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

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1. Introduction

DOE-PETC has initiated at the Yale HTRC Laboratory a systematic three-year experimental and theoretical research program directed toward providing engineers with the 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. 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 also wish to quantify 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 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 - *e.g.* deep tube bundles ('banks') (see, *e.g.*, Rosner, 1986).
- c. Necessary extensions of available particle deposition rate theory (see, *e.g.*, Park and Rosner, 1988).

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

- d. Useful, yet 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).

To be able to develop tractable but realistic/rational 'subroutines' to predict the evolution of wall deposits, it will also be necessary to intensify communication with more empirically oriented engineers/chemists who have the necessary boiler fouling/slagging experience. If successful, we will 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).

3. Research Progress

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

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

A real-time laser light-reflectivity technique (see, e.g., Rosner and Kim, 1984) is being used to study simultaneous thermophoretic and inertial influences on the deposition behavior of MgO particles produced *via* ultrasonic nebulization (submicrometer range). The deposition surface (a concave platinum ribbon) is exposed to a high velocity/temperature jet of alkali sulfate-free combustion products exiting from a seeded ($\text{C}_3\text{H}_8/\text{air}$) microcombustor (110 cm^3). The reflectivity data were calibrated against deposition rates obtained from SEM pictures of the target, and were normalized with the *nominal* particle feed rate, in order to obtain the mass transfer Stanton number, St_m , trends depicted in Figure 1. For the submicron (*ca.* $0.7 \mu\text{m}$) particles inertial effects appear to set in at Stokes (St_k) numbers of $O(10^{-2})$ (an order of magnitude lower than the ones needed for 'pure' inertial *impaction*), affecting significantly the dominant thermophoretic deposition mechanism (Fig. 1). A first order (in St_k) theoretical analysis of the problem in which particle inertia is treated as equivalent to 'pressure diffusion', (see e.g. Fernandez de la Mora and Rosner, 1982), cannot explain the observed dependence of the deposition rate on St_k . We are presently formulating a Lagrangian approach, valid for all values of St_k , in order to interpret these data. In addition, a Single Particle Counter (SPC) and Transit Time Velocimeter (TTV), (Holve *et al.*, 1981; Holve, 1982) are being developed, to allow more precise measurements of particle feed rates and velocities.

3.2 *Relation between Deposit Microstructure and Particle Deposition Mechanism*

Based on feedback from AIChE J. reviewers we have extended our earlier Monte-Carlo simulations of particulate deposit microstructure in three ways:

- a) going from 2 to 3 dimensions;
- b) allowing the 'jump-distance' of the arriving particles to be an arbitrary multiple of the particle dimension;
- c) going from "on-lattice" to "off-lattice" simulations.

Preliminary results were reported at the AIChE National Meeting, November '88 in Washington D.C. Our revised paper is being submitted to AIChE J. in early December 1988. We believe this work will provide a long sought route to relating particulate deposit *microstructure* to deposition *mechanism*. In our future studies we plan to systematically examine the effects of deposit sintering and vapor condensation, both theoretically and experimentally.

3.3 Theory of Particle Deposition from 'Polydispersed' Aerosols

We have recently generalized the results of Rosner (1988) (to appear, AIChE J. early in 1989) to include log-normal particle size distributions of arbitrary 'spread' parameter (cf. 'self-preserving' mainstream particle size distributions). A convenient and efficient method for computing total mass deposition rates for arbitrary size-dependent particle mass transfer coefficient and mainstream particle size spectra is also being developed, using 'piecewise' analytical results.

