MS&T 2013

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

Dr. Peter Witting, Bruce Dover

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

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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
      - $Re = \rho v D / \mu$
      - μ is the viscosity, a temperature dependent property
        - Temperature may change by 1 order of magnitude
        - Gas mixtures: use mixing rule
        - $\mu_{mixture} = \Sigma(y_i \mu_i / \Sigma y_j \Phi_{ij})$
        - $\Phi_{ij,\mu} = 8^{-1/2} (1 + M_i/M_j)^{-1/2} (1 + (\mu_i/\mu_j)^{1/2} / (M_i/M_j)^{-1/4}))^2$

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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, $\Psi = A_{particle} / A_{sphere,\ same\ volume}$
        - $\Psi_{tetrahedron} = 0.671$
        - $C_D = 24/Re\ (1 + 8.1716\ e^{-4.0655\Psi}\ Re^{0.0964 + 0.5565\Psi}) + 73.69\ e^{-5.0748\Psi}\ Re / (Re + 5.378\ e^{6.2122\Psi})$

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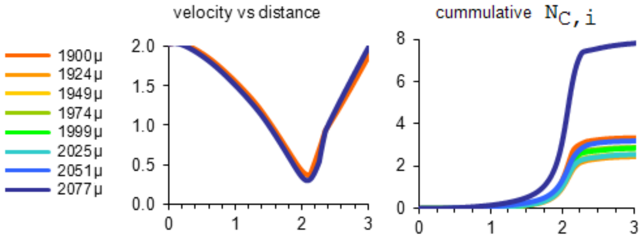
The Force Balance

- The Force Balance:
  - The particle's momentum is substantial (dense, large, etc.)
    - Acceleration must be accounted for
  - Particle acceleration
    - $\boldsymbol{a}_i = (\boldsymbol{F}_{Di} + (\pi(\rho_i\text{-}\rho_{gas})D_i^3/6)\boldsymbol{g})/(\pi\rho_i D_i^3/6)$
    - 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

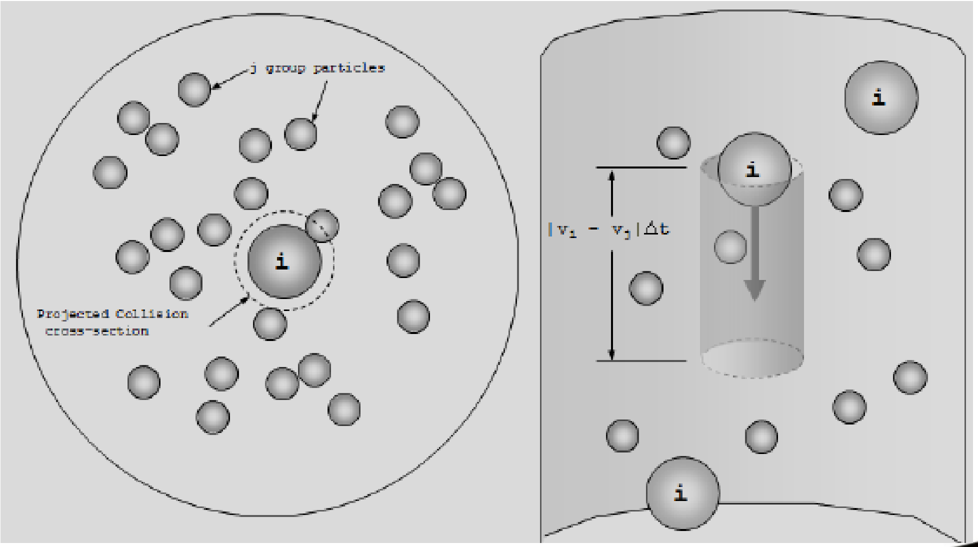
Collision Counting

- 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, η_i)
      - At all points along length
    - Define Collisions / Volume
    - Count collisions
      - Along length
      - Above cut-off temperature



