



## MS&T 2013

Modeling very high temperature, dense cloud, free-fall heating for particles with wide particle size distributions

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# Outline

- Rationale
- Theory
  - The Force Balance
  - Collision Counting
  - Thermal Model
    - Radiation
    - Gray bodies
    - Convective Heat Transfer:
- Examples
- “Harper equipment examples” and questions
- Any questions slides / will be around all day....

# Rationale

- Harper manufactures vertical free-fall reactors
  - Broad range of
    - Temperatures
    - Materials
    - Sizes
      - of furnaces
      - of particles
  - High T = High CAPEX
    - Need good modeling of unexplored parameter sets for appropriate estimation of system



# The Particle Force Balance

- The Force Balance:
  - Gas properties change substantially and with temperature
  - The particle's momentum is substantial (dense, large, etc.)
    - Acceleration is accounted for
- Drag Coefficient
  - The drag force on the particle is
    - $F_D = C_D A_P \rho v^2 / 2$
    - $A_p$  is the particle's projected area
    - $C_D$  is a function of the particle's Reynolds number
      - $Re = \rho v D / \mu$
      - $\mu$  is the viscosity, a temperature dependent property
        - Temperature may change by 1 order of magnitude
        - Gas mixtures: use mixing rule
        - $\mu_{\text{mixture}} = \Sigma(y_i \mu_i / \Sigma y_j \Phi_{ij})$
        - $\Phi_{ij, \mu} = 8^{-1/2} (1 + M_i/M_j)^{-1/2} (1 + (\mu_i/\mu_j)^{1/2} / (M_i/M_j)^{-1/4}))^2$

# The Particle Force Balance

- Drag Coefficient

- The drag force on the particle is

- $F_D = C_D A_P \rho v^2 / 2$

- $C_D$  is a function of the particle's Reynolds number

- For spherical particles...  $\Psi = 1$

- For non-spherical particles

- Sphericity,  $\Psi = A_{\text{particle}} / A_{\text{sphere, same volume}}$

- $\Psi_{\text{tetrahedron}} = 0.671$

- $$C_D = \frac{24}{\text{Re}} (1 + 8.1716 e^{-4.0655\Psi} \text{Re}^{0.0964 + 0.5565\Psi}) + \frac{73.69 e^{-5.0748\Psi} \text{Re}}{(\text{Re} + 5.378 e^{6.2122\Psi})}$$

# The Force Balance

- The Force Balance:
  - The particle's momentum is substantial (dense, large, etc.)
    - Acceleration must be accounted for
  - Particle acceleration
    - $a_i = (F_{Di} + (\pi(\rho_i - \rho_{gas})D_i^3/6)g)/(\pi\rho_i D_i^3/6)$ .
    - velocity is  $v_i(y+\Delta y) = v_i(y) + a_i\Delta t$
    - Substitute  $\Delta t = \Delta y/v_i$ 
      - unstable for  $v_i$  approaching zero
      - however,  $v_i = 0$  is a plugged reactor

# Collision Counting

- Collisions: because different size particle have different speeds

- Interesting if sticky particles

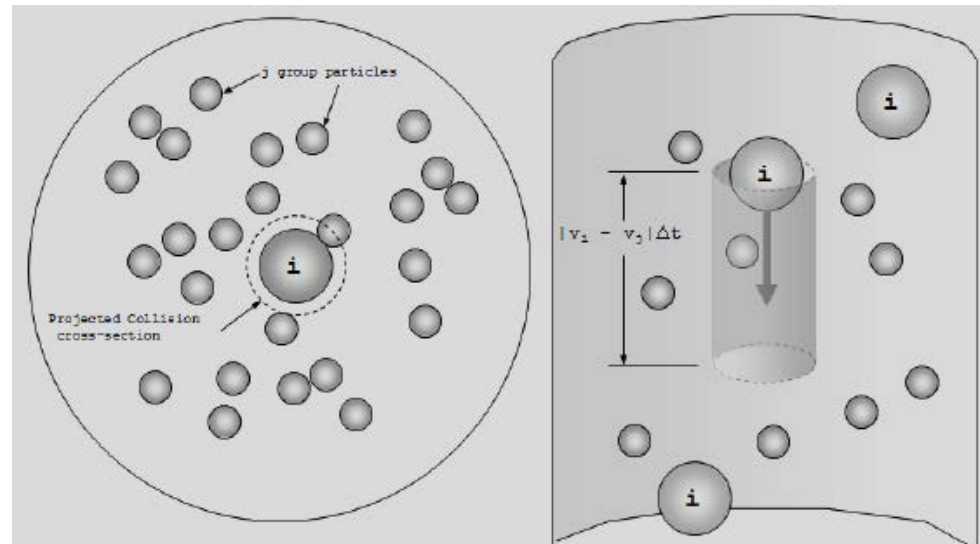
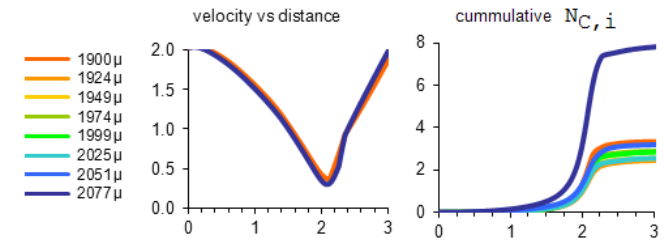
- non-sticky particles: collisions not so important
- non-sticky don't NEED free-fall

