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THEORY OF DEPOSITION OF CONDENSIBLE IMPURITIES ON SURFACES IMMERSED IN COMBUSTION GASES

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1. INTRODUCTION AND RESEARCH OBJECTIVES

Gas turbine development is being impeded by performance losses and "hot corrosion" of components resulting from the deposition of inorganic salts (e.g. Na_2SO_4) and oxides present in the combustion products. Engine operating experience and captive engine tests have provided valuable clues to such phenomena, but smaller-scale laboratory experiments under more precisely controlled conditions, coupled with necessary advances in deposition rate theory, will be necessary to obtain an improved understanding of the mechanisms of deposition on which future control measures can be based [KOHL, et al (1979); ROSNER, SESHADRI, et al (1979)].

We describe here recent theoretical studies directed at providing a sufficiently general, rational framework for future predictions of salt/ash deposition rates in the gas turbine (GT) and related combustion environments. A review of previous work on the mechanisms of deposition reveals that inadequate attention has been paid to the effects of multicomponent vapor transport, thermophoretic transport of vapors and small particles to actively cooled surfaces, variable fluid properties within mass transfer boundary layers, and free stream turbulence. Moreover, insufficient attention has been paid to the transition between vapor transport ($Sc = 0(1)$) behavior and particle transport ($Sc >> 1$) behavior (illustrated below for the case of sodium sulfate capture from seeded combustion gases) and interactions between the mechanisms of concentration diffusion, thermal diffusion and impaction. In the present report, we summarize recent results of a long-range basic research program at Yale directed at obtaining an improved theoretical understanding of ash/salt deposition rate phenomena in combustion systems. Clearly, a reliable, well-grounded predictive scheme in this area could be used to guide the:

- *setting of rational fuel purity standards;
- *selection of engine materials and optimum engine operating conditions;
- *development and optimization of fuel additive systems;
- *development of simulation test facilities and and interpretation of their data;
- *development and signal interpretation of on-line deposition detectors.

2. RECENT ADVANCES IN THE THEORY OF SALT/ASH DEPOSITION FROM COMBUSTION GASES

Our research during the present reporting period has been focused on three areas:

a. Extension of exact laminar boundary layer mass transport theory† into the high Schmidt number (small particle) domain;

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†Page proofs of our first paper in this series [SRIVASTAVA and ROSNER (1979)] have been corrected and returned. The journal version should appear in print this fall.

b. Critique of Vermes' thermophoretic deposition theory [VERMES (1978)] and the development of a comprehensive turbulent boundary layer theory including thermophoresis in a self-consistent way;

c. Application of our CFBL deposition rate theory to conditions anticipated in future, high pressure test facilities.

Additionally, we have developed and exploited useful correlation of inertial impaction efficiencies for cylinders in cross flow, to account for the effects of departures from Stokes' drag law.

Our preliminary results for predicted deposition rate behavior over the entire particle size range from monomeric vapor to particles for which inertial effects predominate (cf. Table 1) are summarized in Figure 1, constructed for conditions anticipated in a high pressure test facility with cylindrical targets in cross flow [ROSNER, D.E. and FERNANDEZ de la MORA, J. (1979)]. Shown plotted is the deposition rate of a particle containing g-Na_2SO_4 monomer units normalized by the corresponding monomer (vapor) value at the same mainstream mass fraction. Note that <u>in the absence of thermophoresis</u> the deposition rate drops to a value more than 3-decades below the corresponding vapor rate before the onset of inertial capture at a (pressure-level dependent) particle radius between 0.1 and 1.0 μm. Irrespective of wall cooling, for sufficiently large particles the inertial deposition rate sharply rises to values <u>ca</u>. 2-decades <u>above</u> the vapor value, assuming each incident particle "sticks." Clearly, for an uncooled surface a fairly sharp minimum deposition would therefore occur at a particle size just prior to the onset of inertial capture. We anticipate that this situation will be drastically modified by the phenomenon of <u>thermophoresis</u> accompanying surface cooling. Using CFBL theory, this is indicated in Figure 1 for two collector cooling conditions at a test pressure level of 12 atm. Thermophoresis is seen to "arrest" the decline in Brownian deposition rate accompanying increased particle size, and for T_w/T_∞ (stag) = 0.8 is expected to increase the deposition rate of <u>ca</u>. 1 μm diam. particles by almost 2-decades above the uncooled surface case. This thermophoretically augmented deposition rate is in fact at a level "only" about 1½ decades beneath the anticipated vapor value under otherwise identical aerodynamic conditions.* While the underlying theory is still under intense development, it is clear that the ability to accurately predict such phenomena, and provide perspective on the overall deposition process, could be of significant value in future engine development involving synthetic (alternate) fuels. It should also be remarked that the information displayed in Figure 1 is essential to predict deposition rates from a <u>particle size distribution</u> (PSD) in the mainstream. In that case Figure 1 provides the "weighting factors" which dictate how efficiently each size range will be captured. The implications with regard to total capture from a PSD, and the falsification of a PSD (<u>via</u> electron microscopy on the sampled material) will be discussed elsewhere.

