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PREDICTIVE MODELLING OF BOILER FOULING

QUARTERLY TECHNICAL PROGRESS REPORT

**For the Period
January 1, 1992 - March 31, 1992**

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1.0 PROGRAM OBJECTIVE AND SCOPE OF WORK

The primary objective of this work is the development of a comprehensive numerical model describing the time evolution of fouling under realistic heat exchanger conditions. As fouling is a complex interaction of gas flow, mineral transport and adhesion mechanisms, understanding and subsequently improved controlling of fouling achieved via appropriate manipulation of the various coupled, nonlinear processes in a complex fluid mechanics environment will undoubtedly help reduce the substantial operating costs incurred by the utilities annually, as well as afford greater flexibility in coal selection and reduce the emission of various pollutants. In a more specialized context, the numerical model to be developed as part of this activity will be used as a tool to address the interaction of the various mechanisms controlling deposit development in specific regimes or correlative relationships. These should prove of direct use to the coal burning industry.

The Statement of Work comprises a series of related and logically structured tasks described as follows:

Phase I

Task 1

Perform semi-quantitative evaluations of solution and algorithmic details of Higher Level Simulation (HLS) techniques applicable to flow in and around a tube bundle.

Task 2

Assess (quantitatively) HLS predictions for flow and turbulence characteristics of related, simpler problems.

Task 3

Reformulate the algorithm to predict flow details around a cylinder in an isothermal, but otherwise representative environment.

Task 4

Predict heat transfer characteristics for the problem in Task 3.

Task 5

Generalize the algorithm to predict flow, turbulence and heat transfer details for multi-tube configurations including in-line and staggered arrangements.

Task 6

Provide project management and financial control with the required technical and financial reports and documentation.

Phase II

Task 1

Develop an appropriate multi-phase, multi-species transport algorithm for a "frozen" gas aerothermal field.

Task 2

Develop sub-modules for surface related processes including adherence and removal.

Task 3

Provide project management and financial control with the required technical and financial reports and documentation.

Phase III

Task 1

Extend the algorithm to couple multi-species, multi-phase transport and deposition models with a comprehensive HLS of flow and heat transfer in a tube bundle for a representative case.

Task 2

Perform pertinent parameter variation studies and develop improved engineering correlations to model fouling in practical boiler configurations and operating environments.

Task 3

Provide project management and financial control with the required technical and financial reports and documentation.

2.0 SUMMARY OF PROGRESS TO DATE

In this reporting period, efforts were initiated to supplement the comprehensive flow field description obtained from the RNG-Spectral Element Simulations by incorporating, in a general framework, appropriate modules to model particle and condensable species transport to the surface.

Specifically, a brief survey of the literature revealed the following possible mechanisms for transporting different ash constituents from the host gas to boiler tubes as deserving prominence in building the overall comprehensive model.

i) Flame-volatilized species, chiefly sulfates, are deposited on cooled boiler tubes via the mechanism of classical vapor diffusion. This mechanism is more efficient than the particulate ash deposition, and as a result there is usually an enrichment of condensable salts, chiefly sulfates, in boiler deposits.

ii) Particle diffusion (Brownian motion) may account for deposition of some fine particles below 0.1mm in diameter in comparison with the mechanism of vapor diffusion and particle depositions, however, the amount of material transported to the tubes via this route is probably small.

iii) Eddy diffusion, thermophoretic and electrophoretic deposition mechanisms are likely to have a marked influence in transporting 0.1 to 5 μ m particles from the host gas to cooled boiler tubes.

iv) Inertial impaction is the dominant mechanism in transporting particles above 5 μ m in diameter to water and steam tubes in pulverized coal fired boiler, where the typical flue gas velocity is between 10 to 25 m/s. Particles above 10 μ m usually have kinetic energies in excess of what can be dissipated at impact (in the absence of molten sulfate or viscous slag deposit), resulting in their entrainment in the host gas.

