NASA Contractor Report 168329



# COMPUTER PROGRAM FOR THE CALCULATION OF MULTICOMPONENT CONVECTIVE DIFFUSION DEPOSITION RATES FROM CHEMICALLY FROZEN BOUNDARY LAYER THEORY

Süleyman A. Gökoğlu

Analex Corporation
Cleveland, Ohio

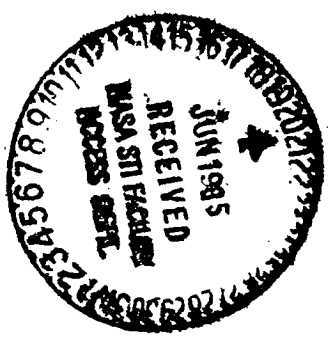
and

Bor-Kuan Chen and Daniel E. Rosner

Yale University
New Haven, Connecticut



January 1984




Prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
Lewis Research Center
Under Contract NAS3-23293 and Grant NAG3-201

ENTER:D 85N27164

DISPLAY 85N27164/2

85N27164*# ISSUE 16 PAGE 2781 CATEGORY 34 RPT#: NASA-CR-168329 E-1971 NAS 1.26:168329 CNT#: NAS3-23293 NAG3-201 84/01/00 35 PAGES UNCLASSIFIED DOCUMENT

UTTL: Computer program for the calculation of multicomponent convective diffusion deposition rates from chemically frozen boundary layer theory TLSP: Final Report

AUTH: A/GOEKOGLU, S. A.; B/CHEN, B. K.; C/ROSNER, D. E.

CORP: Analex Corp., Cleveland, Ohio.; Yale Univ., New Haven, Conn.

AVAIL.NTIS SAP: HC A03/MF A01

Washington Prepared in cooperation with Yale Univ., New Haven, Conn.

MAJS: /*COMPUTER PROGRAMS/*THERMODYNAMIC PROPERTIES/*TRANSPORT PROPERTIES/*VAPOR DEPOSITION

MINS: / BOUNDARY LAYERS/ HEAT TRANSFER/ HOT CORROSION/ MASS TRANSFER/ PREDICTION ANALYSIS TECHNIQUES/ USER MANUALS (COMPUTER PROGRAMS)

ABA: Author

ABS: The computer program based on multicomponent chemically frozen boundary layer (CFBL) theory for calculating vapor and/or small particle deposition rates is documented. A specific application to perimter-averaged Na2SO4 deposition rate calculations on a cylindrical collector is demonstrated. The manual includes a typical program input and output for users.

ENTER:P

PAGE

PAGING COMPLETED. PLEASE ENTER *DISPLAY* FOR NEXT ITEM

# COMPUTER PROGRAM FOR THE CALCULATION OF MULTICOMPONENT CONVECTIVE DIFFUSION DEPOSITION RATES FROM CHEMICALLY FROZEN BOUNDARY LAYER THEORY†

Süleyman A. Gökoğlu*

Analex Corporation
Cleveland, Ohio 44135

and

Bor-Kuan Chen** and Daniel E. Rosner***

Yale University
Chemical Engineering Department
New Haven, Connecticut 06520

## SUMMARY

The computer program developed based on multicomponent chemically frozen boundary layer (CFBL) theory for calculating vapor and/or small particle deposition rates is documented. A specific application to perimeter-averaged $Na_2SO_4$ deposition rate calculations on a cylindrical collector is demonstrated. The manual includes a typical program input and output for users.

E-1971

## I. INTRODUCTION

A wide variety of different engineering fields-including chemical coating of metals, solid state electronics device fabrication, filtration, aircraft icing, corrosion and fouling of gas turbine blades, heat exchangers, etc.-deal with vapor and particle capture, either to exploit or to suppress it, depending on the context. A comprehensive but tractable convective diffusion deposition rate theory has been developed at Yale University based on the assumption of a multicomponent "chemically frozen" boundary layer (CFBL) as outlined in Rosner et al. [1]. The theory which makes full use of available transport coefficient and property information is not only applicable under conditions of multicomponent vapor transport (e.g., CVD applications), but it is also intrinsically capable of simultaneously dealing with particle transport provided the particles are small enough to be considered heavy molecules. The purpose of this manual is to document a simple but useful computer code based on CFBL

---

†Supported by NASA Lewis Research Center Contract NAS3-23293 (Analex Corp.) and Grant NAG3-201 (Yale Univ.).

*Research scientist.

**Present address: E.I. du Pont de Nemours and Co., Biochemicals Dept. E335, Wilmington, Delaware 19898.

***Professor of Chemical Engineering, Director, High Temperature Chemical Reaction Engineering Laboratory.

theory for calculating alkali sulfate deposition rates. We hope that the manual will prevent further misapplications of CFBL theory as has been encountered in the literature [2]. Detailed description of this program, with specific application to perimeter-averaged $Na_2SO_4$ deposition rate calculations on a cylindrical collector is given below. Typical program input and output is included with explanations. The manual contains the program listing in Appendix C.

## SYMBOLS

| | |
|---|---|
| $B_T$ | thermophoretic parameter, equation (35) |
| C | nozzle discharge coefficient |
| $C_{mh}$ | coefficient defining relative sensitivity of mass transfer and heat transfer to variable properties, equation (37) |
| $c_p$ | heat capacity per unit mass at constant pressure |
| $c_v$ | heat capacity per unit mass at constant volume |
| D | Fick diffusion coefficient |
| d | collector (target) diameter |
| $d_j$ | nozzle jet diameter |
| F | function |
| f | fuel to air mass flow rate ratio |
| I | mainstream turbulence intensity |
| K | coefficients of curve-fit in equation (11) |
| k | Boltzmann constant |
| L | mainstream turbulence length scale |
| Le | Lewis number (ratio of Fick to thermal diffusivity) |
| $\underline{M}$ | molecular weight |
| M | average molecular weight of the mixture |
| $\dot{m}''$ | deposition mass flux |
| $\underline{Nu}$ | Nusselt number |
| Nu | Perimeter-averaged Nusselt number |
| P | pressure |
| Pr | Prandtl number (ratio of kinematic viscosity to thermal diffusivity) |
| R | universal gas constant |
| Re | Reynolds number |
| S | spin parameter, equation (33) |
| s | defined by equation (31) |
| Sc | Schmidt number (ratio of kinematic viscosity to Fick diffusivity) |
| T | absolute temperature |
| U | velocity |
| v | sonic velocity |
| $W_a$ | air mass flow rate |
| X | mole fraction |

Greek Symbols:

| | |
|---|---|
| $\alpha_T$ | thermal diffusion factor |
| $\alpha_{T,\infty}$ | thermal diffusion factor at infinite temperature |
| $\alpha_{T,-1}$ | coefficient of $T^{-1}$ in power series expansion of $\alpha_T$ |
| $\epsilon$ | Lennard-Jones molecular interaction energy (well-depth) parameter |
| $\gamma$ | specific heat ratio, $c_p/c_v$ |
| $\lambda$ | thermal conductivity |
| $\mu$ | viscosity |
| $\nu$ | number of Na atoms in species i |

| | |
|---|---|
| $\Phi$ | Wilke-Wassiljewa coefficients, equation (21) |
| $\rho$ | density |
| $\sigma$ | Lennard-Jones molecular size parameter |
| $\omega$ | angular speed of the collector (target) |
| $\Omega$ | collision integral |

Subscripts:

| | |
|---|---|
| av | averaged quantity |
| cL | centerline |
| cp | constant properties |
| D | pertaining to Fick diffusion coefficient |
| h | heat transfer |
| i | species i |
| j | jet exit plane, location "j" in figure 1 |
| k | species k |
| m | mass transfer |
| mix | gas mixture |
| o | stagnation conditions |
| t | mainstream turbulence |
| w | target surface (wall) |
| $\mu$ | pertaining to viscosity |
| $\infty$ | mainstream, location "$\infty$" in figure 1 |

Miscellaneous:

| | |
|---|---|
| CEC | chemical equilibrium code |
| CFBL | chemically frozen boundary layer |
| CVD | chemical vapor deposition |

## II. DESCRIPTION OF PROGRAM WITH APPLICATION TO $Na_2SO_4$ DEPOSITION

The CFBL computer code was developed for and is being used to interpret $Na_2SO_4$ deposition experiments at NASA Lewis Research Center, Cleveland, Ohio [3] because of its importance in hot corrosion. Therefore, here we specifically concentrate on $Na_2SO_4$ deposition rate prediction via the transport of many Na containing species to the collector, although the theory is general in that other salts can easily be incorporated. For a typical burner rig and collector configuration, and station nomenclature shown in figure 1, where any Na containing salt is seeded into the combustor, the deposition rate of $Na_2SO_4$ can be shown to be:

$$\dot{m}''_{Na_2SO_4} = \frac{1}{2} \cdot \frac{M_{Na_2SO_4}}{\bar{M}} \cdot F(\text{turb}) \cdot \frac{\rho_\infty}{d} \cdot \sum_i \left\{ \nu_i \cdot D_{i,\infty} \cdot \overline{Nu}_{m,i} \cdot F_i(\text{Soret}) \right.$$

$$\left. \cdot \left[ (X_{i,\infty} - X_{i,w}) - X_{i,w} \cdot \frac{B_{T,i}}{F_i(\text{Soret})} \cdot \left( \frac{Le_{i,w}}{Le_{i,\infty}} \right)^{0.6} \cdot \frac{c_{p,\infty}}{c_{p,w}} \cdot \frac{1}{C_{mh,i}} \right] \right\} \qquad (1)$$

The multicomponent nature of the problem is reflected by the appearance of summations which include each Na carrier species i. The present program

considers four different possible Na carriers: Na, NaOH, $Na_2SO_4$ and NaCl. Note the implicit assumption (checked below via the element flux ratio constraint) that once Na arrives at the surface of the collector by any of Na carriers, there is always enough sulfur available (e.g., supplied to the system by fuel) to form $Na_2SO_4$.