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*It is interesting to note that for still colder walls, and especially at lower pressures, we predict that the deposition rate can actually <u>increase</u> slightly with particle size, for reasons totally unrelated to particle inertia. Thus, well below the onset of inertial effects we anticipate a (weak) minimum in the deposition rate, corresponding to an <u>optimum particle size</u> (<u>ca</u>. 10^{-2} μm radius in the present case) <u>for minimum deposition rate on highly cooled walls</u>.

TABLE 1
Characteristics of Deposition Over the Spectrum of Particle Sizes[a]

Size	Deposition Mechanism	Typical Characteristics
vapors (1-10Å)	Fick diffusion	dp less than mainstream temperature
	eddy diffusion	low apparent deposition efficiency
	Soret diffusion	
		weak thermophoretic (Soret) effect
		dep rate plateau at T_w well below dp
submicron	Brownian diffusion	apparent dp equal to mainstream T
	eddy diffusion	
	thermophoresis	lowest deposition (collection) efficiency
		large thermophoretic effect—rate more linear in $T_\infty - T_w$
supermicron	inertial impaction	no apparent dp
		highest deposition efficiency ($\rightarrow$100%)
		no thermophoretic effect—rate insensitive to $T_\infty - T_w$

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[a] Taken from ROSNER and FERNANDEZ de la MORA (1979).

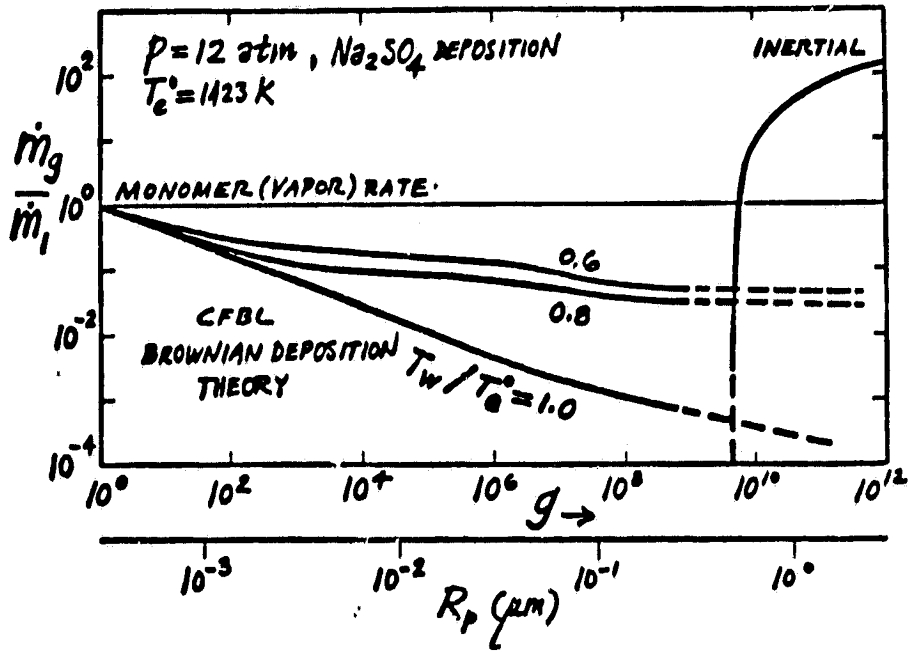

Figure 1. Predicted dependence of Na_2SO_4 deposition rate on particle size in a proposed high pressure burner facility (normalized by monomer (vapor) rate); p = 12 atm

