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GAS-SOLID REACTIONS. PART I. EXTERNAL DIFFUSION-CONTROLLED REAC--ETC(U)
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Similarity Parameters

The partial differential equations governing various transport processes can be simplified by similarity analysis. The various independent variables of the transport problem are combined by dimensional analysis into dimensionless numbers, each of which is a similarity parameter or scaling factor that characterizes some aspect of the problem under investigation. The cogent similarity parameters of this report are:

$$\text{Pr} \quad \text{Prandtl Number} = \frac{\text{kinematic viscosity}}{\text{thermal diffusivity}}$$

$$\text{Re} \quad \text{Reynolds Number} = \frac{\text{inertial forces}}{\text{viscous forces}}$$

$$\text{Sc} \quad \text{Schmidt Number} = \frac{\text{kinematic viscosity}}{\text{mass diffusivity}}$$

$$\text{Le} \quad \text{Lewis Number} = \frac{\text{Pr}}{\text{Sc}}$$

Notation

M = Mass

L = Length

t = Time

E = Energy

T = Temperature

A	area	L^2
C_D	drag coefficient	
\hat{C}_P	constant pressure heat capacity	E/MT
C_T	total concentration	moles/ L^3
\bar{D}_i	effective diffusivity of species i	L^2/t
H	slab thickness	L
\vec{J}_i	molar flux of species i	moles/ L^2t
K	rate constant	
k	thermal conductivity	E/tLT
M	molecular weight	
N_i	moles of species i	
n	stoichiometric coefficient	
U_∞	terminal velocity	L/t
\vec{V}	local molar average velocity	L/t
w	width	L
X_i	mole fraction of species i	
ρ	density	M/L^3
ψ	stream function	L^2/t
μ	dynamic viscosity	M/Lt
ν	kinematic viscosity	L^2/t

**GAS-SOLID REACTIONS PART I:
EXTERNAL DIFFUSION-CONTROLLED REACTIONS**

I) Introduction

This report is concerned with the description of exothermic chemical reactions between gaseous reactants and macroscopic solid surfaces. The observed rate of reaction (global rate) is assumed to be governed by external diffusion of gaseous reactants to the surface. Since these reactions are heterogeneous, any intrinsic chemical kinetics enter into the mathematical formulation as boundary conditions for the coupled partial differential equation describing mass transport to the surface. At the reacting surface, the molar flux (moles/cm²-sec) of reactant *i* can be equated to the rate of chemical reaction:

$$[\bar{D}_i C_T \frac{\partial X_i}{\partial y}]_S = [K(C_T X_i)^{\ell} C_S^m]_S, \quad (I-1)$$

or in dimensionless variables

$$\left[\frac{\bar{D}_i}{KC_T^{\ell-1} C_{SL}^m} \frac{\partial X_i}{\partial y} \right]_S = (X_i)_S^{\ell}.$$

At elevated temperatures the reaction rate constant (*K*) is augmented much more by the temperature increment than the effective diffusivity (\bar{D}_i). Consequently, the ratio

$$\frac{\bar{D}_i}{KC_T^{\ell-1} C_{SL}^m} = \frac{\text{diffusion rate}}{\text{chemical rate}} \ll 1,$$

and the appropriate boundary condition for the mole fraction of species *i* (X_i) on the reaction surface is:

$$(X_i)_S = 0. \quad (I-2)$$

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As the reaction proceeds, the macroscopic reaction surface recedes at a rate simply dependent upon how fast the gaseous reactants are able to arrive. From a microscopic point of view, the actual surface area of the solid reactant at any particular instant of time is unknown. However, if the reacting solid maintains a certain geometric shape during the majority of available reaction time an approximate analysis of the system's time evolution is possible. The primary effect of the solid reactant geometry is the modification of the hydrodynamic flow of gaseous reactants.

Consider the combustion of a chunk of charcoal in a flowing stream of air. Imagine that this chunk of charcoal is tightly enclosed within a geometric surface, which is not in actual contact with the solid. The integral of the oxygen flux over this closed surface equals the accumulation of gaseous reactant (O_2) within the volume. If the chemical rate of reaction is sufficiently rapid so that there is no accumulation inside the volume or, in other words, the solid acts as an oxygen sink, then the integral of the flux over the closed surface is zero:

$$\oint \vec{J}_i \cdot d\vec{S} = 0. \quad (I-3)$$

This formulation is equivalent to a steady-state approximation in the gas phase. The validity of such an approximation is discussed in Appendix A.

