Mathematical modeling of pulverized coal combustion based on transported PDF methods

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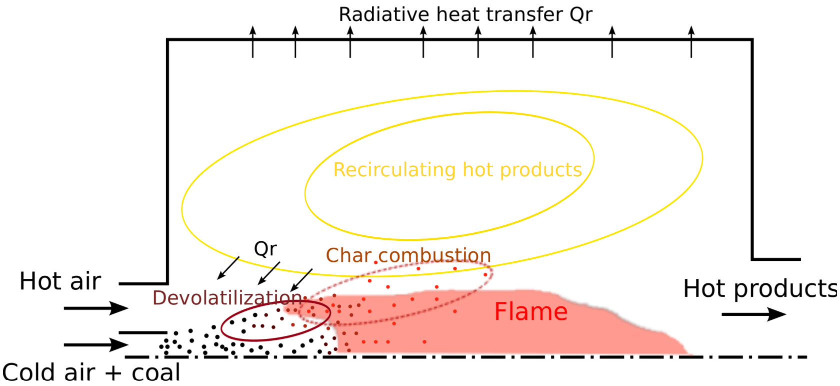
Outline

Outline

Pulverized coal combustion and gasification



Main modeling approaches for coal combustion

Industrial furnace

- Gas phase RANS equations closed with turbulence model for gas phase
- Lagrangian particle tracking with dispersion modeling and PSI-method for phase exchange
- Turbulence-Chemistry interaction model
  1. "Eddy-Break-Up" model
  2. Mixture fraction + assumed shape PDF method (Smith USU, Smoot BYU)

1 “Eddy-Break-Up” model

Solving equations for mean fuel and oxygen mass fraction, $\widetilde{Y}_F$, $\widetilde{Y}_O$:

$$\frac{\partial \widetilde{Y}_F}{\partial t} + \widetilde{u}_j \frac{\partial \widetilde{Y}_F}{\partial x_j} = \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_j} \left(\langle \rho \rangle \frac{\nu_{eff}}{Sc_t} \frac{\partial \widetilde{Y}_F}{\partial x_j} \right) + \widetilde{S}_F^c + \widetilde{S}_F^{coal}$$

$$\widetilde{S}_F = -A_1 \overline{\rho} \frac{\varepsilon}{k} \min(\widetilde{Y}_F, \widetilde{Y}_O)$$

Main issue: $A_1 = 2$ to $A_1 = 32$ used in applications

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2 “Mixture fraction” method

- Based on the assumption that reactions are mixing controlled
- Three stream mixing problem of volatiles, char, and air

- Char mixture fraction $Z_1 = \dfrac{m_c}{m_{ox} + m_c + m_v}$
- Volatile mixture fraction $Z_2 = \dfrac{m_v}{m_{ox} + m_c + m_v}$
- Enthalpy

Assume chemical equilibrium: e.g. $T = T(Z_1, Z_2, h)$

Presume the shape of the Favre PDF $\widetilde{f}_{Z_1,Z_2,h}$

$$\widetilde{T}(\mathbf{x}, t) = \iiint T(\hat{Z}_1, \hat{Z}_2, \hat{h})\widetilde{f}_{Z_1,Z_2,h}(\hat{Z}_1, \hat{Z}_2, \hat{h}; \mathbf{x}, t) \cdot d\hat{Z}_1 \cdot d\hat{Z}_2 \cdot d\hat{h}.$$

2 "Mixture fraction" method

To presume the shape of the joint PDF

- Assume statistical independence of Z_1, Z_2, h
- Neglect fluctuations of h

$$\widetilde{f}_{Z_1,Z_2,h}(\hat{Z}_1, \hat{Z}_2, \hat{h}; \mathbf{x}, t) \approx \widetilde{f}_{Z_1}(\hat{Z}_1; \mathbf{x}, t)\widetilde{f}_{Z_2}(\hat{Z}_2; \mathbf{x}, t)\delta(h - \widetilde{h})$$

