This report summarizes the results of a basic research program in the High Temperature Chemical Reaction Engineering (HTCRE) Laboratory at Yale University. Dealing broadly with chemical and physical phenomena at/near interfaces in high temperature systems, during this reporting period we have obtained further results in the areas of thermal diffusion effects on vapor and small particle mass transport across nonisothermal boundary layers, and inertial effects on particle deposition.
INTERFACIAL CHEMICAL REACTIONS AND TRANSPORT PHENOMENA IN FLOW SYSTEMS

Principal Investigator: Daniel E. Rosner


High Temperature Chemical Reaction Engineering Laboratory
Yale University
Department of Chemical Engineering
P. O. Box 2159YS
New Haven, Connecticut 06520, USA

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1. Introduction:

This interim report summarizes a 14-month basic research program in the High Temperature Chemical Reaction Engineering (HTCRE) Laboratory at Yale University. Our concern is primarily with chemical and physical phenomena near interfaces in high temperature systems, and during this reporting period we have obtained further results in the areas of (i) surface-catalyzed combustion, (ii) the influence of particle thermophoresis on mass transport across nonisothermal boundary layers, and (iii) inertial effects on particle deposition to cooled targets in convective flow. These phenomena constitute a central part of advanced engineering systems containing dispersed condensed phases, or where the condensed phases are used for fluid confinement. The design of advanced propulsion systems requires fundamental data in these broad categories, and it is hoped that the research results and techniques reviewed here will continue to be widely used in the fields of aeronautical, metallurgical, chemical, and mechanical engineering (see Section 5 and 6).

Because of the current or impending availability of our papers in the archival scientific and/or engineering literature, detailed summaries of their contents would be redundant. However, the nature of the information resulting from this program is conveyed in Section 7 via a listing of publications prepared and/or appearing since 1 October 1980. If required, reprints of these papers can be obtained by writing the author. Information on further applications of this work by other workers (regardless of their field) will be especially welcome. Also included is a listing of the 16 talks given during this reporting period, verbally communicating our techniques and results.

The author would also like to acknowledge the many valuable contributions to this program made by his colleagues in the Chemical Engineering Department of Yale University, and elsewhere. This includes Professors Nordine and Halpern, my graduate students: J. Fernandez de la Mora, R. Israel, S. Gokoglu, R. Nagarajan, my postdoctoral research colleagues: R. Atkins and S. S. Kim, and the other research associates listed in Section 8.

2. Technical Objective:

Materials technologies for turbine blades and combustion chambers, re-entry heat shields and rocket nozzles are seriously lacking in both theoretical understanding and reliable experimental data on basic gas-solid reactions at high temperatures and laws governing mass/heat exchange with the surface. This research will provide to systems and materials engineers theoretical understanding and fundamental data on interfacial rate processes, both for gas-surface and gas-particle interactions, with emphasis on high temperature (high performance) systems.

3. Approach:

We are currently developing theoretical methods to generalize the laws of convective mass and energy transfer to include thermophoresis (particle drift down a temperature gradient), and particle inertial effects in systems with heterogeneous chemical reaction, phase change or particle (e.g. soot, ash) deposition on actively cooled solids (e.g. gas turbine vanes, blades). Experi-
mental work will develop new optical methods for studying small particle (soot, ash) deposition to celled targets in combustion gases and extend the capability of the filament flow reactors to the catalytic oxidation of vapor fuels.

### Table 1
Subject Matter of Papers Listed in Section 7

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<th>Subject</th>
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*Titles and complete bibliographic information are given in Section 7.*

4. Progress (Selected Results, Conclusions) October 1980–December 1981

Ongoing research on thermophoretically and inertially modified vapor and small particle deposition reveals that:

R1. Our preliminary H₂/air surface-catalyzed combustion experiments demonstrate that thermal (Soret) diffusion enhances the transport rate of the light fuel H₂ to the hot catalyst surface by more than a factor of 1.15.

R2. Soot, salt or ash particle deposition by convective diffusion on actively cooled surfaces (e.g. GT blades) can be increased by about 100-fold due to thermophoresis (i.e., particle drift down a temperature gradient.

