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DIFFUSION OF A CHEMICAL SPECIES THROUGH A VISCOUS BOUNDARY LAYER

Jay Keller

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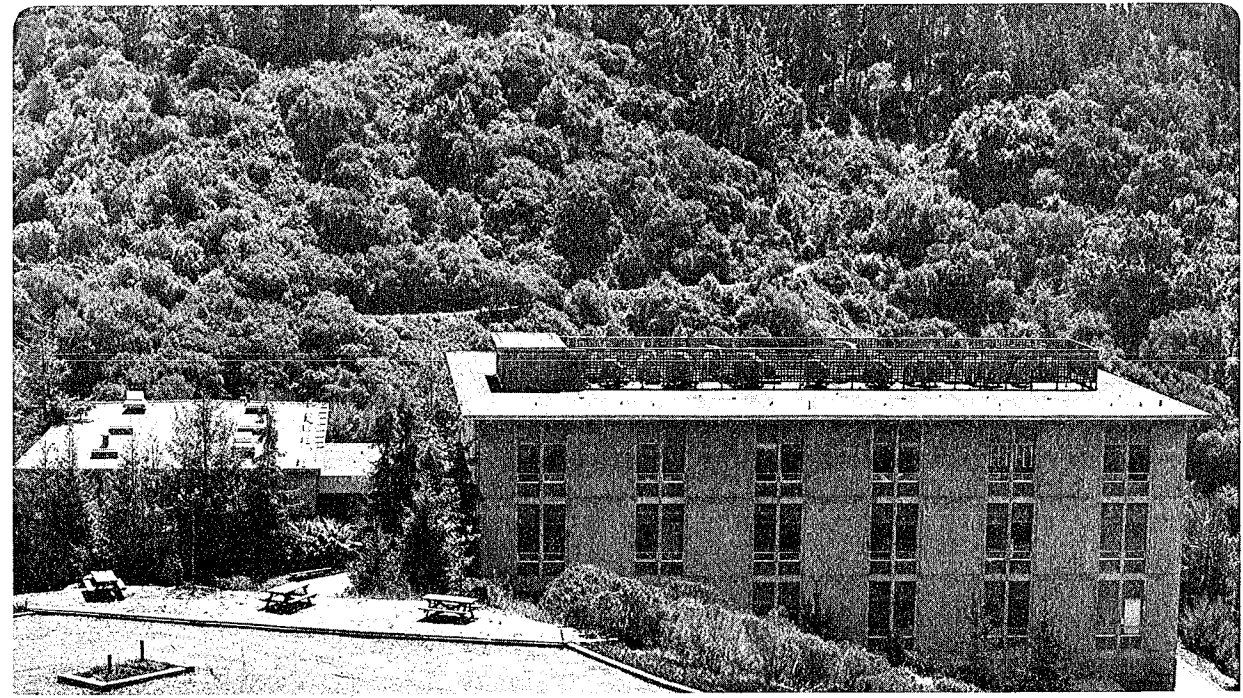
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ABSTRACT

The energy and species equation can be made to reduce to the same form under suitable assumptions. This result is discussed and used to determine the concentration difference of  $H_2S$  in a highly corrosive coal gasification mixture. It is shown that the reaction rate is kinetically controlled and not diffusion limited.

The possibility of using boundary layer control to prevent corrosion of the container walls is also investigated. It is shown that with a suitable injection gas the concentration of  $H_2S$  at the surface can be reduced to a low enough level to stop the corrosion process.

## Preface

In view of the present energy shortage the technical world is developing new energy related technologies. To ease the dependence on petroleum, the United States is turning to its large coal reserves as one potential source of energy. Processing coal into liquid or gas products could be a beneficial way to utilize this fuel. To do so requires that a new high temperature technology be developed. The erosion and corrosion behavior of the materials in a coal conversion plant must be determined in order to design a plant with an economical service life. The corrosion rates alone can be so high that a part will fail after a few weeks in operation. Erosion degradation can reduce the useable life of the component still further. The fluid flow field which supplies reactive gas to the materials surface needs to be defined to establish the actual gas composition at the gas-solid reaction site. This definition of gas composition requires an understanding of the diffusion process and how the viscous fluid motion affects the diffusion of the reacting gas to the wall surface.