By the application of Gauss's theorem, the surface integral can be converted into a volume integral:

$$\oint \vec{J}_i \cdot d\vec{S} = \oint \nabla \cdot \vec{J}_i dV = 0. \quad (I-4)$$

Since the integration volume is arbitrary, the integrand of (I-4) must equal zero:

$$\nabla \cdot \vec{J}_i = 0 .$$

(I-5)

This partial differential equation is an equation of continuity for the gaseous reactant flux. Its derivation rests upon the assumptions of a steady-state profile in the gas phase, instantaneous chemical reactions at the adsorption sites, and the absence of homogeneous reactions.

The preceding formulation of the continuity equation is analogous to the application of Gauss's Law in electrostatics to a dipole. The net charge (accumulation) contained within the Gaussian surface is zero. The integral of the electric field intensity (flux) over the closed surface is zero. However, local regions of the Gaussian surface have electric fields associated with them. In other words, the condition expressed by (I-3) does not imply that the local flux on a portion of the surface must vanish. The determination of this local flux is facilitated by the presence of symmetry and the judicious selection of a coordinate system for the gradient operator.

The calculation of this local reactant flux will provide an approximate analysis of the reacting gas-solid system. For purposes of the model calculations, a Gaussian surface is selected so as to approximate the macroscopic geometry of the reacting solid. Bulk portions of the solid are assumed to be inert, so as to maintain an approximate geometry during reaction in the flowing gas stream. In particular, we will consider a reacting slab whose edges and one face are made inert by a nonreactive coating such as a metal foil. In this model the surface reaction can be considered as occurring on a mathematical plane, whose position is a function of time. The details of what happens to species i once it crosses the local reaction surface and reacts with the individual microscopic components contained within

the solid are neither necessary nor relevant to the description of the external diffusion-controlled process.

This external diffusion occurs through a thin gaseous layer adjacent to the reacting surface termed a boundary layer.¹ Within the boundary layer, there are sharp gradients of flow velocity, temperature, and composition. The thickness of the boundary layer is a function of geometry and the Reynolds number (Re). Outside of the boundary layer, the gaseous reactant mixture is assumed to have a uniform composition and temperature. In this outer region, the flow velocity of the gaseous mixture can be calculated as the gradient of a scalar potential function. This region is called the potential flow region and it provides part of the boundary conditions for the partial differential equations (Appendix B) describing transport processes within the boundary layer.

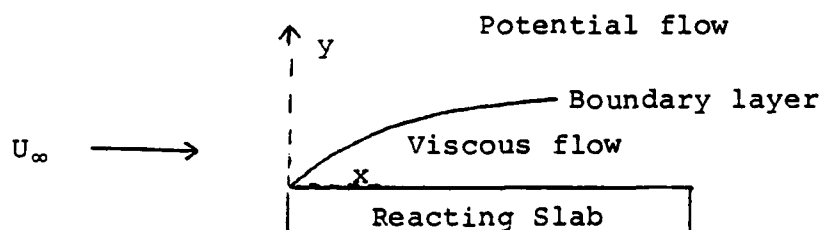
One of the primary objectives of this report is to establish a rational procedure to calculate the local reactant fluxes from known bulk gas stream properties. We are dealing with reactant gases whose physical properties such as density, viscosity, and thermal conductivity vary with temperature. Since these gases react exothermically with a surface, they encounter a substantial temperature gradient. This temperature gradient is in turn determined by the reactant flux to the surface. Once this procedure has been established, the reactant flux will be used to calculate the total available reaction time for a proposed amount of material to be completely reacted. Temperature-time evolution of the reacting system is then determined with the inclusion of convective and radiative losses. Quantitative calculations are presented for the oxidation of graphitic carbon.

II) Calculation of Local Gaseous Reactant Flux

The molar flux (\vec{J}_i) of a chemical species i is a vector quantity which denotes the number of moles of species i that pass through a unit area per unit time. In a stationary coordinate system the molar flux is given by:

$$\vec{J}_i = C_T [X_i \vec{V} - \bar{D}_i \nabla X_i] \quad (II-1)$$

This equation shows that there are two contributions to the molar flux of any species i . The first term is the molar flux of i resulting from the bulk motion of the fluid with a local molar average velocity \vec{V} . The second term is the molar flux due to molecular diffusion (Fick's Law) superimposed on the bulk flow.



Along the x direction, the dominant transport mechanism is bulk flow. This can be made evident by consideration of the x component of equation (II-1):

$$J_{ix} = C_T [X_i V_x - \bar{D}_i \left(\frac{\partial X_i}{\partial x} \right)] \quad (II-2)$$

A typical value for an effective diffusivity (\bar{D}_i) is 2.2×10^{-4} ft²/sec. At a flow rate of 5 ft/sec over a distance of one inch, the ratio of bulk flow in the x direction to molecular diffusion is approximately 2000; therefore, the molar flux of species i along the x direction is given by:

$$J_{ix} \approx C_T X_i V_x \quad (II-3)$$

This flux relation is valid in both the potential flow and viscous flow regimes.