- Conceptual framework:

- Break Particle Size Distribution (PSD) into discrete slices
- Define volumetric number density for each ...
  - Particle size (range,  $\eta_i$ )
  - At all points along length
- Define Collisions / Volume
- Count collisions
  - Along length
  - Above cut-off temperature

$$\eta_j = \Delta t \, m \, X_j / (\Delta t \, v_j \, \pi/4 \, D_i^2) = N_j / (v_j \, \pi/4 \, D_i^2)$$

$$N_j = (m \, X_j / (\pi \rho_j D_j^3/6))$$





# Thermal Model: Radiation

## Thermal Model: Radiation

### View Factors

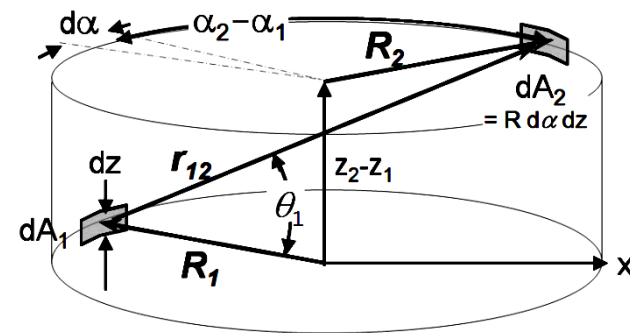
- of tube to self
- of tube to particles
- of particles to particles
  - of one size group to another

### Volumetric density of particle projected area

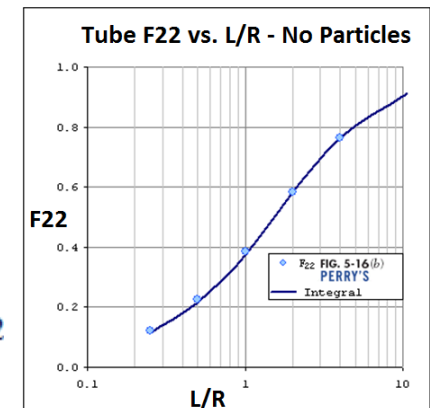
- $\beta = \sum_i \beta_i = \sum_i \eta_i \pi D_i^2 / 4$
- has units of  $L^{-1}$
- $A_{\text{tube}} F_{\text{tube, tube}} = \text{integral over volume element } \pi R_1^2 \Delta y$
- of  $\exp(-\beta |r_{12}|) (|r_{12} \cdot R_1| / |r_{12}| |R_1|)^2 (1/\pi r_{12}^2) R_1 d\alpha_1 dz_1 R_2 d\alpha_2 dz_2$

### Monte Carlo method to view factor calculations

- Comparison to published curve



$$dA_1 \cos(\theta_1) dA_2 \cos(\theta_2) / \pi r_{12}^2$$





# Thermal Model: Radiation

- View of Tube to Tube (through cloud) vs.  $\beta$

- $$\frac{A_{\text{tube}}}{A_{\text{total}}} = \frac{\pi D_t dy}{(\pi D_t dy + \pi/4 D_t^2 dy \times 4\beta)}$$

$$= 1/(1 + \beta D_t)$$

- View of Tube to Particles:

- PSD is broken into 8 groups

- Without radial separation,  $F_{tp} dA_2 = \beta r dr d\alpha dz$
- Distribution across PSD:
- $i=1$  is tube,  $1 < i < 10$  is particles