3. ADMINISTRATIVE INFORMATION

The work described herein is primarily due to the writer and his students, J. Fernandez de la Mora, S. Gokoglu, and A. Zydney. The primary focus for the period covered was the preparation of our paper for the DOE/EPRI Conference [ROSNER and FERNANDEZ de la MORA (1979)].* Our participation in this conference was not only valuable in alerting the gas turbine community to our NASA-supported theoretical and experimental work, but also in making contact with industrial R&D groups (GE, Westinghouse, Pratt and Whitney, Solar, etc.) facing similar technological problems. Some of the key developments reported were the result of A. Zydney's NASA-sponsored participation in the Yale Engineering and Applied Science Summer Research Program. An abstract of Mr. Zydney's talk, presented at the final conference for this program (8-9 August 1979), is included (Section 5.2).

Our comprehensive paper on chemically frozen boundary layer (CFBL) theory [ROSNER, CHEN, FRYBURG and KOHL (1979)] has just been published in <u>Combustion Science and Technology</u> (Vol. 20, Nos. 3, 4, p. 87 ff) and reprints will be transmitted to NASA in a few weeks.

During the next semi-annual period attention will be focused on the development of turbulent boundary layer theory for small particle deposition in the important general case of nonunity $\alpha \cdot Le$ product. A portion of this period (October through December) will be spent at the University of California - Santa Barbara, where the writer will investigate new laser probing techniques to be used in future experiments aimed at testing our vapor and particle deposition rate theories.

4. REFERENCES

KOHL, F.J.; SANTORO, G.J.; STEARNS, C.A.; FRYBURG, G.C.; and ROSNER, D.E., "Theoretical and Experimental Studies of the Deposition of Na_2SO_4 from Seeded Combustion Gases." J. Electrochemical Soc. <u>126</u>, 1054-1061; June 1979.

ROSNER, D.E.; CHEN, B-K; FRYBURG, G.C.; and KOHL, F.J. "Chemically Frozen Multicomponent Boundary Layer Theory of Salt and/or Ash Deposition Rates from Combustion Gases." Combustion Science and Technology (in press); 1979

ROSNER, D.E. and FERNANDEZ de la MORA, J. "Recent Advances in the Theory of Salt/Ash Deposition in Combustion Systems," Proc. DOE/EPRI Conference on Advanced Materials/Alternate Fuel Engines, U.S. Govt. Printing Office (in Press); 1980.

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*Our abstract for this paper is given in Section 5.1. The paper will appear in The Proceedings of the Conference, to be published in 1980 by the U.S. Government Printing Office. The participation of Mr. Fernandez de la Mora was jointly sponsored by NASA and the Yale University Department of Engineering and Applied Science.

ROSNER, D.E.; SESHADRI, K.; FERNANDEZ de la MORA, J.; FRYBURG, G.C.; KOHL, F.J.; STEARNS, C.A.; and SANTORO, G.J. "Transport, Thermodynamic and Kinetic Aspects of Salt/Ash Deposition Rates from Combustion Gases." *Proc. 10th Materials Research Symposium: Characterization of High Temperature Vapors*, U.S. Govt. Printing Office; 1979.

SRIVASTAVA, R. and ROSNER, D.E. "A New Approach to the Correlation of Boundary - Layer Mass Transfer Rates with Thermal Diffusion and/or Variable Properties." IJHMT (in press); 1979.

VERMES, G. "Thermophoresis-Enhanced Deposition Rates in Combustion Turbine Blade Passages." ASME Paper No. 78-WA/GT-1, presented at Winter Annual Meeting ASME, San Francisco; Dec. 10-15, 1978.