In the potential flow region, there is no component of velocity in the y direction. The y component of flux in this region is entirely due to molecular diffusion. Within the viscous flow region, there are large gradients of reactant concentration and velocity. Consequently, both terms in equation (II-1) are of comparable magnitude; and the y component of flux is given by:

$$J_{iy} = C_T [X_i V_y - \bar{D}_i \left(\frac{\partial X_i}{\partial y} \right)]. \quad (\text{II-4})$$

Substitution of (II-3) and (II-4) into (I-5) gives an equation for the mole fraction of species i (X_i) as a function of the spatial coordinates x and y:

$$\frac{\partial}{\partial x} [X_i C_T V_x] + \frac{\partial}{\partial y} [X_i C_T V_y] = \frac{\partial}{\partial y} [C_T \bar{D}_i \frac{\partial X_i}{\partial y}]. \quad (\text{II-5})$$

By application of the principle of total mass conservation (B-1), equation (II-5) can be written in the form:

$$\rho V_x \frac{\partial X_i}{\partial x} + \rho V_y \frac{\partial X_i}{\partial y} = \frac{\partial}{\partial y} [\rho \bar{D}_i \frac{\partial X_i}{\partial y}]. \quad (\text{II-6})$$

In order to develop the solution to this convective diffusion equation, it is necessary to calculate the fluid velocity profiles near the reaction surface. These profiles are governed by equation (B-1), the conservation of total mass and (B-2), the conservation of momentum.

The total mass conservation equation can be formally satisfied by the introduction of a stream function (ψ):

$$\rho V_x = \rho_\infty \frac{\partial \psi}{\partial y} \quad \rho V_y = -\rho_\infty \frac{\partial \psi}{\partial x} \quad (\text{II-7})$$

In order to solve the variable property Navier-Stokes equation, a similarity transformation is employed. This technique converts a partial differential equation into an ordinary differential equation with an independent variable which is some combination of the original independent variables.

As a convenient similarity parameter let us define:²

$$\eta \equiv \frac{1}{2} \sqrt{\frac{U_\infty}{\nu_\infty x}} \int_0^y \frac{\rho(z')}{\rho} dz' . \quad (\text{II-8})$$

This particular combination of variables allows for the variation of gas density across the boundary layer with temperature. Substitution of relation (II-8) into (B-2) converts the Navier-Stokes equation into the following third-order ordinary differential equation:

$$\frac{d}{d\eta} \left[\left(\frac{\mu \rho}{\mu_\infty \rho_\infty} \right) \frac{d^2 f}{d\eta^2} \right] + f(\eta) \frac{d^2 f}{d\eta^2} = 0, \quad (\text{II-9})$$

with boundary conditions

$$f(0) = f'(0) = 0 \quad \lim_{\eta \rightarrow \infty} f'(\eta) = 2,$$

where f is related to the stream function by

$$f(\eta) = \psi / \sqrt{U_\infty \nu_\infty x} . \quad (\text{II-10})$$

The dynamic viscosity (μ) of gases at low density increases with temperature roughly as the 0.6 to 1.0 power of the temperature. Since the density (ρ) decreases inversely with temperature, the product $\rho\mu$ should be roughly constant. In particular, a least squares analysis of the ratio for air over a 1000 K temperature range gave:

$$\frac{\rho\mu}{\rho_\infty \mu_\infty} = 1.14 - 4.92 \times 10^{-4} T. \quad (\text{II-11})$$

This equation fits the tabulated experimental data within 5% over most of the temperature range.

The actual temperature variation is less than 10% over the fitted interval and will be regarded as a perturbation:

$$\frac{\rho\mu}{\rho_{\infty}\mu_{\infty}} = 1.0 + \varepsilon G(T). \quad (\text{II-12})$$

$\varepsilon \ll 1$

In a zero-order approximation, equation (II-9) can be written as:

$$\frac{d^3 f_0}{d\eta^3} + f_0(\eta) \frac{d^2 f_0}{d\eta^2} = 0. \quad (\text{II-13})$$

The solution of this differential equation has been tabulated by Blasius³ for a constant property fluid:

$$f_0(\eta) = \frac{\alpha\eta^2}{2!} - \frac{\alpha^2\eta^5}{5!} + \frac{11\alpha^3\eta^8}{8!} - \frac{375\alpha^4\eta^{11}}{11!} + \dots \quad (\text{II-14})$$

$$\alpha \equiv 1.32824.$$

The velocity profiles can now be determined from (II-14), (II-10) and (II-7).

