Implementing General Framework in MFiX for Radiative Heat Transfer in Gas–Solid Reacting Flows DE-FE0030485

NETL Crosscutting Research – Project Review April 9-11, 2019, Pittsburgh

V M K Kotteda, Presenter
Postdoctoral Researcher
University of Wyoming

David Tobin
Master Student
University of Wyoming

Michael Stoellinger, PI
Associate Professor of Mechanical Engineering
University of Wyoming

UNIVERSITY OF WYOMING

NATIONAL ENERGY TECHNOLOGY LABORATORY

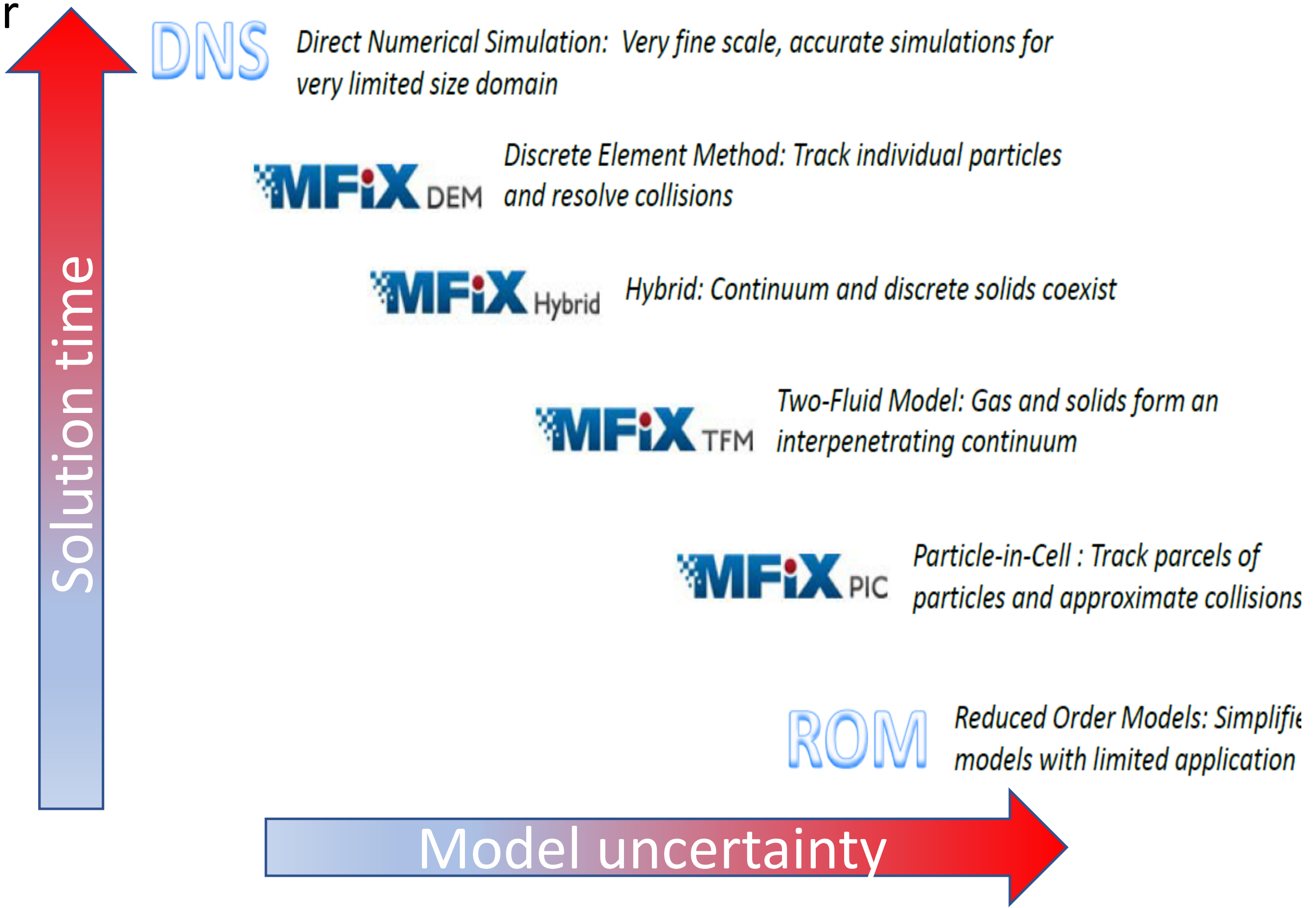
Outline

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

1. Project Description and Objectives

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



DNS *Direct Numerical Simulation: Very fine scale, accurate simulations for very limited size domain*

MFiX DEM *Discrete Element Method: Track individual particles and resolve collisions*

MFiX Hybrid *Hybrid: Continuum and discrete solids coexist*

MFiX TFM *Two-Fluid Model: Gas and solids form an interpenetrating continuum*

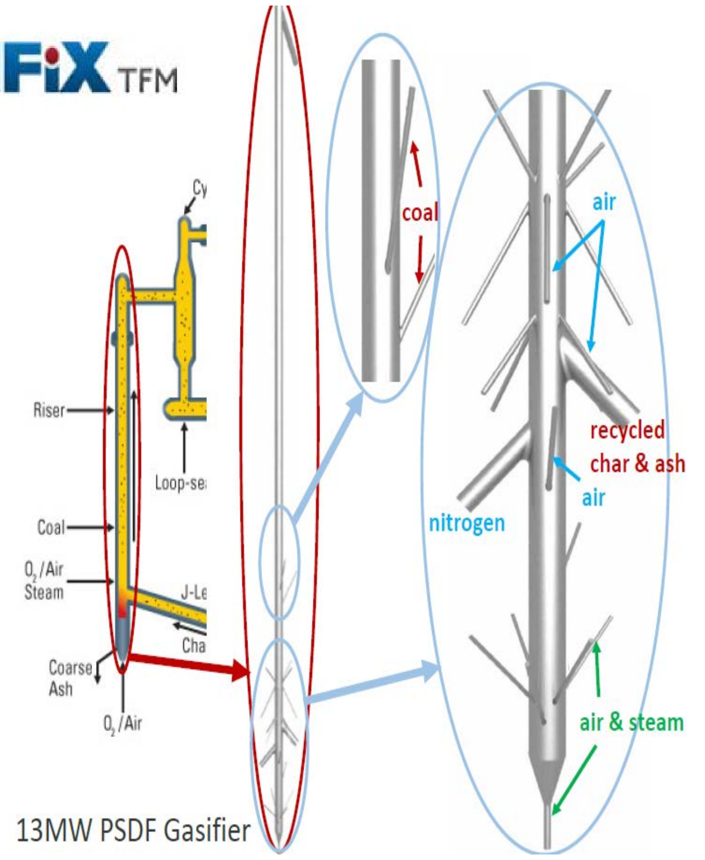
MFiX PIC *Particle-in-Cell : Track parcels of particles and approximate collisions*