This paper will discuss the diffusion of a gaseous component,  $H_2S$ , in a complex gas mixture. The effects of the fluid flow in the fully developed and entrance regions for both laminar and turbulent flow conditions will be examined. The diffusion profiles for the conditions of an operating coal gasifier will be discussed. Finally the potential use of boundary layer control to dictate the concentration of the reacting species at the surface will be examined.



## 1.0 CONCENTRATION PROFILES

### 1.1 Analogy Between Heat and Mass Transfer

An accurate description of this flow field is extremely complex. The four conservation equations (Continuity, Conservation of momentum, Conservation of energy, and Conservation of species) are all inter-related. The complexity of the problem can be drastically reduced by making a number of suitable approximations.

In this problem we are concerned with the effect of the flow field on the diffusion of  $H_2S$  toward the container walls. The primary reaction in the gas concerning  $H_2S$  is the dissociation reaction:  
 $H_2 + \frac{1}{2}S_2 \rightleftharpoons H_2S$ : this can be assumed to be infinitely fast (with respect to the diffusion process) and thus  $H_2S$  will always be in equilibrium. Since the dissociation reaction will replenish  $H_2S$  in the flow as it is used up at the walls, the effect will be to reduce any gradients which the diffusion process creates. Hence if we assume that the concentration of  $H_2S$  is unchanged by chemical reactions occurring in the gas phase (frozen composition), it will yield a worst case for this study.

W. M. Kays<sup>1</sup> develops a simplified theory for mass transfer. If we assume:

- 1) Bulk viscosity is negligible
- 2) Constant properties
- 3) Viscous dissipation negligible
- 4) Pressure gradient diffusion negligible
- 5) Dufour and Soret effects negligible

- 6) Radiation negligible
- 7) Ficks law applies
- 8) No heat generation terms (no chemical reaction)
- 9) Steady flow.

The energy equation can be written:

$$\rho(\vec{V} \cdot \vec{V})_i - \vec{\nabla} \cdot (k\vec{\nabla}T) - \vec{\nabla} \cdot \left( \sum_j (\rho D_j \vec{\nabla} m_j) i_j \right) = 0 \quad (1)$$

and the conservation of species equation can be written:

$$\rho(\vec{V} \cdot \vec{V}) m_j - \vec{\nabla} \cdot [\rho D_j \vec{\nabla} m_j] = 0. \quad (2)$$

It can be shown that under the assumption of  $Le = \alpha/D_i = 1$ , and those given above, these equations will reduce to

$$\rho(\vec{V} \cdot \vec{V}) p - \vec{\nabla} \cdot (\lambda \vec{\nabla} p) = 0 \quad (3)$$

where  $p$  is a "conserved" property.

$p = m_j, i$  and for constant specific heats  $p = T$  as well.

$\lambda = k/c_p$  or  $\rho D_i$  which ever is appropriate.

$\rho =$  is the mean density of the fluid,  $\vec{V}$  denotes the mean velocity vector,  $m_j$  represents the mass concentration of the  $j^{\text{th}}$  species,  $i$  denotes the mixture enthalpy,  $D_j$  gives the diffusion coefficient of species  $i$ ,  $k$  is the mixture thermal conductivity,  $c_p$  represents the specific heat at constant pressure,  $T$  is the temperature, and  $\alpha$  is the thermal diffusivity.

The boundary condition at the interface can be written

$$\dot{m} = \frac{\lambda \frac{\partial p}{\partial y} \Big|_w}{p_w - p_t} \quad (4)$$

where  $p_t$  is the value of  $p$  at the "Transferred substance state",  $p_w$  is the value of  $p$  at the wall. \*

---

\* The Transferred substance state is the state far enough into the boundary such that all transfers occur by convection and hence there are no gradients of any kind. This is explained well in Ref. 7.

For  $p = m_j$ ,  $m_{j_t} = p_t = \dot{m}_{j_t} / \dot{m}$  this equation can be considered a definition of  $m_{j_t}$ .  $\dot{m}$  denotes the mean mass flux away from the surface. Now we can define a mass transfer conductance  $g$  and a driving potential  $B$  such that:

$$\dot{m} = g B$$

where  $B = (p_\infty - p_w) / (p_w - p_t)$ .