The mole fraction of each Na carrier species in the free stream and at the collector surface ($X_{i,\infty}$ and $X_{i,w}$) is supplied to the program by the user. The theory leads to simple algebraic flux relations for each species since it assumes that there is thermo-chemical equilibrium at stations "$\infty$" and "w", although the boundary layer itself is chemically frozen. In the applications to $Na_2SO_4$ deposition experiments at NASA LeRC, the Chemical Equilibrium Code (CEC) developed at NASA LeRC [4] is used to obtain the equilibrium compositions after combustion at specified temperatures and pressures. However, the CFBL code is by no means restricted to coupling with CEC, and the user may provide $X_{i,\infty}$ and $X_{i,w}$ values by any other means available.

Conditions prevailing at station "w" require the imposition of one additional constraint other than vapor/condensate equilibrium [1,5]. Because $Na_2SO_4$ is being deposited, the molar fluxes of Na and S must stand in the ratio 2:1 at the prevailing vapor compositions. The element mass fractions of the inorganic constituents characterizing the free stream are dictated by the experimental conditions; however, the situation at station "w" is more complicated because transport across the boundary layer contributes to element "segregation." Therefore, the element mass fractions at the surface of the collector generally will not be the same as those in the free stream [5]. Hence, the CFBL program also calculates the total S molar flux to the surface with the same formulation given in equation (1). The dominant S carriers to the surface are chosen to be $SO_2$, $SO_3$, and $H_2S$. Therefore, the user has to provide $X_{i,\infty}$ and $X_{i,w}$ values for $SO_2$, $SO_3$, and $H_2S$ as inputs to the program. For any particular set of $X_{i,\infty}$ and $X_{i,w}$ values, obtained from equilibrium calculations and input to the CFBL program, the output gives the calculated Na to S molar flux ratio. In order to satisfy both the thermodynamic (chemical equilibrium) and the transport (molar flux ratio) constraints, the user has to iterate on $X_{i,w}$ values obtained from equilibrium calculations with clever choices of element mass fractions. Finally, the properly chosen element mass fractions will give the proper equilibrium compositions of Na and S carriers at station "w" which in turn will satisfy the 2:1 Na to S molar flux ratio constraint. Experience with the CFBL program indicates that in cases where the system contains excess S, the predicted $Na_2SO_4$ deposition rates are practically insensistive to the fulfillment of the transport requirement except close to the dew point temperature.†

Modification of the CFBL program for application to the multicomponent chemical vapor deposition of condensates other than $Na_2SO_4$ is conceptually straightforward. It requires the proper choice of dominant carrier species and provision of relevant thermodynamic and transport parameters to the program. Generalized versions of the present CFBL code are being developed and applied to $Na_2SO_4 + K_2SO_4$ and $Na_2SO_4 + K_2SO_4 + Li_2SO_4$ solution condensate deposition situations used at Yale University [5] and NASA LeRC.

---

†For the discussion of the fact that "dew-point" is not a pure thermodynamic quantity, the reader is referred to references [5] and [6].

## III. EVALUATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES

Description of the property calculations given below assumes that the following information is supplied to the program by the user as input for a typical configuration given in figure 1:

| | |
|---|---|
| $d_j$ | jet exit diameter, cm |
| $d$ | diameter of cylindrical collector (target), cm |
| $f$ | fuel to air mass flow rate ratio |
| $P_j$ | jet exit (ambient) pressure, atm |
| $P_o$ | stagnation pressure, atm |
| $T_o$ | stagnation temperature, K |
| $T_w$ | collector surface (wall) temperature, K |
| $W_a$ | air mass flow rate, g/sec |

Note that we are assuming a circular jet and a cylindrical collector. For other geometries proper characteristic dimensions must be supplied to calculate the jet exit area, the Reynolds number and mass transfer Nusselt number.

The combustion is assumed to be complete and dominated by the reaction:

$$CH_2 + 3/2\ O_2 \rightarrow CO_2 + H_2O \tag{2}$$

Hence, starting with air of initial composition: 79.05 mole percent $N_2$ and 20.95 mole percent $O_2$, we estimate the composition of combustion product gases by:

$$X_{N_2} = \frac{0.7905}{1 + 1.0331f} \tag{3}$$

$$X_{O_2} = \frac{0.2095 - 3.0993f}{1 + 1.0331f} \tag{4}$$

$$X_{CO_2} = X_{H_2O} = \frac{2.0662f}{1 + 1.0331f} \tag{5}$$

All other species present in the combustion product gas stream are assumed to be of trace amounts and are neglected in the property calculations.

### A. Calculation of $\bar{M}$, $\gamma$, $T_j$ and $U_j$

Average molecular weight of the combustion gases is obtained from:

$$\bar{M} = X_{N_2}M_{N_2} + X_{O_2}M_{O_2} + X_{CO_2}M_{CO_2} + X_{H_2O}M_{H_2O} \tag{6}$$

where $X$ is the mole fraction of each indicated species.

The ratio of heat capacity at constant pressure to heat capacity at constant volume of the mixture is calculated by:

$$\gamma = \frac{c_{p,mix}}{c_{v,mix}} = \frac{c_{p,mix}}{c_{p,mix} - (R/\bar{M})} \tag{7}$$

where $R$ is the universal gas constant (1.9872 cal/mole - K), and the calculation of $c_{p,mix}$ is described below. Assuming an isentropic jet, the temperature and the velocity at the jet exit plane is given by:

$$T_j = T_o \left(\frac{P_j}{P_o}\right)^{(\gamma-1)/\gamma} \tag{8}$$

and

$$U_j = \frac{RT_j}{P_j \bar{M}} \cdot \frac{W_a(1 + f)}{\left(\pi \frac{d_j^2}{4}\right) \cdot C} \tag{9}$$

where $R$ is the universal gas constant (82.057 atm-cm$^3$/mole-K), and $C$ is the discharge coefficient of the jet nozzle to be supplied by the user. The discharge coefficient depends on the geometric shape of the nozzle and the Reynolds number based on the nozzle diameter. If no information is available for the nozzle discharge coefficient, then the program automatically assigns unity as the value of $C$. Note that the velocity calculated from equation (9) based on the total mass flow rate and the effective area of the nozzle exit should agree with the velocity which can be calculated also from the prevailing Mach number based on the isentropic jet assumption as:

$$U_j = v \cdot \left[\left(\frac{T_o}{T_j} - 1\right) \frac{2}{\gamma - 1}\right]^{1/2} \tag{9a}$$

where $v$ is the sonic speed in the gas mixture at $T_o$. In equation (9) it is assumed that the mixture obeys the ideal gas law, so that the density of the mixture is simply:

$$\rho_j = \frac{P_j \bar{M}}{RT_j} \tag{10}$$

### B. Calculation of $c_p$, $\lambda$, $\mu$, and $D_i$

The dimensionless heat capacity of each dominant species is computed from a curve fit:

$$\left(\frac{c_{p,i} M_i}{R}\right) = K_{5,i}T^4 + K_{4,i}T^3 + K_{3,i}T^2 + K_{2,i}T + K_{1,i} \tag{11}$$

where $R$ is the universal gas constant (1.9872 cal/mole - K). Two different sets of constants, K, are used for $T \geq 1000$ K and $T < 1000$ K for a better fit.

