White Paper:

Modeling Very High Temperature, Dense Cloud, Free-Fall Heating for Particles with A Wide Particle Size Distribution

By: Bruce Dover, Senior Process Technology Engineer
Harper International

Abstract

Harper manufactures vertical free-fall reactors for a broad range of material. As temperatures increase, the CAPEX becomes more important. It is important therefore to employ a modeling tool to properly size the equipment for the target production rate. The model is discussed, noting the simplifying assumptions and the rigorous algorithms. The model considers heavy particles (acceleration), semi-opaque clouds (efficiency vs. efficacy), collisions between particles in different size (or shape) families (in case sticking is anticipated), and temperature dependent properties of the gases and solids (to account for phase changes).

Introduction

The objective is to create a physically rigorous model to simulate the heating of powder(s) with various particle sizes. This can be used, then, as a design tool to estimate the productivity of a given system.

At extreme temperatures furnace interior volume is very expensive. This requires investigating the smallest diameter and shortest possible geometries. In order to push productivity to its limit, mass through-put should be as high as possible without compromising quality or operability. Dense clouds of falling powder can be relatively opaque. This is rigorously modeled. Also, particularly with a distribution of particle sizes and where agglomeration may occur, the number of collisions between particles is an important consideration.

Limits

Several strong assumptions are made. For example, the model uses a uniform distribution of particles across the diameter of the tube. The model also assumes a uniform axial gas velocity. This is certainly not the case. Modeling the effect of the falling particles on a developing velocity profile was considered too complicated at this stage. The radiation heat transfer calculation neglects axial radiation. This is not reasonable with large diameter tubes. The heat transfer problem stops at the particle surface. For coarse, insulating particles the relaxation time for temperature gradients (R^2/α) may be on the same order as the free fall time. In these cases it will be necessary to extend the model along the particles' radii.

Model

The physics of the problem can be modeled up to certain limits. The model takes the general form of an explicit numerical solution of a system of nonlinear partial differential equations. In explicit integration the future value of any variable is a function of the current state. The accuracy is improved as the time step is made smaller. For some variables it is more convenient to integrate directly over space steps instead of time.

The Force Balance

Weight = (mass of particle – mass of displaced fluid) x g (gravitational acceleration constant, 9.806 m/s²). The other force is drag from friction and pressure between the particle and the fluid (gas) due to the different velocity of the gas and the particle (s). The drag coefficient, C_D , is a dimensionless number that allows the force to be related to the Reynolds number, Re. Re is also a dimensionless number that is –roughly- the ratio of inertial to viscous forces exerted on the particle by the flow around the particle. The drag force, F_D , is related to C_D and is in the opposite direction of the relative velocity.

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

A_P is the projected area of the particle in the direction of motion, $A_P=\pi R^2$ for a sphere, ρ is the density of the fluid, sometimes the fluid film, around the particle and v is the relative velocity between the particle and the fluid.

The Reynolds number is $Re = \rho v D / \mu$. Where D is the diameter, in this case, of the particle and μ is the dynamic viscosity of the fluid, sometimes the fluid film, around the particle. Identifying the correct viscosity to use is important because the gas temperature changes by approximately and order of magnitude along the length of the system.

The mixing rule used for viscosity is Wilke's.

$$\mu_{mixture} = \Sigma(y_i\mu_i/\Sigma y_j\Phi_{ij})$$

$$\Phi_{ij,\,\mu} = 8^{-½} (1+ M_i/M_j)^{-½} (1 + (\mu_i/\mu_j)^{½} / (M_i/M_j)^{-¼}))^2$$

M_i is the molecular weight of species i.
The example mixture is 80%Ar, 20% H_2 by volume.

The raw material may be crushed, crystalline or spherical. The sphericity, Ψ, of a particle is the ratio of the surface area of a sphere with the same volume as the given particle to the surface area of the particle. The sphericity of a sphere is, by definition, 1. The shapes like cubes, octahedra, tetrahedra, etc. that one might expect to find in a crushed hard material are 0.806, 0.846 and 0.671, respectively.