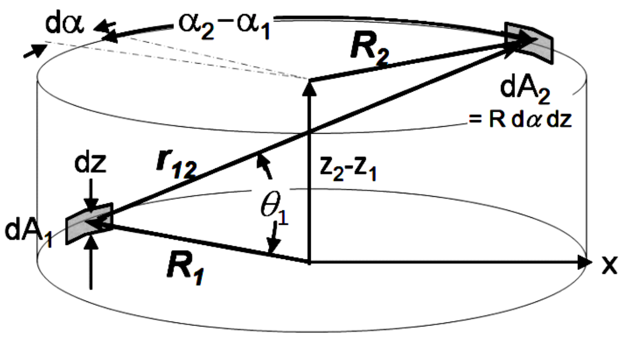
$$\eta_j = \Delta t\, m\, X_j / (\Delta t\, v_j\, \pi/4\, D_t^2) = N_j / (v_j\, \pi/4\, D_t^2)$$

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

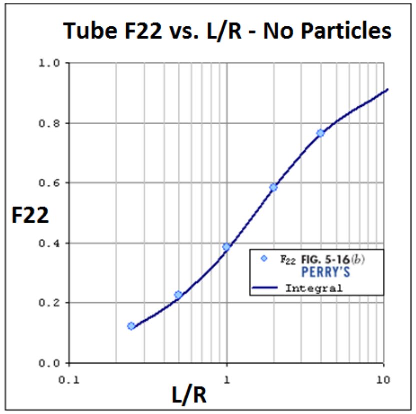


Thermal Model: Radiation

- 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
    - $\beta = \Sigma_i \beta_i = \Sigma_i \eta_i \pi D_i^2 / 4$
    - has units of L^{-1}
    - $A_{tube} F_{tube, tube}$ = integral over volume element $\pi R_1^2 \Delta y$
    - of $\exp(-\beta|\boldsymbol{r}_{12}|)(|\boldsymbol{r}_{12} \cdot \boldsymbol{R}_1|/ |\boldsymbol{r}_{12}| |\boldsymbol{R}_1|)^2 (1/\pi r_{12}^2) R_t d\alpha_1 dz_1 R_t d\alpha_2 dz_2$
  - Monte Carlo method to view factor calculations
    - Comparison to published curve



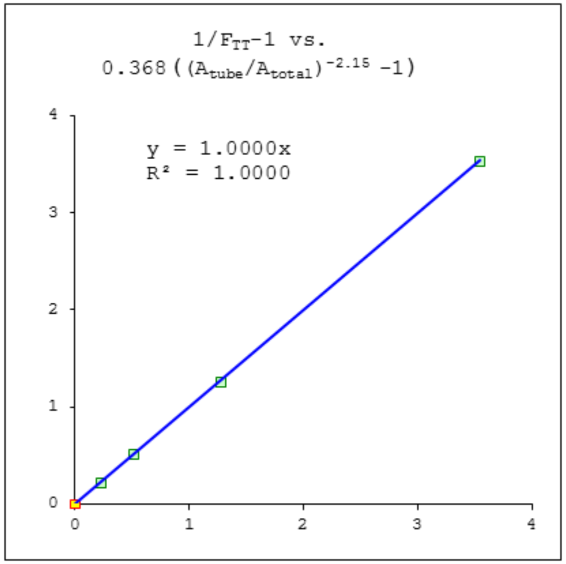
$dA_1 \cos(\theta_1)\, dA_2 \cos(\theta_2)/\pi r_{12}^2$



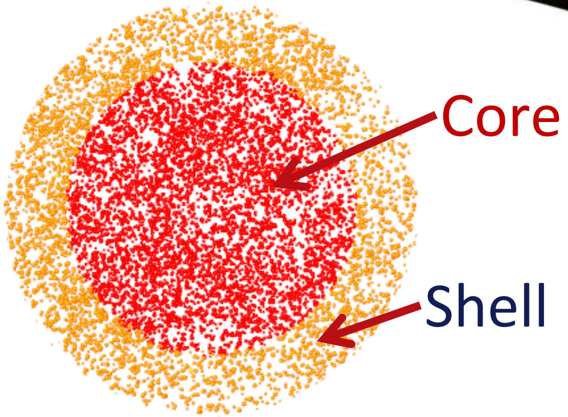
Thermal Model: Radiation

- View of Tube to Tube (through cloud) vs. β
  - $A_{tube}/A_{total} = \pi D_t\, dy / (\pi D_t\, dy + \pi/4\, D_t^2\, dy \times 4\beta)$
    $= 1/(1 + \beta D_t)$
- 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
  - $A_t F_{ti} = A_t F_{tp} A_i / \Sigma_{j\neq 1} A_j$
  - $F_{pt} = F_{tp} A_t / \Sigma_{j\neq 1} A_j$