Viscosity, $\mu_i$, and thermal conductivity, $\lambda_i$, of dominant species are calculated using Chapman-Enskog theory:

$$\mu_i = 2.6693 \times 10^{-5} \frac{\sqrt{M_i T}}{\sigma_i^2 \Omega_{\mu,i}} \quad \text{(g/cm-sec)} \tag{12}$$

$$\lambda_i = \frac{R}{M_i}\left[\frac{15}{4} + 1.32\left(\frac{c_{p,i} M_i}{R} - \frac{5}{2}\right)\right]\mu_i \quad \text{(cal/cm-sec-K)} \tag{13}$$

where $\sigma_i$ is the Lennard-Jones molecular size parameter of the species and $\Omega_{\mu,i}$ is the collison integral for viscosity which is a function of the dimensionless temperature $kT/\epsilon_i$ where $k$ is the Boltzmann constant and $\epsilon_i$ the Lennard-Jones molecular interaction energy (well-depth) parameter for species $i$.

The binary Fick diffusion coefficient of trace species $k$ in each of dominant species $i$ is also calculated from Chapman-Enskog theory:

$$D_{kj} = 0.0018583 \frac{\sqrt{T^3\left(\frac{1}{M_k} + \frac{1}{M_i}\right)}}{P\sigma_{ki}^2 \Omega_{D,ki}} \quad \text{(cm}^2\text{/sec)} \tag{14}$$

where

$$\sigma_{ki} = \frac{1}{2} \cdot (\sigma_k + \sigma_i) \quad \text{(Å)} \tag{15}$$

and $\Omega_{D,ki}$ is the collision integral for diffusion coefficient which (just like $\Omega_{\mu,i}$) is also a function of $kT/\epsilon_{ki}$ where:

$$\frac{\epsilon_{ki}}{k} = \frac{\sqrt{\epsilon_k \epsilon_i}}{k} \quad \text{(K)} \tag{16}$$

The dimensionless thermal diffusion factor for trace species $i$ is conveniently expressed below after a curve-fit to calculations based on Chapman-Enskog theory.

$$\alpha_{T,i} = \alpha_{T,\infty,i} + \frac{\alpha_{T,-1,i}}{T} \tag{17}$$

The resulting least-squares constants, $\alpha_{T,\infty,i}$ and $\alpha_{T,-1,i}$ for a number of species are given in reference [7].

It should be noted that unless experimentally determined, the uncertainties involved in the estimation of $\sigma$ and $\epsilon/k$ are directly reflected in $\mu$, $\lambda$, $D$, and $\alpha_T$ values [8]. Therefore the accuracy of prediction of the CFBL program is limited by the accuracy of such transport parameters.

## C. Calculation of Mixture Properties

Specific heat of the gas mixture is simply given by:

$$c_{p,mix} = \sum_i X_i c_{p,i} \tag{18}$$

where $X_i$ is the mole fraction of species $i$. Viscosity and thermal conductivity of the mixture are calculated from similar formulae

$$\mu_{mix} = \sum_i \frac{X_i \mu_i}{\sum_k X_k \Phi_{ki}} \tag{19}$$

$$\lambda_{mix} = \sum_i \frac{X_i \lambda_i}{\sum_k X_k \Phi_{ki}} \tag{20}$$

where $\Phi_{ki}$ are the Wilke-Wassiljewa coefficients given by:

$$\Phi_{ki} = \frac{1}{\sqrt{8}} \cdot \left(1 + \frac{M_i}{M_k}\right)^{-1/2} \cdot \left[1 + \left(\frac{\mu_i}{\mu_k}\right)^{1/2} \left(\frac{M_k}{M_i}\right)^{1/4}\right]^2 \tag{21}$$

The diffusion coefficient of species $i$ in the mixture is calculated from:

$$D_{i,mix} = \left(\sum_k \frac{X_k}{D_{i,k}}\right)^{-1} \tag{22}$$

The reader is referred to reference [9] for the details of thermodynamic and transport property calculations.

# IV. DIMENSIONLESS NUMBERS

The dimensionless numbers given below are evaluated either at station "$\infty$" or "w" depending on relevance. The static temperature at station "$\infty$", $T_\infty$, is assumed to be equal to $T_j$, calculated in Section III.A. The collector surface temperature (or a representative average temperature if the collector is not isothermal) and the ambient pressure, $P_\infty (=P_j)$, are supplied as inputs by the user.

$$Pr = \frac{c_{p,mix}\mu_{mix}}{\lambda_{mix}} \tag{23}$$

$$Sc_i = \frac{\mu_{mix}}{\rho D_{i,mix}} \tag{24}$$

$$Le_i = \frac{Pr}{Sc_i} = \frac{D_{i,mix}}{[\lambda_{mix}/(\rho c_{p,mix})]} \tag{25}$$

$$Re = \frac{\rho U_\infty d}{\mu_{mix}} \tag{26}$$

Calculation of the Reynolds number requires knowledge of $U_\infty$. Although $U_j$ is obtained in Section III.A, $U_\infty$ is not necessarily the same as $U_j$ depending on the jet velocity profile and the jet divergence angle. For jet diameters larger than the collector diameter (usually) the case), one needs the centerline velocity at station "$\infty$" for the proper calculation of Re. However, $U_j$ calculated in Section III.A. is the average velocity at station "j". Therefore, two corrections are needed; first, to correct average $U_j$ to centerline $U_j$, F (shape), and second, to correct centerline $U_j$ to centerline $U_\infty$, F (div). These corrections take into account the boundary layer effects and the flow area variation from station "j" to station "$\infty$" depending on jet divergence angle. Hence:

$$U_\infty = U_j \cdot F\ (shape) \cdot F\ (div) \tag{27}$$

where F (shape) and F (div) are defined as:

$$F\ (shape) \equiv \left(\frac{U_{cL}}{U_{av}}\right)_j \tag{28}$$

$$F\ (div) \equiv \frac{U_{cL,\infty}}{U_{cL,j}} \tag{29}$$

F (shape) and F (div) are optional inputs to the program. If no information is available, the program automatically assigns unity for both. Based on available data for fully developed turbulent flow in smooth circular ducts, a suggested estimate for F (shape) is:

$$F\ (shape) \cong \frac{(s + 1)\ (2s + 1)}{2s^2} \tag{30}$$

where

$$s \cong 6.349\left(\frac{Re_i}{10^4}\right)^{0.0465} \tag{31}$$

The mass transfer Nusselt number correlations depend, among other things, on the geometry of the collector used. In the NASA LeRC experiment [3], a cylindrical collector was used. The example program listing given at the end of this manual also assumes a cylindrical collector. By making the replacement $Pr \rightarrow Sc_i$, the perimeter averaged mass transfer coefficient, $Nu_{m,i}$, becomes based on the heat transfer correlations recommended for stationary infinitly long cylinders [10]. The additional effects of variable properties and Mach number are approximated by incorporating a post-multiplier term based on the recommendations of references [11] and [12].

$$\overline{Nu}_{m,i} = (0.40\ Re^{1/2} + 0.06\ Re^{2/3})\ (Sc_i^{0.4})\left(\frac{T_w}{T_o}\right)^{0.04} \tag{32}$$

It should be noted that if a different collector geometry is used and/or the surface roughness of the collector can have an appreciable effect on mass transfer, the equation (32) may not be applicable, and the user has to modify the program to supply the best available corresponding mass transfer Nusselt number correlation from the literature.

In many experiments, uniformity of collector surface temperature is obtained by collector rotation and this requires additional modifications of the formulation given by equation (1). In the NASA LeRC deposition experiments the rotational speeds of the smooth collectors used have been neglected based on reference [13], which suggests that if one defines a "spin" parameter

$$S \equiv \frac{\omega d}{2U_\infty} \tag{33}$$

where $\omega$ is the angular speed of the target, then equation (1) (or eq. (32)) should be corrected by the multiplier

$$F\ (spin) \cong (1 + 2S^2)^{0.315} \tag{34}$$

## V. THERMAL (SORET) DIFFUSION EFFECT, F (SORET)

Inclusion of thermal (Soret) diffusion in the mass transfer calculations introduces a nondimensional thermophoretic parameter, [14], which can be expressed as:

$$B_{T,i} \cong -\alpha_{T,i,w} \cdot (Le_{i,w})^{0.4} \cdot \left(\frac{T_o - T_w}{T_w}\right) \tag{35}$$

The effects of thermal (Soret) diffusion ("thermophoresis" for small particles) is thoroughly discussed and correlated in references [7, 14-17] for both vapor and small particle mass transfer. For the current applications of the CFBL program to NASA LeRC deposition experiments, the emphasis has been on vapor

deposition. Therefore, the "sink" effect of thermal diffusion is justifiably neglected, and only the "suction" effect is considered, i.e.:

$$F_i \text{ (Soret)} \cong F_i \text{ (suction)} \cong \frac{-B_{T,i}}{1 - \exp(B_{T,i})} \tag{36}$$

For small particle mass transfer applications where inertial effects are not important, the user should modify the program to include the "thermophoretic sink" effect as described in references [14] and [16]. For such applications a method for estimating small particle transport properties ($D_i$, $\alpha_{T,i}$, etc.) is given in reference [17].