In the vicinity of cooled tubes, alkali sulfates, formed prior to entry in the boiler by conversion of primarily alkali hydroxides and chlorides, may condense on ash, fume and fly ash or alternatively through self-nucleation owing to the large supersaturation in the boundary layer. Thus, a comprehensive nucleation model may be required to predict the size distribution and composition of aerosols formed from condensation of ash

vapor/alkali sulfates. Such a model should be formulated to incorporate significant mechanisms of homogeneous/heterogeneous nucleation, agglomeration and adsorption as dictated by kinetic processes. Coupling of nucleation/agglomeration with the deposition mechanisms outlined in (i) to (iv) should duly account for a combination of simultaneous deposition processes and hence enable to accurately predict fouling phenomena for this practically important operating range.

Typical range of particle sizes for normal boiler operating experience comprises particles $>0.1\mu\text{m}$ and $40\mu\text{m}$; hence a judiciously formulated model incorporating a non-linear combination of transport processes including inertial impaction, turbulent eddy diffusion and possible thermophoresis is strictly warranted.

On the question of the particle equation of motion, the analysis presented by Maxcy and Riley regarding the equation of motion of a small rigid sphere in a non-uniform flow, i.e.,

$$\begin{aligned} \frac{d\bar{v}}{dt} = & \frac{2(\rho-1)}{2\rho+1} \bar{g} + \frac{2}{2\rho+1} \left(\frac{D\bar{u}}{Dt} + \frac{1}{2} \frac{d\bar{u}}{dt} + \frac{r^2}{20} \frac{d\nabla^2\bar{u}}{dt} \right) \\ & - \frac{9/(r^2 \text{Re})}{2\rho+1} \left(\bar{v} - \bar{u} - \frac{r^2}{6} \nabla^2\bar{u} \right) \\ & - \frac{9/(r\sqrt{\pi \text{Re}})}{2\rho+1} \\ & \times \int_0^t \frac{(d/d\tau) \left[\bar{v} - \bar{u} - (r^2/6) \nabla^2\bar{u} \right]}{(t-\tau)^{1/2}} d\tau \end{aligned} \quad (1)$$

needs to be appropriately simplified for incorporation in the RNG-Spectral Element code. In the above $\bar{v}$ is the velocity of the sphere, $\bar{u}$ is the velocity of the undisturbed fluid evaluated at the center of the sphere, t is the time, r is the radius of the sphere, ρ is the ratio of the density of the sphere to the density of fluid, d/dt denotes a time derivative following the sphere, and D/Dt denotes a time derivative using the undisturbed fluid velocity as the convective velocity. The variables in Equation (1) have been made

dimensionless in terms of a characteristic length D_c and velocity u_0 of the undisturbed flow and $Re = u_0 D_c / \nu$ where ν is the kinematic viscosity of the fluid.

In the above equation, if it is assumed that the density of the particle is sufficiently great compared to the density of gas, virtual mass effects are unimportant. Furthermore, for a sufficiently small particle, the Bassett history terms and the buoyancy terms should be small compared to the Stokes drag term. The same reasoning would suggest that the Saffman lift term (which does not appear explicitly in the above equation of motion) should be small compared to the Stokes drag term, and this is generally the case, except in the viscous sublayer where the combination of a large normal component of velocity and a large normal gradient of the streamwise component of the velocity can make the lift term significant for particles in certain size ranges.

The Saffman lift force takes the form:

$$f_s = 6.46 \mu r^2 \left[\left(\frac{1}{\nu} \right) \left| \frac{du_x}{dy} \right| \right]^{1/2} (v_x - u_x) \quad (2)$$

In equation (2) f_s is the lift force acting on a rigid spherical particle in a uni-directional time dependent shear flow that points in the x direction and is a function of y . The sign of the right hand side of (2) is valid provided that (du_x/dy) is positive.