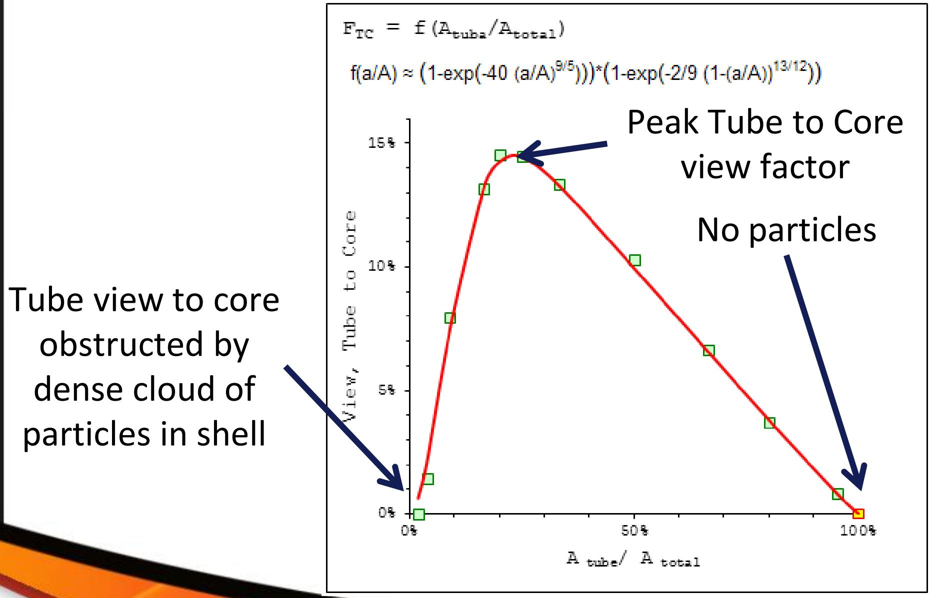
$$A_i F_{it} = A_t F_{Ti} = A_t F_{tp} A_i / \Sigma_{j\neq 1} A_j$$
$$F_{pp} = 1 - F_{pt},$$
$$A_i F_{ij} = A_i F_{pp} A_j / \Sigma_{k\neq 1} A_k$$

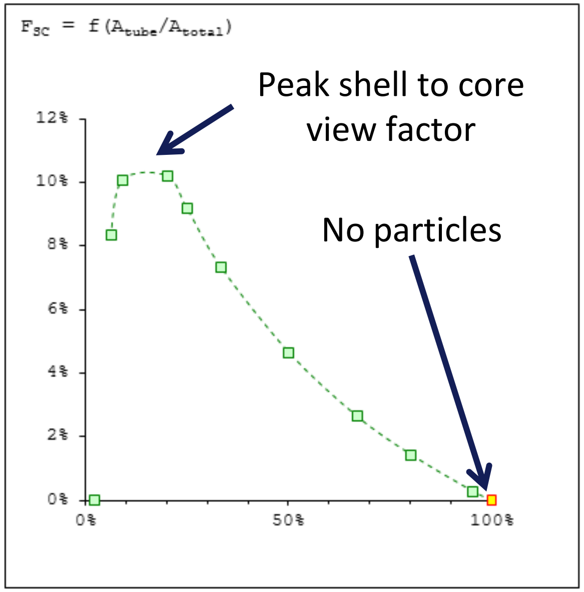


Thermal Model: Radiation



- 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
      - $F_{sc}=A_cF_{cs}/A_s$, $F_{cc}=1-(F_{ct}+F_{cs})$, 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