In the program the user also has the option of completely "turning off," if so desired, the thermal diffusion effect from inclusion in the calculations by specifying the input variable "FSORET" as "false". In this simple way we can demonstrate the relative importance of thermal diffusion mass transport in any multicomponent CVD situation.

It is known that variable properties across the boundary layer affect mass transfer rates in a somewhat different manner than they do the better known heat transfer rates. In case of thermal diffusion, this effect is in addition to the one already incorporated in the perimeter-averaged Nusselt number (eq. (32)). Certainly, the effect will be different depending on the temperature dependence of the transport properties of the species in question and the characteristics of the mass transfer boundary layer. Therefore, it is convenient to introduce a new dimensionless parameter, $C_{mh,i}$, defined as:

$$C_{mh,i} \equiv \frac{(Nu_m/Nu_{m,cp})_i}{(Nu_h/Nu_{h,cp})} \tag{37}$$

Simple engineering correlations to predict the effect of variable properties on mass transfer (the numerator in eq. (37)) and on heat transfer (the denomenator in eq. (37)) are given in reference [12]. However, if the space reserved for $C_{mh,i}$ in the input data is left blank, the program automatically assigns a value of unity for each $C_{mh,i}$.

## VI. MAINSTREAM TURBULENCE EFFECT, F (turb)

It is known that mainstream turbulence, apart from turbulence within the boundary layer, influences the transport rates to surfaces [18-19]. Although there is considerable quantitative disagreement among various researchers, the CFBL program uses the correlation given in reference [20] based on perimeter-averaged heat transfer measurements for cylinders in cross flow. If one has knowledge of free stream turbulence intensity, $I_t$, and axial macroscale of turbulence, $L_t$, then the correlation at a particular Re for a cylinder of diameter d is given in the separable form:

$$F \text{ (turb)} \cong 1 + fct_1(I_t Re) \cdot fct_2(L_t/d) \tag{38}$$

where $fct_1$ and $fct_2$ are presented in graphical form in reference [20]. The CFBL program uses the following curve fits for $fct_1$ and $fct_2$.

$$\text{fct}_1(I_t\text{Re}) \cong \begin{cases} 12.375\left[1 - \left(1 - \dfrac{I_t\text{Re}}{10^4}\right)^{3/2}\right] & \text{if } I_t\text{Re} \le 10^4 \\ 9.0 + 3.375\text{x}10^{-4}\, I_t\text{Re} & \text{if } I_t\text{Re} > 10^4 \end{cases} \tag{39}$$

$$\text{fct}_2(L_t/d) \cong \begin{cases} 0.124\text{x}10^{-3}[(L_t/d) - 11.0]^2 + 2.0\text{x}10^{-3} & \text{if } L_t/d > 2 \\ -4.0\text{x}10^{-3}[(L_t/d) - 1.75]^2 + 12.25\text{x}10^{-3} & \text{if } L_t/d \le 2 \end{cases} \tag{40}$$

F (turb) probably also depends on $Sc_i$, but the information is not yet sufficient in the literature to incorporate it into the present formalism. The user has three options in using the F (turb) factor:

1. If one chooses not to use the F (turb) factor, then leave the variable "TURB" blank in input data, in which case the program automatically assigns the value of unity for F (turb).
2. If the particular F (turb) to be used by the program is known, then that value should be read in as input for the variable "TURB", but leave the variables "TURIN" and "TURL" blank.
3. If one has knowledge of $I_t$ and $L_t$ and chooses to use the correlation supplied by the program based on equations (38) to (40), then input data for "TURB" is dummy, but "TURIN" (percent $I_t = I_t/100$) and "TURL" input values must be read in.

## VII. ROUTINES

The names and functions of the subroutines used in the program are given below:

| | |
|---|---|
| MAIN | calculates the deposition rate based on equation (1) |
| PARAM | provides $\epsilon/k$, $\sigma$, and molecular weight of dominant species in the gas mixture |
| CALESL | provides the dimensionless heat capacity of dominant species in the gas mixture from a curve fit |
| CALMIX | calculates $c_{p,mix}$ in cal/g-K |
| COLINT | evaluates $\Omega_\mu$ and $\Omega_D$ from a curve fit to the already supplied $kT/\epsilon$ versus $\Omega_\mu$ and $\Omega_D$ data [8]. Also calculates $\mu_i$ and $\lambda_i$ for dominant species |
| MIXPRO | calculates $\mu_{mix}$ and $\lambda_{mix}$ |
| COEDIF | calculates $D_{ki}$ of trace species k in i |
| DIF | calculates $D_{i,mix}$ |
| TMDF | calculates F (Soret) |
| NUM | calculates $Nu_{m,i}$ |
| TURBL | calculates F (turb) |

## VIII. DESCRIPTION OF PROGRAM INPUT

The input data to the CFBL program is read in three different stages. The first stage reads in one card which contains the following information according to the format specified.

```
  READ(5,1) IRUN, ITYPE, F, WA, TW, TO, PO, PJ, DC, WOBS, FSORET
1 FORMAT(2I2, 8F9.0, 3X, L1)
```

| | |
|---|---|
| IRUN | The user can use this variable for his own purposes (e.g., to keep track of which experiment, which run, etc.). |
| ITYPE | The user can use this variable for his own purposes (e.g., to keep track of the type of salt fed to the combustor, etc.). |
| F | Fuel to air mass flow rate ratio |
| WA | Air flow rate, g/sec |
| TW | Collector (target) surface temperature, K. Give an average temperature if the collector surface is not isothermal. |
| TO | Stagnation temperature, K |
| PO | Stagnation pressure, atm |
| PJ | Jet exit (ambient) pressure, atm |
| DC | Discharge coefficient of jet nozzle. Optional input. Leave blank if no information is available. See Section III.A. |
| WOBS | Experimentally observed deposition rate. Used in calculating the percent error in the prediction, mg/hr. |
| FSORET | Logical variable. Specify as 'T' if thermal diffusion is desired to be included in the calculations, or as 'F' if otherwise. |

The second stage reads in one card which contains the following information according to the format specified:

```
    READ(5,998) DIAW, LW, DJ, TURB, TURIN, TURL, SHAPE, DIV
998 FORMAT(8F10.0)
```

| | |
|---|---|
| DIAW | Diameter of the cylindrical target, cm |
| LW | Length (height) of the cylindrical target, cm |
| DJ | Diameter of circular jet nozzle exit plane, cm |
| TURB | Turbulence enhancement factor, F (turb). Optional input.<br>(a) Leave blank if no consideration is required.<br>(b) Give your own estimate if information is available, but then leave "TURIN" and "TURL" blank, |
| TURIN | Percent mainstream turbulence intensity ($I_t$/100). Optional input.<br>(a) Leave blank if no consideration is required.<br>(b) Leave blank if you supply your own "TURB".<br>(c) Give your estimate if program consideration is desired, but then specify "TURL", too. |
| TURL | Axial macroscale of mainstream turbulence, cm. Optional input.<br>(a) Leave blank if no consideration is required.<br>(b) Leave blank if you supply your own "TURB".<br>(c) Give your own estimate if program consideration is desired, but then specify "TURIN", too. |
| SHAPE | F (shape). Optional input. Leave blank if no information is available. See Section IV. |
| DIV | F (div). Optional input. Leave blank if no information is available. See Section IV. |

The third stage reads in seven cards, one for each species. The order is given by:

1 = NaOH
2 = Na
3 = $Na_2SO_4$
4 = $SO_2$
5 = $SO_3$
6 = NaCl
7 = $H_2S$

Note that this input is specific to $Na_2SO_4$ deposition only, and must be modified for other salts and/or salt solutions accordingly. Each card contains the following information according to the format specified.

```
  READ(5,2) XW(I), XJ(I), CMH(I)
2 FORMAT(2E15.4, F10.0)
```

XW(I) Equilibrium mole fraction of species i at station "w"
XJ(I) Equilibrium mole fraction of species i at station "j" or equivalently at station "∞"
CMH(I) Ratio of effect of variable properties on mass transfer to heat transfer. Optional input. See Section V.

A typical input data set is given in Appendix A.