Since there is a mass flux toward the boundary, this flux effects the flow field in much the same way as blowing or suction at the walls. Hence it is convenient to define  $g^*$  as the mass transfer conduction without blowing:

$$g^* = \lim_{B \rightarrow 0} \left( \frac{\dot{m}}{B} \right). \tag{5}$$

The ratio  $g/g^*$  is primarily a function of  $B$ . It should be noted that for  $B = 0$ ,  $g/g^* = 1$ . It is assumed a priori that for this problem  $B \cong 0$  and hence  $g/g^* \cong 1$ .

With the assumptions made, the mass transfer and the heat transfer problems are the same. Now we can draw on the vast background in heat transfer to solve the problem at hand. To use this information all we need do is recognize.

$$St = \frac{h}{\rho U c_p} = \frac{g}{\rho U}$$

$$Nu = \frac{hd}{k} = Sh = \frac{gd}{\rho D_i}$$

$$g = h/c_p$$

by the assumption ( $Le = 1$ ) we have  $\alpha = D_i$  and finally  $m_i = T$ .

St is the Stanton number, Nu denotes the Nusselt number, Sh is the

Sherwood number,  $Le$  denotes the Lewis number,  $h$  is the heat transfer coefficient,  $U$  denotes a characteristic velocity, and finally  $d$  is the pipe diameter. Recall it is assumed that  $g^* = g$ ; thus we can use the data for the case of no blowing.

### 1.1.1 Boundary Conditions

Solving for the mass flux rate at the wall it is assumed that the rate of chemical reaction at the wall is far less than the rate at which the reacting component is diffusing through the gas. In other words, the diffusion rate is sufficiently large to assure there will always be a reactive molecule at the material's surface. Thus, the boundary condition is one of a constant mass flux toward the material's surface. The magnitude of this flux is then given by the reaction rate of the corrosive agent with the surface of the material in question.

## 1.2 Solutions to the Mass Transfer Problem

### 1.2.1 Laminar Flow

Solutions to the energy equation are well documented. The important features of these results are:

- 1) For fully developed pipe flow the  $Nu$  is a constant, and for constant heat flux boundary conditions the  $Nu = 4.364$ .<sup>1,2</sup>
- 2) When considering a fully developed velocity profile and a developing thermal profile, we see that the  $Nu$  decreases from a very large value ( $Nu = \infty$ ) asymptotically approaching 4.364.

- 3) The case of both profiles developing (the entrance to a heated pipe) is similar to case 2 above; however, when both profiles are developing together, the value of the  $Nu$  is higher than if only the temperature profile is developing.<sup>1</sup>

With the assumptions made, we have  $Nu = Sh = gd/\rho D_i$ . Hence from case 3 the conductance decreases from  $\infty$  to a value of  $g = 4.364 \rho D_i/d$ . (Recall  $\dot{m} = gB$  so as  $g$  tends to  $\infty$ ,  $B$  tends to 0 provided  $\dot{m} = \text{constant}$ .)

### 1.2.2 Turbulent Flow

The assumptions made in reducing the governing equations to the conserved property equation required the  $Le = 1$ . If we invoke Reynolds analogy (Reynolds analogy basically states that the eddy diffusivities are equal  $\epsilon_{\text{heat}} = \epsilon_{\text{momentum}} = \epsilon_{\text{species}}$ ), we see  $Le_{\text{turb}} = 1$  and hence this formulation is still valid.

The trends for turbulent flow are similar to those of laminar flow. Analytical solutions are available for the case of fully developed profiles as well as the case of a developing thermal profile.<sup>1</sup> Extensive work has been done by Boelter, Young and Iverson<sup>3</sup> on combined hydrodynamic and thermal entrance region. Their data show the same trends as in laminar flow. Indeed the results indicate that the  $Nu$  increases due to the effects of turns and irregular entrances. Figures 9-14 of Kays<sup>1</sup> gives a summary of these results.