ROM *Reduced Order Models: Simplifie models with limited application*

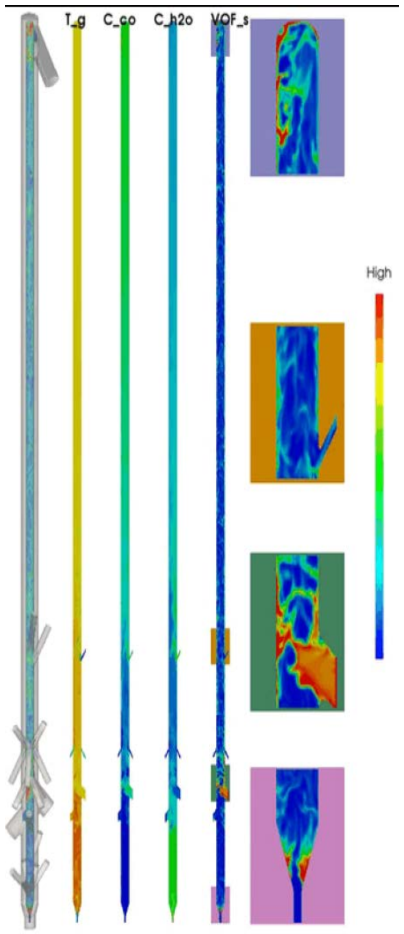
1. Project Description and Objectives

Status of the beginning of the project

MFiX TFM



13MW PSDF Gasifier



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

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

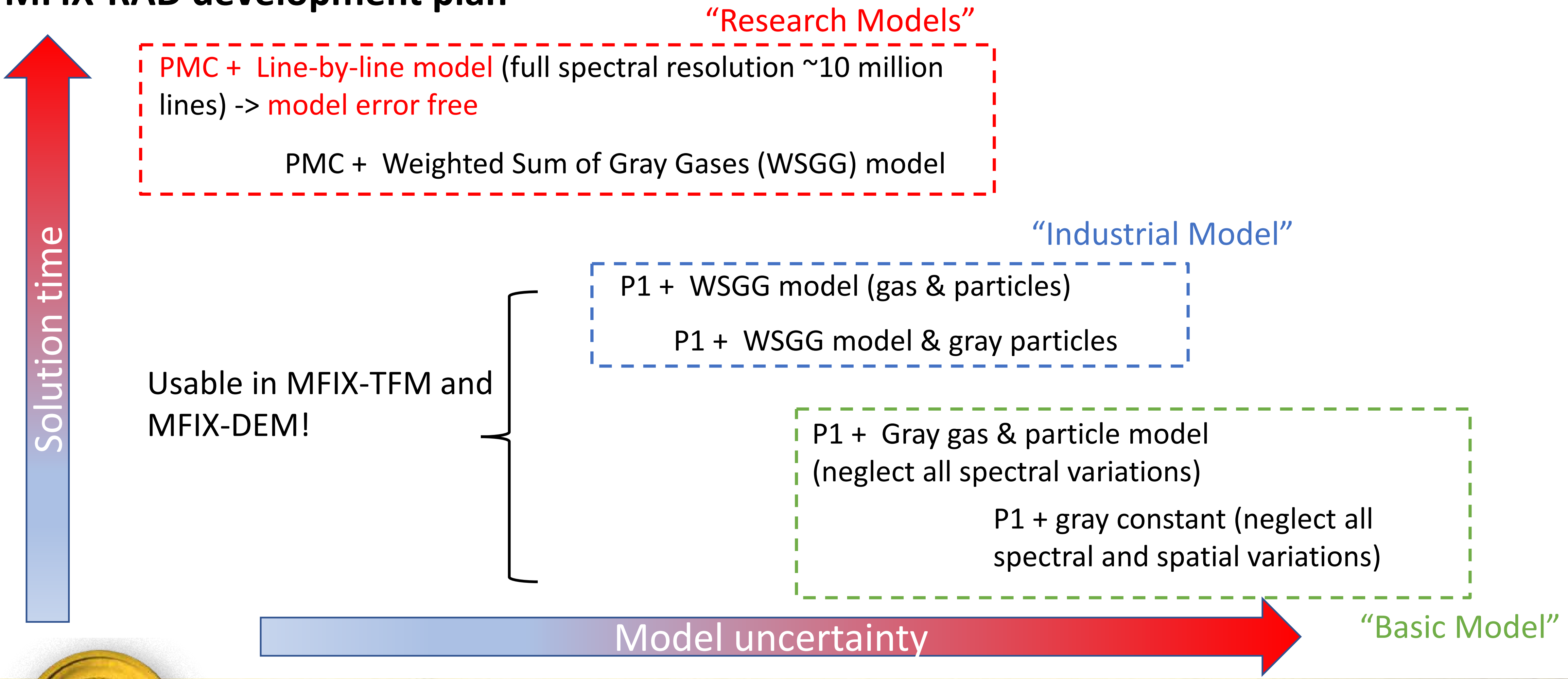
1. Project Description and Objectives

Technology benchmarking: comparing three popular CFD packages

Capability	MFiX	OpenFOAM (open source)	ANSYS-FLUENT (commercial)
TFM reacting	yes	yes	yes
DEM reacting	yes	no	no
Radiative Heat transfer	no	Gray, P1, DOM	Gray, simple WSGG, P1, DOM

1. Project Description and Objectives

MFIX-RAD development plan



“Research Models”

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

PMC + Weighted Sum of Gray Gases (WSGG) model

“Industrial Model”

P1 + WSGG model (gas & particles)

P1 + WSGG model & gray particles

Usable in MFIX-TFM and MFIX-DEM!

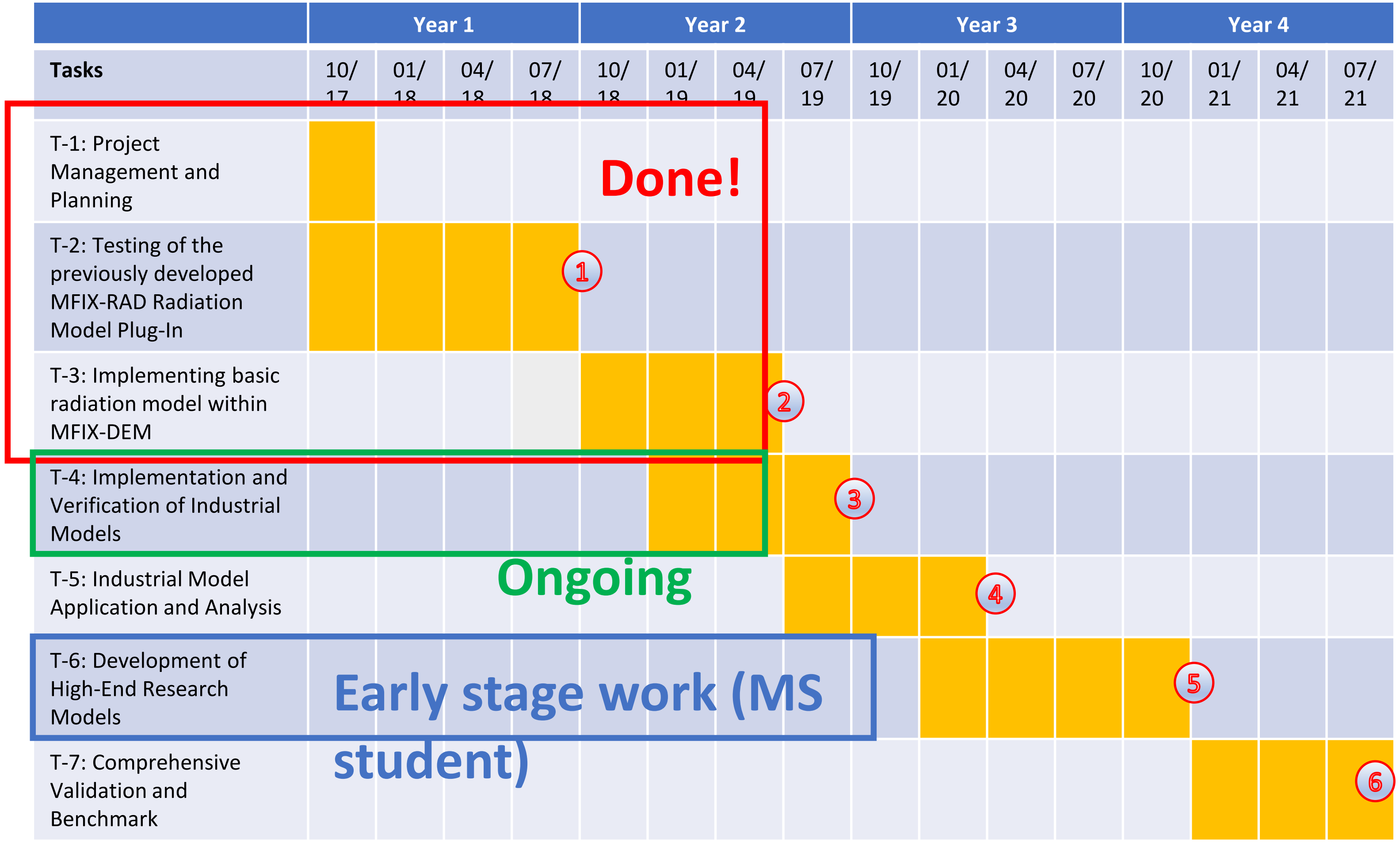
P1 + Gray gas & particle model (neglect all spectral variations)