## IX. DESCRIPTION OF PROGRAM OUTPUT

The program output contains all the information read into the program as input. Description of the additional variables printed out is given below:

| | |
|---|---|
| D(I) | Diffusion coefficient of species i in gas mixture, $D_{i,mix}$, in $cm^2/sec$ |
| NU(I) | Mass transfer Nusselt number of species i, $Nu_{m,i}$ |
| SC(I) | Schmidt number of species i, $Sc_i$, at station "∞" |
| TAU(I) | Thermophoretic parameter of species i, $B_{T,i}$ |
| F(SORET)(I) | $F_i$(Soret) of species i |
| M(I) | Equivalent $Na_2SO_4$ deposition rate of species i mass transfer rate in mg/hr |
| YNAJ | Total Na mole fraction in flame |
| YNAW | Total Na mole fraction at station "w" |
| YSJ | Total S mole fraction in flame |
| YSW | Total S mole fraction at station "w" |
| AM | Average molecular weight of gas mixture (neglects trace species) |
| TURB | F(turb) |
| RE | Reynolds number at station "∞" |
| SUM | Total Na mass flux to the surface in $g/cm^2$-sec |
| SMS | Total S mass flux to the surface in $g/cm^2$-sec |
| RATIO | Na to S molar flux ratio at the surface |
| ERROR | Percent error between experimentally observed and predicted $Na_2SO_4$ deposition rates |
| GM | $\gamma = c_{p,mix}/c_v$ |
| PR | Prandtl number at station "∞" |

| | |
|---|---|
| X(I) | Mole fraction of dominant species in flame |
| TJ | Jet exit static temperature, $T_j = T_\infty$, K |
| RHOJ | Density of gas mixture at station "j" or equivalently "$\infty$" in $g/cm^3$ |
| UJ | Jet exit velocity, $U_j$, in cm/sec |
| ETAMIX | $\mu_{mix}$ at station "$\infty$" in g/cm-sec |
| LAMIX | $\lambda_{mix}$ at station "$\infty$" in cal/cm-sec-K |
| CMIX | $c_{p,mix}$ at station "$\infty$" in cal/g-sec |

A typical output data set is given in Appendix B.

```
12345678901234567890123456789012345678901234567890123456789012345678901234567890**** REFERENCE LINE

         F          WA          TW          TO          PO          PJ          DC        WOBS     FSORET
19 2  0.0481   20.0214       900.0      1885.5       1.068       1.000       1.000       27.00          T
  DIAW              LW          DJ        TURB       TURIN        TURL       SHAPE                   DIV
 1.905          1.2649        2.54         0.0         0.0         0.0         0.0                   0.0
        XW(I)                   XJ(I)      CMH(I)
     6.9810E-14          6.3810E-06         0.0
     3.1280E-20          8.2740E-07         0.0
     3.6060E-12          2.6170E-13         0.0
     8.0742E-06          2.4994E-05         0.0
     1.3345E-05          4.8236E-08         0.0
     0.0                 0.0                0.0
     5.9210E-31          1.1600E-14         0.0

12345678901234567890123456789012345678901234567890123456789012345678901234567890**** REFERENCE LINE
```

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

ALL GAS PROPERTIES PERTAIN TO TJ,PJ

IRUN =19
ITYPE = 2
F = 0.048100
TW (K) = 900.000
TO (K) = 1885.500
PO (ATM) = 1.068000
PJ (ATM) = 1.000000
DC = 1.000000
WOBS (MG/HR) = 27.0000
FSORET =T
WA (G/SEC) = 20.02139
DIAW (CM) = 1.90500
LW (CM) = 1.26490
DJ (CM) = 2.54000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000
SHAPE = 0.0000
DIV = 0.0000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

| I | D(I) | NU(I) | SC(I) | X(I),J | X(I),W | TAU(I) | F(SORET),I | M(I) |
|---|---|---|---|---|---|---|---|---|
| 1 | 0.29905E 01 | 0.78633E 02 | 0.10820E 01 | 0.63810E-05 | 0.69810E-13 | 0.73861E-01 | 1.03738 | 0.10364E 02 |
| 2 | 0.37881E 01 | 0.71538E 02 | 0.85418E 00 | 0.82740E-06 | 0.31280E-19 | -0.23133E-01 | 0.98848 | 0.14756E 01 |
| 3 | 0.18316E 01 | 0.95670E 02 | 0.17666E 01 | 0.26170E-12 | 0.36060E-11 | 0.26800E 00 | 1.13998 | -0.64711E-05 |
| 6 | 0.25178E 01 | 0.84235E 02 | 0.12851E 01 | 0.00000 | 0.00000 | 0.15291E 00 | 1.07840 | 0.00000 |

| YNAJ | YNAW | YSJ | YSW |
|---|---|---|---|
| 0.720840E-05 | 0.728181E-11 | 0.250422E-04 | 0.214192E-04 |

AM = 28.81070
TURB = 1.00000
RE = 12913.625
SUM (G/CM**2/SEC) = 0.14063E-06
SMS (G/CM**2/SEC) = 0.26371E-06
RATIO = 0.7437
PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 11.83948
ERROR (%) = -56.1501
GM = 1.26601
PR = 0.689647
X(N2) = 0.753079
X(O2) = 0.057563
X(H2O) = 0.094679
X(CO2) = 0.094679
TJ (K) = 1859.6157

| RHOJ(G/CM**3) | UJ(CM/S) | ETAMIX(POISE) | LAMIX(CAL/CM/K/S) | CMIX(CAL/G/S) |
|---|---|---|---|---|
| 0.188806E-03 | 0.219344E 05 | 0.610923E-03 | 0.290277E-03 | 0.327682E 00 |