### 1.2.3 Summary

In Sections 1.1 and 1.2 the analogy between mass and heat transfer was discussed. It was seen that for a variety of problems the solutions to the energy equation are also solutions to the mass diffusion equation. The solutions covered in Section 1.2 are for a wide range of flow conditions which vary from fully developed laminar flow to the entrance region in a developing turbulent flow field.

## 1.3 Determination of the Physical Problem

### 1.3.1 Reaction Rate

It has been shown that the mass flux is proportional to the concentration difference. Thus for the largest possible mass concentration difference, we need to examine the case which yields the largest mass flux (or chemical reaction rate at the wall). The reactive agent at the wall is  $S_2$ . The amount of  $S_2$  present is given by the dissociation reaction  $H_2 + 1/2S_2 \rightleftharpoons H_2S$ . The degree of dissociation is an increasing function of temperature.

We assume that the chemical reaction rate is of the Arrhenius form:

$$K(T) = A \exp\left(-\frac{E_A}{RT}\right)$$

where  $E_A$  denotes the activation energy;  $R$  denotes the universal gas constant;  $A$  is a constant (in reality  $A$  is a weak function of temperature);  $K(T)$  is the rate constant.

Then for the global reaction  $1/2S_2 + Fe \rightarrow FeS$ , the reaction rate is given by:

$$\frac{d[FeS]}{dt} = K(T) [S_2]^{1/2} [Fe]$$

where  $[A_i]$  denotes concentration of  $A_i$  species.

Therefore the worst case is given by using the highest temperature in the system (1255°K) and a representative concentration of  $H_2S$ . This will yield the highest mass flux of  $H_2S$  to the surface for this concentration of  $H_2S$ .

The reaction rate can be found if we first assume that there is no concentration difference across the stream. Then the concentration at the wall can be assumed to be that of the free stream. With this, the reaction rate can be found and, using the results of Section 1.1 and 1.2, the concentration differences can be found. The reaction rate is found by using the results of Rao and Nelson<sup>4</sup> "Sulfidation of 310 Stainless Steel at Sulfur Potentials Encountered in Coal Conversion Systems".

In order to extrapolate the rate data from the data of Rao and Nelson, it is necessary to determine the partial pressure of  $S_2$  ( $P_{S_2}$ ) from the mixture  $H_2O$ ,  $H_2S$ ,  $H_2$ ,  $CO$ , and  $CO_2$  gases and the equilibrium expression for the gas phase reaction:

$$\begin{aligned} & (H_2 + 1/2S_2 \rightleftharpoons H_2S) \\ P_{H_2S} &= 1.22 \text{ ATM} \\ P_{H_2} &= 1.24 \times 10^1 \text{ ATM} \\ K_{eq} &= \frac{P_{H_2S}}{P_{H_2} P_{S_2}^{1/2}} = 15.54 \\ P_{S_2} &= 4.05 \times 10^{-5} \text{ ATM.} \end{aligned}$$

Over a period of about five hours,  $5.66 \text{ mg/cm}^2$  has been gained giving an approximate reaction rate of  $1.89 \times 10^{-2} \text{ mg/cm}^2 \text{ min.}$

The approximate elemental analysis of the surface scale<sup>4</sup> is 40 w% S, 35 w% Fe, 18 w% Cr, and 7 w% Ni. This corresponds to a generalized mole formula of  $\text{NiFe}_5\text{Cr}_3\text{S}_{10}$  which yields a molar rate of reaction of approximately  $3.872 \times 10^{-10} \text{ moles/cm}^2 \text{ sec.}$  Therefore:

$$K = \text{Approximate reaction rate} = 3.872 \times 10^{-10} \text{ moles/cm}^2 \text{ sec.}^*$$

### 1.3.2 Physical Properties

It has been shown that the presence of particles does not have a large effect on the transport properties of the gas.<sup>5</sup> Thus the transport properties of a gas mixture of:

$\text{H}_2$ ;	$\chi = .182$ mole fraction
$\text{H}_2\text{O}$ ;	$\chi = .5$
$\text{CO}$ ;	$\chi = .15$
$\text{CO}_2$	$\chi = .15$
$\text{H}_2\text{S}$ ;	$\chi = .018$

were calculated by using kinetic theory.\*\*  $\chi$  denotes the mole fraction of the given species.