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

“Basic Model”

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!

Ongoing

Early stage work (MS student)

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

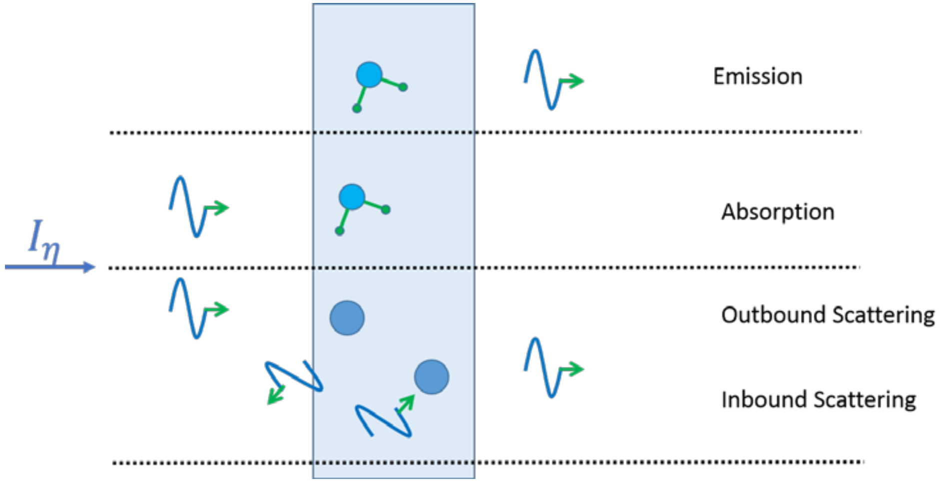
$$\varepsilon_{s_m} \rho_{s_m} c_{ps_m}\left(\frac{\partial T_{s_m}}{\partial t} + u_{s_m} \,.\, \Delta T_{s_m}\right) = \nabla q_{s_m} + \sum_{m=1}^{M} H_{gsm} - \Delta H_{rs_m} - \nabla . \vec{q}_{rs_m}$$

Single particle Energy equation for MFiX-DEM

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

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

2. Project Update



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

$$-a_\eta I_\eta$$

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

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:

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

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

Gray P1 model assumptions

$$\frac{dI_\eta}{ds} = \vec{s}\cdot\nabla I_\eta = a_\eta I_{b\eta} - a_\eta I_\eta - \sigma_{s\eta} I_\eta + \frac{\sigma_{s\eta}}{4\pi}\int I_\eta(\vec{s}')\Phi_\eta(\vec{s},\vec{s}')d\Omega$$

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)

Gas phase absorption

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

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

Solid phase absorption

Gas phase emission

Solid phases emission

2. Project Update

“Distributing the source terms”

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

Continuous phase

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

Gray models for a_g

- “gray constant” $a_g = const$ (user input)
- “gray” => Planck mean absorption using CO_2 and H_2O

Dispersed phase m (M total)

$$a_s = \sum_{m=1}^{M} a_{s,m} \qquad E_s = \sum_{m=1}^{M} E_{s,m} = \sum_{m=1}^{M} a_{s,m}\,\frac{\sigma\,T_{s,m}^4}{\pi}$$

$$-\nabla\cdot q_{rs} = \sum_{m=1}^{M} a_{s,m}\,G - 4\pi\sum_{m=1}^{M} a_{s,m}\,\frac{\sigma\,T_{s,m}^4}{\pi} = \sum_{m=1}^{M}\left(a_{s,m}G - 4a_{s,m}\sigma\,T_{s,m}^4\right) = \sum_{m=1}^{M} -\nabla\cdot q_{rs,m}$$

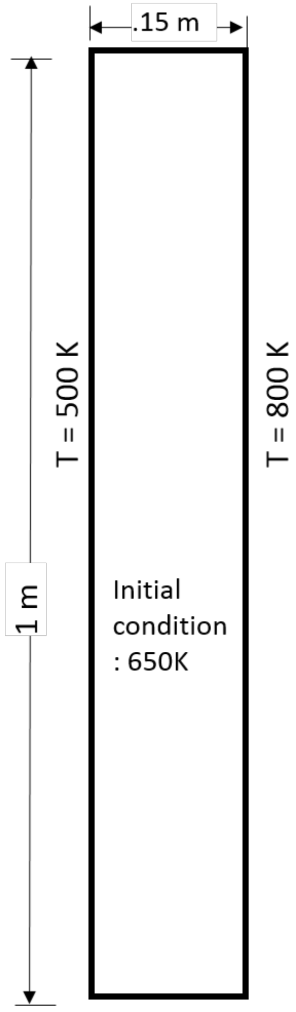
$$\boldsymbol{-\nabla\cdot q_{rs,m}} = \boldsymbol{a_{s,m}}\boldsymbol{(G - 4\sigma\,T_{s,m}^4)}$$

Gray models for $\boldsymbol{a_{s,m}}$

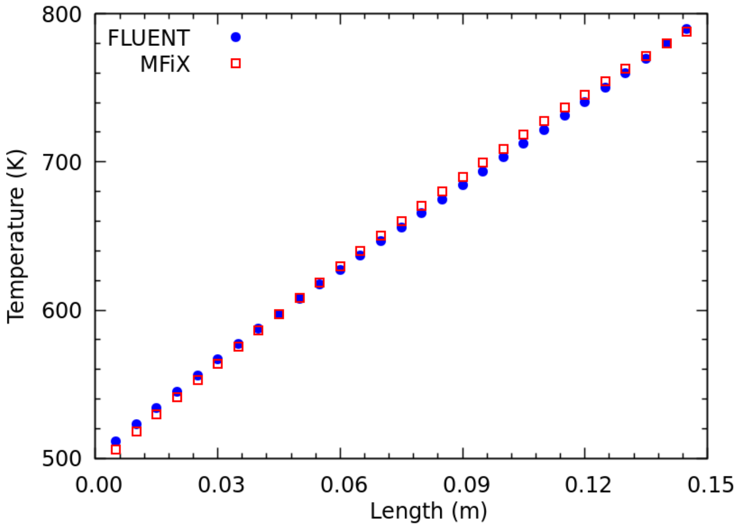
- “gray constant” based on constant emissivity and diameter of particles
- “gray” based on Buckius-Hwang correlation (depends on refractive index, mean particle size, void fraction and temperature)