# APPENDIX C

```
0000100 C
0000200 C*************************************************************************************
0000300 C
0000400 C
0000500 C                    V A R I A B L E   N A M E   L I S T
0000600 C                    ---------------   -------   -------
0000700 C
0000800 C
0000900 C  VARIABLE                          DESCRIPTION
0001000 C
0001100 C  ADT          = TEMPORARY STORAGE VALUE FOR KT/E
0001200 C  AII,AJJ      = TEMPORARY STORAGE VALUE FOR DATOS(3,I)
0001300 C  AJ           = AREA OF JET NOZZLE (CM**2)
0001400 C  ALPA(79)     = KT/E AS INPUT PERMANENT DATA
0001500 C  ALPHA(I)     = THERMAL DIFFUSION COEFFICIENT FOR TRACE SPECIES I
0001600 C  AM           = MEAN MOLEC. WEIGHT OF GAS MIXTURE(NEGLECTS TRACE SPECIES)
0001700 C  APHMIX       = THERMAL DIFFUSIVITY OF MIXTURE AT STATION J
0001800 C  APHW         = THERMAL DIFFUSIVITY OF MIXTURE AT STATION W
0001900 C  AW           = AREA OF THE COLLECTOR(TARGET), (CM**2)
0002000 C
0002100 C  C            = CMIX INTERMEDIATE
0002200 C  CJ           = DIMENSIONLESS HEAT CAPACITY
0002300 C  CMIX         = MIXTURE HEAT CAPACITY AT STATION J (CAL/(G*K))
0002400 C  CMH(I)       = RATIO OF EFFECT OF VARIABLE PROP. ON MASS TO HEAT TRANS.
0002500 C                   OPTIONAL INPUT.LEAVE BLANK IF NO INFORMATION AVAILABLE.
0002600 C  COEF1        = COEFFICIENTS FOR COMPUTING HEAT CAPACITY (1000K<T<5000K)
0002700 C  COEF2        = COEFFICIENTS FOR COMPUTING HEAT CAPACITY (300K<T<1000K)
0002800 C  CONDT        = THERMAL CONDUCTIVITY (TEMPORARY) , (CAL/(CM*SEC*K))
0002900 C  CP           = MIXTURE HEAT CAPACITY AT STATION W (CAL/(G*K))
0003000 C
0003100 C  D            = TEMPORARY STORAGE FOR BINARY DIFF. COEF. (CM**2/SEC)
0003200 C  DC           = DISCHARGE COEFFICIENT OF JET NOZZLE. OPTIONAL INPUT.
0003300 C                   LEAVE BLANK IF NO INFORMATION IS AVAILABLE, IN WHICH
0003400 C                   CASE THE PROGRAM AUTOMATICALLY ASSIGNS UNITY AS ITS VALUE
0003500 C  DA           = DIFF. COEFF. OF TRACE SPECIES AT STATION J (CM**2/SEC)
0003600 C  DATOS(1,I)= E/K FOR SPECIES I
0003700 C  DATOS(2,I)= SIGMA FOR SPECIES I (COLLISION DIAMETER PARAMETER)
0003800 C  DATOS(3,I)= MOLECULAR WEIGHT OF SPECIES I
0003900 C  DEN          = DENOMINATOR
0004000 C  DIAW         = DIAMETER OF THE CYLINDERICAL COLLECTOR (CM)
0004100 C  DIFF         = TEMPORARY STORAGE FOR BINARY DIFF. COEF. (CM**2/SEC)
0004200 C  DIV          = DIVERGENCE FACTOR FOR NOZZLE JET DEFINED AS THE RATIO
0004300 C                   OF CENTERLINE VELOCITY AT COLLECTOR LOCATION TO
0004400 C                   CENTERLINE VELOCITY AT JET EXIT. DEPENDS ON THE JET
0004500 C                   DIVERGENCE ANGLE. OPTIONAL INPUT, LEAVE BLANK IF NO
0004600 C                   INFORMATION AVAILABLE.
0004700 C  DJ           = DIAMETER OF JET NOZZLE EXIT PLANE (CM)
0004800 C  DW           = DIFF. COEF. OF TRACE SPECIES AT STATION W (CM**2/SEC)
0004900 C
0005000 C  E/K          = RATIO OF MOLECULAR INTERACTION ENERGY PARAMETER
0005100 C                   (LENNARD-JONES) TO BOLTZMANN CONSTANT (K)
0005200 C  EOKI,EOKJ = TEMPORARY STORAGE FOR DATOS(1,I)=E/K
0005300 C  EOVKIJ       = E/K, SQUARE ROOT OF EOKI*EOKJ
0005400 C  EPSOVK      = DATOS(1,I)=E/K
```

```
0005500 C  ERN         = DIFFERENCE BETWEEN PREDICTED AND OBSERVED DEPO. RATES
0005600 C  ERROR       = PERCENT ERROR BETWEEN PREDICTED AND OBSERVED DEP. RATE
0005700 C  ET          = EXPONENTIAL(-TAU), SORET INTERMEDIATE
0005800 C  ETA         = MIXTURE VISCOSITY AT STATION W (G/(CM*SEC))
0005900 C  ETAMJ       = TEMPORARY VALUE FOR MIXTURE VISCOSITY (G/(CM*SEC))
0006000 C  ETAMIX      = MIXTURE VISCOSITY AT STATION J (G/(CM*SEC))
0006100 C
0006200 C  F           = FUEL TO AIR RATIO (BY MASS)
0006300 C  FSORET      = LOGICAL VALUE PLACED INTO THE INPUT DATA FILE.  IF IT IS
0006400 C                SET TO 'T' THEN THE SORET EFFECT WILL BE INCLUDED.  IF IT
0006500 C                IS SET TO 'F' THEN THE SORET EFFECT WILL BE EXCLUDED.
0006600 C
0006700 C  GM          = GAMMA
0006800 C  GMR         = (GAMMA-1.)/GAMMA
0006900 C  G           = WASSILJEWA-WILKE FACTOR
0007000 C
0007100 C  ITYPE       = NOT USED BY PROGRAM. OPTIONAL FOR USER PURPOSES.
0007200 C  IRUN        = NOT USED BY PROGRAM. OPTIONAL FOR USER PURPOSES.
0007300 C
0007400 C  LAMDA       = MIXTURE THERMAL CONDUCTIVITY AT STATION W (CAL/(CM*SEC*K))
0007500 C  LAMP        = TEMPORARY THERMAL CONDUCTIVITY (CAL/(CM*SEC*K))
0007600 C  LAMIX       = MIXTURE THERMAL CONDUCTIVITY AT STATION J (CAL/(CM*SEC*K))
0007700 C  LEJ         = LEWIS NUMBER FOR TRACE SPECIES AT STATION J
0007800 C  LOD         = RATIO OF MAINSTREAM TURBULENCE LENGTH SCALE TO COLLECTOR DIAM.
0007900 C  LW          = LENGTH OF THE CYLINDERICAL COLLECTOR (CM)
0008000 C  LEW         = LEWIS NUMBER FOR TRACE SPECIES AT STATION W
0008100 C
0008200 C  M           = DATOS(3,1)=MOLECULAR WEIGHT OF SPECIES I
0008300 C  M(I)        = EQUIVALENT NA2SO4 DEPOSITION RATE OF TRACE SPECIES MASS
0008400 C                TRANSFER RATE (MG/HR)
0008500 C
0008600 C  NU          = NUSSELT NUMBER FOR MASS TRANSFER
0008700 C
0008800 C  OMEDT,OVDT= COLLISION INTEGRALS
0008900 C  OMED(79)    = COLLISION INTEGRAL FOR MASS DIFFUSIVITY
0009000 C  OME (79)    = COLLISION INTEGRAL FOR VISCOSITY OR THERMAL CONDUCTIVITY
0009100 C
0009200 C  PHI         = F(TURB) INTERMEDIATE RELATED TO TURBULENCE INTENSITY
0009300 C  PJ          = JET EXIT PLANE PRESSURE (ATM)
0009400 C  PO          = STAGNATION PRESSURE (ATM)
0009500 C  PR          = PRANDTL NUMBER AT STATION J
0009600 C  PROV        = INTERMEDIATE  IN CALCULATION OF ETAMIX
0009700 C  PSI         = F(TURB) INTERMEDIATE RELATED TO TURBULENCE LENGTH SCALE
0009800 C
0009900 C  R           = GAS CONSTANT=1.9872 CAL/(GMOLE*K)
0010000 C  RATIO       = SODIUM TO SULFUR MOLAR FLUX RATIO
0010100 C  RE          = REYNOLDS NUMBER AT COLLECTOR LOCATION
0010200 C  REJ         = REYNOLDS NUMBER AT OUTLET OF JET
0010300 C  RHOJ        = DENSITY OF MIXTURE AT JET OUTLET
0010400 C  RHOW        = DENSITY OF MIXTURE AT WALL
0010500 C
0010600 C  SC          = SCHMIDT NUMBER FOR TRACE SPECIES AT STATION J
0010700 C  SHAPE       = SHAPE FACTOR (CENTERLINE VELOCITY)/(AVERAGE VELOCITY)
0010800 C                OPTIONAL INPUT. LEAVE BLANK IF NO INFORMATION AVAILABLE.
```

```
0010900 C   SIGMA      = MOLECULAR SIZE PARAMETER (LENNARD-JONES)
0011000 C   SIGI,SIGJ = TEMPORARY STORAGE FOR DATOS(2,I)=SIGMA
0011100 C   SIGK,SIGL = TEMPORARY STORAGE FOR DATOS(2,I)=SIGMA
