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

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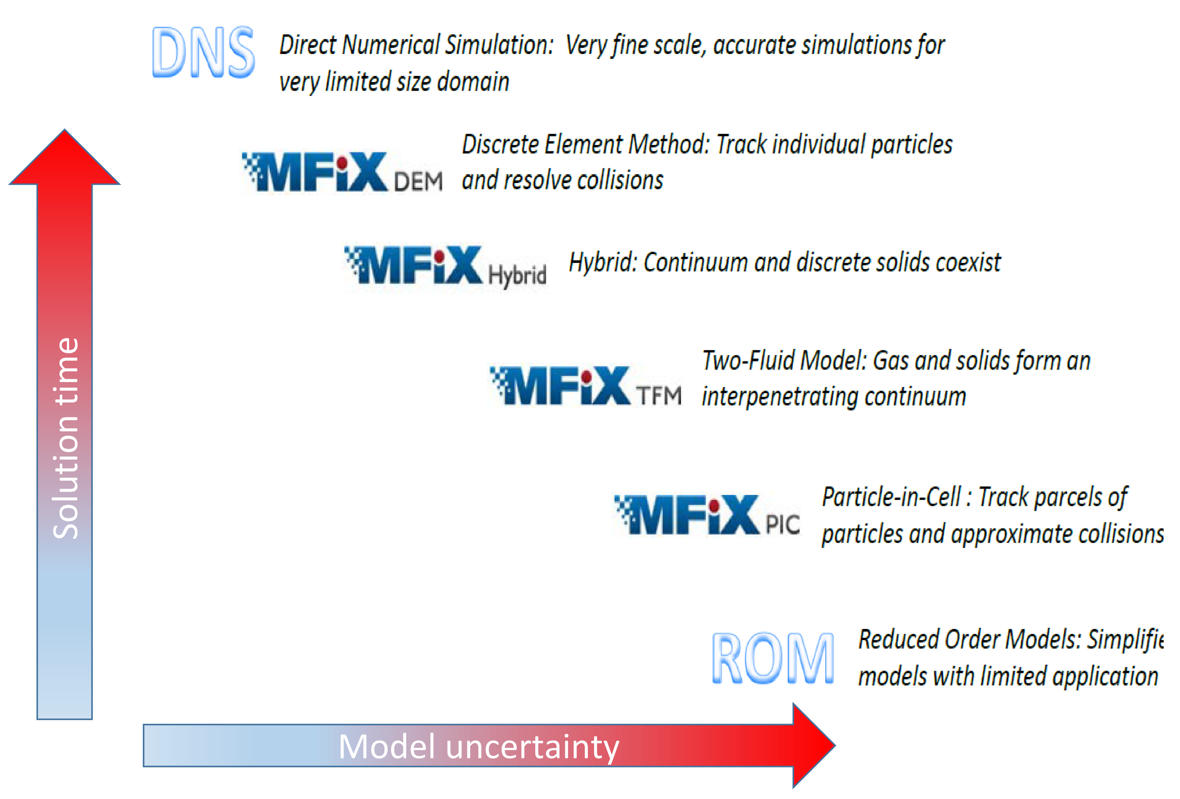
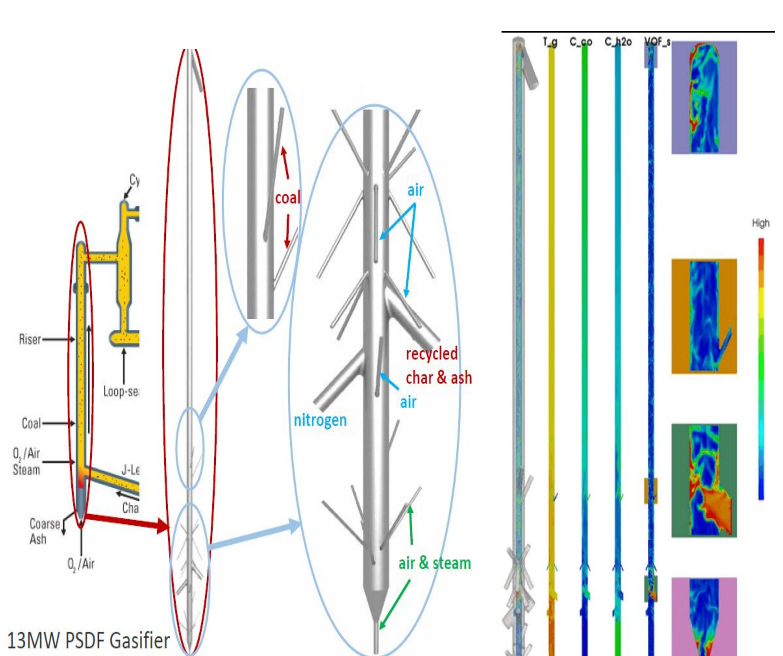
1. NETL's MFIX suite: Tradeoffs between uncertainty and CPU cost



2. Multiphase Flow Modeling

MFiX TFM **Application: 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 the in the model?