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

Despite the demonstrated importance of *thermophoresis* in delivering submicron ash to heat exchanger surfaces (see e.g. Rosner and Kim, 1984) no reliable, relevant experimental measurements of the thermophoretic diffusivity ($\alpha_T D_p$) of such particles have been reported. For this reason we have been developing an experimental technique to determine inorganic particle thermophoretic diffusivities in high temperature combustion gas environments using a seeded counterflow laminar diffusion flame operated at low strain rate. In our previous (preliminary) experiments (Gomez, Smooke and Rosner, 1988) the particle thermophoretic diffusivity was estimated by: i) measuring the temperature field using a fine thermocouple; ii) measuring the thickness of a thermophoretically-induced particle-free zone using He-Ne laser light scattering; iii) numerically computing the convective velocity at the particle stagnation planes (PSP). Since buoyancy effects, not accountable for in the numerical code (iii), seem to cause a systematic spatial shift along the axial direction between the measured and calculated temperature profiles, we are now also *experimentally* determining the axial component of the gas convective velocity, v_z , at the PSP. To this end, we have: i) measured the particle *radial* velocity components by laser velocimetry (LDV) at a given radial location as a function of axial position in the flame; ii) calculated the gas density at the corresponding locations (from the temperature measurements); and iii) determined v_z by applying mass conservation to a cylindrical control volume extending from each burner mouth to the corresponding particle stagnation plane. Our results for submicron TiO_2 particles exhibit good agreement (ca. 10%) between the inferred particle thermophoretic diffusivities and the maximum values calculated from the gas kinetic theory of Waldmann (see e.g. Garcia-Ybarra and Rosner, 1988). Experiments are now under way to study the dependence of the particle thermophoretic diffusivity on the host gas momentum diffusivity by replacing N_2 with He, as the inert diluent in our CH_4/O_2 flames. Our experimental findings for submicron particles of TiO_2 and Al_2O_3 will be summarized in a publication now in preparation.

3.5 Role of Photophoresis in Combustors with High Radiative Heat Fluxes

Using the recent photophoretic predictions of Dr. Mackowski (1988), we have computed the deposition rates of spherical particles by convection, thermophoresis and photophoresis across laminar boundary layers, with emphasis on the commonly encountered case in which both thermophoresis and photophoresis act to accelerate the deposition rate. A short account of this work will be presented at the April 1989 ACS-Div. Fuel Chem. Mtg. in Dallas, TX (Castillo, Mackowski and Rosner, 1989). In follow-on theoretical studies we are investigating the photophoretic properties of non-spherical particles and the optical properties of *deposited* particles.

4. Administrative Information

During this reporting period (Fall '88 research leave from Yale), the PI has presented 12 lectures on Yale-HTCRE research in the areas of deposition and heterogeneous kinetics to universities and government laboratories in Australia and New Zealand. These lectures are itemized in Appendix A, which begins with a 3 hour summary of our DOE-sponsored research at a Workshop on Fouling and Slagging organized by the Australia/New Zealand Combustion Institute for Oct. 11, 1988 at U. Sydney. The booklet cover sheet, contents, and lecture outline are include here as Appendices B and C, with the complete booklet being available from Dr. B. Young, CSIRO, PO Box 136, N. Ryde, NSW 2113, Australia at cost (*ca.* 17 \$USA + postage). The resulting exchange of technical information that took place during Fall '88 will help us direct our future deposition research to have the greatest practical impact on the pulverized coal power generation community in the USA. Opportunities for future research collaboration have also been identified.

We have also received and corrected the pageproofs of 6 HTCRE-Lab papers supported, in part, by this program. The resulting publications will appear in Spring '89 in the journals: Chemical Engineering Science, Chemical Engineering Communications, AIChE J, PhysicoChemical Hydrodynamics, International J. of Heat and Mass Transfer and International J. of Multiphase Flow. M. Tassopoulos presented an account of our recent research on the deposit microstructures (Tassopoulos *et al.*, 1988) at the AIChE National Mtg, Washington D.C., November 28-December 2, 1988. A revised version of this manuscript has just been submitted to the AIChE J. for review and ultimate publication. We have also submitted a short manuscript on particle deposition by combined convection, thermophoresis and photophoresis for the 9-14 April '89 ACS Meeting in Dallas TX (Symposium on Ash Deposition).

Based on the advances made in the first two years of this three-year program (see, *e.g.*, Section 3), it would be timely to discuss/define attractive extensions of this DOE-research program. This will be done during the next quarterly report period. In the meantime, our research in each of the areas discussed in Section 3 will be brought as far as possible and published, subject, of course, to our available funding (to 8/31/89).