- View of Particles to Particles

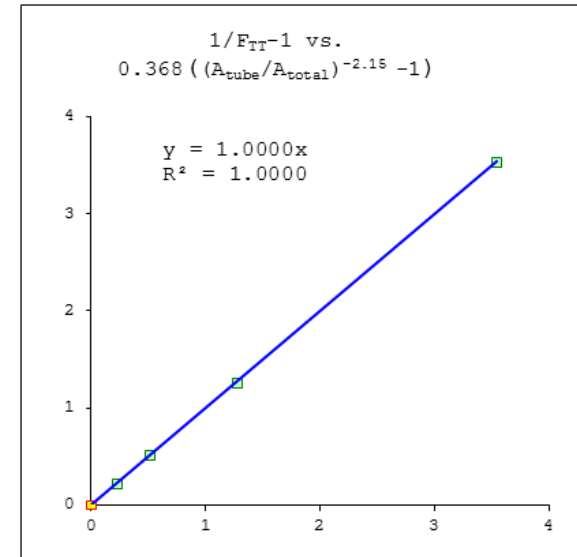
- $$A_t F_{ti} = A_t F_{tp} A_i / \sum_{j \neq 1} A_j$$

- $$F_{pt} = F_{tp} A_t / \sum_{j \neq 1} A_j$$

$$A_i F_{it} = A_t F_{Ti} = A_t F_{tp} A_i / \sum_{j \neq 1} A_j$$

$$F_{pp} = 1 - F_{pt},$$

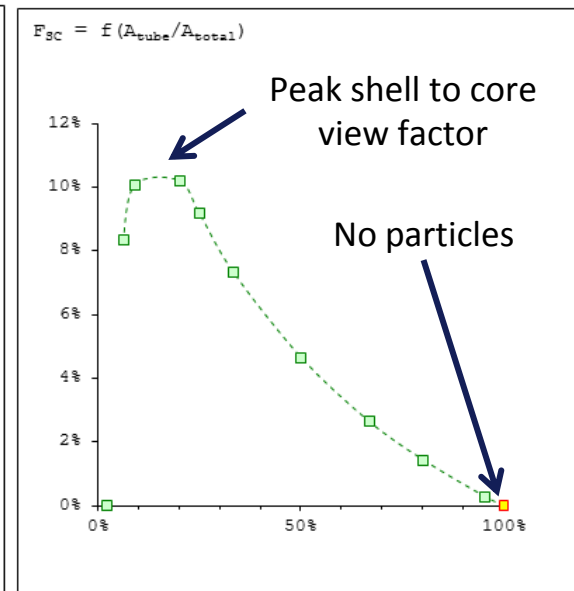
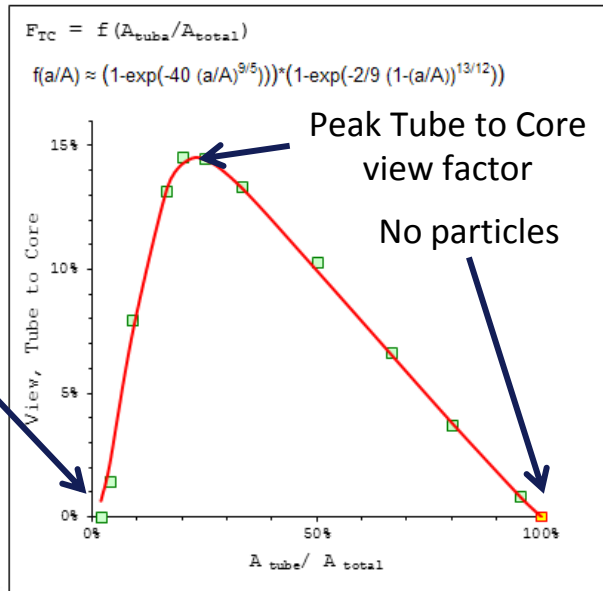
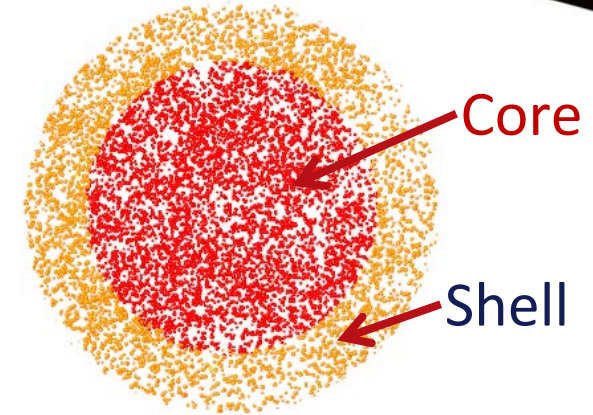
$$A_i F_{ij} = A_i F_{pp} A_j / \sum_{k \neq 1} A_k$$



