DOE/PC/90756--T12

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DE93 003899

QTR #11

**Research on Thermophoretic and Inertial Aspects of Ash
Particle Deposition on Heat Exchanger Surfaces in
Coal-Fired Equipment**

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Quarterly Technical Report on: DE-FG22-86 PC 90756

Total Contract Period: 9/1/86 - 8/31/89

Quarterly Period Covered: 3/1/88¹ - 5/31/89

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1. Introduction

DOE-PETC initiated at the Yale HTRC Laboratory a systematic three-year experimental and theoretical research program directed toward providing engineers with data, methods, and rational correlations needed to improve the generality and accuracy of prediction of inorganic particle *deposition rates* under typical coal combustion conditions (*i.e.*, those leading to the importance of thermophoretically-enhanced diffusion (submicron mode) and the inertially-enhanced "impaction" (supermicron mode), often in the presence of simultaneous alkali salt vapor condensation. After a brief statement of objectives (Section 2) we outline our experimental and theoretical progress during this quarterly reporting period (Section 3), with our results summarized in the references documented in Section 5 and Appendix A. Section 4 gives relevant administrative information (personnel, research plans).

2. Background Statement: Objectives

The goal of our research in the area of ash *transport* is to advance the capability of making reliable engineering predictions of the dynamics of net deposit growth for surfaces exposed to the products of coal combustion. To accomplish this for a wide variety of combustor types, coal types, and operating conditions, this capability must be based on a quantitative understanding of each of the important mechanisms of mineral matter transport, as well as the nature of the interactions between these substances and the prevailing "fireside" surface of the deposit. This level of understanding and predictive capability could ultimately be translated into very significant cost reductions for coal-fired equipment design, development and operation.

Our emphasis in the present program: "Research on Thermophoretic and Inertial Aspects of Ash Particle Deposition on Heat Exchanger Surfaces in Coal-Fired Equipment" is on developing and experimentally validating* rational, theoretical methods of predicting the role of *inertia* and ash particle *thermophoresis* in determining net deposition rates (see, *e.g.*, Rosner, 1985; 1986). We are also quantifying how simultaneous *vapor* deposition (*e.g.*, alkali sulfate) can influence the sticking and erosion associated with impacting particles. Specifically, as a result of this DOE-PETC supported program, we believe that it will be possible for us to develop:

- a. An improved understanding of the factors governing impacting particle capture and deposit erosion probabilities, leading to rational correlations (see, *e.g.*, Rosner and Nagarajan, 1987).
- b. Ways of applying recent *mass* transfer theories (developed for idealized geometries) and available *heat* and *momentum* transfer data to develop prediction methods for important practical situations — *eg.* deep tube bundles ('banks') (see, *eg.*, Rosner, 1986).

* Our previous DOE-METC supported experiments have been confined to vapor and submicron particle systems in the absence of inertial phenomena (*e.g.* Rosner, 1989a). For an overview of convective mass transfer, see the PI's recent textbook (Rosner, 1986, 1988), especially Chapters 6, 8.

- c. Necessary extensions of available particle deposition rate theory (see, e.g., Park and Rosner, 1989) and the phoretic properties of particles (García-Ybarra and Rosner, 1989; Mackowski, 1989).
- d. Useful, rational correlations to generalize the results of actual or numerical experiments and make them suitable for engineering design calculations (Israel and Rosner, 1983; Wessel and Righi, 1988).
- e. The beginnings of an understanding of the interrelationship between deposition *mechanism*, deposit *microstructure* and deposit *properties* (eg. thermal resistance, ...).

To develop tractable but realistic/rational procedures for predicting the evolution of wall deposits, we also have intensified communication with more empirically oriented engineers/chemists who have the necessary boiler fouling/slagging experience. Thus, based on the insights gained from the present program we should ultimately be able to recommend economical 'subroutines' (compatible with practical requirements of global computer codes, recent deposition research results and cumulative empirical observations) to predict the evolution of wall deposits for, say, design studies of coal-fired furnaces and boilers (see, e.g., Gokoglu and Rosner, 1984; and, also, Appendix A3).