The binary diffusivities are given by<sup>6</sup>

$$D'_{ij} = \frac{.002628 [T^3 (M_i + M_j)]^{1/2}}{P \sigma_{ij}^2 \Omega_{ij}^{(1,1)} (T_{ij}^*)} \quad (6)$$

---

\* Note Rao's data already includes the diffusion through the gas; thus this analysis gives a worse case.

\*\* This is the gas composition typically found in an HyGas plant.



where  $D_{ij}^!$  denotes the binary diffusivity of the  $i^{\text{th}}$  species through the  $j^{\text{th}}$  species;  $M_i$  molecular weight of  $i^{\text{th}}$  species;  $P$  is the pressure;  $\sigma_{ij}$  denotes the collision diameter ( $\text{\AA}$ ); and  $\Omega_{ij}^{(1,1)}(T_{ij}^*)$  is the potential energy integral (tabulated in Ref. 6).

The Diffusion Coefficient for a gas mixture can be approximated with high accuracy by Eq. 7

$$D_i = \frac{1 - \chi_i}{\sum_{i \neq k}^n \chi_k / D_{ik}} \quad (7)$$

The coefficient of viscosity was found by the relationship<sup>6</sup>

$$\mu = 266.93 \times 10^{-7} \frac{[MT]^{1/2}}{\sigma_{\Omega}^{2(2,2)}(T^*)} \quad (8)$$

where  $\Omega^{(2,2)}(T^*)$  denotes the collision cross section integral.

The approximate mixing formula (Eq. 9) employed binary diffusivities and proved to be easier than the more precise formula employing large matrices.<sup>6</sup> The approximate relationship still gives good results as compared with experimental data.<sup>6</sup>

$$u_{\text{mix}} = \sum_i^{\Gamma} \left[ \frac{X_i^2}{\frac{X_i^2}{u_i} + 1.385 \sum_{k \neq i}^{\Gamma} X_i X_k \frac{RT}{PM_{i ik}}} \right]. \quad (9)$$

Finally the thermal conductivity was calculated by Eq. 10:

$$k_i = 1989.1 \frac{\sqrt{T/M}}{\sigma_{\Omega}^2(2,2)(T^*)} \left[ 1 \times 10^{-7} \right]. \quad (10)$$

A simple weighted arithmetic average is used (Eq. 11) to find the thermal conductivity for the mixture.

$$k = \sum_{i=1}^{\Gamma} X_i k_i. \quad (11)$$

The results are given in Table 1.3.

Table 1.3. Calculated values using Equations 6-11.

Species	$D_{H_2S, i}$ cm <sup>2</sup> /sec	k cal/cm sec °K	$\mu$ g/cm sec	$C_p$ cal/g °K
H <sub>2</sub> O	$3.611 \times 10^{-2}$	$8.444 \times 10^{-4}$	$2.284 \times 10^{-4}$	.5901
H <sub>2</sub>	$1.031 \times 10^{-1}$	$1.535 \times 10^{-4}$	$3.711 \times 10^{-4}$	3.698
CO	$2.741 \times 10^{-2}$	$1.228 \times 10^{-4}$	$4.615 \times 10^{-4}$	.293
CO <sub>2</sub>	$2.148 \times 10^{-2}$	$7.777 \times 10^{-5}$	$4.593 \times 10^{-4}$	.307
H <sub>2</sub> S	$2.186 \times 10^{-2}$	$8.163 \times 10^{-5}$	$3.733 \times 10^{-4}$	.341
Total	$3.458 \times 10^{-2}$	$4.817 \times 10^{-4}$	$3,973 \times 10^{-4}$	1.064

The parameters which characterize this problem are:

- 1) Pipe diameter = 91.44 cm
- 2) Flow velocity = 1524 cm/sec
- 3) Pressure = 68.046 ATM.
- 4) Temperature = 1255.57°K
- 5) Composition
  - $x_{H_2O} = .5$
  - $x_{H_2} = .182$
  - $x_{CO} = x_{CO_2} = .15$
  - $x_{H_2S} = .018$
- 6) Average molecular weight  $M = 20.791$  g/g mole. From the table the following can be calculated.