The sphericity is a parameter in the relation between C_D and Re.

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

For spherical particles the above relation is replaced by the much simpler relation:

$$C_D = 24/Re\,(1 + 0.14Re^{0.7}) \text{ valid for } 0.1<Re<1000$$

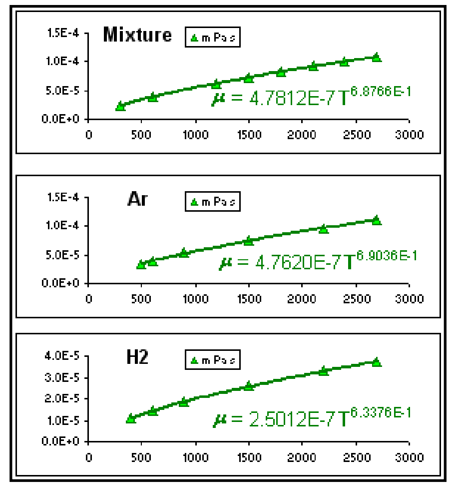


Figure 1: Viscosity of Argon H2 Mixture as function of Temperature

For the simulations that extend to melting the particles the sphericity changes. Presumably at some temperature in the melting range (or, at some extent of melting) the particle coalesces into a sphere. Its drag, at that point becomes that of a sphere (or less due to motion of the molten fluid).

The acceleration, $\boldsymbol{a}_i$, is $(\boldsymbol{F}_{Di} + (6\pi(\rho_i-\rho_{gas})D_i^3)\boldsymbol{g})/(6\pi\rho_i D_i^3)$. $\boldsymbol{F}_{Di}$, $\boldsymbol{a}_i$, and $\boldsymbol{g}$ are vectors ($\boldsymbol{F}$ up and $\boldsymbol{g}$ down). The weight force is modified by buoyancy. The velocity is $v_i(y+\Delta y) = v_i(y) + a_i\Delta t$. Substitute $\Delta t = \Delta y/v_i$. This is unstable for v_i approaching zero. Note, however, $v_i = 0$ is a plugged reactor.

Accounting for the velocity gradient in the fluid and its possible effect on the distribution of particles across the tube cross-section is currently beyond the scope of this investigation.

Collisions are counted to evaluate the effects of crowding other than the effect it may have on radiation heat transfer. The mechanical effects of collisions are beyond the scope of this investigation.

The continuous particle size distribution (PSD) is discretized and it is assumed that all of the particles in a size-group move at the same speed and reach the same temperatures along the length. The PSD for an example is given in the figure.

Assuming a uniform gas velocity across the tube cross-section (a strong assumption – likely not true), the velocity of any particle in a given size range (modeled as a single group with all members identical) is the same as all other particles in the group at that vertical position.

Particles in different groups, however, may be moving at different velocities. For example, a large group i particle moving relative to a large number of smaller group j particles will collide with, on average, the volumetric number density of j particles times the volume swept out by the i particle in a given time increment Δt. The particle drop simulation is an explicit integration along the length. The length increment is Δy. Therefore, the time step is $\Delta y/v_i$ (different for each particle group).

The length in the moving coordinate system defined by the relative velocity is, however, $|v_j-v_i|\Delta t$. The volume swept by the i particle with respect to collisions with j group particles is

$$V_{C,ij} = \pi/4(D_i + D_j)^2\Delta t|v_j-v_i| = \pi/4(D_i + D_j)^2 |v_j - v_i| \Delta y/ v_i.$$