# Thermal Model: Radiation

## ■ View of Tube to Particles:

- Radial gradient:  $dA_2 = \beta r \, dr \, d\alpha \, dz$ 
  - separate powder into shell and core (equal volumes)
  - Calculate,  $F_{tc}$  and  $F_{cs}$  and generate the rest
    - $F_{sc} = A_c F_{cs} / A_s$ ,  $F_{cc} = 1 - (F_{ct} + F_{cs})$ , etc.
  - No radial gradient in volumetric loading of powder
  - $i=1$  is tube,  $i=2$  to  $5$  is shell,  $i=6$  to  $9$  is core
  - $IF(i=1, IF(j=1, F_{tt}, IF(j<6, F_{st}, F_{ct})), IF(j=1, IF(i<6, F_{ts}, F_{tc}), IF(j<6, IF(i<6, F_{ss}, F_{sc}), IF(i<6, F_{cs}, F_{cc}))))$



# Grey Bodies

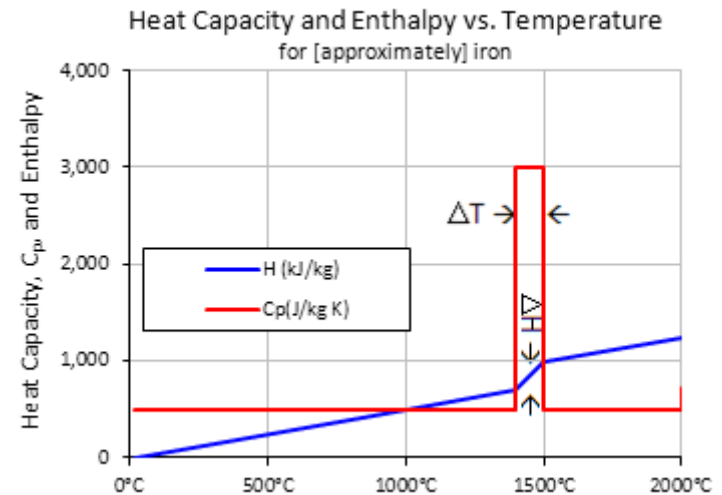
- Grey: emissivity,  $\varepsilon$ , less than 1 and not a function of wavelength
  - Some radiation is absorbed, some reflects
  - Radiosity Vector (effective temperature)
    - $\{W_i, i=1, 2, ..N\} = \{N \times N\}^{-1} \{f(A_i, \varepsilon_i, T_i)\}^T$
    - Radiation transfer to an i particle =  $\sigma \pi D_i^2 \varepsilon_i / (1 - \varepsilon_i) (W_i - T_i^4)$
  - Inverting a Matrix in each step of an explicit integration
    - $W_i = \left( (A_i^T \mathbf{A} \mathbf{F}_{ij} - \delta_{ij} A_i / (1 - \varepsilon_i))^{-1} \times (-A_i * (\varepsilon_i / (1 - \varepsilon_i)) * T_i^4)^T \right)^T$
    - $\mathbf{A} \mathbf{F}_{ij} = \text{if}(i=1, 1, A_i / (\sum A_i - \pi D_{\text{tube}} \Delta y)) * F_{ij}$
    - $F_{ij} = \text{if}(i=1, \text{if}(j=1, F_{tt}, F_{tp}), \text{if}(j=1, F_{pt}, F_{pp}))$

# Convective Heat Transfer

- Convective Heat Transfer:
  - Transfer Coefficient,  $h$ 
    - $Nu_i = 2 + 0.6Re_i^{1/2} Pr^{1/3}$ 
      - $h_i = Nu_i k_i / D_i$
      - $k$  (gas thermal conductivity) has a subscript because the film temperature is used for gas transport properties
  - The model has logic that deals separately with
    - Upward flowing gas
    - Downward flowing gas
    - No net gas flow
  - Gas temperature calculation
    - For flowing gas,  $T(y \pm \Delta y)$  is integrated along each  $\Delta y$
    - For non-flowing gas,  $T_g = \Sigma_i (h_i A_i T_i) / \Sigma_i (h_i A_i)$