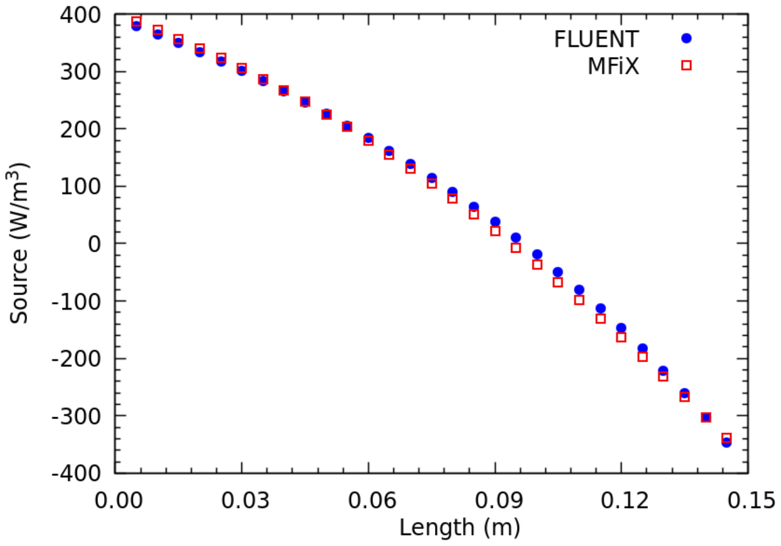
2. Project Update

Basic Verification of the P1 implementation

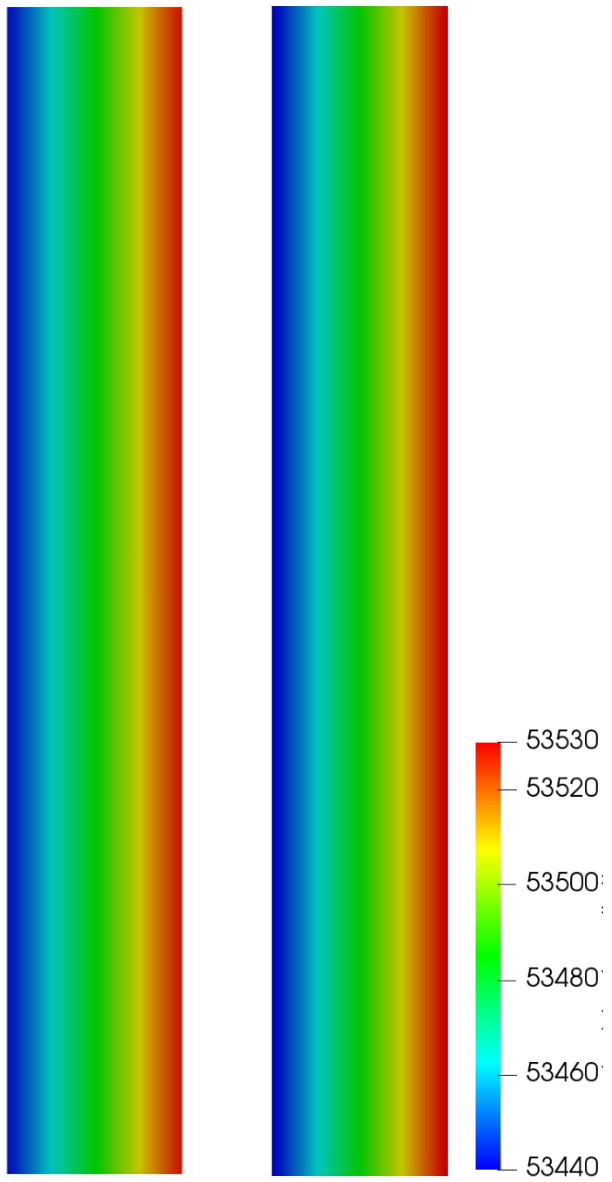


- 2D Steady, single phase
- Heat transfer via radiation (P1, $a_g = 0.01 m^{-1}$) and diffusion
- Mesh: 30x200
- Use Ansys-Fluent solver for verification