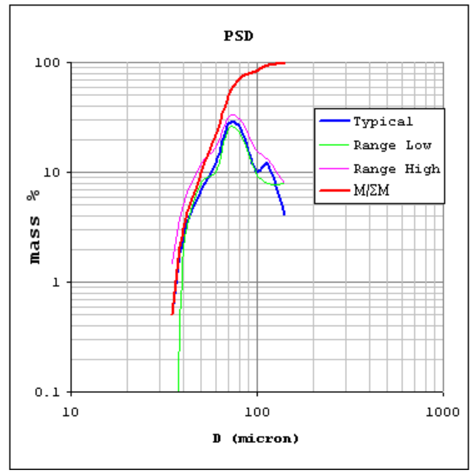


Figure 2: Continuous Particle Size Distribution

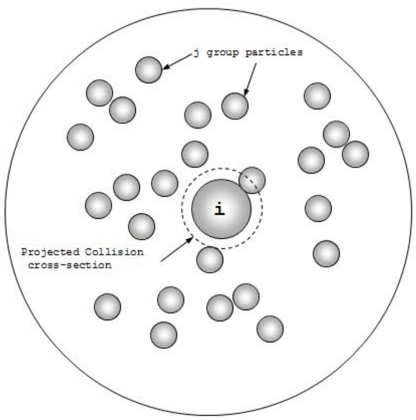


Figure 3a: Radial Cross Section

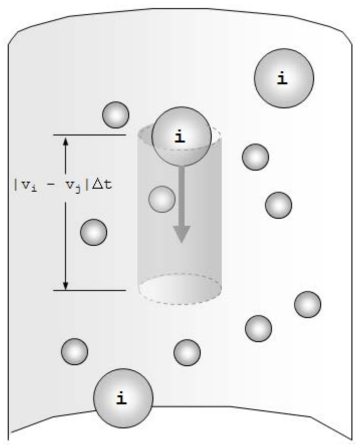


Figure 3b: Centerline Cross Section

The volumetric number density of particles of group j, η_j, is the number, $\Delta t\ N_j$, divided by the volume the particles move in a infinitesimal time step, Δt

$$\eta_j = \Delta t\ m\ X_j / (\Delta t\ v_j\ \pi/4\ D_t^2) = N_j / (v_j\ \pi/4\ D_t^2) \qquad (1)$$

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

Where m is the total mass rate (production rate), X_j is the fraction of m that is in group j, $6\pi\rho_i D_j^3$ is the j group particle's mass, $\Delta t\ N_j$ is the number of j particles moving past any horizontal plane in the time Δt and $(\Delta t\ v_i\ \pi\ D_t^2 / 4)$ is the volume of the tube over length $\Delta t\ v_i$.

The average number of collisions that the single i particle has with j group particles along length increment Δy is, therefore,

$$V_{C,ij} \times \eta_j = \pi/4(D_i+D_j)^2|v_j-v_i|\ \Delta y/ v_i\ \ N_j / (v_j\ \pi/4\ D_t^2)$$

$$= N_j\ (D_i+D_j)^2|v_j-v_i|/(D_t^2\ v_j v_i)\ \Delta y$$

Summing over j, the total number of collisions for one i particle over length Δy, $N_{C,i}$, is

$$N_{C,i} = \{C_{ij}\}\ \{N_j\}\ \Delta y,$$

where $C_{ij} = (D_i + D_j)^2|v_j - v_i|/(D_t^2\ v_j v_i)$ and $\{N_j\} = \{N_i\}^T.=\{0, N_2, N_3,...\}$, index 0 is the tube.

This can be explicitly integrated along the length. Furthermore, logic can be added that suppresses the count below some arbitrary collision cut-off temperature on the presumption that no agglomeration from contact occurs below that temperature.

The thermal energy balance is also integrated explicitly over time, $T(t+\Delta t) = f(T(t))$. The $\Delta t = \Delta y/v_i$ does not work here. The slower smaller particles need a smaller Δt for numerical stability. The treatment below deals, first, with blackbody radiation, then, absorption of radiation by a semi-opaque cloud of particles, then grey body radiation and finally convection.

Black Bodies

Radiation heat transfer is calculated between the furnace (tube) and the particles and radiation between the particles that **may**, due to their different sizes may be at different temperatures along the length of the free-fall.