Radiative heat transfer!

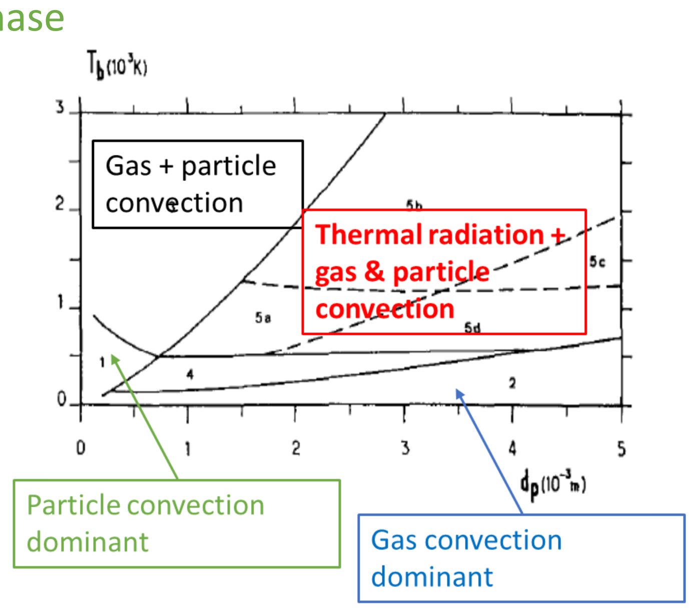
3. Relevance of radiative heat transfer

Main modes of heat transfer in two-phase flow applications

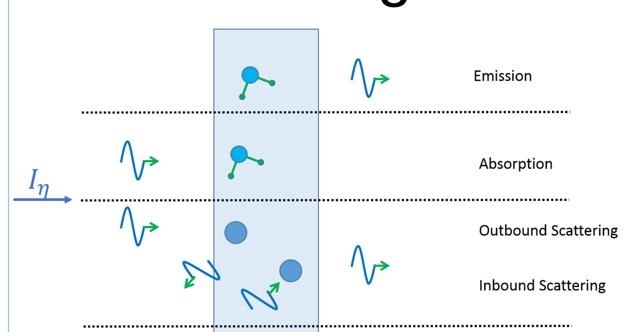
- Convection of particulate phase
- Convection of gas
- Thermal radiation

Application: Heat transfer in non-reacting fluidized bed

Theoretical estimate: G. Flamant et al, (Powder Technology 69 (1992)



4. Describing radiative heat transfer



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

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

Source term in the energy equation:

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

Solution approach:

- 3 spatial dimensions (x,y,z): CFD discretization
- 2 directional dimensions (ϕ,ψ): RTE solvers
- 1 spectral dimension (η): spectral models

5. Modeling challenges for radiative heat transfer

RTE solvers

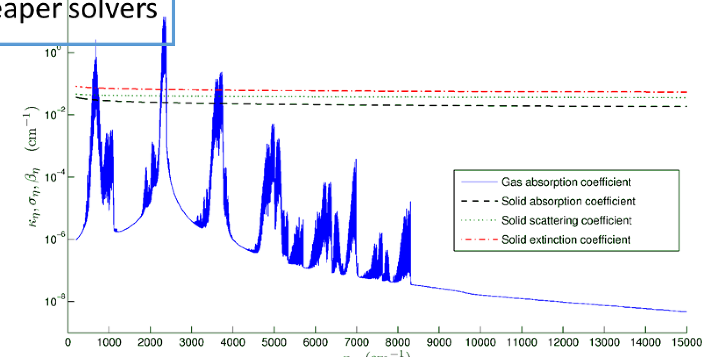
- Spherical Harmonics (**P1**, P2, .. PN)
- Discrete Ordinate Method (DOM)
  - easy to extend to high orders
  - expensive to model scattering
- Photon Monte Carlo (PMC)
  - random sampling of photon bundles
  - expensive but arbitrarily accurate
  - used for validation of cheaper solvers