3. Research Progress

Our most recent results can be conveniently divided into the following five sub-areas:

3.1 *Experimental and Theoretical Studies of Particle Deposition in the Simultaneous Presence of Inertia and Thermophoretic Effects*

3.1.1 To derive the maximum amount of information from our deposition rate experiments it remains for us to calibrate our mainstream particle concentrations and velocities. Toward this end we have been gaining experience with the Single Particle Counter / Transit Time Velocimeter (SPC/TTV) developed during the previous months, testing it in a cold flow environment using nebulized solutions of MgSO_4 (droplet size *ca.* $3\ \mu\text{m}$) as well as ZrSiO_4 particles dispersed with an improved version of our syringe feeder. Attempts to use the SPC/TTV with submicron ($0.7\ \mu\text{m}$) MgO particles suspended in our hot micro-jet, showed that the signal/noise ratio of the present system is not adequate for this size range. We are presently examining ways to overcome this difficulty (e.g. optimizing the arrangement of the optics, using more sensitive photodetectors or perhaps switching to a higher power laser than the currently used, 7mW He-Ne).

3.1.2. We have developed numerical and asymptotic models to account for the simultaneous effects of inertia and thermophoresis on the transport of particles across LBL's with *streamwise curvature* which will be compared with our experimental data once the abovementioned measurements of particle concentration and velocity in the micro-jet are completed. In addition, we have derived analytically useful asymptotic ($Sc \gg 1$, $Re^{1/2} \gg 1$, $Stk \ll 1$) results for the effect of inertia on Brownian diffusion deposition rates on curved surfaces from isothermal LBL flows. This analysis can now be extended to include thermophoresis and thereby clarify the role of inertia in modifying the thickness of 'dust-free' zones near submerged hot 'objects' and the role of Brownian diffusion in 'smearing' out the apparent discontinuity in the particle concentration (cf. our parallel measurements of $\alpha_T D_p$ in the counter-flow gaseous diffusion flame configuration).

3.1.3. Our survey of rational theories of particle sticking and the effects thereupon of liquid layers, shows that for modest collision velocities [of $O(1 \text{ m/s})$] of micron sized particles with thin liquid layers [when the elastohydrodynamic collision and rebound theory of Davis *et al.* (1986) is applicable) the critical energy E^* required for rebound scales asymptotically ($Re_{pp}/\rho_g \ll 1$) with the fifth power of the liquid layer thickness, illustrating the significant effect that liquid layers are expected to have on the sticking probability, s (in general, s is an increasing function of E^*). A micromechanical model of sticking on, and erosion of, deposits can be formulated following recent developments in the field of partially saturated granular media (see, *e.g.* Gili and Alonso, 1988). While a lower priority item for the present (more experimentally oriented) project, such an approach now looks very promising to us and warrants a feasibility study planned for the immediate future.

3.2 Relation between Deposit Microstructure and Particle Deposition Mechanism

As an extension of our earlier Monte-Carlo study of the relation between particulate deposit microstructure and particle deposition mechanism (Tassopoulos, O'Brien and Rosner, 1989, to appear during the next reporting period), we are investigating alternative dynamical sticking laws, and performing associated three-dimensional off-lattice simulations to assess their influence on the resulting deposit microstructure. In the simplest version we assume that every particle arrives at the target with a velocity specified *a priori* both in magnitude and direction. An energy balance at the point of impact between the moving and fixed particle (taking into account energy losses due to elastic/plastic deformation in the radial direction and friction in the tangential direction) determines whether the moving particle sticks or escapes. If the particle bounces, its new initial velocity is computed, and the particle is followed to its next contact with deposit. We repeat this sequence until the particle sticks. In another version, particle sticking is determined in a similar manner but we further superimpose a flow field that drives the particles towards the target. For computational simplicity we have illustrated this approach using a potential flow along the stagnation line. We find that both models result in *denser* deposits than those obtained using our previous (relatively "unrestricted") active site model. We also compute and report the evolution of the surface roughness, and other higher order descriptors such as void-void and void-solid correlation functions, associated with such deposits. A paper describing these situations and their practical implications will be presented at the AIChE Annual Mtg, November 1989 in San Francisco. The associated abstract appears as Appendix A -3.

3.3 Theory of Particle Deposition from 'Polydispersed' Aerosols

Our paper on the rapid prediction of total mass deposition rates from log-normally distributed aerosol populations of arbitrary spread (Rosner and Tassopoulos, 1989) contains results of the type shown in Fig. 1, applicable to convective diffusion of particles in the 'continuum regime'. Here m_{ref}'' is the 'reference' deposition rate, viz. the rate one would expect if all the particles had the mean particle volume $\bar{v} \equiv \phi_p/N_p$. Results such as these dramatically simplify the prediction of total mass deposition rates from 'polydispersed' dust-laden streams when one or several deposition mechanisms occur over important portions of the log-normal size spectrum. We have thus succeeded in generalizing my previous study (Rosner, 1989) which provided simple results for a 'single' mechanism (*eg.* convective-diffusion) and 'coagulation-aged distribution'.