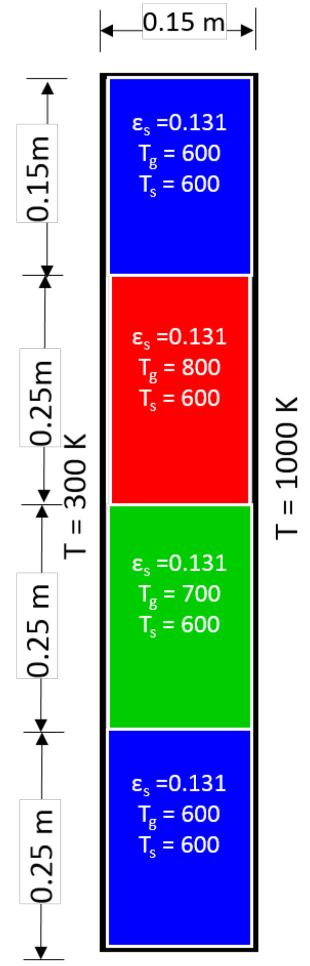
Incident radiation G $[W/m^2]$ fields



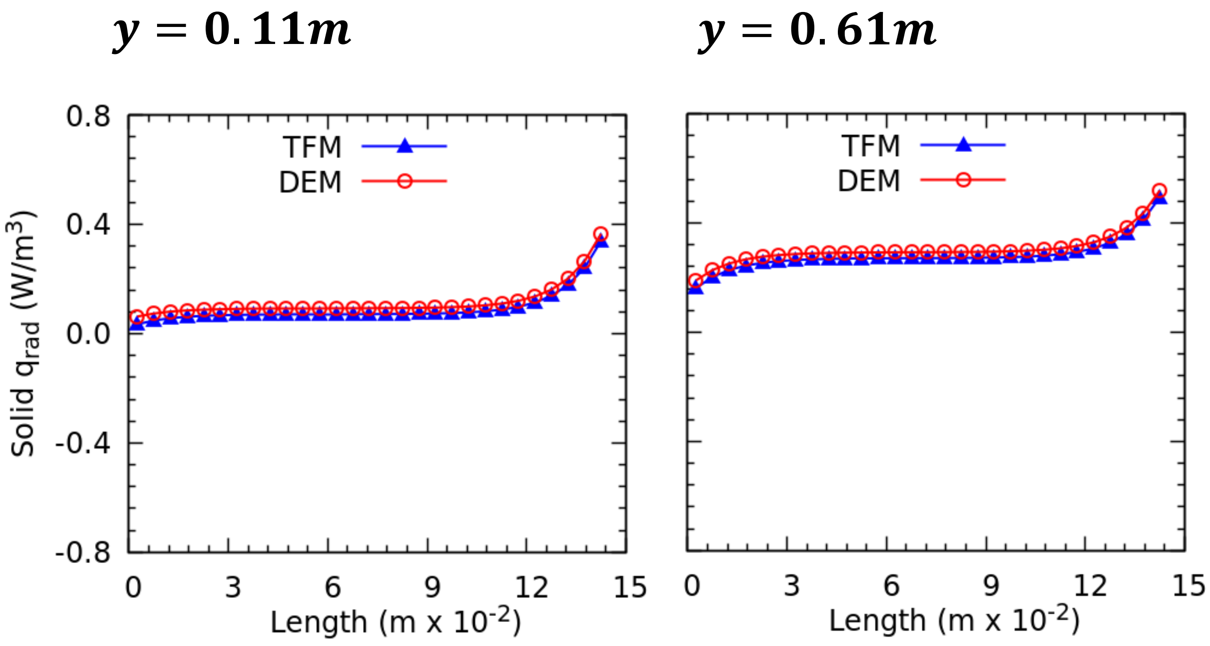
FLUENT MFIiX

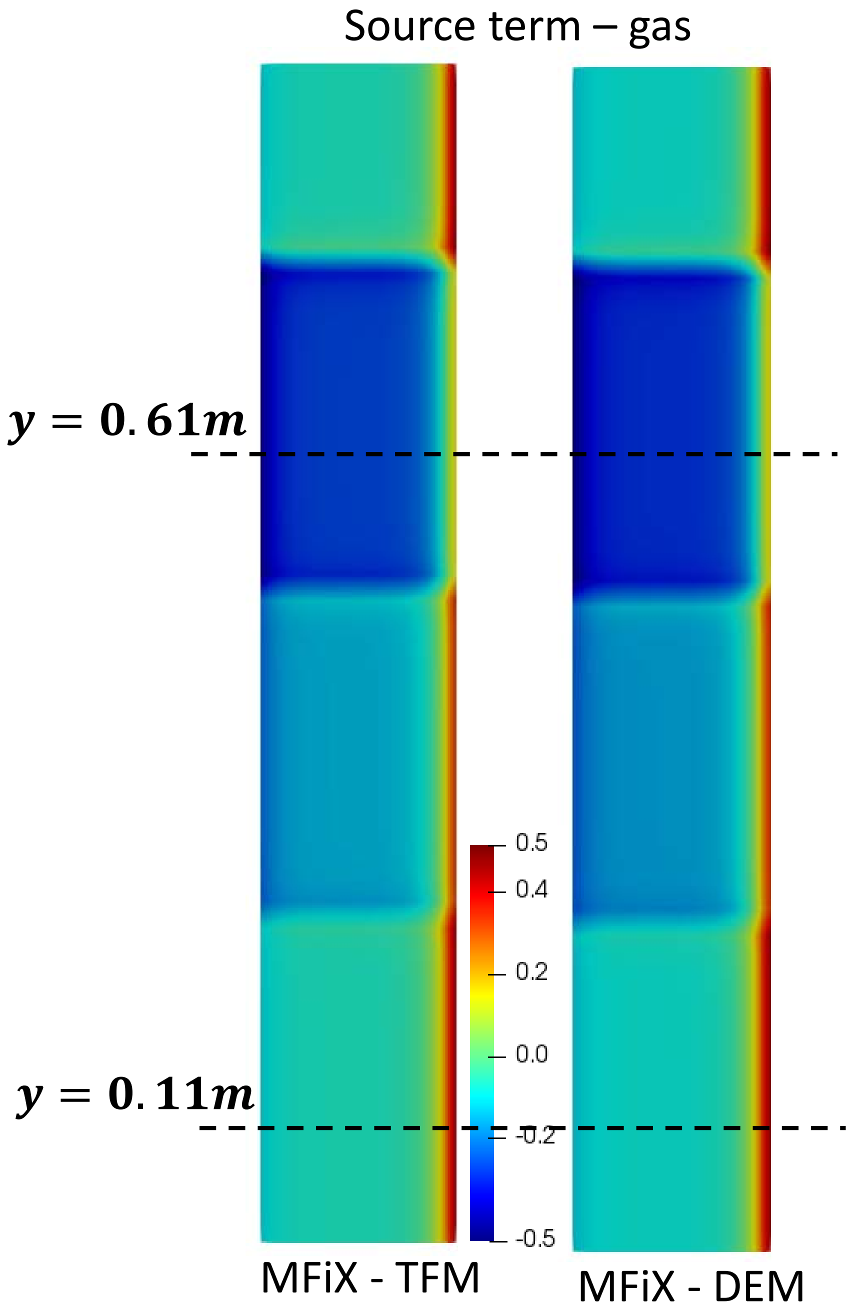
2. Project Update

Verification of the P1 - DEM implementation



- 2D, Radiation only (frozen "fields"), 30x90 cells
- Compare TFM and DEM results => should be identical
- Gas phase $a_g = 0.3cm^{-1}$
- one particle per cell ($d_p = 1mm$, $em_s = 0.6$ =>$a_s = 0.6cm^{-1}$





2. Project Update

Relevance of thermal radiation in Lab-Scale reactors (54kWth)

- **Two Fluid Model**
  - 2 solid phases (cold and hot char)
  - 5 gas phases ($N_2, O_2, CO, CO_2, soot$)
  - Neglect convective heat transfer
- **Geometry**
  - 2D Cylindrical
  - 20 x 60 cells

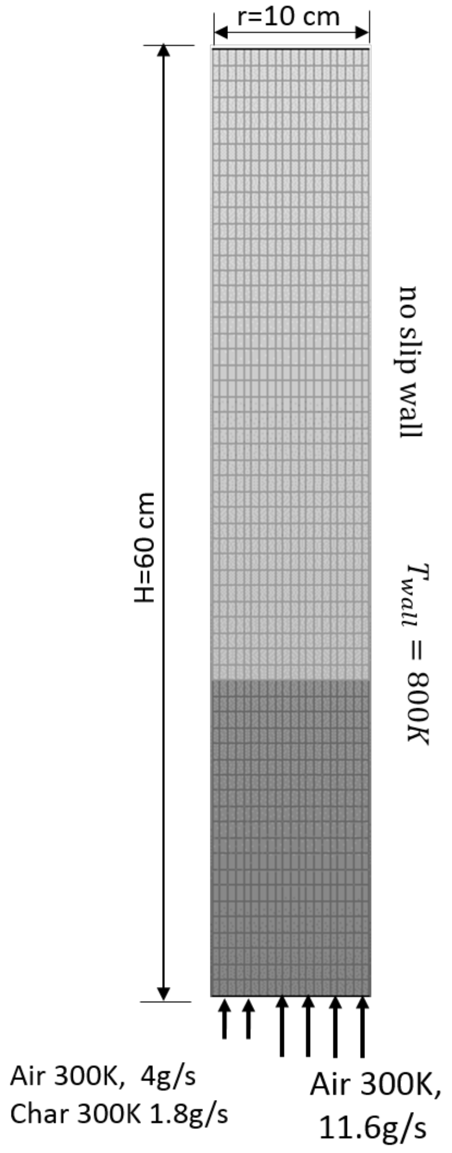
Compare results with and without radiative heat transfer!