By the application of the similarity transformation (II-8) to the convective diffusion equation (II-6), the following second-order ordinary differential equation is obtained:

$$\frac{d}{d\eta} \left[\frac{\rho\mu}{\rho_{\infty}\mu_{\infty}} \frac{1}{Sc} \frac{dX_i}{d\eta} \right] + f(\eta) \frac{dX_i}{d\eta} = 0$$

$$\lim_{\eta \rightarrow \infty} X_i = X_i^{\infty} \quad \lim_{\eta \rightarrow 0} X_i = 0. \quad (\text{II-15})$$

The zero-order solution for this equation is:

$$x_i(\eta) = \frac{x_i^\infty \int_0^\eta \exp[-Sc \int_0^\beta f_0(z) dz] d\beta}{\int_0^\infty \exp[-Sc \int_0^\beta f_0(z) dz] d\beta} \quad (\text{II-16})$$

Since we are primarily interested in the flux of reactant i near the reaction surface ($\eta = 0$), only the first term in the Blasius solution (II-14) need be retained. Substitution of this term into (II-16) gives the mole fraction profile through the boundary layer in terms of an incomplete gamma function:⁴

$$x_i(\eta) = \frac{x_i^\infty \int_0^\eta \exp[-Sc(\alpha n^3/3!)] dn}{\int_0^\infty \exp[-Sc(\alpha n^3/3!)] dn} \quad (\text{II-17})$$

$$\sim x_i^\infty (.6774 Sc^{1/3}) \int_0^\eta \exp[-Sc(\alpha n^3/3!)] dn.$$

The flux of reactant species i across the reaction surface can be calculated by the application of the chain rule to equation (II-17):

$$\begin{aligned} J_{iy} &= [\bar{D}_i C_T \frac{\partial x_i}{\partial y}]_{y=0} = [\bar{D}_i C_T \frac{dx_i}{dn} \frac{\partial \eta}{\partial y}]_{y=0} \quad (\text{II-18}) \\ &= \frac{[\bar{D}_i C_T \rho]_{y=0}}{\rho_\infty} \frac{x_i^\infty}{2} \left(.6774 Sc^{1/3} \right) \sqrt{\frac{U_\infty}{\nu_\infty x}}. \end{aligned}$$

The effective diffusivity, total gas concentration, and density in equation (II-18) are to be evaluated at the temperature of the reaction surface. Since this temperature is itself dependent upon the flux, the problem does not seem soluble at first sight. However, equation (II-18) can be simplified by the introduction of a dimensionless Nusselt number evaluated for gas properties in the bulk flow region:

$$Nu_{\infty} = \frac{J_{iy} x}{C_T^{\infty} D_i^{\infty}} = \left(\frac{\bar{D}_i C_T \rho}{\bar{D}_i^{\infty} C_T^{\infty} \rho_{\infty}} \right) \frac{X_i^{\infty}}{2} \sqrt{\frac{U_{\infty} x}{\nu_{\infty}}} (.6774 Sc^{1/3}). \quad (II-19)$$

The effective diffusivity of gases varies as the square of the temperature. Since both the density and species concentration are inversely proportional to temperature, the product of these three variables is independent of temperature and equal to a constant. Equation (II-19) can now be written as:

$$Nu_{\infty} = \frac{1}{2} \sqrt{\frac{U_{\infty} x}{\nu_{\infty}}} X_i^{\infty} (.6774 Sc^{1/3}). \quad (II-20)$$

This is a central result of the calculation. It indicates that the flux at the highly exothermic reaction surface can be calculated from known bulk fluid properties far from the reaction zone. The flux at the reaction surface is given by:

$$J_{iy} = \frac{(.6774 Sc^{1/3})}{2} C_T^{\infty} D_i^{\infty} X_i^{\infty} \sqrt{\frac{U_{\infty} x}{\nu_{\infty}}}. \quad (II-21)$$

It is to be noted that the reaction surface for this specified orientation is not uniformly accessible from a diffusional point of view. In particular, the leading edge ($x=0$) has an infinite flux. This explains ignition at the forward edge of the gas flow. If the slab were oriented so that its surface would be normal to the gas flow (stagnation flow) the flux would be reduced about 15%, but the reaction surface would be uniformly accessible. Stagnation flow geometry is the preferred orientation in experimental work where the external transport problem is coupled with intrinsic chemical kinetics.