When divided by the particle mass and expressed in a dimensionless form, the Saffman lift force contributes an additional term to the right hand side of Equation (1) of the form:

$$f_s / m_p = - \left(\frac{0.343}{\rho r Re} \right) \left| \frac{du_x}{dy} \right|^{1/2} (v_x - u_x) \quad (3)$$

As is shown above, while the large/intermediate size region of the spectrum can be conveniently treated using a Lagrangian formulation with due regard to eddy diffusion, Figures (1) through (4), sub/micron particle deposition rates are strongly influenced by thermophoretic effects and typical particle deposition rates are enhanced by many orders of magnitude over the inertial deposition rates. Furthermore, particle diffusion can no longer be neglected; thus the merits of an approach that treats them in a Eulerian framework needs to be evaluated. Generally, the mass loading of submicron particles as

well as the vapor phase constituents is negligibly small, allowing the possibility of employing an approach that treats them as trace species, semi-independent of the main bulk motion. The extent to which the behavior of the two distinct trace species is coupled to each other is presently unclear. There are indications that condensation of vapor phase constituents forms a "glue-like" material which then determines the sticking and erosion probability of impacting particles. Assuming that such interactions can be modelled or experimentally determined, it should, in principle, be feasible to incorporate in a comprehensive model the combined influence of micron, submicron and aerosol or vapor phase constituents for multi-species deposition. When formulating such a model, for turbulent flow problems where embedded laminar sublayers cannot be resolved adequately owing to excessive computational requirements, means have to be provided to couple the relevant "wall transfer and deposit" processes to bulk flow computations. Here, a first order treatment might be conveniently employed that utilizes turbulent boundary layer correlations for particle deposition rates in a fashion analogous to the use of turbulent wall boundary conditions for the treatment of wall shear stress calculations.

3.0 TECHNICAL APPROACH

The following discussion develops criteria to assess the significance of simultaneous presence of both condensable vapors and aerosol particles on mass transfer (deposition) rates.

It has been proposed in the literature that the simultaneous presence of aerosol particles and condensable vapors in a saturated boundary layer may affect deposition rates to subcooled surfaces because of vapor-particle interactions. Scavenging of condensable vapors by aerosol particles may lead to increased particles size (and mass) and decreased vapor mass fraction, thus altering both vapor and particle deposition rates. Particles, if sufficiently concentrated may also coagulate. Analysis presented below to assess the significance of such phenomena assumes particles are already present in the mainstream and are not created inside the boundary layer via homogeneous nucleation.

The boundary layer mass conservation equations for the condensable vapor and aerosol particles (dilute) in two dimensions (for clarity) can be expressed as: (assuming sufficiently small particles, incapable of inertially impacting on surfaces):

$$\rho u \frac{\partial w_i}{\partial x} + \rho v \frac{\partial w_i}{\partial y} = \rho D_i \frac{\partial^2 w_i}{\partial y^2} - \dot{r}''' \quad (4)$$

(condensable species i)

$$\rho u \frac{\partial w_p}{\partial x} + \rho(v + v_T) \frac{\partial w_p}{\partial y} = \rho w_p \frac{\partial v_T}{\partial y} + \dot{r}''' \quad (5)$$

where v_T is the aerosol particle thermophoretic velocity given by:

$$v_T = \alpha_{T,p} D_p \frac{\partial \ln T}{\partial y} \cong -\alpha_{T,p} D_p \frac{\Delta T}{T_w} \frac{1}{\delta_h} \quad (6)$$

and $\dot{r}'''$ denotes the mass of vapor locally scavenged by the aerosol particles per unit time and volume. If one approximates the shapes of the aerosol particles by spheres, neglects the relative velocity of condensable vapors with respect to aerosol particles, and takes the

largest possible mass transfer driving force, the $(\dot{r}''')_{\max}$ can be expressed in terms of the diffusion flux of condensable vapors onto the surfaces of aerosol particles, i.e.,

$$\begin{aligned}
 (\dot{r}''')_{\max} &= \left(2 \frac{D_i}{d_p} \rho w_{i,\infty} \right) \pi d_p^2 \left(\frac{\rho w_{p,\infty}}{\frac{\pi}{6} d_p^3 \rho_p} \right) \\
 &= 12 \frac{D_i}{d_p^2 \rho_p} \rho w_{i,\infty} \rho w_{p,\infty}
 \end{aligned} \tag{7}$$