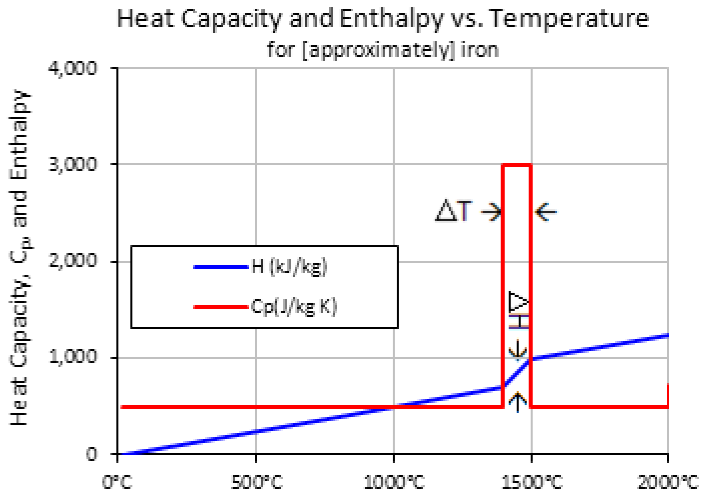
- Grey: emissivity, ε, less than 1 and not a function of wavelength
  - Some radiation is absorbed, some reflects
  - Radiosity Vector (effective temperature)
    - $\{W_i, i=1, 2, ..N\} = \{N \times N\}^{-1}\{f(A_i,\varepsilon_i,T_i)\}^T$
    - Radiation transfer to an i particle = $\sigma\pi D_i^2\varepsilon_i/(1-\varepsilon_i)\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

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 Δy
    - For non-flowing gas, $T_g = \Sigma_i (h_i A_i T_i)/\Sigma_i (h_i A_i)$

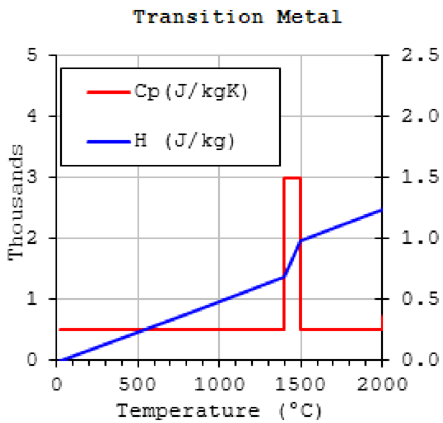
Particle Temperature

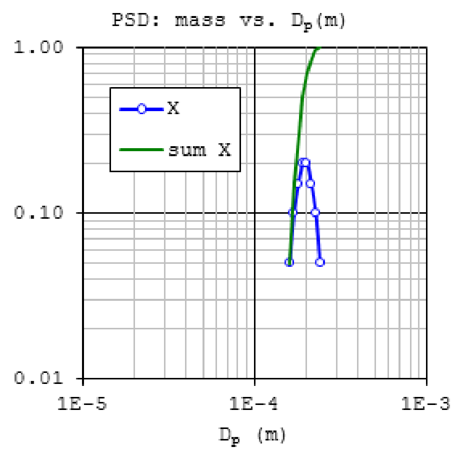
- Explicit Integration:
  - $T(t+\Delta t) = T(t) + \Sigma q/mC_p$
    - Σq is the sum of the radiation and convection heats
    - m, the particle mass, is $\pi D^3\rho/6$
    - C_p is the heat capacity, $C_p = dH/dT$
    - Phase changes can be modeled
      - Melting iron over 100C° range