The consumption rate of species i (in moles per second) at the reaction surface is given by:

$$\frac{dN_i}{dt} = -\int_0^w dz \int_0^L J_{iy} dx = -.6774 Sc^{1/3} (C_T^\infty X_i^\infty \bar{D}_i) w \sqrt{\frac{U_\infty L}{V_\infty}} \quad (II-22)$$

The decrease in moles of solid per second may be equated to this rate:

$$\frac{dN_i}{dt} = \frac{1}{n} \frac{dN_S}{dt} = \frac{1}{n} \frac{d}{dt} [C_S V_S] = \frac{\rho_S}{n M_S} (Lw) \frac{dH}{dt} \quad (II-23)$$

Equations (II-23) and (II-22) can be combined to give a differential equation for the slab thickness (H) as a function of time:

$$\frac{dH}{dt} = -.6774 Sc^{1/3} \sqrt{Re_L} \left[\frac{C_T^\infty X_i^\infty \bar{D}_i M_S n}{\rho_S} \right] \quad (II-24)$$

This equation is readily integrated to give:

$$H(t) = H_0 (1 - t/t_c) \quad (II-25)$$

where the total available reaction time (t_c) is given by

$$t_c = \frac{H_0 \rho_S L (1.477)}{M_S n (\bar{D}_i X_i^\infty C_T^\infty) \sqrt{Re_L} (Sc)^{1/3}} \quad (II-26)$$

III) Temperature-Time Profiles

In order to describe the temperature-time profile, the system is treated by a lumped thermal analysis. In such an analysis, internal temperature gradients are neglected and the object is assumed to have a mass-averaged temperature. The validity of this approach can be established by consideration of a dimensionless ratio known as the Biot modulus. The Biot modulus is the ratio of internal heat flow resistance to external heat flow resistance. If the Biot modulus is

less than 0.1, the resulting error in the temperature calculation is less than 5%.

Since the slab is assumed to be quite thin (H_0 - 15 mils) and have a finite thermal conductivity, the internal heat flow resistance is small. For convective cooling with air flow rates of 5.5 ft/sec, the Biot modulus is approximately .14 which justifies a lumped analysis.

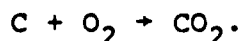
The accumulation of thermal energy inside the slab can be written as a simple energy balance:

$$(\text{Interior Energy Accumulation}) = (\text{Energy Input}) - (\text{Energy Output}).$$

The energy input (Q) is provided by the highly exothermic surface reaction. The rate of heat generation is determined from equation (II-24):

$$Q = (-\Delta H^{\circ}) \frac{dN_S}{dt} = -\Delta H^{\circ} \frac{A_0 S}{M_S} \frac{dH}{dt} \quad (\text{III-1})$$

The enthalpy of reaction (ΔH°) varies with temperature. From thermodynamics, this temperature dependence can be calculated through differences in the heat capacities of the products and the reactants. For the carbon systems in the present calculations, this enthalpy variation is less than 1% and is neglected. All calculations are performed with $\Delta H^{\circ} = -94.0$ Kcal/mole. The reaction is assumed to be:



The energy output mechanisms are convection and radiation. Convective losses tend to dominate the energy balance in the first few seconds until the system attains steady-state behavior. The convective loss coefficients (\bar{h}_Q) are evaluated through bulk fluid properties in exact analogy to the mass transfer problem developed

in Section II.

The radiative losses depend upon the values assumed for the emissivities. Since one surface is assumed to be an inert metal foil, its emissivity is held constant at .2 which is typical of oxidized aluminum. The emissivity of the reacting surface is allowed to vary from 0 to 1.0. Steady-state temperatures are plotted against the sum of the two surface emissivities in Appendix C. For the carbon system, realistic values of this sum are probably anywhere from .9 to 1.1. Such a total emissivity corresponds to a steady-state temperature of roughly 650°C. If the total emissivity is above .3, radiative losses exceed convective losses for an air flow rate of 5.5 ft/sec. Realistic values of the radiative losses appear to be about 65%.

A typical temperature-time profile is presented in Appendix C. The energy balance equation is a nonlinear ordinary differential equation. The total available reaction time is first determined from (II-26), then broken down into 100 steps, and numerically integrated by a fourth-order Runge-Kutta procedure. The approach of the system to a steady-state temperature is governed by the slab thickness and material heat capacity.

APPENDIX A

Terminal Velocities and the Steady-State Approximation

In order to understand the hydrodynamically induced transport of oxygen to the reaction surface, it is necessary to determine the fluid velocity profiles near the falling object. These velocity profiles are governed by the appropriate solution of the Navier-Stokes equation which is regarded as the mathematical formulation of the conservation of fluid momentum. If steady-state profiles are assumed for the fluid flow, there is a substantial simplification of the Navier-Stokes equation.