0011200 C   SIG2       = DATOS(2,I)=SIGMA
0011300 C   SIG        = SIGMA VALUE FOR SPECIES I
0011400 C   SM(I)      = MASS FLUX OF TRACE SPECIES I (G/CM**2/SEC)
0011500 C   SMS        = TOTAL SULFUR MASS FLUX TO THE SURFACE (G/CM**2/SEC)
0011600 C   SUM        = TOTAL SODIUM MASS FLUX TO THE SURFACE (G/CM**2/SEC)
0011700 C
0011800 C   T          = TEMPERATURE (K)
0011900 C   TAU        = SORET SUCTION PARAMETER FOR SPECIES I
0012000 C   TO         = STAGNATION TEMPERATURE (K)
0012100 C   THERM      = THERMAL DIFFUSION FACTOR FOR SPECIES I
0012200 C   TJ         = JET (STATIC) TEMPERATURE (K)
0012300 C   TURB       = TURBULENCE ENHANCEMENT FACTOR. OPTIONAL INPUT.
0012400 C                  A) LEAVE BLANK IF NO CONSIDERATION REQUIRED.
0012500 C                  B) GIVE YOUR OWN ESTIMATE IF INFORMATION AVAILABLE, BUT
0012600 C                     LEAVE 'TURIN' AND 'TURL' BLANK IF YOU DO SO.
0012700 C   TURIN     = PERCENT MAINSTREAM INTENSITY. OPTIONAL INPUT.
0012800 C                  A) LEAVE BLANK IF NO CONSIDERATION REQUIRED.
0012900 C                  B) LEAVE BLANK IF YOU SUPPLY YOUR OWN 'TURB'.
0013000 C                  C) GIVE YOUR ESTIMATE IF PROGRAM CONSIDERATION DESIRED,
0013100 C                     BUT THEN GIVE AN ESTIMATE FOR 'TURL',TOO.
0013200 C   TURL       = MAINSTREAM LENGTH SCALE (MACRO) , CM. OPTIONAL INPUT.
0013300 C                  A) LEAVE BLANK IF NO CONSIDERATION REQUIRED.
0013400 C                  B) LEAVE BLANK IF YOU SUPPLY YOUR OWN 'TURB'.
0013500 C                  C) GIVE YOUR ESTIMATE IF PROGRAM CONSIDERATION DESIRED,
0013600 C                     BUT THEN GIVE AN ESTIMATE FOR 'TURIN',TOO.
0013700 C   TW         = WALL TEMPERATURE (K)
0013800 C
0013900 C   UJ         = JET EXIT VELOCITY
0014000 C
0014100 C   VISC(I)    = VISCOSITY OF SPECIES (G/(CM*SEC))
0014200 C   V(I)       = NUMBER OF SODIUM ATOMS IN TRACE SPECIES I
0014300 C
0014400 C   WA         = AIR FLOW RATE (G/SEC)
0014500 C   WI,WJ      = TEMPORARY STORAGE VALUES FOR DATOS(3,I)
0014600 C   WPRED      = PREDICTED NA2SO4 DEPOSITION RATE (MG/HR)
0014700 C   WOBS       = EXPERIMENTALLY OBSERVED NA2SO4 DEPOSTION RATE (MG/HR)
0014800 C
0014900 C   XJ(I)      = MOLE FRACTION OF SPECIES I IN FLAME
0015000 C   XI         = TURIN*RE/100,F(TURB) INTERMEDIATE
0015100 C   XW(I)      = MOLE FRACTION OF SPECIES I AT WALL
0015200 C   X(4)       = MOLE FRACTION OF DOMINANT SPECIES IN MIXTURE
0015300 C
0015400 C   YNAJ       = TOTAL SODIUM MOLE FRACTION IN FLAME
0015500 C   YNAW       = TOTAL SODIUM MOLE FRACTION AT STATION W
0015600 C   YSJ        = TOTAL SULFUR MOLE FRACTION IN FLAME
0015700 C   YSW        = TOTAL SULFUR MOLE FRACTION AT STATION W
0015800 C
0015900 C
0016000 C*************************************************************************************
0016100 C
0016200 C
```

```
0016300 C  SODIUM VERSION OF CHEMICALLY FROZEN BOUNDARY LAYER THEORY
0016400 C  USED FOR SODIUM SULFATE DEPOSITION RATE CALCULATIONS
0016500 C
0016600 C  MAIN PROGRAM
0016700 C
0016800       REAL LAMIX,LAMDA,LEW,LEJ,NU,LW
0016900       REAL M(7)
0017000       DIMENSION V(7),XW(7),XJ(7),SM(7),ALPHA(7),CMH(7)
0017100       COMMON/VA/DATOS(3,5)
0017200       LOGICAL FSORET
0017300       COMMON FSORET
0017400       COMMON/GFR/X(4)
0017500       DATA V/ 1.0 , 1.0 , 2.0 , 0.0 , 0.0 , 1.0 , 0.0 /
0017600 C
0017700       WRITE(6,490)
0017800   490 FORMAT(10X,'CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE',/)
0017900       WRITE(6,900)
0018000   900 FORMAT(10X,'ALL GAS PROPERTIES PERTAIN TO TJ,PJ',/)
0018100 C
0018200 C*****************************************************************
0018300 C                                                               *
0018400 C     PAY SPECIAL ATTENTION TO THE FORMAT OF THE INPUT PARAMETERS *
0018500 C     SEE 'VARIABLE NAME LIST' ABOVE FOR DESCRIPTION OF VARIABLES *
0018600 C                                                               *
0018700 C*****************************************************************
0018800 C
0018900 C  DOMINANT SPECIES IN THE MIXTURE
0019000 C  1=NITROGEN , 2=OXYGEN , 3=WATER , 4=CARBON DIOXIDE
0019100 C
0019200 C  TRACE SPECIES IN THE MIXTURE
0019300 C  1=NAOH , 2=NA , 3=NA2SO4 , 4=SO2 , 5=SO3 , 6=NACL , 7=H2S
0019400 C
0019500 C
0019600 C  INPUT : 1
0019700 C
0019800       READ(5,1)IRUN,ITYPE,F,WA,TW,TO,PO,PJ,DC,WOBS,FSORET
0019900     1 FORMAT(2I2,8F9.0,3X,L1)
0020000 C
0020100 C  INPUT : 2
0020200 C
0020300       READ(5,998) DIAW,LW,DJ,TURB,TURIN,TURL,SHAPE,DIV
0020400   998 FORMAT(8F10.0)
0020500 C
0020600 C  INPUT : 3
0020700 C
0020800       DO 502 I=1,7
0020900       READ(5,2) XW(I),XJ(I),CMH(I)
0021000     2 FORMAT(2E15.4,F10.0)
0021100   502 CONTINUE
0021200 C
0021300 C  OUTPUT OF INPUT PARAMETERS
0021400 C
0021500       WRITE(6,978) IRUN,ITYPE,F,TW,TO,PO,PJ,DC,WOBS,FSORET
0021600   978 FORMAT(10X,'IRUN =',I2,/,10X,'ITYPE =',I2,/,10X,'F =',          -
```

```
0021700       *F10.6,/,10X,'TW (K) =',F10.3,/,10X,                -
0021800       *'TO (K) =',F10.3,/,10X,'PO (ATM) =',F10.6,/,10X,'PJ (ATM) =',F10.6-
0021900       *,/,10X,'DC =',F9.6/10X,'WOBS (MG/HR) =',F10.4,/,10X,'FSORET =',L1)
0022000        WRITE(6,988) WA,DIAW,LW,DJ,TURIN,TURL,SHAPE,DIV
0022100    988 FORMAT(10X,'WA (G/SEC) =',F10.5,/,10X,'DIAW (CM) =',F10.5,      -
0022200       */,10X,'LW (CM) =',F10.5,/,10X,'DJ (CM) =',F10.5,/,10X,           -
0022300       *'TURIN =',F8.4,'  PERCENT',/,10X,'TURL (CM) =',F10.5,/,10X,       -
0022400       *'SHAPE =',F7.4,/,10X,'DIV =',F7.4)
0022500        WRITE(6,939)
0022600    939 FORMAT(/,10X,'I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL',/)
0022700 C
0022800 C   ASSIGN E/K,SIGMA AND MOLECULAR WEIGHT OF DOMINANT SPECIES
0022900 C
0023000        DATOS(1,1)=71.4
0023100        DATOS(2,1)=3.798
0023200        DATOS(3,1)=28.0134
0023300        DATOS(1,2)=106.7
0023400        DATOS(2,2)=3.467
0023500        DATOS(3,2)=31.9988
0023600        DATOS(1,3)=356.0
0023700        DATOS(2,3)=2.649
0023800        DATOS(3,3)=18.0152
0023900        DATOS(1,4)=195.2
0024000        DATOS(2,4)=3.941
0024100        DATOS(3,4)=44.0098
0024200 C
0024300 C   THERMAL DIFFUSION FACTOR OF TRACE SPECIES
0024400 C   I==NAOH,I=2=NA,I=3=NA2SO4,I=4=SO2,I=5=SO3,I=6=NACL,I=7=H2S
0024500 C
0024600        ALPHA(1)=0.1592*(1.-429.5/TW)
0024700        ALPHA(2)=-0.0607*(1.-551.2/TW)
0024800        ALPHA(3)=0.7828*(1.-476.2/TW)
0024900        ALPHA(4)=0.3131*(1.-198.2/TW)