$$\begin{aligned}
 Pr &= \nu/\alpha = .8775 & \rho &= 1.374 \times 10^{-2} \text{ g/cm}^3 \\
 Le &= \alpha/D_i = .9527 & Re &= Ud/\nu = 4.818 \times 10^6 \\
 Sc &= \nu/D_i = .836
 \end{aligned}$$

### 1.3.3 Summary

The Lewis number for this gas is about 1 (the molecular Lewis number = .9527, the turbulent  $Le=1$ ) and all the other assumptions listed in Section 1.1.1 are reasonable for this case. From Fig. 32 (page 7-36 of Ref. 2) the local Nu number ranges from  $\infty$  to 300 and thus the concentration difference ( $m_c - m_w$ ) goes from 0.0 to  $1.862 \times 10^{-7}$  moles/cm<sup>3</sup>.\* Indeed the assumption of a small concentration difference used to calculate the reaction rate is valid, and it is concluded that there is no significant concentration difference between the main stream and the wall caused by the fluid motion. It should be noted that the Reynolds number for this flow is well above the critical Re for pipe flow; hence this flow can be assumed to be turbulent.

## 2.0 CONTROLLING THE CONCENTRATION PROFILE

The remainder of this survey discusses the results of various authors covering the effects of injection through a porous wall. The effect of the heat transfer and thus the mass diffusion for both laminar and turbulent profiles will be described. Finally the condition of a typical coal gasifying plant will be investigated.

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\* This is for a  $Re = 200,000$  so the actual difference will be less, since the Nu scales as  $Re^{.8}$  for turbulent flow. It is assumed that for turbulent flow the law of the wall type profile is appropriate. Hence the profile is such that the concentration at infinity (for flow over a flat plate) and the center line concentration (for flow in a pipe) will be about equal.

## 2.1 Laminar Flow

### 2.1.1 Effect of Injection on Heat Transfer

S. W. Yuan and A. B. Finkelstein discuss the problem of heat transfer in a porous laminar pipe flow.<sup>7</sup> They found for small injection rates that the heat transfer coefficient decreased with increased injection. Yuan and Finkelstein made a hypothesis that for large blowing rates the value of the Nu would approach an asymptotic value instead of its apparent linear dependence on the injection rate as their results have shown. This hypothesis was shown to be correct in the work done by Leo F. Carter and William N. Gill.<sup>8</sup> They examined the effects of blowing and suction in horizontal and vertical conduits.\*

## 2.2 Turbulent Flow Conditions

### 2.2.1 The Effect of Heat Transfer

It is expected that the effects of coolant injection in turbulent flow will be similar to the effect for the laminar case. Indeed this is what S. W. Yuan and A. Barazotti have shown.<sup>10</sup> The effect of injection is to reduce the temperature gradient at the wall and thus the heat transferred to the wall.

It should be noted that for both the laminar and turbulent case the drag coefficient increases while the heat transfer coefficient decreases. Thus the Reynolds analogy between the drag coefficient and the heat transfer coefficient is not valid for injection through a porous tube.

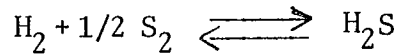
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\* According to Schlichting, pipe flow can be approximated by flow in a rectangular conduit for large pipe diameters.<sup>9</sup>

### 2.3 Evaluation of a Coal Gasification Atmosphere

The purpose of using boundary layer control is to prohibit the corrosive materials from reaching the container wall. In order to determine the amount of injection necessary to stop the formation of FeS, the following procedure was used.