We are presently generating the universal functions needed to apply 'moment' methods to aerosol evolution problems in which the PSD may be approximated as a log-

normal (in particle volume) and wall loss processes participate. As a by-product this leads to short-cut methods for predicting the parameters governing both the PSD parameters governing the *deposited* aerosol as well as the aerosol that escapes capture. We plan to apply these results/methods shortly to problems involving particle-laden flows in ducts and deep tube banks.

3.4 *Application of Counterflow Diffusion Flames to the Determination of Inorganic Particle Thermophoretic Diffusivities*

Our initial experiments on N₂-diluted counterflow gaseous diffusion flames, stabilized at an average strain rate of 13 s⁻¹, indicated the existence of a 1.5 mm thick thermophoretically-induced *particle-free (dark) zone*, which can be used to make measurements of the particle thermophoretic diffusivity. Replacing N₂(g) with He (g) in these flames imposed operation at a much larger strain rate, $a=28\text{ s}^{-1}$, more than double that of the nitrogen diluted flame, because of stabilization difficulties. To a first approximation the velocity gradients in the He-flame are twice those in the N₂-flame, which would result in a smaller dark zone thickness than those previously measured in the N₂ case, if the particle thermophoretic diffusivity, $\alpha_T \cdot D_p$, were the same. In contrast, we experimentally determined a dark-zone thickness of 2.8 mm, about 90% greater than in the N₂ flame. Results from kinetic theory ($Kn \gg 1$) indicate a direct proportionality between $\alpha_T \cdot D_p$ and the momentum diffusivity, μ , of the host gas. Replacing N₂ by He dramatically increases the momentum diffusivity of the host gas, which explains why the dark zone phenomenon is dramatized despite the larger strain rates.

Quantitative determination of $\alpha_T \cdot D_p$ requires accurate knowledge of the gaseous convective velocity at the particle stagnation plane (PSP). In our original approach we computed this velocity from a numerical code accounting for full molecular transport and chemical kinetics. However, discrepancies between experiments and calculations in the position of the flame (probably due to buoyancy effects) obliged us to develop an experimental technique to infer the axial velocity at the PSP from LDV measurements of the radial velocity component at a fixed radial location, as a function of axial coordinate, and exploiting overall mass conservation. These measurements have now been initiated and will be analyzed during the next reporting period. Uncertainties due to composition effects on local gas density and multicomponent momentum diffusivity will be evaluated.

3.5 *Role of Photophoresis in Combustors with High Radiative Heat Fluxes*

Our results on photophoresis (Mackowski, 1989; and Castillo, Mackowski and Rosner, 1989) reveal significant transport effects, mainly for particles which are carbonaceous (char-like, soot-like) rather than ash-like. Figure. 2 shows the predicted dimensionless transport coefficient (proportional to the ordinary Stanton number for mass transfer ;see,e.g. Rosner,1986,1988)) as a function of radiation/convective flux ratio (q_R/q_F) and carbonaceous particle radius for laminar boundary layer flow past a wall cooled to 70% of the mainstream temperature, subjected to a radiative energy spectrum appropriate to a black-body source at *ca.* 1800K. One sees that large effects on the particle deposition rate are produced if the radiative flux is comparable to or exceeds the ordinary (Fourier) energy flux. We are now extending this work to include the effects of inevitable particle *asymmetries*, including agglomerate (shape) effects, and the role that energy transfer (eg. radiative cooling of larger particles in a population) might play in the coagulation dynamics (Mackowski, Rosner and García-Ybarra, 1989) and deposition dynamics of such aerosol populations.

4. Administrative Information

Based, in part, on this DOE-PETC-supported program at Yale during this reporting period:

- 4.1 We have corrected the pageproofs of four papers dealing with a) the deposition dynamics of nucleating vapors (Liang, Gomez, Castillo and Rosner, 1989), b) deposit microstructure/mechanism interrelations (Tassopoulos and Rosner, 1989a), c) coagulation of particles in non-isothermal laminar boundary layers (Park and Rosner, 1989a) and d) the coupling between thermophoretic and inertial effects in particle deposition (Park and Rosner, 1989b). These papers should appear during the next reporting period. (See Appendices A1, A5, A6, A7.)
- 4.2 We have submitted 3 abstracts for presentations at future meetings: Rosner and Tassopoulos, 1989; Tassopoulos, O'Brien and Rosner, 1989b; and Mackowski, Rosner and Garcia-Ybarra, 1989. (See Appendices A3, A8.)
- 4.3 We presented and have revised our ACS-Symposium paper (Ash Deposition, April 9-14, 1989, Dallas, TX) on photophoretic effects on particle deposition to be suitable for the corresponding special issue of *Progress in Energy and Combustion Science* (Castillo, Mackowski and Rosner, 1989). This paper will be submitted for peer review in June.
- 4.4 Dr. Mackowski's paper on the photophoretic properties of small spherical particles (in both the free-molecule and near-continuum limits) has just appeared in *Int. J. Heat Mass Xfer.* (See Appendix A4.)
- 4.5 We continued working on the preparation of a research proposal to be submitted to DOE-PETC (ca. mid-September) to allow us to extend the most promising aspects of our present research on ash deposition fundamentals.