MFIX-RAD settings in mfix.dat

```
# Radiation Model
 RAD_ON = .T.
 RAD_EMIS_W = 1.0 1.0 1.0 1.0
 RAD_T_W = 300 300 800 800
 RAD_NQUAD = 1
 RAD_SKIP = 0
 RAD_NRR = 10
 RAD_RTE = 'P1'
 RAD_SPECTRAL = 'GRAY'
```

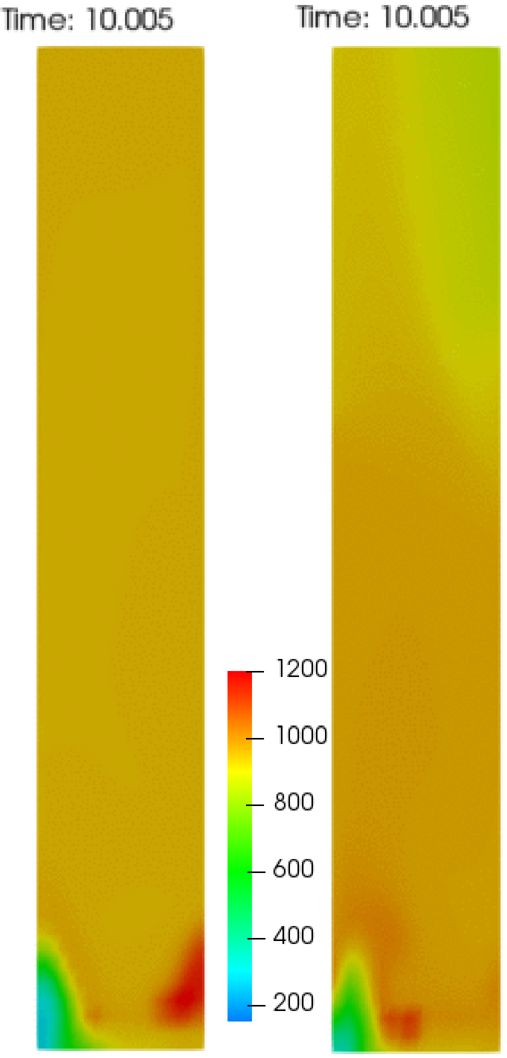
Gas & solid phase reactions

2*CO --> Soot + CO2
2*CO --> Soot + CO2
CO + 0.5*O2 --> CO2
2*FC1 + O2 --> 2*CO
FC1 + CO2 --> 2*CO
2*FC2 + O2 --> 2*CO
FC2 + CO2 --> 2*CO
FC2 --> FC1
Ash2 --> Ash1



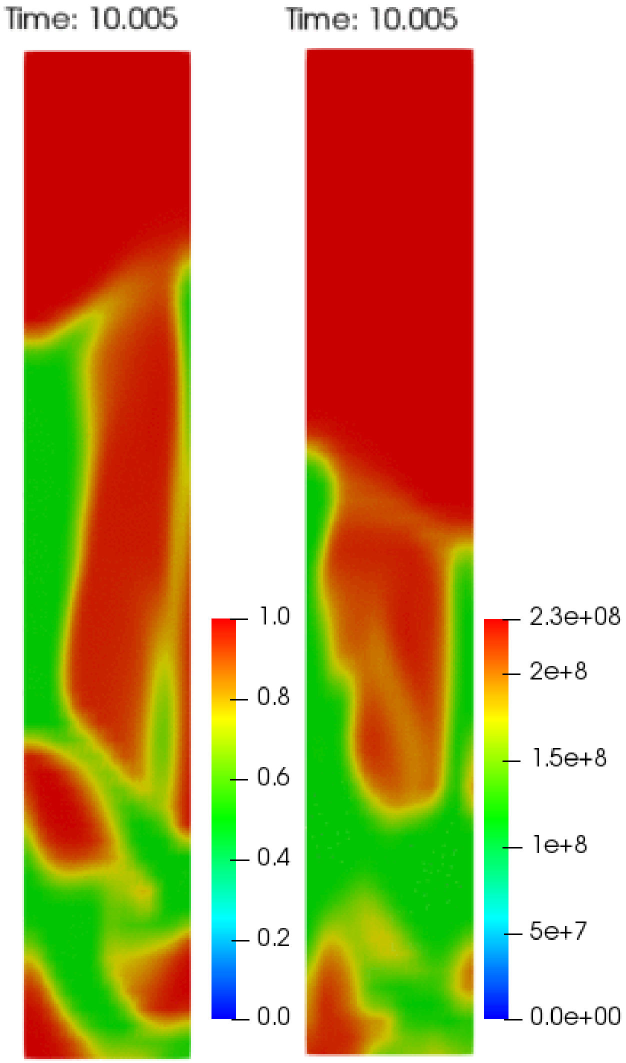
2. Project Update

Gas Temperature [K]