5. APPENDICES (5.1)

RECENT ADVANCES IN THE THEORY OF SALT/ASH DEPOSITION IN COMBUSTION SYSTEMS[a, b]

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ABSTRACT

Gas turbine development is being impeded by performance losses and "hot corrosion" of components resulting from the deposition of inorganic salts (e.g. Na_2SO_4) and oxides present in the combustion products. Engine operating experience and captive engine tests have provided valuable clues to such phenomena, but smaller-scale laboratory experiments under more precisely controlled conditions, coupled with necessary advances in deposition rate theory, will be necessary to obtain an improved understanding of the mechanisms of deposition on which future control measures can be based.

We describe here recent theoretical and experimental studies directed at providing a sufficiently general, rational framework for future predictions of salt/ash deposition rates in the gas turbine GT and related combustion environments. A review of previous work on the mechanisms of deposition reveals that inadequate attention has been paid to the effects of multicomponent vapor transport, thermophoretic transport of vapors and small particles to actively cooled surfaces, variable fluid properties within mass transfer boundary layers, and free stream turbulence. Moreover, insufficient attention has been paid to the transition between vapor transport ($Sc = O(1)$) behavior and particle transport ($Sc \gg 1$) behavior (illustrated here for the case of sodium sulfate capture from seeded combustion gases) and interactions between the mechanisms of concentration diffusion, thermal diffusion and impaction. Recent advances in some of these areas are described, along with information derived from new experimental techniques based on the on-line use of optical methods to rapidly probe deposition onset and rates in combustion systems. We conclude with an assessment of research needs highlighted both by this program and the increased interest in "synthetic fuels."

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[a] Supported in part by NASA-Lewis Research Center/Materials and Structures Division, under Grants NSG-3107 and 3169.

[b] Proceedings DOE-EPRI Conference on Advanced Materials/Alternate Fuel Engines (Castine, Maine (1979) (in press).

[c] Professor of Chemical Engineering and Applied Science; Director of HTCRE Lab.

[d] Graduate student.

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PREDICTED INORGANIC VAPOR AND PARTICLE DEPOSITION RATES FROM COMBUSTION GASES TO COOLED SURFACES* Andrew Zydney, Yale University [Advisor: D.E. Rosner]

The problem of corrosion of gas turbine materials, known to be associated with the formation of a condensate layer,[1] has motivated our interest in predicting inorganic vapor and particle deposition rates. For example, when the fuel contains sulfur impurities and the injested air contains NaCl, hot corrosion caused by Na_2SO_4(c) will occur if the turbine blades are at temperatures below the dew point of sodium sulfate.

Deposition rates can be predicted by a "chemically frozen" boundary layer (CFBL) theory, based on the assumption that negligible amounts of chemical reaction and/or condensation occur within the mass transfer boundary layer,[2,3] and an inertial capture theory. These theories include the coupled effects of Fick (concentration) diffusion and Soret (thermal) diffusion.

One of our goals is to predict the deposition rates of Na_2SO_4(c) from a seeded laboratory burner now being designed at the NASA-Lewis Research Center. This test facility will operate at stagnation pressures well above one atmosphere, will have velocities near sonic, and will use five adjacent cylindrical cooled targets to measure deposition rates. Some interesting features of this problem are the appearance of Na_2SO_4 particles (g-mers) in the mainstream, non-negligible effects of thermophoresis, the importance of viscous dissipation, and the interference caused by the proximity of the cylindrical targets. The computer program required to incorporate these effects has been constructed in modular form to allow for possible future refinement and application to other related systems.

For vapor deposition an interesting corollary of CFBL theory is that the dew point is not a purely thermodynamic quantity but is influenced by thermal and multicomponent diffusion. In fact there is more than one "dew point" depending upon its operational definition: one defined by extrapolating the mass deposition rate as a function of temperature curve to zero deposition and one defined by the temperature at which a clean (condensate-free) surface will first exhibit a stable condensate upon cooling. We are investigating the magnitude of the difference between these two "dew points", as well as the approximate dew point predicted solely on the basis of thermodynamics using mainstream chemical element ratios.

*Supported in part by NASA Grant 3107

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