Assume marginal β-PDF (parametrized by first two moments):

$$\frac{\partial \widetilde{Z_2}}{\partial t} + \widetilde{u}_j \frac{\partial \widetilde{Z_2}}{\partial x_j} = \frac{1}{\langle\rho\rangle} \frac{\partial}{\partial x_j} \left(\langle\rho\rangle \frac{\nu_{eff}}{Sc_t} \frac{\partial \widetilde{Z_2}}{\partial x_j} \right) + \widetilde{S}_{dev}$$

$$\frac{\partial \widetilde{Z_2''^2}}{\partial t} + \widetilde{u}_j \frac{\partial \widetilde{Z_2''^2}}{\partial x_j} = \frac{1}{\langle\rho\rangle} \frac{\partial}{\partial x_j} \left(\langle\rho\rangle \frac{\nu_t}{Sc_t} \frac{\partial \widetilde{Z_2''^2}}{\partial x_j} \right) + 2\frac{\nu_t}{Sc_t} \frac{\partial \widetilde{Z_2''^2}}{\partial x_k} \frac{\partial \widetilde{Z_2''^2}}{\partial x_j} - C_\phi \frac{\epsilon}{k} \widetilde{Z_2''^2} + \widetilde{Z_2''^2 S_{dev}''}$$

Main issues:

- Enthalpy fluctuations might be significant
- Statistical independence questionable

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Alternative: Transported PDF method

Solve a transport equation for $\widetilde{f}_{Z_1,Z_2,h}(\hat{Z}_1, \hat{Z}_2, \hat{h}; \mathbf{x}, t)$

Advantages:

- No independence assumption necessary
- Fluctuations of all scalars included
- Can be easily extended to better chemistry models

Refined chemistry models:

- Two or more different volatile streams
- Finite rate chemistry by using skeletal/detailed reaction mechanism

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Gas phase PDF transport equation

- Consider one point mass density function (MDF) $\mathcal{F}_g(\mathbf{v},\psi;\mathbf{x},t)=\rho(\psi)f_g(\mathbf{v},\psi;\mathbf{x},t)$
- $\int \mathcal{F}_g(\mathbf{v},\psi;\mathbf{x},t)d\psi d\mathbf{v}=\alpha_g(\mathbf{x},t)\left\langle\rho(\mathbf{x},t)\right\rangle=\overline{\rho}(\mathbf{x},t)$
- Derive the exact transport equation for $\mathcal{F}_g$ from the Navier-Stokes equation for tow phase flow

$$\frac{\partial\mathcal{F}_g}{\partial t}+v_j\frac{\partial\mathcal{F}_g}{\partial x_j}+\frac{\partial}{\partial v_i}\left[\frac{1}{\overline{\rho}}\left(-\frac{\partial\overline{p}}{\partial x_i}+\overline{\rho}g_i+\langle S_{u_i}\rangle\right)\mathcal{F}_g\right]$$
$$=-\frac{\partial}{\partial v_i}\left[\langle a_i|\,\mathbf{v},\psi\rangle\mathcal{F}_g\right]-\frac{\partial}{\partial\psi_\alpha}\left[\langle\theta_\alpha|\,\mathbf{v},\psi\rangle\mathcal{F}_g\right]-\frac{\partial}{\partial\hat{h}}\left[\langle S_{rad}|\,\mathbf{v},\psi\rangle\mathcal{F}_g\right]$$
$$-\frac{\partial}{\partial\hat{h}}\left[\left\langle\dot{h}_{cr}\middle|\,\mathbf{v},\psi\right\rangle\mathcal{F}_g\right]+\frac{1}{\rho(\psi)}\langle S_m|\,\mathbf{v},\psi\rangle\mathcal{F}_g$$

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Main difficulties with the PDF equation