The view of a finite length of tube to itself without any particles blocking the radiation is the integral over the area of the view from each infinitesimal area element. It is, therefore a double integral. In cylindrical coordinates, the areas, dA are simply $R_t d\alpha dz$. dA_1, is held while dA_2 is sweeps over the entire inner surface, $\pi D_T \Delta Z$. The process is repeated for dA_1 over the surface.

For an empty tube the integrand is $dA_1 \cos(\theta_1)\ dA_2 \cos(\theta_2)/\pi \mathbf{r_{12}}^2$. The $\cos(\theta_2)$ term accounts for the projection of dA_2 in the direction of dA_1. It can be shown that $\cos(\theta_1) = \cos(\theta_2)$. $\boldsymbol{r_{12}}$ is the vector from dA_1 to dA_2.

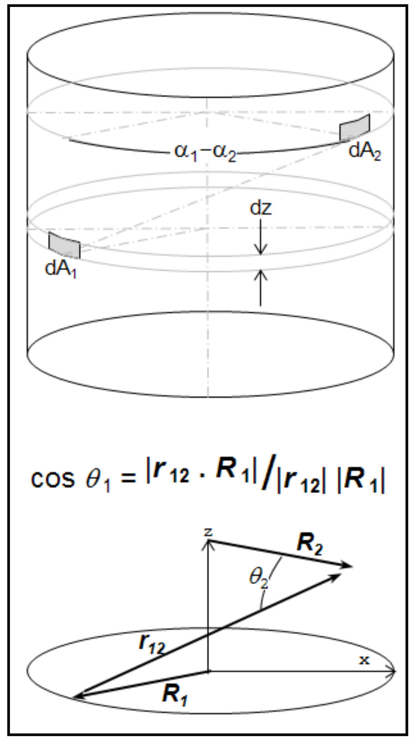


Figure 4: Cylindrical Geometry for Integration

The cloud density parameter is the volumetric density of the projected area of the particles (The projected area of a sphere is the area of disk of the same diameter; the particle's shadow or silhouette.) Strictly, the convention is that for individual particles that "see none of themselves" i.e. no concavities, the projected area is one fourth of the surface area (exactly the case for spheres).

The volumetric density of projected area, β, is defined based of the previously defined number density, η_i (see section on collisions, equation 1). $\beta = \Sigma_i \beta_i = \Sigma_i \eta_i \pi D_i^2 / 4$, β has units of L^{-1} $(=L^2/L^3)$.

The intensity, I, of collimated light changes by $dI = -\beta I dx$. Integrated over finite length, L, $I(L) = I(0) e^{-\beta L}$. Applying the shading of the particles to the radiation view factor calculation we get a new integrand

$$\exp(-\beta|\boldsymbol{r_{12}}|)(|\boldsymbol{r_{12}} \cdot \boldsymbol{R_1}|/ |\boldsymbol{r_{12}}|\ |\boldsymbol{R_1}|)^2\ (1/\pi \mathbf{r_{12}}^2)\ R_t d\alpha_1 dz_1\ R_t d\alpha_2 dz_2.$$

This was integrated with a Monte Carlo style algorithm. The result was checked against published values. The $r/R=0$ intercepts from the referenced graph are used to generate the points. The curve is calculated with b=0 at varied L/R:

Fitting the values to a function that can be used over the length of the free-fall is necessary. Small fitting errors can be magnified by the relationships used to get the views, for example, of the particles to the tube and the particles to themselves. A different measure of the cloud density is used which is related to β by this simple relation: $A_{tube}/A_{total} = \pi D_t dy / (\pi D_t dy + \pi/4 D_t^2 dy \times 4\beta) = 1/(1 + \beta D_t)$. A bit of manipulation gets a relationship where $f(F_{tt})$ and $g(A_{tube}/A_{total})$ satisfy $f(1) = g(1) = 0$.

