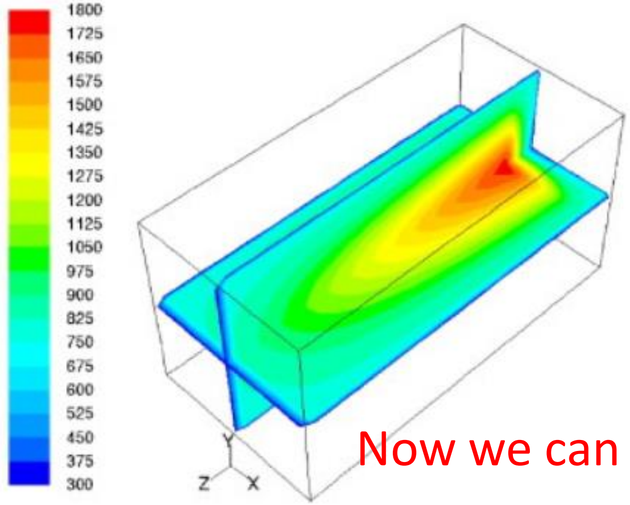


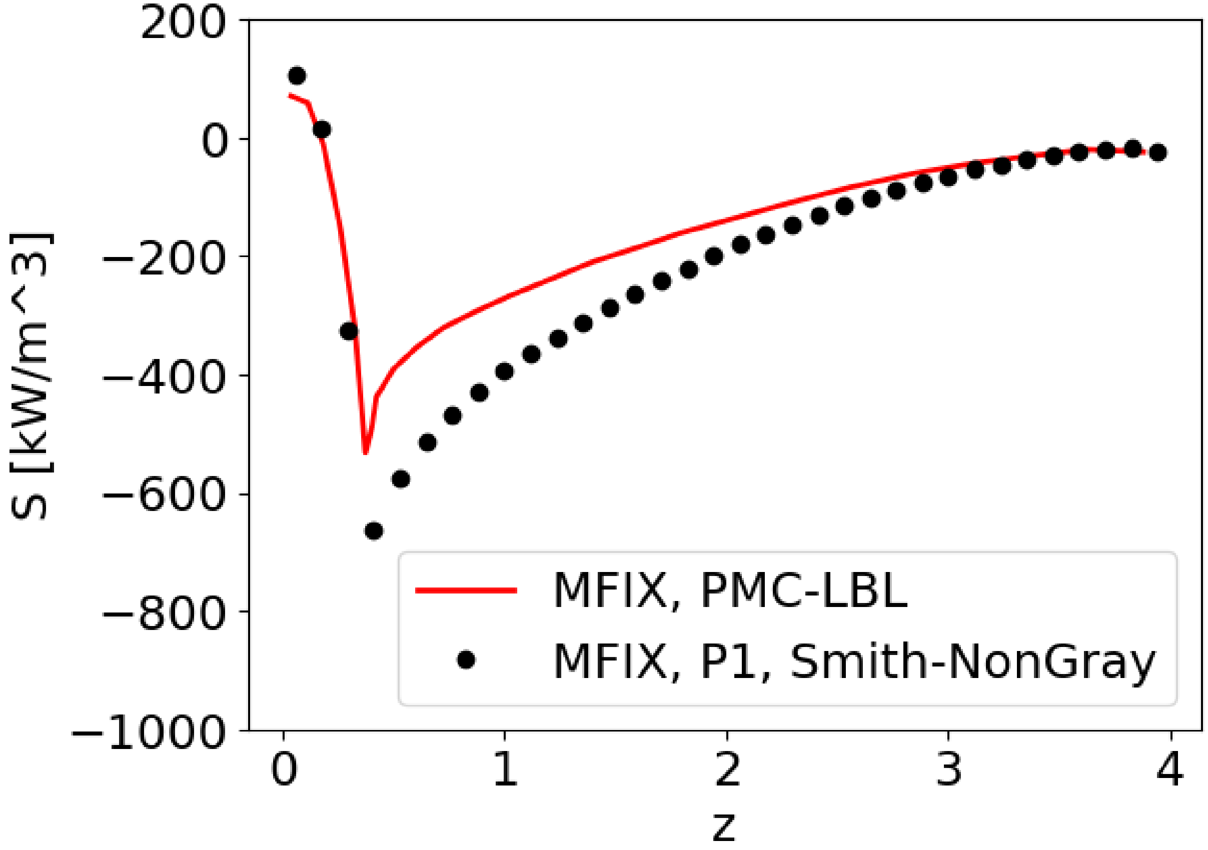


2. Project Update

T6: Development of High-End Research Models

- 3D Steady, single phase
- $x_{CO_2} = 0.1, x_{H_2O} = 0.2$
- Varying wall emissivity
- Mesh: 17x17x34, tracked $N = 10^9$ rays
- LBL with 1.2 million lines, 20 temeperatures





Now we can finish Task 7 “Comprehensive Validation and Benchmark”:

Is the observed error of the industrial model (P1, WSGG-NonGray) due to

- the simplified P1 RTE solver (test my using PMC with WSGG-NonGray)
- the simplified spectral WSGG-NonGray model -> test alterative WSGG models

3. Preparing Project for Next Steps

- 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)
- Integrate MFIX-RAD Plug-In into main MFIX distribution (start mid-June)

3. Preparing Project for Next Steps

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Submitted paper

"Study the thermal radiation effects in gas-solid flows with gray and non-gray P1 models implemented in MFIX" (Powder Technology)

Remaining tasks

- 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
  - Comparison of PMC-LBL and PMC-ngWSGG results will reveal WSGG model errors
  - Such an analysis is only possible with PMC!

Second paper

"Analysis of non-gray WSGG models for multiphase flows through PMC-LBL benchmark data"

Acknowledgements

Acknowledgment: "This material is based upon work supported by the Department of Energy Award Number DE-FE0030485"

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