- Conditional acceleration

$$-\frac{\partial}{\partial v_i}\left[\langle a_i | \mathbf{v}, \psi\rangle \mathcal{F}_g\right] = -\frac{\partial}{\partial v_i}\left[\frac{1}{\rho(\boldsymbol{\psi})}\left\langle -\frac{\partial p'}{\partial x_i} + \frac{\partial \tau'_{ij}}{\partial x_j} + S'_{u_i}\middle| \mathbf{v}, \psi\right\rangle\right]$$

- Micro mixing

$$-\frac{\partial}{\partial \psi_\alpha}\left[\langle \theta_\alpha | \mathbf{v}, \psi\rangle \mathcal{F}_g\right] = \frac{\partial}{\partial \psi_\alpha}\left[\frac{1}{\rho(\boldsymbol{\psi})}\left\langle -\frac{\partial J_j^{\alpha\prime}}{\partial x_j}\middle| \mathbf{v}, \psi\right\rangle\right]$$

- Conditional phase exchange terms $\left\langle \dot{h}_{cr}\middle| \mathbf{v}, \psi\right\rangle, \langle S_m | \mathbf{v}, \psi\rangle$

- High dimensionality $(dim = 2 + 2 + 3 = 5)$

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Numerical solution of the PDF equation

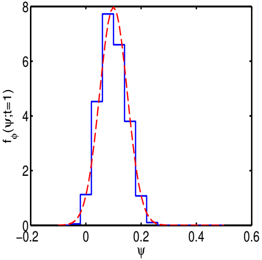
PDF equation $\Longleftrightarrow$ **Monte Carlo method**

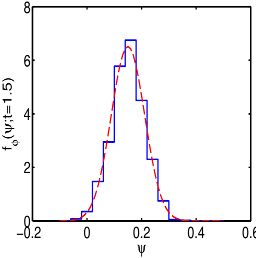
$$\frac{\partial f_\phi}{\partial t} = -a\frac{\partial f_\phi}{\partial \psi} + D\frac{\partial^2 f_\phi}{\partial \psi^2}, \quad D = \frac{b^2}{2}, \text{ on } \psi \in (-\infty, \infty)$$

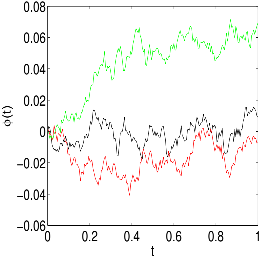
$$f_\phi(\psi; t=0) = \delta(\psi)$$

$$d\phi(t;\omega_i) = a\,dt + b dW_t(\omega_i), \quad \phi^{(i)}(t=0) = 0$$

dW_t increments of a Wiener process: normal random variables with $\mathcal{N}(0, dt)$







Trajectories of 3 realizations for $a = 0.1$, $b = 0.05$:
Euler-Maruyama scheme with $\Delta t = 0.005$

Gas phase Monte Carlo model

- Position $dx_i^* = u_i^* dt$

- Velocity (SLM-model)

$$du_i^* = \left(-\frac{1}{\rho^*} \left[\frac{\partial \overline{p}}{\partial x_i} \right]^* + g_i + \frac{\langle S_{u_i} \rangle}{\rho^*} \right) dt$$
$$- \left(\frac{1}{2} + \frac{3}{4} C_0 \right) \left[\frac{1}{\tau} \right]^* \left(u_i^* - [\widetilde{u}_i]^* \right) dt + \left(C_0 \, [\varepsilon]^* \right)^{1/2} dW_i$$

- Composition (LMSE-model)

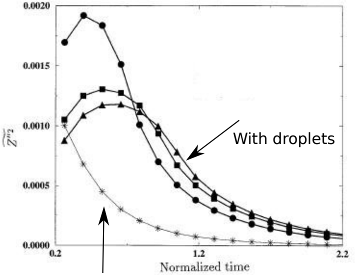
$$dZ_i^* = -\frac{[\omega_\phi]^*}{2} \left(Z_i^* - \left[\widetilde{Z}_i \right]^* \right) dt + S_{Z_i}^* dt$$
$$dh^* = -\frac{[\omega_\phi]^*}{2} \left(h^* - \left[\widetilde{h} \right]^* \right) dt + S_{rad}^* dt + \dot{h}_{cr}^* dt + S_h^* dt$$