Participants in this comprehensive research program on particle deposition from combustion gases include the writer-P.I (D. E. Rosner), Graduate Students A. Konstandopoulos, M. Tassopoulos and P. Yaras, and Drs. J.L. Castillo, P. Garcia-Ybarra, A. Gomez, and D. Mackowski.

5. References

Castillo, J.L. and Rosner, D.E., "Theory of Surface Deposition from a Binary Dilute Vapor-Containing Stream, Allowing for Equilibrium Condensation within the Laminar Boundary Layer", *Int. J. Multiphase Flow*, **15**, [1], 97-118(1989)

Castillo, J.L., Mackowski, D., and Rosner, D.E., "Photophoretic Contribution to the Transport of Absorbing Particles across Combustion Gas Boundary Layers", presented at the Symposium on Ash Deposition, ACS Mtg., Div. Fuel Chem., April 9-14, 1988, Dallas TX; to appear in *Progress in Energy and Combustion Science* (1989).

Davis, R.H. et.al. "Elasto-hydrodynamic Collision of Two Spheres", *J. Fluid Mechanics* **163**, 479 (1986)

Garcia-Ybarra, P., and Rosner, D.E., "Thermophoretic Properties of Nonspherical Particles and Large Molecules", *AIChE J.*, **35**, [1], 139-147 (1989)

Gili J.A. and Alonso E.E. "Discontinuous Numerical Model for Partially Saturated Soils at Low Saturation" in *Numerical Methods in Geomechanics* (Innsbruck, 1988) pp365-372 (1988) Swoboda (ed.) Balkema, Rotterdam.

Gomez, A., Smooke, M.D. and Rosner, D.E., "Application of Counterflow Diffusion Flames to the Determination of Particle Thermophoretic Diffusivities", Presented at the 22nd Int. Combustion Symp. August 1988, Seattle, WA.

Holve, D.J., Tichenor, D., Wang, J. C.F., and Hardesty, D.R., "Design Criteria and Recent Developments of Optical Single Particle Counters for Fossil Fuel Systems", *Opt. Engrg.*, **20** (4), 529-539 (1981).

Holve, D.J., "Transit Timing Velocimetry (TTV) for Two-Phase Reacting Flows", *Comb. and Flame*, **48**, 105-108, (1982).

Israel, R. and Rosner, D.E., "Use of a Generalized Stokes Number to Determine the Aerodynamic Capture Efficiency of Non-Stokesian Particles from a Compressible Gas Flow", *Aerosol Sci. & Tech.* (J. of Amer. Assoc. Aerosol Res.) **2**, 45-51 (1983)

Konstandopoulos, A.G., Goldman, Y. and Rosner, D.E., "Experimental Studies of Inorganic Particle-Laden High Temperature/Velocity Jet Impingement at Collecting Surfaces; Sticking and Deposit Erosion in the Simultaneous Presence of Condensing Alkali Sulfate Vapors", presented at the 18th Annual Meeting of the Fine Particle Society, Symposium on Multiphase Flow, Boston, MA 8/3-7/1987 (in preparation, 1989)

Konstandopoulos, A.G., Goldman, Y. and Rosner, D.E., "Experimental and Theoretical Studies of the Combined Effects of Particle Inertia and Thermophoresis on Deposition Rates across Laminar Combustion Gas Boundary Layers" (in preparation, 1989)

Labowsky M. and Rosner D.E., "The Method of Line Source Images for Solving Interacting Cylinder Diffusion Problems", *I.J.H.M.T.* (in press, 1989)

Liang B., Gomez A., Castillo J. and Rosner D.E., "Experimental Studies of Nucleation Phenomena within Thermal Boundary Layers — Influence of Chemical Vapor Deposition Rate Processes", *Chem. Engrg Communications* (in press, 1989)

Mackowski, D., "Photophoresis of Aerosol Particles in the Free Molecular and Slip-Flow Regimes", *Int. J. Heat Mass Transfer*, **32** [5], 843- (1989)