# Particle Temperature

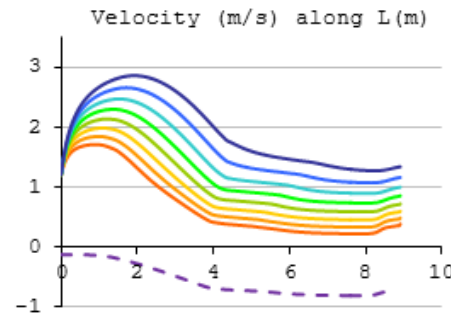
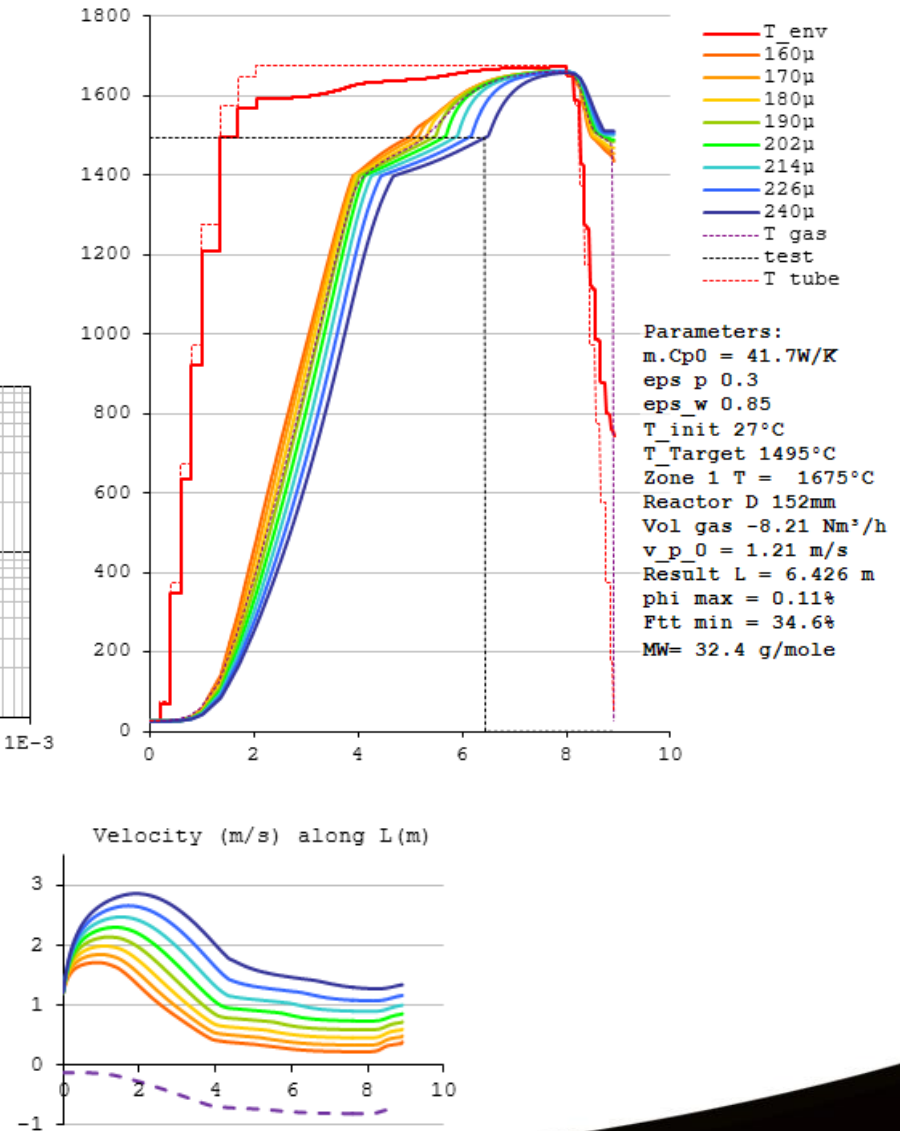
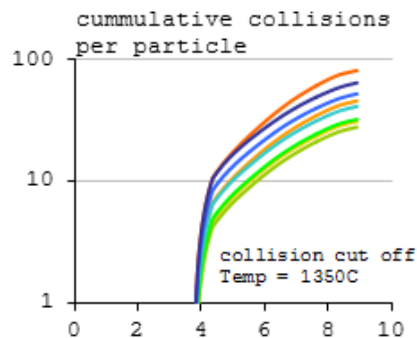
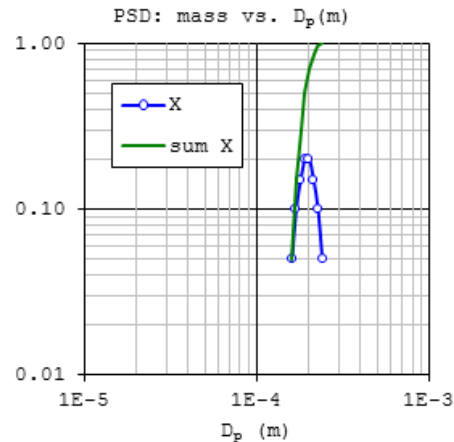
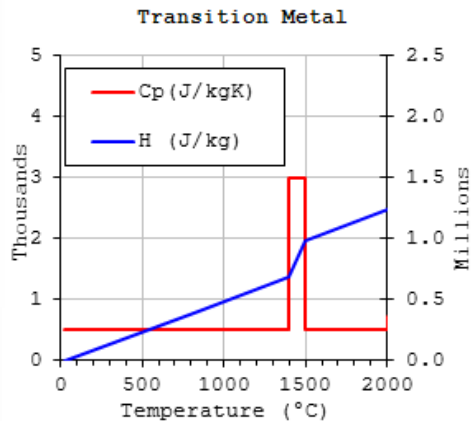
- Explicit Integration:
  - $T(t+\Delta t) = T(t) + \Sigma q/mC_p$ 
    - $\Sigma q$  is the sum of the radiation and convection heats
    - $m$ , the particle mass, is  $\pi D^3 \rho / 6$
    - $C_p$  is the heat capacity,  $C_p = dH/dT$
    - Phase changes can be modeled
      - Melting iron over 100C° range