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- 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, 1988)
- 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, 1988)
- Mackowski, D., "Photophoresis of Aerosol Particles in the Free Molecular and Slip-Flow Regimes", *Int. J. Heat Mass Transfer* (in press, 1988)
- Park, H.M. and Rosner, D.E., "Thermophoretic and Inertial Effects on Particle Deposition Rates for Highly Loaded Dusty Gas Systems -- Laminar Stagnation Point Flow Between Two Parallel Stationary Disks", *Chemical Engineering Science* (under review, 1988)

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Tassopoulos, M., O'Brien, J.A., and Rosner, D.E., "Theoretical Approach to Establish Particle Deposition Mechanism/Deposit Microstructure Relationships " presented at the 1988 Annual AIChE Mtg., Washington, D.C., Nov.27-Dec.2, 1988

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

Figure 1. Submicron (ca. 0.7 μm diam.) MgO particle deposition rates on concave targets exposed to seeded combustion products, inferred from reflectivity measurements under the simultaneous influence of particle inertia ($StkRe^{1/2} > 0$) and thermophoresis (after Konstandopoulos *et al.*, 1988).

APPENDIX A

FALL '88 AUSTRALIA/NEW ZEALAND LECTURES BY PROF. D.E. ROSNER[†]

DATES	HOST	LOCATION	HRS	TOPICS
11 Oct.	Comb. Inst. Australia/New Zealand	U. Sydney, Sydney	3	Deposition rates of inorganic vapors and particles in combustion systems.
13 Oct.	BHP-Central Res. Labs	Newcastle-NSW-Australia	1	Flow reactor studies on the gasification kinetics of refractory solids
27 Oct.	ChE Dept.-U.Sydney	Sydney-NSW-Australia	1	Combustion viewed as chemical reaction engineering
9 Nov.	ME Dept.-U.Sydney	Sydney-NSW-Australia	1	Similitude and correlation methods in engineering
14 Nov.	State Electric Commission. - Victoria	Melbourne-Victoria-Aust.	2	Deposition rates of inorganic vapor and particles in combustion systems
24 Nov.	Dept. ChE-U. Queensland State Electric Commission	Brisbane-Queensland-Aust.	2	Deposition rates of inorganic vapors and particles in combustion systems
28 Nov.	ChE. Dept.-U.Canterbury	Christchurch-New Zealand	1	Deposition rates of inorganic vapors and particles in combustion systems
8 Dec.	ChE. Dept.-U.Auckland	Auckland-New Zealand	1	Deposition rates of inorganic vapors and particles in combustion systems

[†] Research leave, Yale University, Department of Chemical Engineering, New Haven, CT 06520 USA

Appendix B

Fouling and Slagging in Combustors -

Problems and Solutions

Guest Lecturer: Professor Dan E. Rosner
Director High Temperature Chemical Reaction
Engineering Laboratory
Yale University, Connecticut, USA

Sponsored by the Australia and New Zealand Section of the Combustion Institute

Held at the Department of
Chemical Engineering
The University of Sydney
October 11, 1988

Co-ordinators:
Dr B. C. Young
CSIRO Division of Coal
Technology

Associate Professor T.F. Wall
Department of Chemical and
Materials Engineering,
University Of Newcastle

Appendix B (Cont.)

CONTENTS	Page
Preface	v
Recent Research on Fundamental Aspects of Vapor Deposition and Particle Deposition at the Yale University HTCRE laboratory - Topic Outline <i>D. E. Rosner</i>	1
Recent Research on Fundamental Aspects of Vapor Deposition and Particle Deposition - Topic Summaries <i>D. E. Rosner</i>	3
Experimental and Theoretical Research on the Deposition Dynamics of Inorganic Compounds from Combustion Gases <i>D. E. Rosner</i>	5
Mass Transfer across Combustion Gas Thermal Boundary Layers - Power Production and Materials Processing Implications <i>D. E. Rosner</i>	34
Rational Engineering Correlations of Diffusional and Inertial Particle Deposition Behaviour in Non-Isothermal Forced Convection Environments <i>D. E. Rosner</i>	40
Toward a Mechanistic Theory of Net Deposit Growth from Ash-Laden Flowing Combustion Gases: Self-Regulated Sucking of Impinging Particles and Deposit Erosion in the Presence of Vapor Deposited - or Submicron Mist - 'Glue' <i>D. E. Rosner</i>	52
Publications List (1976-1988) <i>D. E. Rosner</i>	60
Transport Processes in Chemically Reacting Flow systems - <i>D. E. Rosner</i> Book Reviews	69
Ash Fusion, Strength and Electrical Resistivity <i>P. Polychroniadis, R.P. Gupta and T.F. Wall</i>	71
Characterisation of Coal Ashes by TMA and by Electrical Resistance <i>B. Anderson and G.C. Ellis</i>	75
Modelling Ash Deposition: A Mechanistic Approach <i>R.P. Gupta, H.B. Vuthaluru and T.F. Wall</i>	79
Gas Turbine Smoke Emission Research at Aeronautical Research Laboratory <i>F.W. Skidmore</i>	86
Characterisation and Major Inorganic Constituent Distribution of Flyash <i>C. Paulson</i>	93
Ash Deposition Effects from Some NSW Coals <i>A. Lowe and R. Boyd</i>	96
Combustion Testing of South Australian Coals and Results <i>C. Taylor, A. Kosminski, R.G. Williams and E.R. Lindner</i>	100
Slagging and Fouling of Australian Coals - Problems, Testing and Prediction <i>A. Conroy and D. Phong-anant</i>	106