- Particle weight

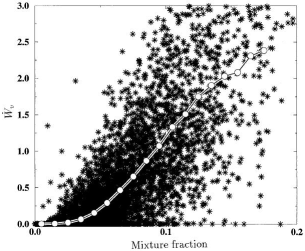
$$\frac{d \, [w^* m^*]}{dt} = \left(S_{Z_1}^* + S_{Z_2}^* \right) [w^* m^*]$$

Mixture fraction source terms

- Mass transfer creates fluctuations in mixture fractions
- Only some DNS results for evaporating droplets available



Reveillon and Vervisch, Comb. and Flame 2000



Reveillon and Vervisch, Comb. and Flame 2000

- Scatter plot of mixture fraction source term
- Line denotes conditional source term $\left\langle S_{Z_2} \middle| Z_2 \right\rangle_p \sim Z_2^2$

Mass transfer terms continued

- We would need $\langle S_{Z_1} | Z_1, Z_2, h \rangle_p, \langle S_{Z_2} | Z_1, Z_2, h \rangle_p$
- Joint gas phase - solid phase statistics not available
- Only $\langle S_{Z_1} \rangle_p , \langle S_{Z_2} \rangle_p$ are available $\Rightarrow$ Need a model

Following Reveillon and Vervisch:

$$S^*_{Z_1} = \langle S_{Z_1} | Z_1, Z_2 \rangle = \begin{cases} \gamma_1 \cdot \left(c_{m1} + Z_1^{*2} \right) \cdot X^*_{O_2} & \text{if } Z_1^* < 0.35 \\ 0 & \text{otherwise,} \end{cases}$$

$$S^*_{Z_2} = \langle S_{Z_2} | Z_2 \rangle = \begin{cases} \gamma_2 \cdot \left(c_{m2} + Z_2^{*2} \right) & \text{if } Z_2^* < 0.2 \\ 0 & \text{otherwise.} \end{cases}$$

- Determine γ_1, γ_2 such that unconditional mean is recovered:

$$\gamma_2(\mathbf{x}, t) = \frac{\bar{\rho} \langle S_{Z_2} \rangle_p}{\int S^*_{Z_2} \mathcal{F}_g d\psi d\mathbf{v}}$$

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Coal particle MDF

Coal particle properties:

- position $\mathbf{X}_p^+(t)$, velocity $\mathbf{u}_p^+(t)$, diameter $D_p^+(t)$, density $\rho_p^+(t)$, temperature $T_p^+(t)$
- the gas velocity "seen" by the particle $\mathbf{u}_s^+(t)$
- the gas composition "seen" by the particle $\phi_s^+(t)$
- for short $[\mathbf{X}_p^+(t), \mathbf{\Phi}^+(t)]$
- particle mass $m_p^+ = \rho_p^+ \pi D_p^{+3}/6$ is a function of $\mathbf{\Phi}^+$.

Coal particle mass density function:

$$\mathcal{F}_p(\mathbf{x}, \mathbf{\Psi}; t) = \left\langle \sum_{+} m_p^+ \delta(\mathbf{X}_p^+(t) - \mathbf{x}) \cdot \delta(\mathbf{\Phi}^+(t) - \mathbf{\Psi}) \right\rangle,$$

such that $\mathcal{F}_p(\mathbf{x}, \mathbf{\Psi}; t) \cdot d\mathbf{\Psi}$ gives the probable mass of coal particles present at $(\mathbf{x}, t)$ with properties in the range $[\mathbf{\Psi}, \mathbf{\Psi} + d\mathbf{\Psi}]$

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Coal particle MDF equation

Now assume:

- laws for $d\Phi_i^+/dt$ and dm_p^+/dt are given
- particle collisions not relevant (dilute particle phase)

$$\frac{\partial \mathcal{F}_p}{\partial t} + v_{p,j}\frac{\partial \mathcal{F}_p}{\partial x_j} = -\frac{\partial}{\partial \Psi_i}\left[\left\langle \frac{d\Phi_i^+}{dt} \middle| \mathbf{x}, \boldsymbol{\Psi}; t \right\rangle_p \mathcal{F}_p\right] + \left\langle \frac{1}{m_p^+}\frac{dm_p^+}{dt} \middle| \mathbf{x}, \boldsymbol{\Psi}; t \right\rangle_p \mathcal{F}_p,$$

- Lagrangian particle evolution laws in general semi-empirical
- No laws known for "seen" gas velocity $\phi_s^+(t)$ and "seen" composition $\phi_s^+(t)$
- MDF transport equation high dimensional

$\Longrightarrow$ Modeling and numerical solution by Monte Carlo method

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Solid phase Monte Carlo method

Consider:

- A set of uniformly distributed Lagrangian parcels (stochastic coal particles)
- Each parcel represents independent realization of the joint properties
- The ensemble provides and approximation of the exact MDF:

$$\mathcal{F}_p(\mathbf{x}, \mathbf{\Psi}; t) \approx \mathcal{F}_p^L(\mathbf{x}, \mathbf{\Psi}; t) = \left\langle \sum_{*} n_p^* m_p^* \cdot \delta(\mathbf{X}_p^*(t) - \mathbf{x}) \cdot \delta(\mathbf{\Phi}^*(t) - \mathbf{\Psi}) \right\rangle_p$$

- A parcel $*$ is not in one-to-one correspondence to a “real” coal particle $\Rightarrow$ hence the weight factor n_p^*

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Solid phase Monte Carlo method

- Position

$$\frac{dX^*_{p,i}}{dt} = u^*_{p,i},$$

- Velocity (Schiller-Neumann drag law)

$$\frac{du^*_{p,i}}{dt} = \frac{u^*_{s,i} - u^*_{p,i}}{\tau^*_p} - \frac{1}{\rho^*_p}\left[\frac{\partial \langle p \rangle}{\partial x_i}\right]^* + g_i.$$

- Seen velocity (given for fluctuating seen velocity $\mathbf{u}^{*\,''}_s = \mathbf{u}^*_s - \widetilde{\mathbf{u}}$)

$$du^{*\,''}_{s,i} = -\left(u^*_{p,j} - \left[\left\langle u^*_{p,j}\right\rangle_{|p}\right]^* + \left[\left\langle u^{*\,''}_{s,j}\right\rangle_{|p}\right]^*\right)\left[\frac{\partial \widetilde{u}_i}{\partial x_j}\right]^* dt$$
$$+ \frac{1}{[\overline{\rho}]^*}\frac{\partial \overline{\rho}\widetilde{u''_i u''_j}}{\partial x_j} dt + G_{s,ij}\, u^{*\,''}_{s,j}\, dt + B_{s,ij} dW_j$$

Solid phase Monte Carlo method

- Temperature (Nusselt according to Ranz-Marshall)

$$\frac{dm_p^* c_{p,p} T_p^*}{dt} = \pi D_p^* \, Nu \, k_m \left(T_s^* - T_p^* \right) + \epsilon_p {D_p^*}^2 \pi \sigma \left(\frac{G}{4\sigma} - {T_p^*}^4 \right)$$

- Seen temperature and composition

$$T_s^* = T^*(i) \quad \text{and} \quad X_{s,ox}^* = X_{O_2}^*(i), \qquad i \sim \mathcal{U}([1, N_{pg,cell}]).$$

- Mass (assume diameter remains constant)

$$\frac{dm_p^*}{dt} = \frac{{D_p^*}^3}{6} \pi \frac{d\rho_p^*}{dt} = \dot{m}_{vol}^* + \dot{m}_{char}^*$$

  - First Devolatilization (single rate according to Badzioch and Hawksley)
  - Then char combustion according to BCURA model