Spectral models

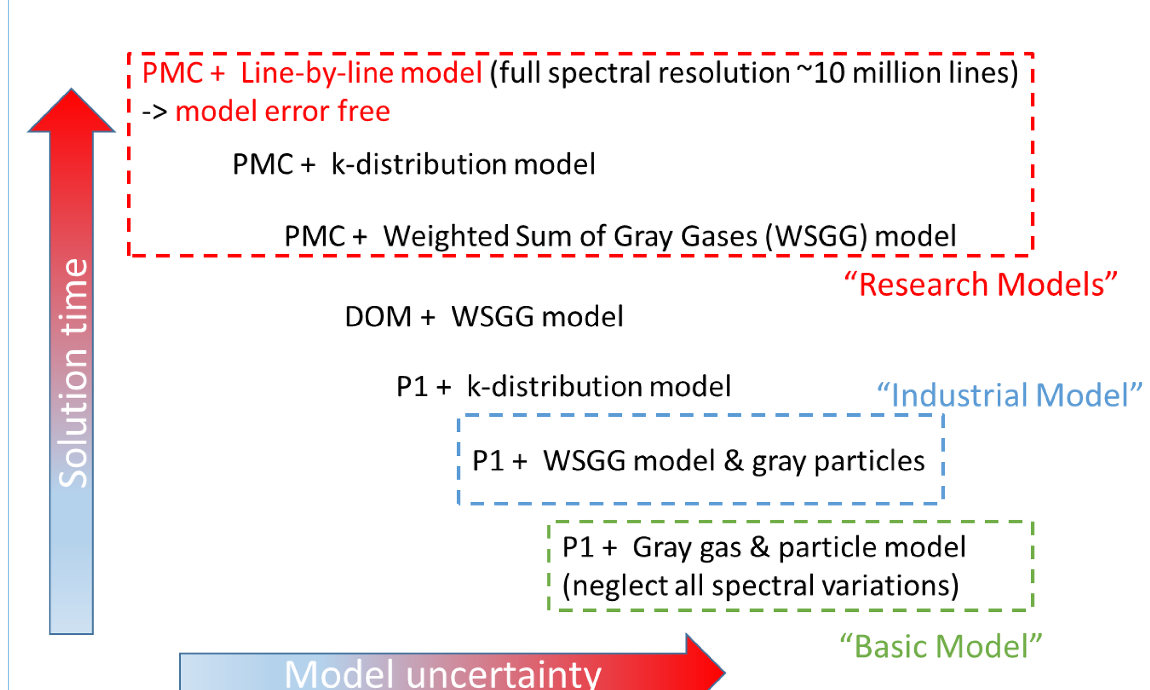
- Gas phase (CO_2, H_2O, CO): shows strong variations with wavelength on multiple scales
- Particle phase: less depend on wavelength but depends on refractive index and size

Example:

- Temperature T=600K
- Gas with 10% CO_2
- Particle
  - $m = 2.2 - 1.12i$
  - $\varepsilon_p = 10^{-3}$
  - $D_p = 0.4mm$



6. Modeling approaches for radiative heat transfer



7. Project technical approach

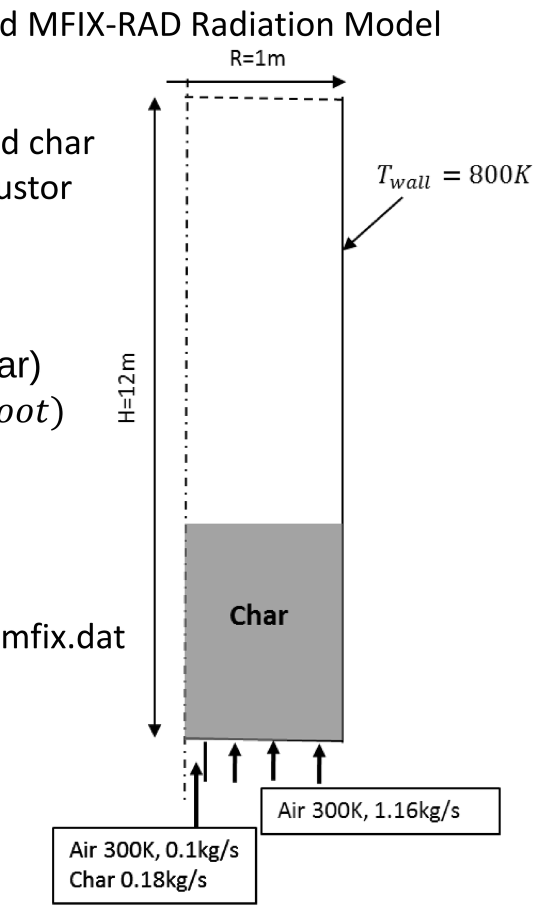
1. Testing of basic MFIX-RAD module (MDFIX-TFM)
   - P1 + Gray Gas & Particles -> completed
   - Parallel implementation finished and currently tested
2. Implementing basic radiation model within MFIX-DEM
   - Enables to use the basic radiation model in the higher fidelity MFXI-DEM approach
3. Implement & verify industrial model
   - P1 + WSGG + Gray particles (MFIX TFM and DEM)
4. Industrial model application and analysis
   - Demonstrate on a large scale gasifier the influence of the radiation model
5. Development of high end research models
   - PMC + LBL with a focus on a HPC suitable implementation in MFX - DEM
6. Comprehensive validation
   - Utilize model-error free PMC results to do this

8. First results

Task 1: "Testing of the previously developed MFIX-RAD Radiation Model Plug-In and basic model"

Simplistic pilot scale 1.5MWth fluidized bed char combustion (modified Spouted Bed Combustor tutorial)

- **Two Fluid Model**
  - 2 solid phases (cold and hot char)
  - 5 gas phases $(N_2, O_2, CO, CO_2, soot)$
- **Geometry**
  - 2D cylindrical axisymmetric
  - 40 x 80 cells



Compiled MFIX-RAD using the 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'
```

T_{gas} [K] no radiation (t=12s)