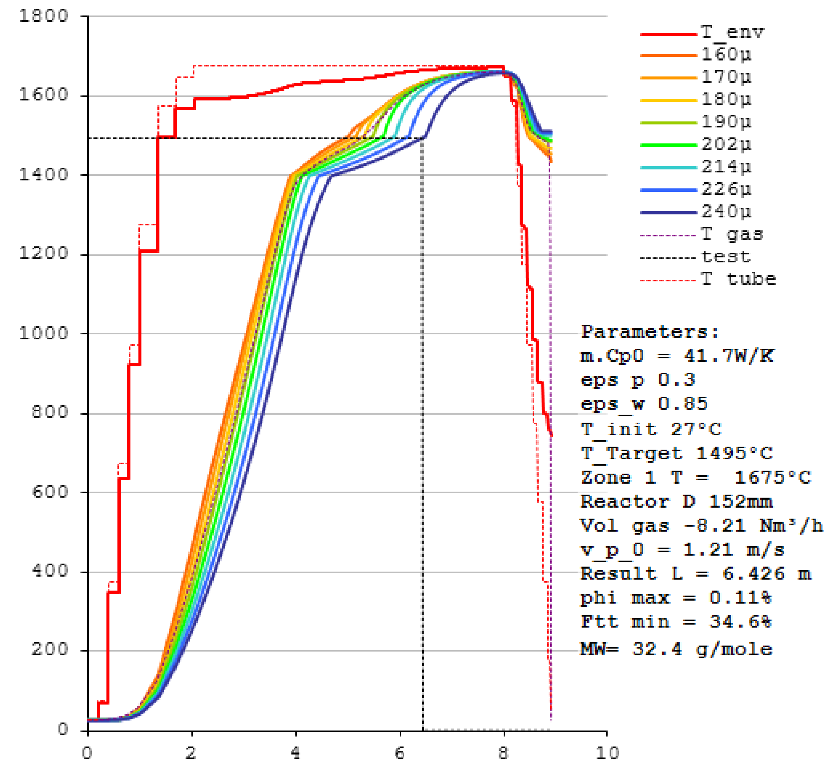


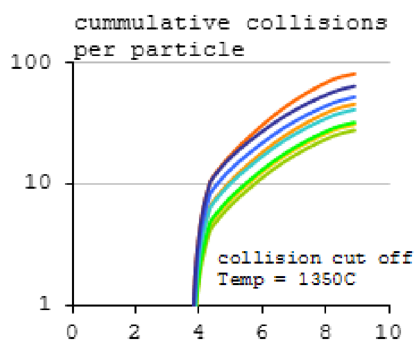
Results/Examples

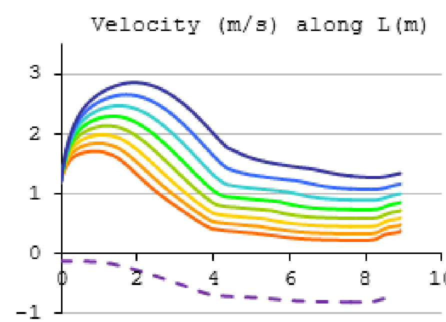
- How to read the output
  - Temperature vs. Length, legend, parameter list
  - C_p and Enthalpy vs. Temperature
  - Particle Size Distribution
  - Collisions per particle (for each size) along length
  - Velocity for each size along length