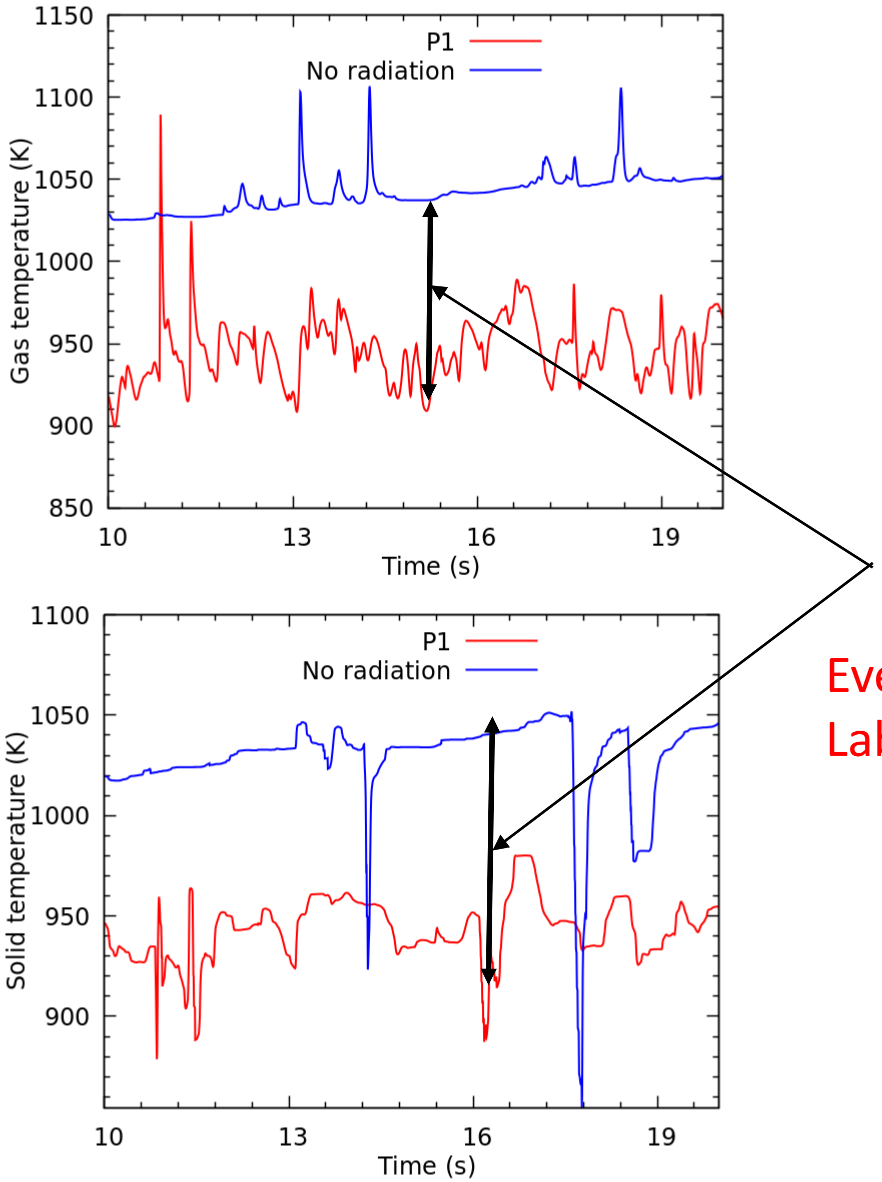
No rad **P1 gray**

Gas volume fraction



No rad **P1 gray**

Mass weighted average temperatures at the outlet



$\Delta T > 110^o C$

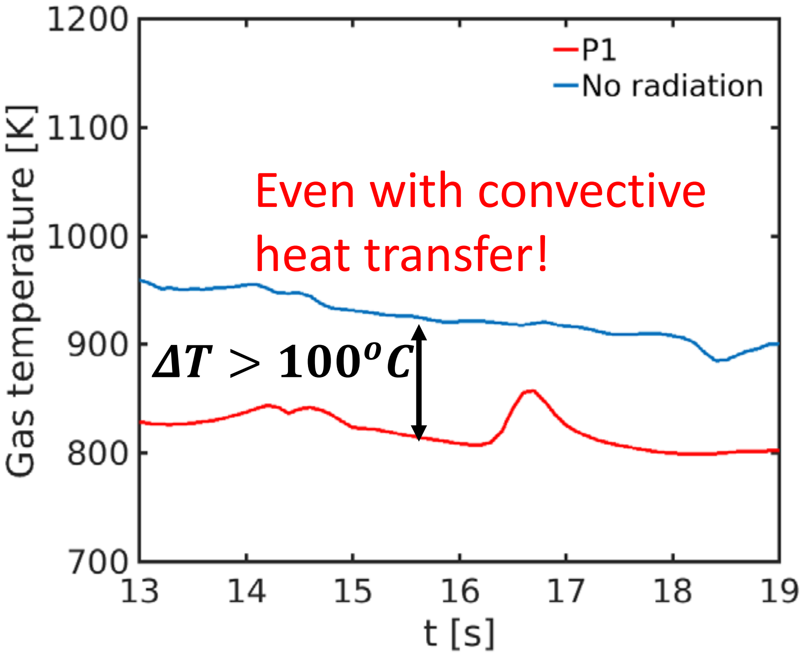
Even in low-Temp Lab scale reactor!

2. Project Update

Relevance of thermal radiation in a Large Scale reactor (5.4 MWth)

- **Same case as before but thermal power scaled up by a factor of 100**
  - Include convective heat transfer to walls using average heat transfer coefficient $h = 14\ W/m^2K$
- **Mesh** 40 x 120 cells

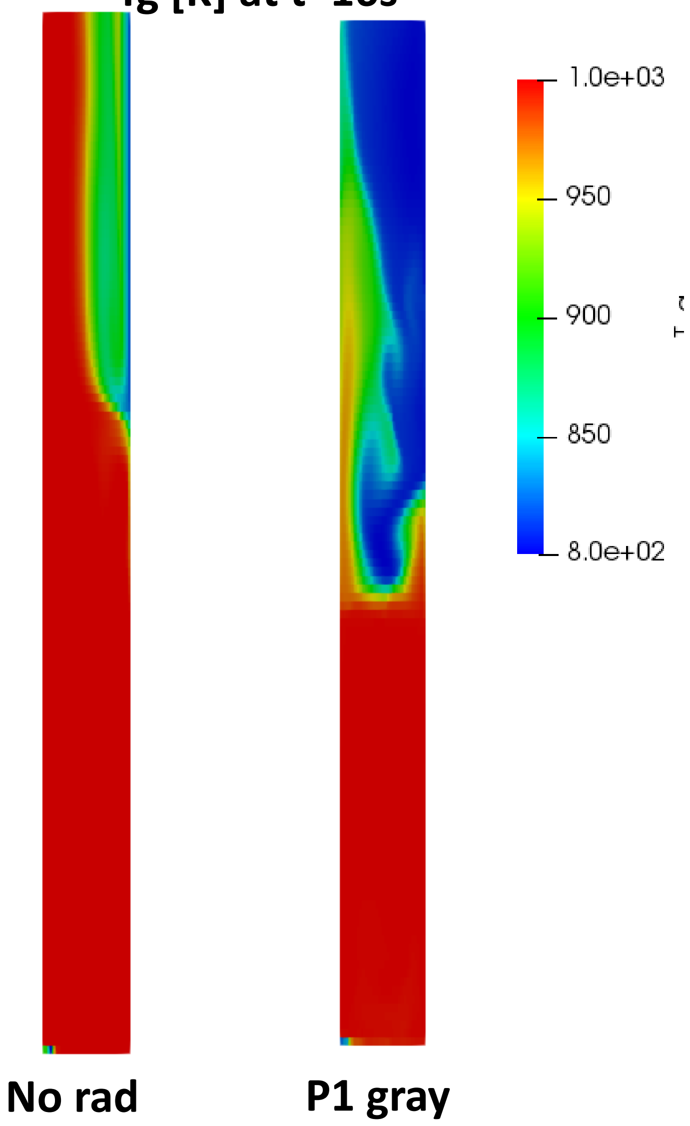
Mass weighted average temperature at the outlet



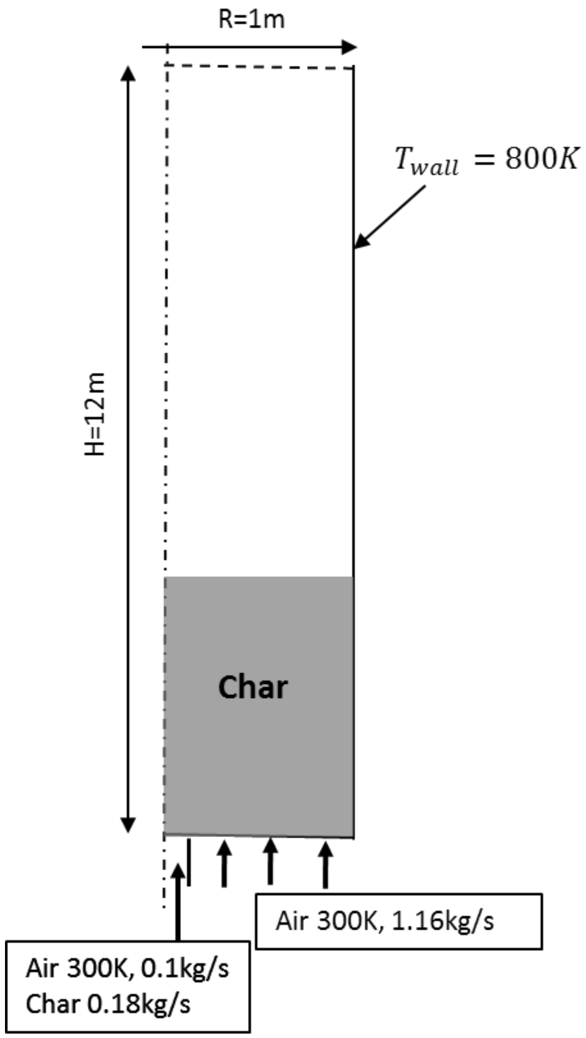
Even with convective heat transfer!