By definition all of the views from any giving body sum to one.

$$\Sigma_j F_{ij} = 1 \quad (2)$$

The view that body 1 has of body 2, F_{12}, is related to the view body 2 has of body 1.

$$A_1F_{12} = A_2F_{21} \text{ or } F_{21} = (A_1/A_2)\, F_{12} \quad (3)$$

For the purpose of calculating heat transfer, each group (by size) of particles is treated as a single body. The disintegration of F_{tp}, the view from the tube to the particles en mass to F_{ti} the view from the tube to the particles in an individual size group, is straightforward.

It is assumed that the particles are uniformly distributed across the tube cross section. The view from the tube to the particles is distributed among the sets of particles according their areas. The total area of the particles is $\Sigma_{j\neq 1} A_j$. The area fraction of a single group, i, is $A_i/\Sigma_{j\neq 1} A_j$.

$$F_{tp} = 1 - F_{tt},$$

from equation 2. To simplify the subscripts let $F_{ti} = F_{tp,\, i}$,

$$A_t F_{ti} = A_t F_{tp}\, A_i/\Sigma_{j\neq 1} A_j,$$

by distribution over areas argument

$$F_{pt} = F_{tp}\, A_t/\Sigma_j A_j,$$

from equation 3

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

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

from equation 2

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

note $F_{ii} \neq 0$, group i particles see each other.

Very dense clouds of particles ($\beta D_t >> 1$) may require the extension of this work to check for a radial gradient. Numerical integration of the view from the tube to particles near the tube wall is very slowly converging. The steadier approach is to find the view from the tube to a core, F_{tc}. Here the core is half the tube cross section ($D_c = D_t/2^{½}$), F_{tc} is shown in the top figure on the left. The area differential changes to $dA_2 = \beta$□r dr dα dz (a volume element times β, the volumetric density of projected area). An additional relationship between the core and shell is required. F_{sc} was calculated by similar additional changes to the integration. The numerical result with no empirical fit is shown lower left. The views of self, F_{cc} and F_{ss}, can be found from the balances, $\Sigma\, F_{ij} = 1$.

This radial gradient was not used in the results.