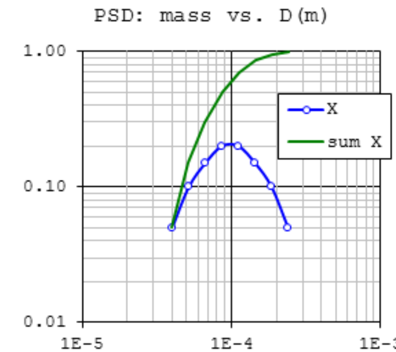


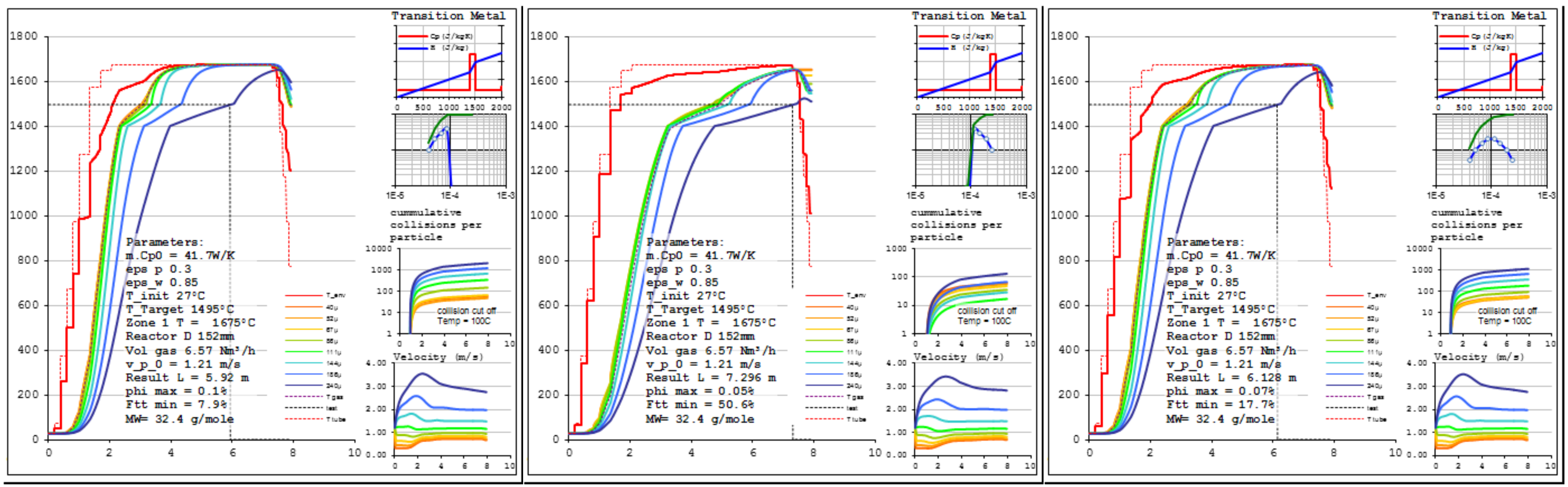




Results/Examples

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

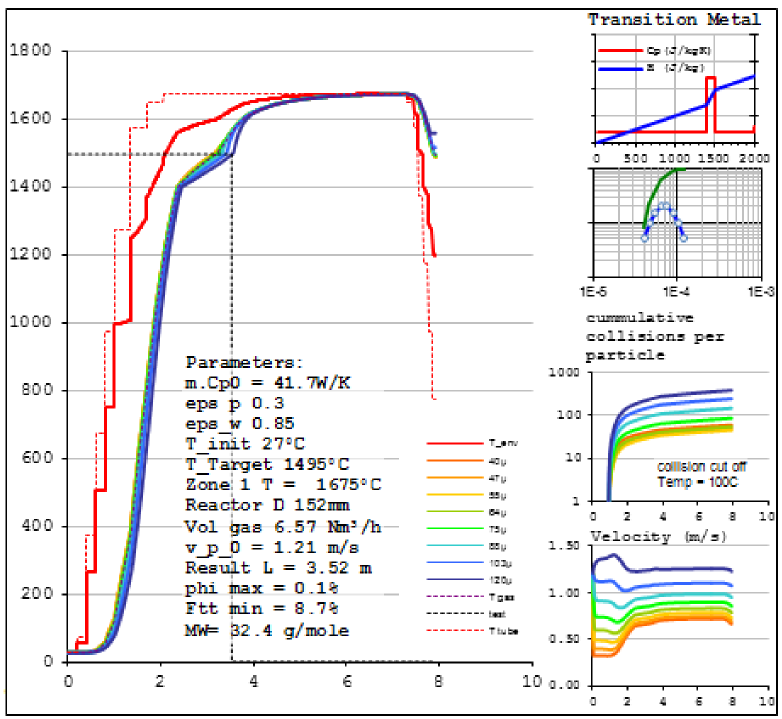


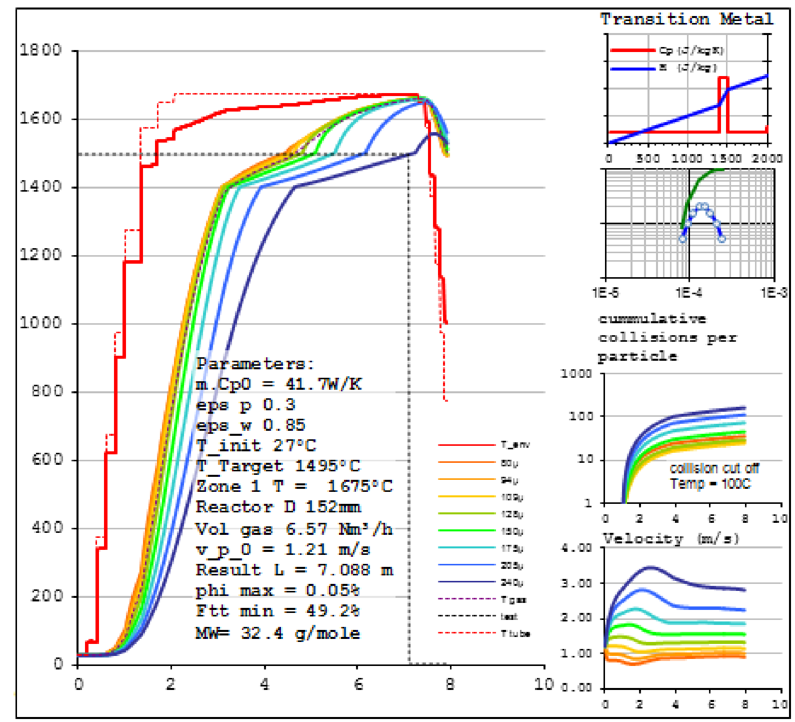


- On the left, fine cut (ignore the big particles) 300kg melts in 3.5m
- Central figure, coarse cut, requires 7.3m
- On the right the full 40-240μ PSD requires 6.1m