$\Delta T > 100^o C$

Tg [K] at t=16s

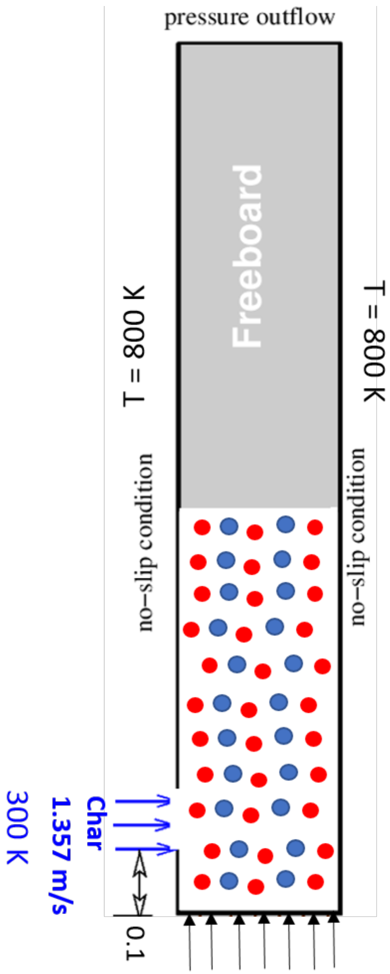


No rad **P1 gray**



2. Project Update

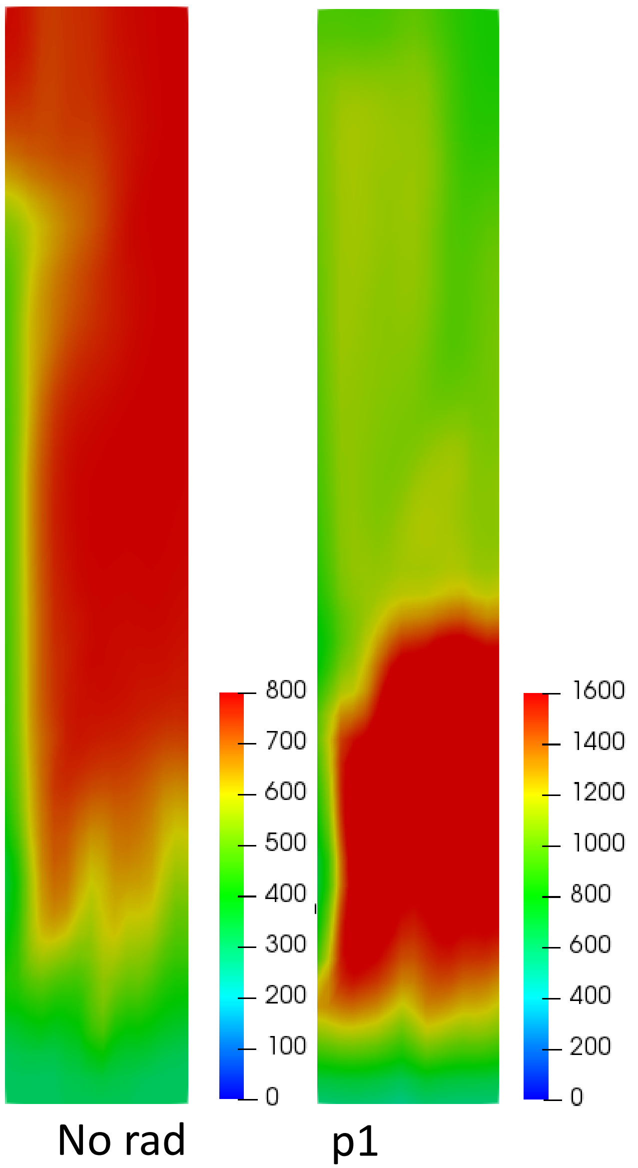
MFiX-DEM with radiation



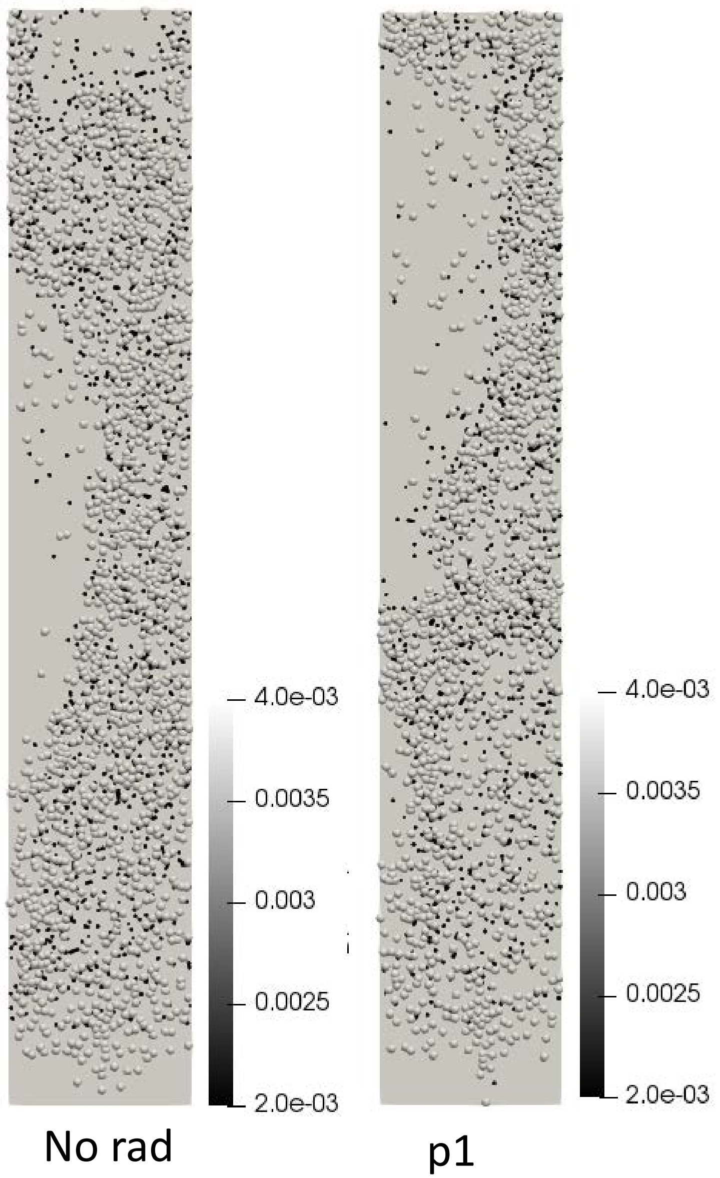
- Only heat transfer (no chemical reactions)
- 2D Cartesian
- Length = 0.15 m, Height = 0.90m, 15 x 45 cells
- Particle diameters 4mm, 2mm
- Particle emissivity $\epsilon_p = 0.6$
- Constant gas phase absorption coefficient $a_g = 3.0m^{-1}$

Time = 0.1s

Gas Temperature



Solid particles location



3. Preparing Project for Next Steps

- **Market Benefits/Assessment**
  - MFiX is widely used the CFD tool for modeling/optimization of reacting multiphase flow
  - MFiX currently has no radiative heat transfer modeling capability
  - For a simple spouted bed combustor, neglecting radiative heat transfer results in temperature differences of $100^o C$
- **Technology-to-Market Path**
  - Basic MFiX-RAD Plug-In is available at GitLab => every MFiX user can download and use it their process modeling!
  - A more accurate spectral model based on WSGG is currently implemented and will be available by the end of May 2019
  - Detailed experimental data for validation is rare in Fluidized Bed Combustors/Gasifiers at larger scale
    - We will use a LBL Photon – Monte Carlo method (model error free) to validate the lower fidelity gray and WSGG models to provide uncertainty values
  - We are seeking industry collaborators who want to use MFiX-RAD in their applications

4. Concluding Remarks

- Basic radiation model (Gray, P1) has been implemented and verified for MFiX-TFM and MFiX-DEM
- First results in low-temperature spouted bed confirm that radiative heat transfer is important

Next Steps

- Extend basic radiation model to be usable in the new and improved MFIX-PIC (v19.1)
- Finish implementation and verification of industrial model (WSGG, P1)
- Implement Photon Monte Carlo solver for detailed validation of lower fidelity models
  - David Tobin (MS student) has started this task and it will be his thesis topic

4. Concluding Remarks

- We have received the detailed (1.4 M cells) MFiX case set up for the 13MW Power Systems Development Facility (PSDF) gasifier => temperature and syngas composition data available at the outlet
  - We will use this case for validation of the models in a large-scale application
  - Expect improvements compared to simulations that neglected radiative heat transfer