where the mass transfer Nusselt number is taken to be 2, corresponding to mass transfer to/from spheres in a quiescent medium. Note that the analysis below will provide a conservative estimate of the significance of the above mentioned effects because use is made of the largest possible reaction (condensation) rate, $\dot{r}'''_{\max}$. In reality, the actual reaction rate $\dot{r}'''$ will be smaller because (a) the local mass fractions of both condensable vapors ω_i and aerosol particles ω_p inside the boundary layer will be smaller than their corresponding mainstream values $\omega_{i,\infty}$ and $\omega_{p,\infty}$ and (b) the driving force for condensation onto the aerosol particle is determined by the difference between the condensable vapor local mass fraction, ω_i in the boundary layer and the mass fraction locally prevailing on the aerosol particle surface at the gas/condensate interface (assumed to be much smaller than ω_i here).

Now considering the effects of the presence of condensable vapors on particle deposition rates, it is seen that the thermophoretic velocity v_T of aerosol particles depends on the thermophoretic diffusivity $\alpha_{T,p} D_p$ as shown in Equation (6). However, because the thermophoretic diffusion faction $\alpha_{T,p}$ is inversely proportional to the Brownian diffusion coefficient, D_p , the thermophoretic velocity is actually independent of D_p (and hence d_p). Therefore, it is known a priori that vapors condensing on aerosol particle surfaces will not affect their thermophoretic velocity. However, the deposition rate of aerosol particles will still be affected because the depositing particles will be larger (heavier). A proper way to measure the significance of this effect is to consider the maximum fraction change in the aerosol particle diameter due to vapor condensation. The rate of change of mass of an aerosol particle $\Delta m / \Delta t$, is given by:

$$\frac{\Delta m}{\Delta t} = \rho_p \left(\frac{\pi \Delta (d_p^3)}{6} \right) = \rho_p \frac{\pi d_p^2}{2} \frac{\Delta d_p}{\Delta t} \quad (8)$$

But $\Delta m/\Delta t$ is also given by the mass deposition rate of saturated vapors condensing on the aerosol particle surface, i.e.,

$$\frac{\Delta m}{\Delta t} = (\pi d_p^2) (\dot{m}_i) = \pi d_p^2 \left(2 \frac{D_i}{d_p} \rho \omega_{i,\infty} \right) \quad (9)$$

Hence,

$$\Delta d_p = 4 \frac{D_i}{d_p} \frac{\rho \omega_{i,\infty}}{\rho_p} \Delta t \quad (10)$$

In (10) Δt is the residence time of the aerosol particles travelling with a thermophoretic speed $|v_T|$ inside the thermal boundary layer of thickness δ_h and can be estimated from:

$$\Delta t \approx \frac{\delta_h}{v_T} \approx \frac{\delta_h}{\alpha_{T,p} D_p \frac{\Delta T}{T_w} \frac{1}{\delta_h}} = \frac{\delta_h^2}{\alpha} \frac{1}{(\alpha_{T,p} Le_p) \Delta T} \frac{T_w}{\Delta T} \quad (11)$$

where α is the thermal diffusivity of the mixture and Le denotes the particle Lewis number. Combining, Equations (10) and (11), the fraction change in the aerosol particle diameter is given by:

$$\frac{\Delta d_p}{d_p} = 4 \frac{Le_i}{(\alpha_{T,p} Le_p)} \frac{T_w}{\Delta T} \frac{\rho \omega_{i,\infty}}{\rho_p} \left(\frac{\delta_h}{d_p} \right)^2 \quad (12)$$

The parameters in Equation (12) can be readily estimated for the prevailing operating conditions to assess the significance of vapor scavenging by particles.