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Phase coupling

- Mass transfer

$$\langle S_{Z_2} \rangle = -\frac{1}{V_{\Omega_k} \overline{\rho}} \sum_{* \in \Omega_k} n_p^* \dot{m}_{vol}^*$$

- Heat transfer

$$\dot{h}_{cr}^* = -\frac{1}{V_{\Omega_k} \overline{\rho}} \sum_{* \in \Omega_k} n_p^* m_p^* c_{p,p} \frac{dT_p^*}{dt}$$

- Enthalpy of the added mass e.g. volatiles

$$h_{vol} = \frac{\sum_{* \in \Omega_k} n_p^* \cdot \dot{m}_{vol}^* \left(c_{p,p} \left(T_p^* - T_{ref,0} \right) + h_{vol}^0 \right)}{\sum_{* \in \Omega_k} n_p^* \dot{m}_{vol}^*}$$

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Radiation model

RTE for gray absorbing, emitting and scattering medium consisting of gas, soot and particles

$$\frac{dI}{ds} = -\left(\kappa_{gs} + \kappa_p + \sigma_p\right) I + \kappa_{gs} I_{b,g} + E_{b,p} + \frac{\sigma_p}{4\pi} \int_0^{4\pi} I(\mathbf{s}')\phi(\mathbf{s}', \mathbf{s}) d\Omega'$$

- Averaging the RTE leads to new unclosed terms $\Rightarrow$ Turbulence Radiation Interaction (TRI)
- PDF approach accounts for exact emission TRI:

$$\langle I_{b,g} \rangle = \frac{\sigma \left\langle T^4 \right\rangle}{\pi}, \langle I_{b,p} \rangle = \frac{1}{V_{\Omega_k}} \left\langle \sum_{* \in \Omega_k} \epsilon^* n_p^* \frac{\pi D_p^{*2}}{4} \frac{\sigma T_p^{*4}}{\pi} \right\rangle$$

RTE solved with Discrete Transfer Method (DTM) for isotropic scattering

- Solve RTE along predetermined number of rays through the domain
- Change of ray intensities in a cell gives radiation heat source
- Source term distributed among particles in cell $\Rightarrow$ S_{rad}^*

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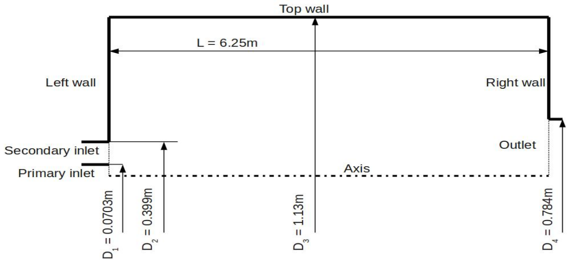
2MW pulverized coal-air flame B1

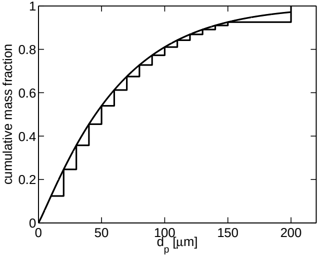
IFRF furnace No. 1, Measurements by Michel and Payne (1980)



- Primary inlet: $U = 40.7m/s$, $\overline{T} = 463K$
- Secondary inlet: $U = 9.6m/s$, $\overline{T} = 773K$
- Coal: high volatile bituminous $Y_{vol} = 0.31$, $Y_C = 0.59$
- $\langle D \rangle = 63\mu m$

Simulation details

- Code: Hybrid Finite Volume - Monte Carlo
- Grid: 2-d axisymmetric 204 $\times$ 56 (axial by radial) cells
- Gas Particles: nominal 50 particles per cell



- Coal Parcels: 10 parcels per cell per size class = 150 parcels per cell
- DTM grid: 41 $\times$ 12 cells, 1024 rays traced from every boundary cell surface

Computational time: 20 hours on a single processor "Core2 Quad 2.4 GHz"