  - Smaller particles help to heat the larger particles

Results

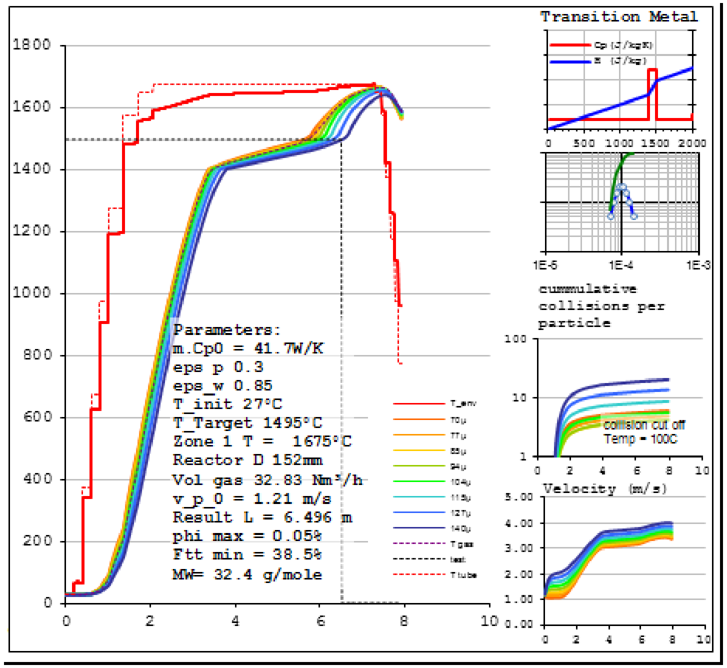
- Results/Examples: 6 slides
  - Alternates of “narrow” particle distributions

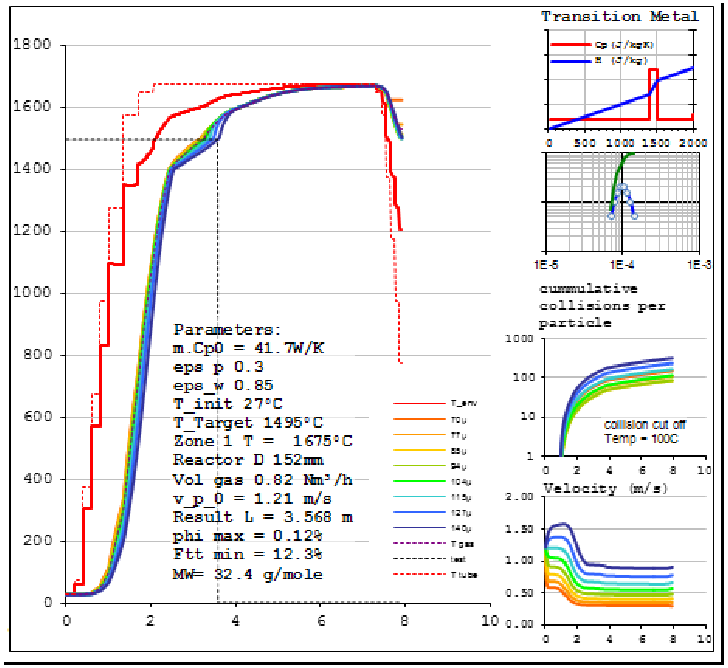




Results

- 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

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Any Questions?