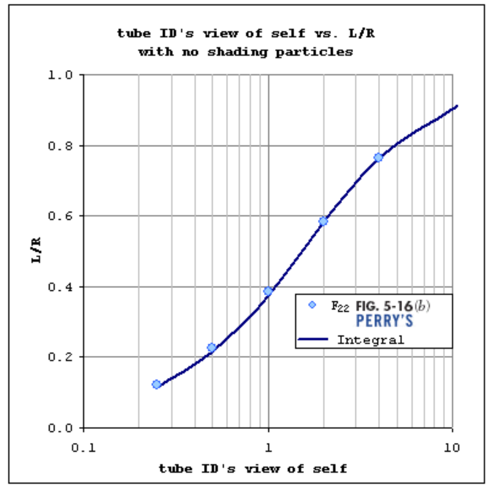


Figure 5: View Factor of Tube on Tube

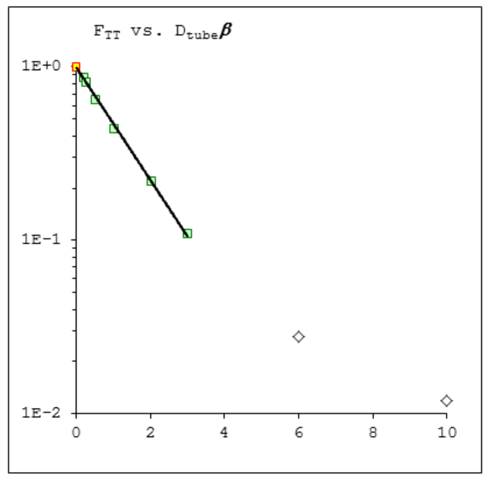


Figure 6: View Factor as a Function of Tube Diameter

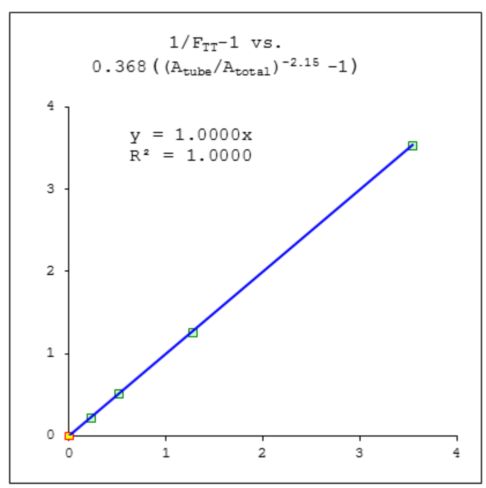


Figure 7: Linear Fit of View Factor to the Fractional Area

Grey Bodies

All of the above is defined for black particles (emissivity = 1). For grey particles (emissivity: independent of wavelength but less than 1) the reflected light must be accounted for. Essentially, a view-area-reflectivity weighted average temperature for each body is calculated. This is the radiosity, $\{W_i\}^T$ below.

$$\begin{bmatrix} \overline{11}-\dfrac{A_1}{\rho_1} & \overline{12} & \overline{1r} & \overline{1s} \\ \overline{12} & \overline{22}-\dfrac{A_2}{\rho_2} & \overline{2r} & \overline{2s} \\ \overline{1r} & \overline{2r} & \overline{rr}-A_r & \overline{rs} \\ \overline{1s} & \overline{2s} & \overline{rs} & \overline{ss}-A_s \end{bmatrix} \begin{bmatrix} W_1 \\ W_2 \\ W_r \\ W_s \end{bmatrix} = \begin{bmatrix} -\dfrac{A_1\varepsilon_1}{\rho_1}E_1 \\ -\dfrac{A_2\varepsilon_2}{\rho_2}E_2 \\ 0 \\ 0 \end{bmatrix}$$

$$\dot{Q}_{i,\mathrm{net}} = (A_i\varepsilon_i/\rho_i)(E_i - W_i)$$

Here (from Perry's Chemical Engineers' Handbook), 11 with an over bar is shorthand for A_1F_{11}, ε_1 is the emissivity of body 1 and ρ_1 ($\rho = 1-\varepsilon$, yet another ρ) is the reflectivity. E_i is the blackbody radiative flux from i, σT_i^4 where σ is the Stefan-Boltzmann constant. In the above, the r and s refer to refractories with no net flux. In our system the right hand side has no 0's. The solution breaks down if the simulated length is so long that the residual temperature differences disappear.

The system of equations is solved for the W_i and these are used to get the net radiation to the surface i. The matrix and vectors can be constructed using index vectors, $\mathbf{i} = \{1, 2, \dots\}$ and $\mathbf{j} = \mathbf{i}^T$.

$\{W_i\}^T = \{\Omega_{ij}\}^{-1}\ \{\Lambda_i\}^T$

$\Omega_{ij} = A_jB_iF_{ij} - \delta_{ij}\,A_i/(1-\varepsilon_i)$

$\Lambda_i = -A_i\ \varepsilon_i/(1-\varepsilon_i)\ T_i^4$

$A_j = A_i^T$, $A_i = \{A_{\text{Tube}}, A_{\text{Particle group 1}}, A_{\text{Particle group 2}} \dots\}$

$B_i = \{B_i\}$: $B_{i=1} = 1$, $B_{i>1} = A_i/(\Sigma_{k\neq 1}A_k))$ …

$F_{ij} = \{F_{ij}\}$: $F_{i=1,\,j=1} = F_{TT}$, $F_{i>1,\,j=1} = F_{TP}$, $F_{i=1,\,j>1} = F_{PT}$, $F_{i>1,\,j>1} = F_{PP}$

$\delta_{ij} = 1$ if $i=j$, 0 otherwise

Notes:

The "i" and "j" here include the tube $(i, j = 1)$.

The ***W*** in the reference and here differ by a factor of σ.