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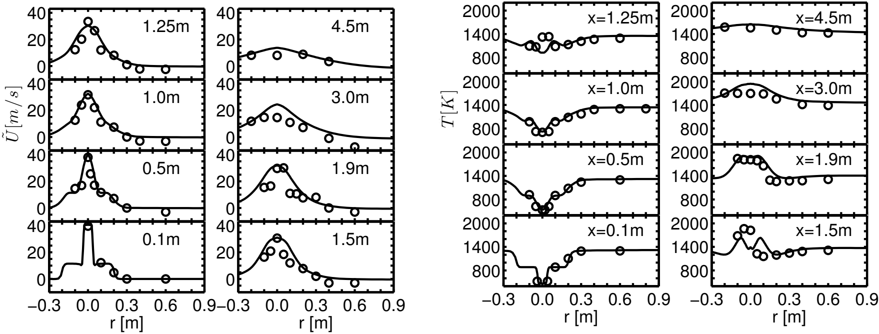
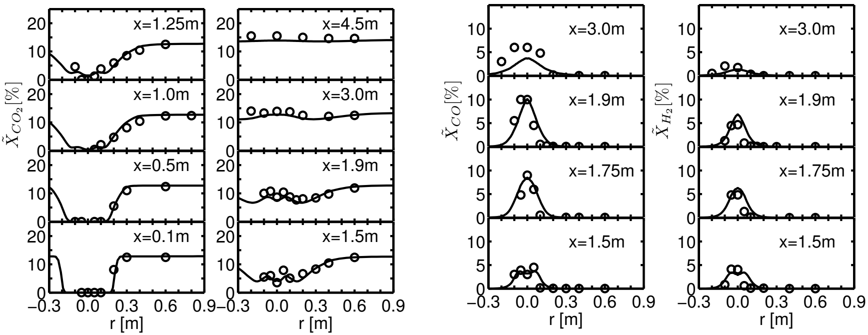
Simulation results: Validation

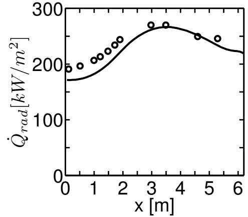


Simulation results: Validation

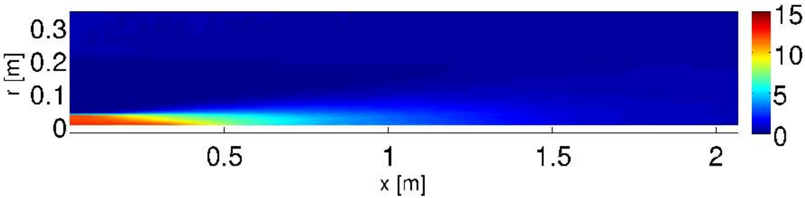


Simulation results: Analysis

Incident radiative wall heat flux

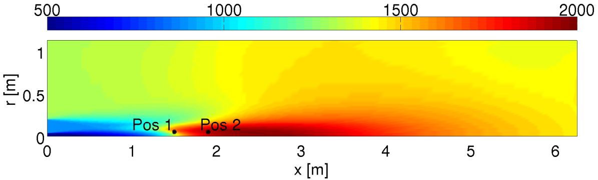


Particle absorption coefficient $[1/m]$

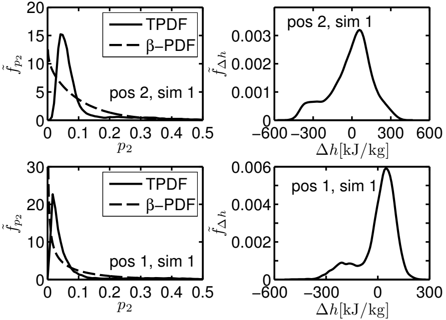


Simulation results: Analysis

Mean temperature:



Marginal PDF's:



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Conclusions

- PDF simulation results agree very well with measurements
- Presumed shape PDF method could be improved using TPDF results
- Probably we should aim at a joint gas phase - particle phase approach
- DNS studies of a simple configuration would greatly aid the modeling effort