# Results/Examples

## How to read the output

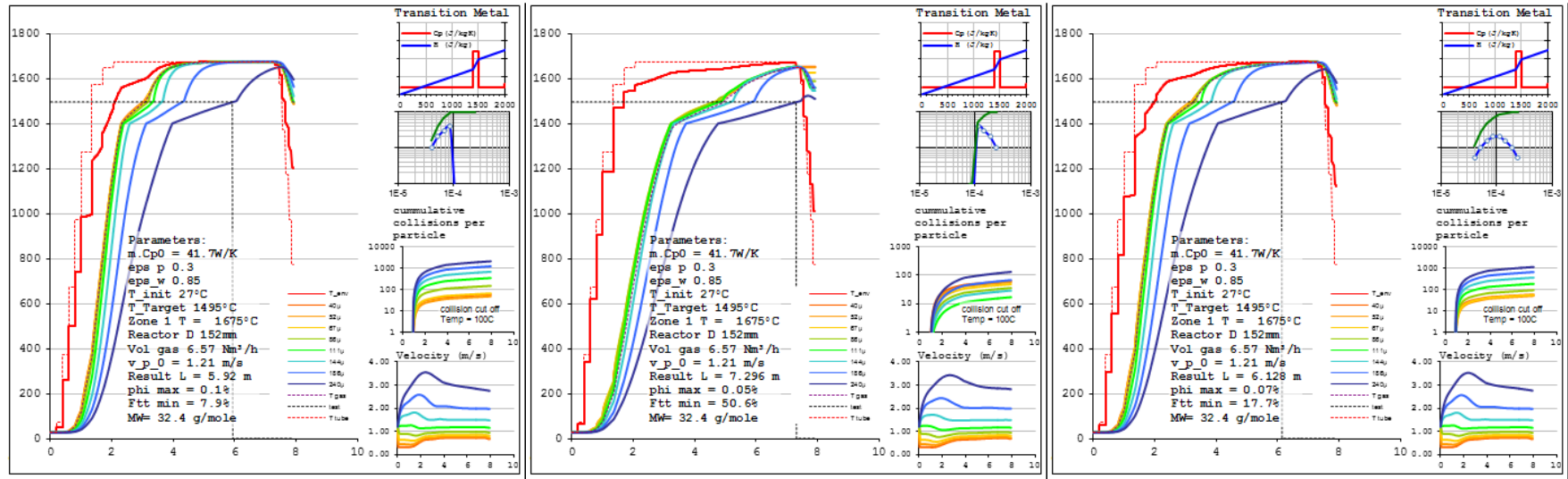
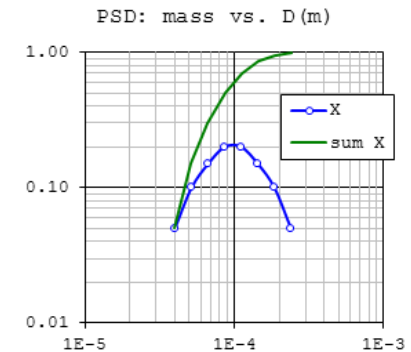
- Temperature vs. Length, legend, parameter list
- $C_p$  and Enthalpy vs. Temperature
- Particle Size Distribution
- Collisions per particle (for each size) along length
- Velocity for each size along length