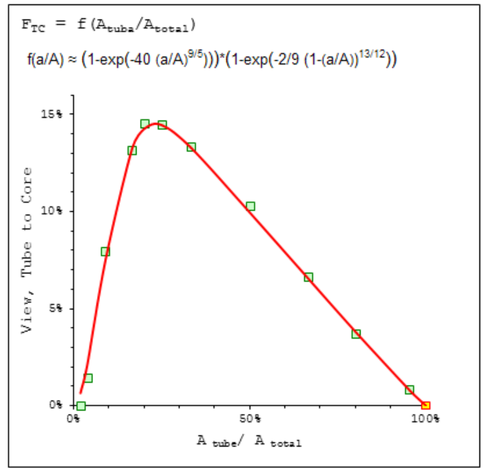


Figure 8a: View Factor of Tube to the Tube's Core as a Function of Fractional Area

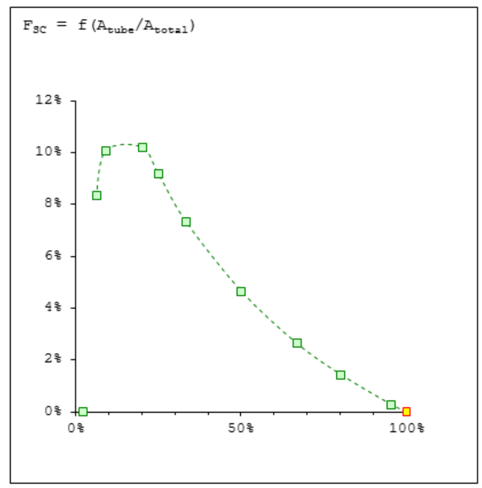


Figure 8b: View Factor of Shell to the Tube's Core as a Function of Fractional Area

The radiation heat transfer to a single particle is $Q_{rad,\,i} = \sigma\pi D_i^2\varepsilon_i/(1-\varepsilon_i)\ (W_i - T_i^4)$

Convective heat transfer between the particles and the fluid is calculated using flow dependent empirical correlations. The assumption is that the flow is relatively undisturbed by the other particles. Most of the simulated cases have a maximum volumetric loading of less than a few percent. Another assumption is that the gas is non-radiating. For systems where the gas is flowing, it is necessary to track/model the gas temperature along the length, as well.

If the gas velocity is zero there can be no net heat transfer to or from the gas. Mathematically, this is stated as "the sum of the heats transferred to the gas is zero" or: $\Sigma_i\, h_i A_i\, (T_i - T_g) = 0$, i h_i, A_i, and T_i are the local heat transfer coefficient, area and temperature of surface "i". Note, again: "i" includes the tube. The no-net-flow gas temperature is

$$T_{g,\,NF} = \Sigma_i\,(h_i A_i T_i)/\,\Sigma_i(h_i A_i).$$

The gas augments heat transfer between the various surfaces in parallel with radiative heat transfer.

Flowing gas can be used by the process in several ways. Gas flowing up past the falling particles will extend the residence time in the hot zone. Gas flowing down, with the particles can reduce the range of velocities, hence reducing the number of collisions.

For flowing gas an explicit integration is a bit more complicated. For the base case of large numbers of fine particles and relative small gas flow, the gas is close to equilibrium with the particles ($T_{g,\,NF}$). For the alternate case, small number of large particle and large counter-flowing gas, the gas temperature can be much different than the temperature of the local solid surfaces.

The solution method that works for both extremes – and the range between them- is to use an integrated form:

$$m._g\, C_{p,g}\, dT_g = \Sigma_i\, h_i dA_i\, (T_i - T_g)$$

Where $dA_i = (A_i/\Delta y)dz$, $m._g$ and $C_{p,g}$ are the mass rate and heat capacity of the gas, respectively. This can be integrated over $0<z<\Delta y$. After some rearrangement, a compact form is

$$T_g(y+\Delta y) = T_g(y) + (T_s - T_g(y))(1-\exp(-HA/\, m._g\, C_{p,g}))$$

$$HA = \Sigma_i(h_i A_i),\; T_s = \Sigma_i\,(h_i A_i T_i)/HA.$$

The results are not particularly sensitive to whether "i" refers to the upstream or local temperature. For high flow cases it is more important to track the heat carried by the gas.