A further effect relates to the influence of the presence of aerosol particles on vapor deposition rates. In this context, a measure of the importance of the presence of ash particles acting as a sink for vapor molecules can be obtained by comparing the

relative magnitude of the reaction (r''') term in Equation (4) to the diffusion term. An effective Damkohler number defined as:

$$Da \equiv \frac{\text{characteristic vapor diffusion time across mass transfer boundary layer}}{\text{characteristic reaction (condensation) time}}$$

is such a quantity. The characteristic vapor diffusion time is given by:

$$t_i = \frac{\delta_{m,i}^2}{D_i} \quad (13)$$

and the characteristic reaction (condensation) time is given by:

$$t_r = \frac{\rho \omega_{i,\infty}}{\dot{r}_{\max}} = \frac{1}{12} \frac{d_p^2 \rho_p}{D_i \rho \omega_{p,\infty}} \quad (14)$$

Thus,

$$Da = \frac{t_i}{t_r} = 12 \frac{\rho \omega_{p,\infty}}{\rho_p} \left(\frac{\delta_{m,i}}{d_p} \right)^2 \quad (15)$$

The quantities in Equation (15) can be estimated for prevailing operating conditions.

Finally, considering the effect of particle coagulation on aerosol particle deposition rates, it is assumed that the residence time of the aerosol particle inside the thermal boundary layer is determined by thermophoretic velocity as the aerosol particle transport is demonstrated by thermophoresis. A comparison of the characteristic particle residence time inside the thermal boundary layer with the characteristic coagulation time is a measure of the significance of particle coagulation. If one assumes a nearly monodisperse system with Brownian coagulation, then the ratio of two characteristic time is given by:

$$\frac{t_{thermophoresis}}{t_{coagulation}} = \frac{\delta_h}{\frac{v_T}{\left(\frac{\beta \rho \omega_{p,\infty}}{\frac{\pi}{6} d_p^3 \rho_p} \right)^{-1}}} \quad (16)$$

$$= \frac{6}{\pi} \left(\frac{\beta}{d_p \alpha} \right) \left(\frac{1}{\alpha_{T,p} Le_p} \right) \left(\frac{T_w}{\Delta T} \right) \left(\frac{\rho \omega_{p,\infty}}{\rho_p} \right) \left(\frac{\delta_h}{d_p} \right)^2$$

where β is the binary coagulation rate constant given by:

$$\beta = \frac{8}{3} \frac{kT}{\mu}$$

Again, the relevant quantities can be readily obtained from operating conditions.

It is tentatively concluded from the above analysis that $(\delta/d_p)^2$ is the single most critical factor to consider in deciding when to neglect vapor-particle interactions for thermophoretically dominated systems.

4.0 CONCLUSION AND PLANS FOR FUTURE WORK

4.1 Conclusions to Date

Good technical progress has been made. Regarding the Saffman lift force on influencing the behavior of the particle in the vicinity of the tube surface, experience to date shows that the lift force has virtually no effect outside the viscous sublayer. The main effect of the lift force is to impart momentum to particles that are moving through the viscous sublayer toward the wall. Although the magnitude of the lift force is small compared to the magnitude of the normal component of the Stokes drag force, the impulse provided by the lift force has a very pronounced effect on the deposition of the particles. The importance of the lift force stems mainly from the fact that it occurs in just the right region - namely, a region in which the normal component of the fluid velocity has fallen to negligible values. The form of the lift force will almost certainly show some Reynolds number dependence, and when the particle gets within a few diameters of the wall, other effects do become important. However, cases tried in this effort, as well as those reported in the literature, show that a considerable increase in the deposition rate can be caused by a relatively small impulse in the viscous sublayer, and, provided that one can estimate the size of the lift force from other measurements or calculations, one can use correlative analyses to estimate the deposition rate.

4.2 Plans for Next Reporting Period

Efforts will be continued to supplement the comprehensive flow field description obtained from the RNG-Spectral Element Simulations by incorporating in a general framework, appropriate sub/models to model particle and condensable species transport to the surface.

Figure 1. Particle Trajectories for the Asymmetric Cylinder in a Channel

Figure 2. Particle Trajectories for the 2x2 Cylinder Array

Figure 3. Particle Trajectories in the Spanwise Direction
for the 2x2 Cylinder Array

Figure 4. Particle Trajectories for the 3x3 Cylinder Array

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