The partial pressure of sulfur corresponding to the largest amount possible and still preventing the formation of FeS is  $P_{S_2} = 1.12 \times 10^{-7}$  atmospheres.<sup>11</sup> This is the largest value of  $P_{S_2}$  for which FeS will not form with 310 stainless steel. The equilibrium constant for the reaction,



at a pressure and temperature of  $P = 68.05$  Atm.,  $T = 1255.37^\circ K$  is  $K_{eq} = 15.54$ . The partial pressure of  $H_2S$  is then found by the mass action law (Eq. 12).\*

$$K_{eq} = \frac{P_{H_2S}}{P_{H_2} P_{S_2}^{1/2}} \quad (12)$$

If the injected gas is assumed to consist of the products of the gasifier with  $H_2S$  removed, then the gas composition would be;

$$\begin{aligned} x_{H_2} &= .185 \\ x_{H_2O} &= .509 \\ x_{CO} &= x_{CO_2} = .153 \end{aligned}$$

---

\* This reaction is assumed to be infinitely fast so that  $H_2 + 1/2 S_2 \rightleftharpoons H_2S$  in equilibrium.

with a product mixture of;

$$\begin{aligned}x_{\text{H}_2} &= .182 \\x_{\text{H}_2\text{O}} &= .5 \\x_{\text{CO}} &= x_{\text{CO}_2} = .15 \\x_{\text{H}_2\text{S}} &= .018.\end{aligned}$$

Since  $\text{H}_2$  appears in both the injected gas as well as an element in the reaction of  $\text{H}_2\text{S}$ , an iterative technique was used to determine the  $P_{\text{H}_2\text{S}}$  at the surface of the material.

The mixture at the surface is then,

$$\begin{aligned}x_{\text{H}_2\text{S}} &= 9.612 \times 10^{-4} \\x_{\text{H}_2} &= .1848 \\x_{\text{H}_2\text{O}} &= .5085 \\x_{\text{CO}} &= x_{\text{CO}_2} = .1529.\end{aligned}$$

Recall from Section 1.3.2 that the mixture density is

$$\rho = 6.609 \times 10^{-4} \text{ gmole/cm}^3.$$

Thus the concentration at the wall is,

$$m_{\text{H}_2\text{S}_w} = \rho x_{\text{H}_2\text{S}} = 6.353 \times 10^{-7} (\text{gmole}_{\text{H}_2\text{S}}/\text{cm}^3).$$

and in the main stream the concentration of  $\text{H}_2\text{S}$  is

$$m_{\text{H}_2\text{S}_c} = 1.189 \times 10^{-5} (\text{gmole}_{\text{H}_2\text{S}}/\text{cm}^3).$$

From the results of S. W. Yuan and A. Barazotti,<sup>10</sup> the ratio  $\frac{m_c - m_w}{m_c - m_o}$  of H<sub>2</sub>S is needed. Thus,

$$\frac{m_c - m_w}{m_c - m_o} = .947.$$

Their data is good to about  $\frac{m_c - m_w}{m_c - m_o} = .9$ .  $m_o$  denotes the concentration in the injected fluid. To extrapolate into the region of interest a curve of the following form is used:

$$\frac{m_c - m_w}{m_c - m_o} = 1 - a \exp \left\{ -b \left\{ \frac{Q}{W} \right\} \right\} \quad (13)$$

By the least squares method the constants a and b were found to be

$$a = .43079$$

$$b = .11182$$

This curve fits the data very well ( $r^2 = .96$ ); thus it is assumed that this curve will give a reasonably accurate extrapolation into the region of interest. Hence

$$\frac{m_c - m_w}{m_c - m_o} = 1 - .43079 \exp \left\{ - .11182 \left\{ \frac{Q}{W} \right\} \right\}$$

and for  $\frac{m_c - m_w}{m_c - m_o} = .947$

$$\begin{aligned} \frac{Q}{W} &= \frac{V_o \rho_o}{U \rho} \\ &= .0187 \end{aligned}$$

where  $V_o$  is the blowing velocity,  $\rho_o$  denotes the density of the injected gas.



Again, from Section 1.3.2; for the center of the stream

$$\begin{aligned}\bar{M} &= 20.791 \text{ g/mole} \quad \text{and} \\ \rho &= 1.374 \times 10^{-2} \text{ g/cm}^3 \\ U &= 1524 \text{ cm/sec.}\end{aligned}$$

Thus the coolant mass rate is,

$$\begin{aligned}Q &= \rho_o V_o \\ &= .3915 \text{ g/cm}^3 \text{ cm/sec.}\end{aligned}$$

The results of Olson and Eckert<sup>12</sup> show that for steady state ( $x/d = 16$ ), the local dimensionless pressure gradient changes from about .02 to about .16 which is an increase of about 700%. Although this technique shows promise in reducing the corrosion problem it does cause an increase in pressure loss and hence a greater pumping requirement.