The correlation used to get the gas-powder heat transfer coefficient is

$$Nu_i = 2 + 0.6 Re_i^{1/2}\, Pr^{1/3},$$

Re is defined previously, Pr – the Prandtl number ($= C_p\, \mu/k$) – is taken to be relatively constant because the viscosity and thermal conductivity of a gas tend to show similar temperature dependence. In the example, the difference over 3000K was about 3%.

$$h_i = Nu_i k_i\, /D_i,\; k_i = k_{T0}\, (\tfrac{1}{2}\,(T_i + T_g)/T_0)^{kA}$$

For the interesting cases where $A_{particles} > A_{tube}$ and $h_{shape} = Nu\; k_{gas}/D_{shape}$ yielding $h_{particle} >> h_{tube}$, convection to and from the tube wall can usually be neglected.

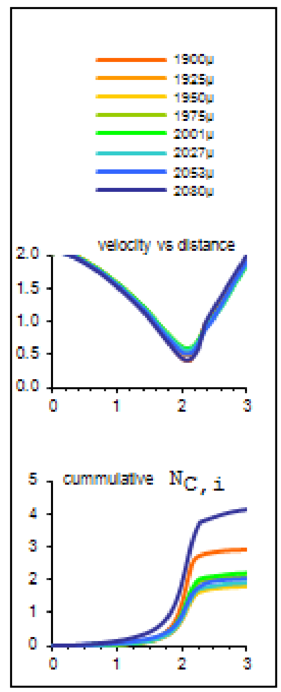


Figure 9: Velocity and Particle Count for various Particle Sizes

The temperature of the particles as a function of time and/or distance is, in explicit numerical integration, a simple algebraic relationship:

$$T(t+\Delta t) = T(t) + \Delta t(\text{net heat transfer rate to particle})/(\text{particle mass x heat capacity})$$

This model allows materials to pass through energetic phase transitions. This is captured mathematically by making the heat capacity a function of temperature. A plot of the enthalpy versus temperature is fit with a $C_p(T)$. The iteration time steps must be small enough and the phase change temperature band wide enough so that the temperature changes a few times as the element passes through the phase change.

Results

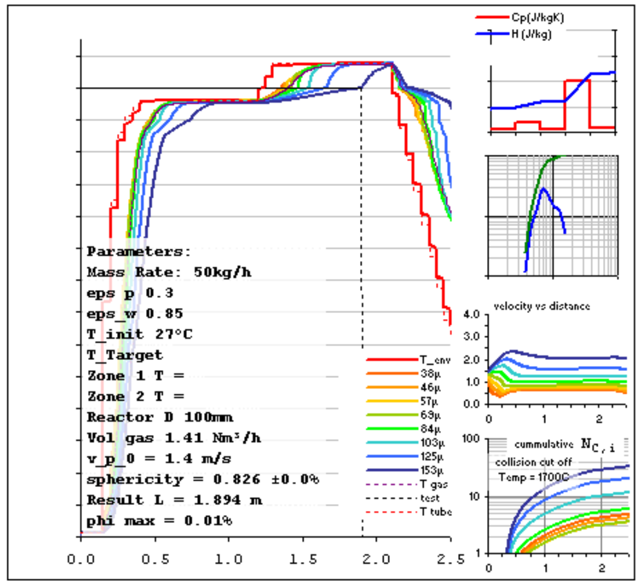
The model produces a set of graphs that show nearly all the input parameters.

For example, this figure shows along with the temperature for each size group and the boundary conditions, the material thermodynamics, the particle size distribution, the particle velocities for each size, the collision count and the complete set of input parameters.

This example is a 2-Zone furnace treating 50kg/h of an example material.

As a test of the collision model, a narrow PSD was nearly brought to zero velocity by a substantial counter-flowing gas.

The collision count spikes at the same point along the length where the velocity is at its minimum.



Another example with a similar PSD going through a phase change explores the use of counter-flowing gas to reduce the collisions.