# Results/Examples

- Two “narrow” particle distributions vs. combined
  - Starting PSD has a  $D_{50}$  of 100 $\mu$
  - Fine cut (below 100 $\mu$ ), Coarse cut (above 100 $\mu$ )
  - Target: melt 300kg/h iron ( $C_p=500\text{J/kgK}$ ,  $\Delta H=250\text{kJ/kg}$  over 100C°)

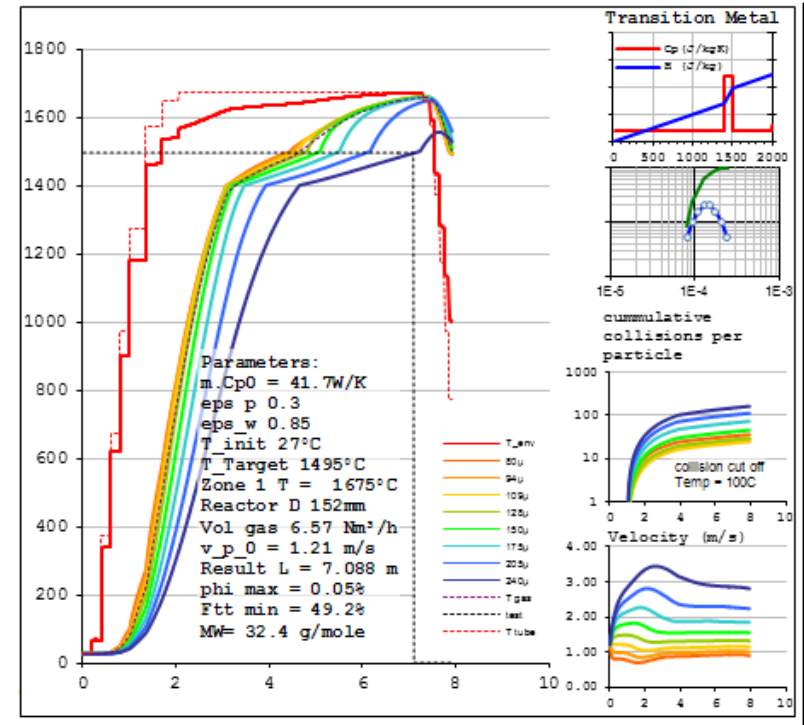
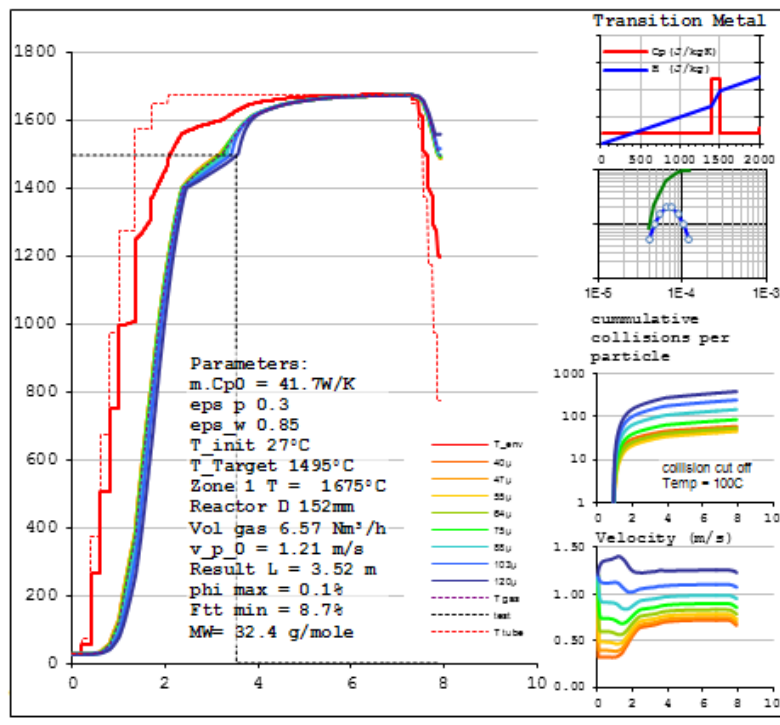