### 3.0 CONCLUSIONS

Using the results of heat transfer analysis, the gas concentration profiles for laminar and turbulent flow fields were found. It was calculated that for the conditions existing in coal gasifiers the concentration difference due to the flow field of  $H_2S$  (the corrosive agent) between the mean flow and the wall was very small, ( $0 \leq (m_c - m_w) \leq 1.862 \times 10^{-7}$  moles/cm<sup>3</sup>). Thus the effects of the concentration gradient due to the fluid flow field can be neglected, and the concentrations of the reactive constituents of the gas can be calculated thermodynamic considerations only.

It was also shown that by injecting an inert gas through the wall the corrosion potential of the gas at the wall surface could be markedly decreased. The formation of FeS could, thereby, be reduced to near 0.

It should be pointed out that the concept of boundary layer control to modify the chemical composition of a reactive gas mixture at the surface of components in coal gasifiers requires further study to determine its feasibility.

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## LIST OF SYMBOLS

$\rho$	density g/cm <sup>3</sup>
$\vec{V}$	velocity vector cm/sec
$D_j$	diffusion coefficient for the j <sup>th</sup> species cm <sup>2</sup> /sec
$m_i$	mass concentration of j <sup>th</sup> species mass of j/total mass
$\dot{m}$	mass flux g/cm <sup>2</sup> -sec
$i_j$	enthalpy of j <sup>th</sup> species cal/g
$\rho$	conserved property
$T$	temperature °K
$k$	thermal conductivity cal/cm-sec-°K
$c_p$	specific heat at constant pressure cal/g-°K
$\alpha_i$	thermal diffusivity of the i <sup>th</sup> species cm <sup>2</sup> /sec
$\alpha$	thermal diffusivity of the mixture cm <sup>2</sup> /sec
$h$	heat transfer coefficient cal/cm <sup>2</sup> -sec-°K
$g$	mass transfer coefficient g/cm <sup>2</sup> -sec
$g^*$	defined by equation (5)
$B$	driving potential (mass transfer number)
$d$	pipe diameter cm
$K(T)$	chemical rate constant
$A$	constant
$E_A$	activation energy cal/gmole
$R$	ideal gas constant 1.986 cal/gmole-°K
$P_i$	partial pressure of the i <sup>th</sup> species atmospheres
$P$	total pressure atmospheres

$K_{eq}$	equilibrium constant
$D_{ij}$	binary diffusivity of the $i^{th}$ species through the $j^{th}$ species
$M_j$	molecular weight of the $i^{th}$ species
$\sigma_{ij}$	collision diameter $\text{\AA}$
$\Omega^{(1,1)}(T_{ij}^*)$	potential energy integral
$\Omega^{(2,2)}(T^*)$	collision cross section integral
$\chi_i$	mole fraction of $i^{th}$ species
$\mu_i$	coefficient of viscosity of the $i^{th}$ species g/cm-sec
$\mu_{mix}$	mixture viscosity g/cm-sec
$\nu$	kinematic viscosity $(\mu/\rho)\text{cm}^2/\text{sec}$
$Q$	injection mass flow rate $\text{g}/\text{cm}^2\text{-sec}$
$U$	mass flux velocity, average flow rate cm/sec
$\epsilon$	eddy diffusivity (turbulent)
$\lambda$	defined by equation 3

### Subscripts

t	transferred substance state
c	center line of the pipe
w	pipe wall
o	injected condition
$\infty$	conditions at infinity

Dimensionless groups

Nu	Nusselt number	$hd/k$		
Sh	Sherwood number	$gd/\rho D_i$		
Re	Reynolds number	$Ud/\nu$		
Sc	Schmidt number	$\nu/D_i$		
St	Stanton number	$h/\rho U c_p$	or	$g/\rho U$
Pr	Prandtl number	$\nu/\alpha$		
Le	Lewis number	$\alpha/D_i$		

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