R3. Systematic comparisons with the results of exact solution to the boundary layer equations reveal that our new "pseudo-blowing/source" correlation successfully predicts the effects of thermal (Soret) diffusion transpiration and/or viscous dissipation on mass transfer rates in laminar or turbulent forced convection situations of interest in the fields of soot or ash deposition in combustors, or gas turbine stages, surface-catalyzed combustion, chemical vapor deposition (CVD) systems,
is now being generalized to allow the treatment of simultaneous particle phoretic effects (e.g. sedimentation, centrifugal drift, electrostatic precipitation, etc.).

4. Particle capture date at supercritical Stokes' numbers can be correlated in terms of an effective Stokes number which incorporates the effects of non-Stokes' particle drag, collector geometry, and gas compressibility.

5. For inertial particle deposition, local particle enrichment or depletion, phenomena can occur even at subcritical Stokes' numbers. An Eulerian particle deposition approach can be used to predict deposition rate distributions on curved targets and extended, using a Fokker-Planck formulation, to explain aerodynamic isotope separation phenomena in low density gases.

6. Optical methods (e.g. change in surface reflectivity) appear to be promising for rapid measurements of deposition (salt, "ash") from seeded combustion gases. Preliminary measurements of micron-sized TiO\textsubscript{2} and MgO-particle deposition reveal significant effects of thermophoresis for radiation cooled ribbon targets in flat hydrocarbon/air flames.

5. **Technological Significance, Relevance:**

A reliable basis for predicting vapor and particle deposition rates from combustion gases should now enable more rational gas turbine fuel purity standards to be set, and allow deposition/corrosion control systems to be selected and optimized. Results of this phase of our research will allow future aircraft gas turbines to be designed to operate efficiently, reliably and economically, using a broader range of liquid fuels, and over a wider variety of environmental conditions (including the ingestion of marine air or desert dust).

6. **Scientific Applications, Research Implications:**

Results of this program continue to be of use to research in the following areas:

* Correlation of heat exchanger tube fouling behavior in pulverized coal-fired combustors (EXXON).

* Hot corrosion and aircraft icing studies (NASA-Levis Research Labs).

* Development of on-line salt dew-point and deposition rate detectors (Argonne National Laboratories).

* Deconvolution of observed particle size spectra to infer mainstream ("undisturbed") size distributions (e.g. soot in flames) (all combustion research labs).

* Feasibility studies of a new class of low pressure drop particle filters for gas turbines (U. S. Naval Ship Engineering Center, Philadelphia).
Exploitation of thermophoresis in the production of optically graded light communication pipes (Bell Labs).

Use of mathematical methods to predict surface-catalyzed combustion rates in forced convection boundary layer situations (French researchers Garo, Ledoux, Gousebet et al.).

Performance of Space Shuttle Orbiter thermal protection system materials (NASA-Houston).

Gasification kinetics of pyrolytic graphite ACT combustor liners by atomic oxygen (H. Nelson, J. Bolsom, A. Bruns, McDonnel-Douglass, St. Louis, MO).

Interpretation of small particle inertial impaction performance under low pressure, transonic jet conditions (Herring, Flagan et al.).


7.1 Papers in Print


P5. Fernandez de la Mora, J.: Deterministic and Diffusive Mass Transfer Mechanisms in the Capture of Vapor and Particles, PhD Dissertation, Yale University, (December (1980)).

7.2 Papers Submitted, or in Press


7.2 Papers Submitted, or in Press - continued


7.3 Papers Presented


7.3 Papers Presented - continued


7.3 Papers Presented - continued


8. Personnel Contributing to this Research:

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<th>Name</th>
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<td>Rosner, D.E.</td>
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<td>Fernandez de la Mora, J.</td>
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<tr>
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<td>Vasenka, J.</td>
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<sup>a</sup>Principal Investigator
<sup>b</sup>Graduate Research Assistant
<sup>c</sup>Summer Research Program - Yale Engineering and Applied Science
<sup>d</sup>Postdoctoral Research Assistant