Mackowski, D. and Rosner, D.E., "Photophoretic Motion of Non-Uniform Particles", Prepared for presentation at the 20th Annual meeting of the Fine Particle Society, Boston, MA, 22-26 August 23 1989

Park, H.M. and Rosner, D.E., "Multiphase Continuum Theory of Dopant Redistribution Across Aerosol-Laden Laminar NonIsothermal Boundary Layers" *Chemical Engrg. Science*, **44** [3] 603-617 (1989a)

Park, H.M. and Rosner, D.E., "Combined Inertial and Thermophoretic Effects on Particle Deposition Rates in Highly -Loaded Dusty Gas Systems", *Chemical Engrg. Science*, (in press, 1989b)

Park, H.M. and Rosner, D.E., "Effect of Coagulation in the Boundary Layer on the Size Distribution of Thermophoretically Deposited Particles", *Chem. Engrg. Science* (in press, 1989c)

Rosner, D.E., "Mass Transfer across Combustion Gas Thermal Boundary Layers — Power Production and Materials Processing Implications", in *Heat Transfer in Fire and Combustion Systems*, HTD 45, ASME, NY-NY, 3-8 (1985)

Rosner, D.E., *Transport Processes in Chemically Reacting Flow Systems*, Butterworths, Stoneham, MA (1986); Second Printing, 1988

Rosner, D.E., "Total Mass Deposition Rates from 'Polydispersed' Aerosols"; *AIChE J.* 35, [1], 164-167 (1989)

Rosner, D.E., "Experimental and Theoretical Research on the Deposition Dynamics of Inorganic Compounds from Combustion Gases"; Invited paper for the *Benjamin G. Levich Memorial Issue of J. PhysicoChemical Hydrodynamics* 10, [5/6], 663-674 (1988)

Rosner D.E. and Günes D., "Theory of Deposit Shape Evolution for Heat Exchanger Surfaces Exposed to the Flow of Fly-Ash Containing Combustion Products", in preparation, (1989)

Rosner, D.E., and Kim, S.S., "Optical Experiments on Thermophoretically Augmented Submicron Particle Deposition from 'Dusty' High Temperature Gas Flows", *The Chemical Engrg. J.* (Elsevier) 29, No.3, 147-157 (1984)

Rosner, D.E., and Nagarajan, R., "Toward a Mechanistic Theory of Deposit Growth from Ash-Laden Flowing Combustion Gases: Self-Regulated Sticking of Impacting Particles and Deposit Erosion in the Presence of Vapor 'Glue'", in *AIChE Symposium Series* 83, No.257, *Heat Transfer-Pittsburgh 1987* (R.W. Lyczkowski, ed.) 289-296 (1987)

Rosner D.E. and Park H.M., "Thermophoretically Augmented Mass, Momentum and Energy Transfer Rates in High Particle Mass-Loaded Laminar Forced Convection Systems", *Chem. Engrg. Science* 43, [10], 2689-2704 (1988)

Rosner D.E. and Tassopoulos M., "Mass Deposition Rates from Streams Containing 'Polydispersed' Particle Populations of Arbitrary Spread", to be presented at the AIChE Annual Meeting, Session on *Fundamentals of Mass Transport*, San Francisco, November 6-10, 1989; *AIChE J.* (to appear Sept. 1989)

Tassopoulos, M., O'Brien, J.A., and Rosner, D.E., "Theoretical Approach to Establish Particle Deposition Mechanism/Deposit Microstructure Relationships", Paper 28f, 1988 Annual AIChE Mtg., Session 28 on *Fundamental Research in Heat and Mass Transfer in Two and Three Phase Systems* (Washington D.C., Nov.27-Dec.2, 1988); *AIChE J.* 35, [6], 967-980 (1989)

Wessel, R.A and Righi, J., "Generalized Correlations for Inertial Impaction of Particles on a Circular Cylinder", *Aerosol Sci. and Tech.* (J. of Amer. Assoc. Aerosol Res.) 9, No. 1, 29-60 (1988)

1. Actual total mass deposition rate (as a fraction of the deposition rate if all particles in the log-normal distribution of spread σ_g had the mean particle volume ϕ_p/N_p) for convective-diffusion of dense particles or fractal agglomerates across laminar or turbulent boundary layers (after Rosner and Tassopoulos, 1989)

Photophoretic Effect on Deposition Rates

2. Effect of radiative flux in modifying the deposition rate of absorbing particles across laminar boundary layers with $T(\text{wall})/T(\text{ambient}) = 0.7$ (after Castillo, Mackowski, and Rosner, 1989)

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