Appendix C

Recent Research on Fundamental Aspects of Vapor Deposition and Particle Deposition at the Yale University HTCRE Laboratory^a

DANIEL E. ROSNER^b

Yale University, Department of Chemical Engineering, New Haven, CT 06520, USA
Fax No. (203) 432-2797

Topic(s)

1. Vapor deposition with and without chemical reaction
 - 1.1 Seeded flame alkali sulfate deposition experiments (See References^c: 142, 150, 166, 167)
 - 1.2 Interpretation based on vapor diffusion BL-theory (See References: 99, 135)
 - 1.3 Dew points and dew point shifts associated with transport phenomena (See References: 101, 126)
 - 1.4 Effect of vapor phase reaction on CVD-rates (See Reference: 157)
2. Submicron particle deposition: Brownian diffusion, thermophoresis and photophoresis
 - 2.1 Seeded flame optical reflectivity studies of submicron MgO(s) deposition (See Reference: 130)
 - 2.2 Thermophoretic boundary layer theory (See References: 101, 117, 119, 129, 131, 132, 133, 140, 144)
 - 2.3 Theory of the thermophoretic coefficient: particle size and shape effects; implications (See Reference: 152)
 - 2.4 Organic soot deposition and "thermophoretic thermometry" (See References: 134, 143)
 - 2.5 Photophoresis for absorbing particles in the presence of high radiation energy fluxes (See Mackowski, 1988)
 - 2.6 Particle deposition from polydispersed aerosol populations (See Reference: 168)
 - 2.7 High particle mass loading effects (see References: 140, 154, 161-163)
3. Inertial effects on particle deposition rates
 - 3.1 Inertial impaction at supercritical Stokes numbers: classical trajectory theory and recent developments/correlations based on Stk_{eff} (See Reference: 116)
 - 3.2 Inertial effects on deposition rates at subcritical Stokes numbers: Eulerian approach, inertial enrichment, centrifugal "suction"/"blowing", "eddy impaction" (See References: 107, 114, 119)
 - 3.3 Inertially-modified particle deposition from polydispersed aerosol populations (See Reference: 168)
4. Interactions between vapor deposition (VD) and particle deposition (PD)
 - 4.1 Vapor nucleation in thermal boundary layers (See References: 149, 160)
 - 4.2 Vapor scavenging by suspended particulate matter (See References: 148, 156)
 - 4.3 Factors determining the sticking probability of impacting particles: self-regulated sticking in the presence of 'glue' (See Reference: 164; and, also, Nagarajan and Anderson, 1988)

^a Prepared for presentation at Oct. 11, 1988 Workshop on Fouling and Slagging, Australian Section of the Combustion Institute, Sydney University, Sydney, Australia.

^b Director, Yale University Chemical Department High Temperature Chemical Reaction Engineering Laboratory; Professor of Chemical Engineering.

^c Reference numbers cited refer to Professor Rosner's Publication List (attached), which identifies HTCRE Lab coworkers in each area of deposition research

Appendix C (Cont.)

Recent Research on Fundamental Aspects of Vapor Deposition and Particle Deposition at the Yale University HTCRE Laboratory (Continued)

5. Research on condensate layer shape, dynamics and deposit microstructures

- 5.1 Fluid dynamics of aerodynamically driven liquid condensate layers (See References: 124, 145)
- 5.2 Shape change effects for solid deposits (See Rosner and Gunes, 1988)
- 5.3 Relation between deposit microstructure/properties and deposition mechanism for particulate deposits (See Reference: 169)

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