- On the left, fine cut (ignore the big particles) 300kg melts in 3.5m
- Central figure, coarse cut, requires 7.3m
- On the right the full 40-240 $\mu$  PSD requires 6.1m
  - Smaller particles help to heat the larger particles



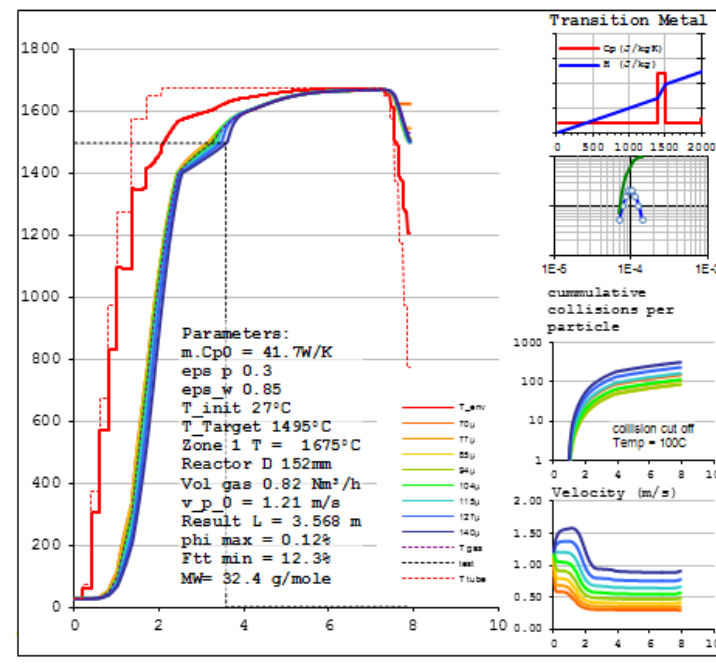
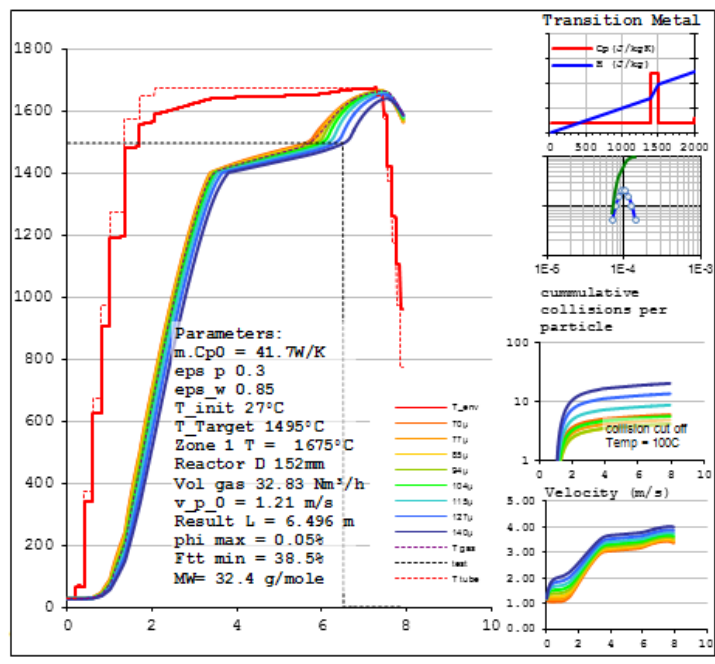
# Results

- Results/Examples: 6 slides
  - Alternates of “narrow” particle distributions



# Results

- Results/Examples: 6 slides
  - Effect of co-flowing gas to reduce collisions
    - 10 fold decrease in collisions and 2 fold increase in length



# Possible Extensions to the Work

- Radial Gradients in powder
  - Distribution over cross section
    - New view factor calculations
  - More annular cuts
- Axial radiation
  - Much larger matrices to invert
    - May need to reformulate program
- Collisions →
  - Agglomeration (above cut-off)
  - Acceleration

# Vertical Systems

- Multiple Tubes Available
  - Alloy, Graphite
  - Quartz, Alumina
  - Monolithic, multi-segment
- Multi-Tube Reactors
  - Think “heat exchanger”



1.25m long, 1 zone  
100-150mm ID “tube”  
1400°C  
2-phase flow  
Multiple tubes



4.5m long, 3 zone  
250mm ID, graphite tube  
2200°C, water cooled

Any Questions?