In this Appendix, we examine the validity of the steady-state approximation for a falling particle and formulate an analysis to determine the effect of particle geometry on the terminal velocity. A general force balance on a particle falling through the atmosphere can be written:

$$\rho_S V_S \frac{dV}{dt} = V_S g (\rho_S - \rho) - F_D. \quad (\text{A-1})$$

The drag force (F_D) due to air resistance is dependent on the projected area (A_S) of the particle in the direction of motion, the kinetic energy, the Reynolds number, and at very high velocities the Mach number. For low velocities, the drag force follows Newton's equation:

$$F_D = \frac{1}{2} \rho V^2 A_S C_D. \quad (\text{A-2})$$

The friction factor or drag coefficient (C_D) has been experimentally determined by Becker⁵ for several particle geometries. Substitution of (A-2) into (A-1), followed by separation of variables, and integration gives the particle velocity as a function of time:

$$V(t) = \sqrt{g/b(1-\rho/\rho_s)} \tanh [\sqrt{gb(1-\rho/\rho_s)}t] \quad (A-3)$$

where

$$b \equiv \frac{1}{2} \left(\frac{A_S}{V_S} \right) \rho / \rho_s C_D \quad (A-4)$$

In expression (A-3), the particle is assumed to start from rest at the origin. In the limit of time approaching infinity, the hyperbolic tangent approaches unity and the terminal velocity is given by:

$$U_\infty = \sqrt{g/b(1-\rho/\rho_s)} \quad (A-5)$$

An identical result could be obtained from (A-1) and (A-2) by setting the acceleration (dv/dt) equal to zero and solving for the velocity.

If we define t_∞ as the time required for the particle to attain 99 percent of its terminal velocity, then we find:

$$t_\infty \equiv \frac{\tanh^{-1}[.99]}{\sqrt{gb(1-\rho/\rho_s)}} = \frac{2.45}{\sqrt{gb(1-\rho/\rho_s)}} \quad (A-6)$$

which provides a quantitative measure of the time required for the falling particle to attain a steady-state velocity. This time is 1 to 2 seconds, which is much less than the available reaction time.

The position of the particle as a function of time is determined from the integral of the velocity over time:

$$z(t) = \frac{1}{b} \text{Log}_e (\cosh[\sqrt{gb(1-\rho/\rho_s)}t]) \quad (A-7)$$

Since the position of a falling object as a function of time can easily be determined experimentally, equation (A-7) provides a transcendental equation for the drag coefficient contained in b.

Appendix B

Variable Fluid Boundary Layer Equations¹

(B-1) Conservation of total mass

$$\nabla \cdot (C_T \vec{V}) = \nabla \cdot (\rho \vec{V}/M) = \frac{1}{M} \nabla \cdot (\rho \vec{V}) = 0$$

(B-2) Conservation of Momentum (Navier-Stokes Equation)

$$\rho V_x \frac{\partial V_x}{\partial x} + \rho V_y \frac{\partial V_x}{\partial y} = \frac{\partial}{\partial y} \left[\mu \frac{\partial V_x}{\partial y} \right]$$

(B-3) Conservation of species i

$$\rho V_x \frac{\partial X_i}{\partial x} + \rho V_y \frac{\partial X_i}{\partial y} = \frac{\partial}{\partial y} (\rho \bar{D}_i \frac{\partial X_i}{\partial y})$$

(B-4) Conservation of energy

$$\rho V_x \hat{C}_p \frac{\partial T}{\partial x} + \rho V_y \hat{C}_p \frac{\partial T}{\partial y} = \frac{\partial}{\partial y} \left[k \frac{\partial T}{\partial y} \right]$$

Appendix C

Typical Input Data, Model Equations, and Calculated Temperatures

Typical Input Data:

Length = 3.0 inches

Width = 1.0 inches

Thickness = 15 mils

Reactant Density = .29 g/cc

Average Molecular Weight = 12

Ambient Temperature = 27 C

Air Viscosity = 16.88×10^{-5} ft²/sec

Air Pressure = 1.00 Atm

Thermal Conductivity of Air = 1.516×10^{-2} Btu/hr-ft-F

Air Flow Rate = 5.5 ft/sec

Enthalpy = 94.0 Kcal/mole

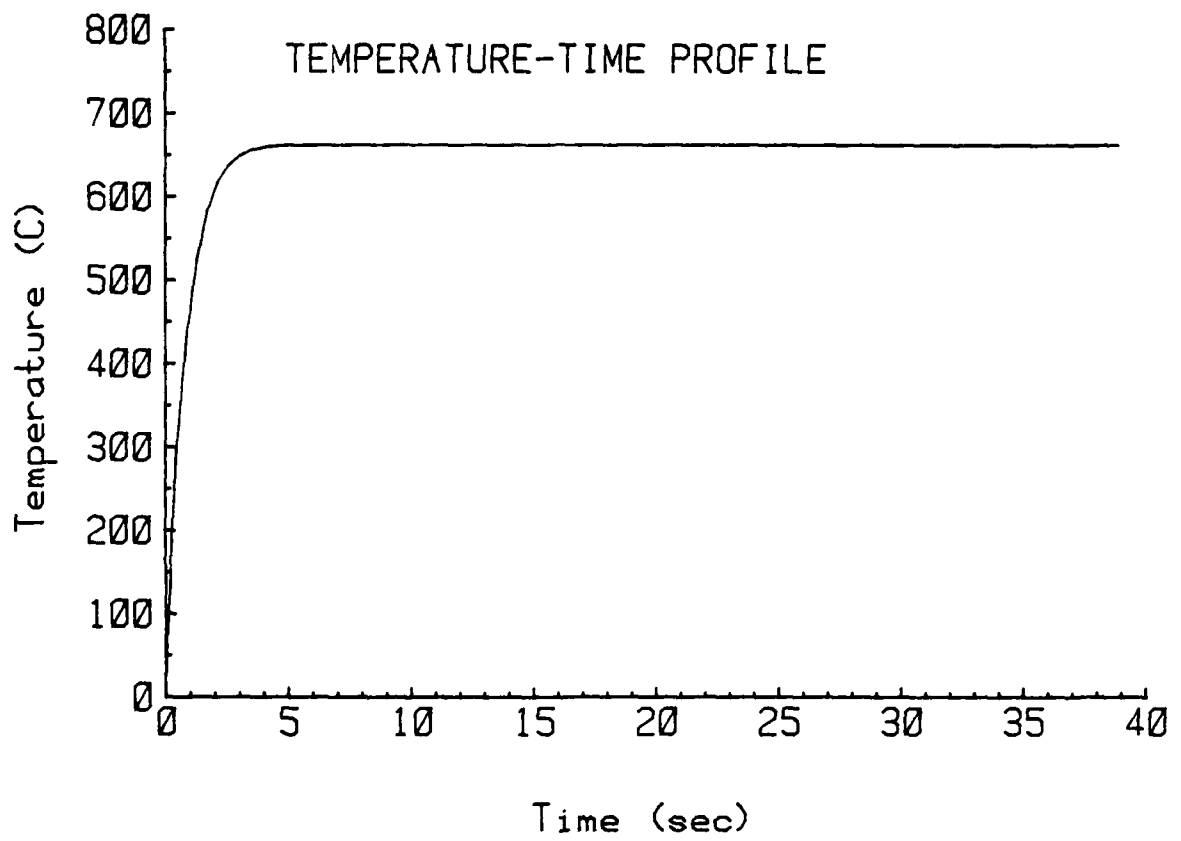
Schmidt Number = Prandtl Number = .708

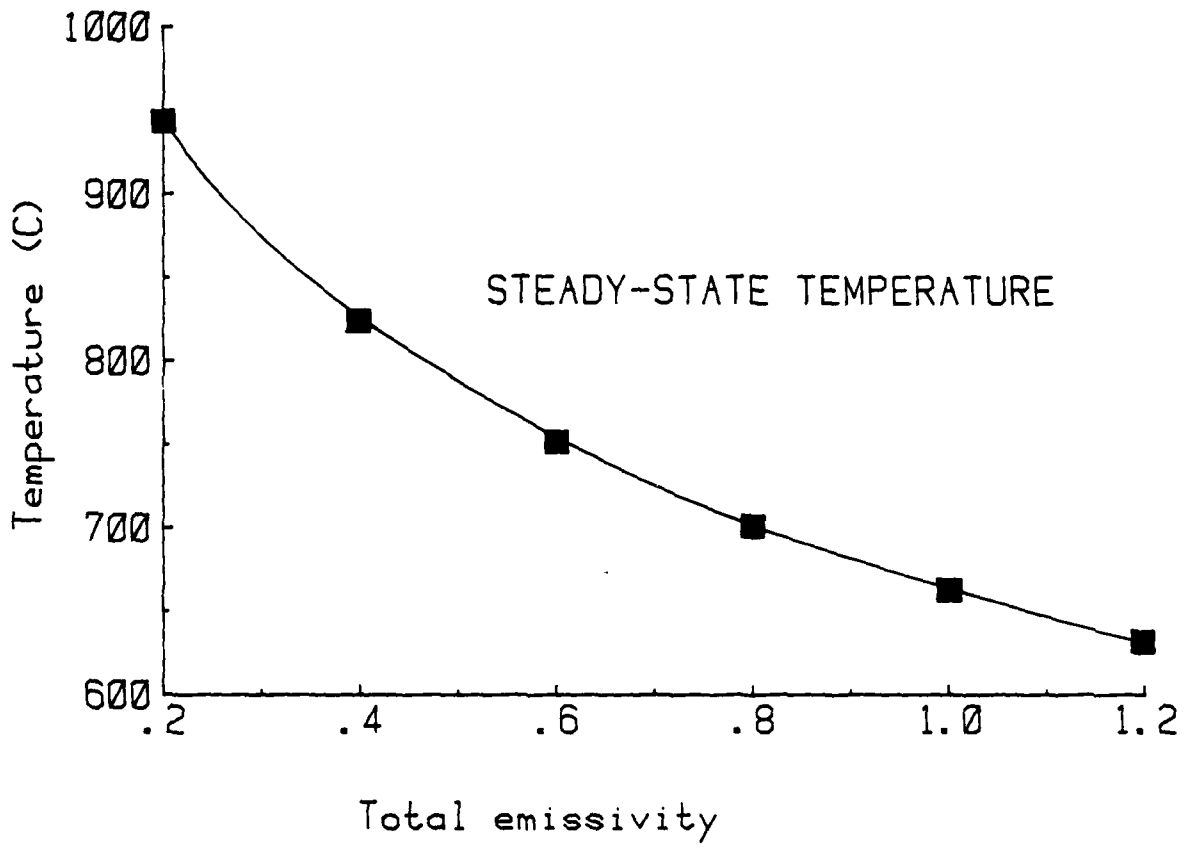
Model Equations:

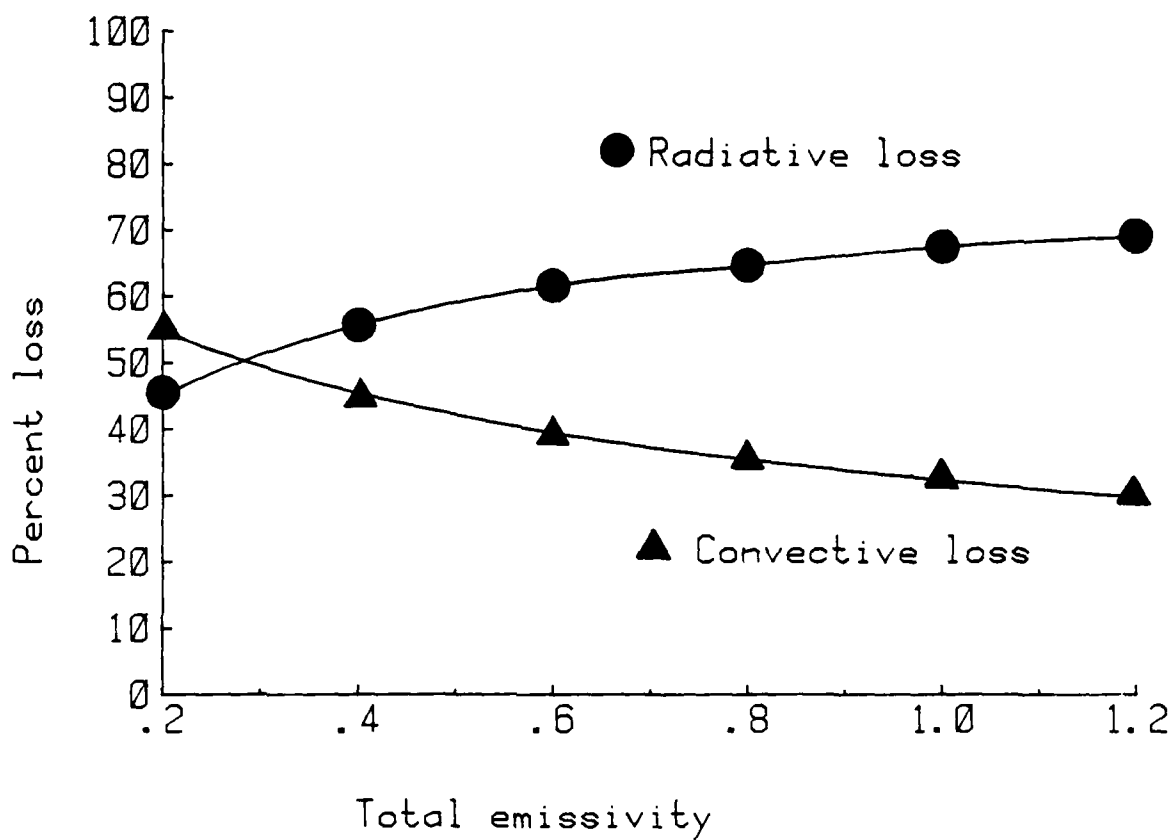
$$\rho_S \hat{C}_p(T) H(t) \frac{dT_S}{dt} = Q - 2\bar{h}_Q (T_S - T_\infty) - \sigma(\epsilon_1 + \epsilon_2) (T_S^4 - T_\infty^4)$$

$$H(t) = H_0 (1 - t/t_c)$$

$$\hat{C}_p(T) = (4.10 + 1.02 \times 10^{-3} T - \frac{2.10 \times 10^5}{T^2}) / 12$$







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