0025000        ALPHA(5)=0.3877*(1.-184.3/TW)
0025100        ALPHA(6)=0.3462*(1.-420.0/TW)
0025200        ALPHA(7)=0.0592*(1.-79.38/TW)
0025300 C
0025400 C   COMPUTE THE AVERAGE MOLECULAR WEIGHT OF MIXTURE
0025500 C   (NEGLECT THE TRACE SPECIES)
0025600 C   1=NITROGEN,2=OXYGEN,3=WATER,4=CARBON DIOXIDE
0025700 C   MOLE FRACTIONS OF DOMINANT SPECIES AFTER COMBUSTION
0025800 C
0025900        DEN=1.+1.0331*F
0026000        X(1)=0.7905/DEN
0026100        X(2)=(0.2095-3.0993*F)/DEN
0026200        X(3)=2.0662*F/DEN
0026300        X(4)=X(3)
0026400        AM=DATOS(3,1)*X(1)+DATOS(3,2)*X(2)+DATOS(3,3)*X(3)+DATOS(3,4)*X(4)
0026500 C
0026600 C   CALCULATE JET EXIT TEMPERATURE,(K), AND VELOCITY,(CM/SEC)
0026700 C
0026800        CALL CALMIX(TO,AM,CMIX)
0026900        GM=CMIX/(CMIX-1.9872/AM)
0027000        GMR=(GM-1.)/GM
```

```
0027100        AJ=3.14159*DJ*DJ/4.
0027200        TJ=TO*(PJ/PO)**GMR
0027220        IF(DC.EQ.0.00) DC=1.00
0027300        UJ=((82.057*TJ)/(PJ*AM))*(WA*(1.+F))/(AJ*DC)
0027400 C
0027500 C   CALCULATE MIXTURE PROPERTIES AT STATIONS J AND W
0027600 C
0027700        RHOJ=PJ*AM/TJ/82.057
0027800        RHOW=PJ*AM/TW/82.057
0027900        CALL CALMIX(TJ,AM,CMIX)
0028000        CALL CALMIX(TW,AM,CP)
0028100        CALL MIXPRO(TJ,ETAMIX,LAMIX)
0028200        CALL MIXPRO(TW,ETA,LAMDA)
0028300        APHMIX=LAMIX/CMIX/RHOJ
0028400        APHW=LAMDA/CP/RHOW
0028500        PR=CMIX*ETAMIX/LAMIX
0028600 C
0028700 C   CALCULATE REYNOLDS NUMBER
0028800 C
0028900        IF(SHAPE.EQ.0.0) SHAPE=1.0
0029000        IF(DIV.EQ.0.0) DIV=1.0
0029100        REJ=RHOJ*UJ*DIAW/ETAMIX
0029200        RE=REJ*SHAPE*DIV
0029300 C
0029400 C   GIVE VALUES OF E/K, SIGMA AND MOLEC. WEIGHT FOR TRACE SPECIES I
0029500 C
0029600        DO 10 I=1,7
0029700     25 IF(I.GT.1) GO TO 5
0029800        DATOS(1,5)=1962.0
0029900        DATOS(2,5)=3.804
0030000        DATOS(3,5)=39.9971
0030100        GO TO 11
0030200      5 IF(I.GT.2) GO TO 6
0030300        DATOS(1,5)=1375.
0030400        DATOS(2,5)=3.567
0030500        DATOS(3,5)=22.98977
0030600        GO TO 11
0030700      6 IF(I.GT.3) GO TO 7
0030800        DATOS(1,5)=2221.
0030900        DATOS(2,5)=5.00
0031000        DATOS(3,5)=142.0371
0031100        GO TO 11
0031200      7 IF(I.GT.4) GO TO 8
0031300        DATOS(1,5)=335.4
0031400        DATOS(2,5)=4.112
0031500        DATOS(3,5)=64.0588
0031600        GO TO 11
0031700      8 IF(I.GT.5) GO TO 9
0031800        DATOS(1,5)=431.4
0031900        DATOS(2,5)=4.207
0032000        DATOS(3,5)=80.0582
0032100        GO TO 11
0032200      9 IF(I.GT.6) GO TO 12
0032300        DATOS(1,5)=1989.
```

```
0032400         DATOS(2,5)=4.186
0032500         DATOS(3,5)=58.4428
0032600         GO TO 11
0032700      12 CONTINUE
0032800         DATOS(1,5)=301.1
0032900         DATOS(2,5)=3.623
0033000         DATOS(3,5)=34.0758
0033100      11 CONTINUE
0033200 C
0033300 C    DIFFUSION COEFFICIENT OF TRACE SPECIES AT STATIONS J AND W
0033400 C
0033500         CALL DIF(TJ,PJ,DA)
0033600         CALL DIF(TW,PJ,DW)
0033700 C
0033800 C    LEWIS NUMBER OF TRACE SPECIES AT STATIONS J AND W
0033900 C
0034000         LEJ=DA/APHMIX
0034100         LEW=DW/APHW
0034200 C
0034300 C    SCHMIDT NUMBER OF TRACE SPECIES AT STATION J
0034400 C
0034500         SC=ETAMIX/RHOJ/DA
0034600 C
0034700 C    MASS TRANS. NUSSELT NO.(PERIMETER-AVERAGED,CYLINDERICAL COLLECTOR)
0034800 C
0034900         CALL NUM(TW,TO,RE,SC,NU)
0035000 C
0035100 C    COMPUTE F(SORET)
0035200 C
0035300         CALL TMDF(I,TW,TO,LEW,ALPHA,TAU,THERM)
0035400 C
0035500 C    COMPUTE F(TURB)
0035600 C
0035700         CALL TURBL(RE,TURB,TURIN,TURL,DIAW)
0035800 C
0035900 C    CALCULATE NA2SO4 DEPOSITION RATE CONTRIBUTED FROM SPECIES I
0036000 C    BY CFBL FORMULATION.
0036100 C
0036200         IF(CMH(I).EQ.0.0) CMH(I)=1.0
0036300         SM(I)=TURB*DA*RHOJ*THERM*((XJ(I)-XW(I))+XW(I)*TAU/THERM*          -
0036400        *(LEW/LEJ)**0.6*CMIX/CP/CMH(I))*NU*DATOS(3,5)/AM/DIAW
0036500         IF(V(I).EQ.0.0) GO TO 10
0036600         AW=3.14159*DIAW*LW
0036700         M(I)=AW*3.600E6*0.5*142.0371/DATOS(3,5)*SM(I)*V(I)
0036800 C
0036900 C    PRINT INTERIM OUTPUT
0037000 C
0037100         IF(I.GT.1) GO TO 546
0037200         IF(FSORET) GO TO 100
0037300         WRITE(6,544)
0037400    544  FORMAT(/,10X,'CALCULATIONS DO NOT INCLUDE THERMAL DIFFUSION',/)
0037500    100  WRITE(6,545)
0037600    545  FORMAT(T2,'I',T11,'D(I)',T25,'NU(I)',T40,'SC(I)',T55,'X(I),-
0037700       CJ',T70,'X(I),W',T85,'TAU(I)',T100,'F(SORET),I',T116,'M(I)')
```

```
0037800   546 WRITE(6,550) I,DA,NU,SC,XJ(I),XW(I),TAU,THERM,M(I)
0037900   550 FORMAT(1X,I1,6E15.5,F15.5,2E15.5,/)
0038000    10 CONTINUE
0038100 C
0038200 C  COMPUTE TOTAL SODIUM(NA) AND SULFUR(S) MASS FLUX
0038300 C     SUM=J(NA), SMS=J(S)
0038400 C
0038500       SUM=SM(1)*22.98977/39.9971+SM(2)*1.0+SM(3)*2.*22.98977            -
0038600      //142.0371+SM(6)*22.98977/58.4428
0038700       SMS=SM(3)*32.06/142.0371+SM(4)*32.06/64.0588+SM(5)*               -
0038800      *32.06/80.0582+SM(7)*32.06/34.0758
0038900 C
0039000 C  COMPUTE SODIUM TO SULFUR MOLAR FLUX RATIO
0039100 C
0039200       RATIO=SUM/SMS*32.06/22.98977
0039300 C
0039400 C  COMPUTE TOTAL NA AND S MOLE FRACTIONS AT STATIONS J AND W
0039500 C
0039600       YNAJ=XJ(1)+XJ(2)+(XJ(3)*2)+XJ(6)
0039700       YNAW=XW(1)+XW(2)+(XW(3)*2)+XW(6)
0039800       YSJ=XJ(3)+XJ(4)+XJ(5)+XJ(7)
0039900       YSW=XW(3)+XW(4)+XW(5)+XW(7)
0040000       WRITE(6,211)
0040100   211 FORMAT(//,T8,'YNAJ',T24,'YNAW',T40,'YSJ',T57,'YSW')
0040200       WRITE(6,212)YNAJ,YNAW,YSJ,YSW
0040300   212 FORMAT(4E16.6,/)
0040400 C
0040500 C  CALCULATE NA2SO4 DEPOSITION RATE (MG/HR)
0040600 C
0040700       WPRED=M(1)+M(2)+M(3)+M(6)
0040800 C
0040900 C  COMPUTE PERCENT ERROR BETWEEN M(PRED) AND M(OBS)
0041000 C
0041100       ERR=WPRED-WOBS
0041200       ERROR=ERR/WOBS*100.
0041300 C
0041400 C  PRINT RESULTS
0041500 C
0041600       WRITE(6,4)AM,TURB,RE,SUM,SMS,RATIO,WPRED,ERROR,GM,PR,X(1),X(2),X(3), -
0041700      *X(4),TJ
0041800     4 FORMAT(/,10X,'AM =',F10.5,/,10X,'TURB =',F10.5,/,10X,'RE =',F10.3,/, -
0041900      *10X,'SUM (G/CM**2/SEC) =',E13.5,/,10X,'SMS (G/CM**2/SEC) =',E13.5,/, -
0042000      *10X,'RATIO =',F10.4,/,10X,                                        -
0042100      *'PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) =',F10.5,/,10X,         -
0042200      *'ERROR (%) =',F10.4,/,10X,'GM =',F10.5,/,10X,'PR =',F10.6,/,10X,  -
0042300      *'X(N2) =',F10.6,/,10X,'X(O2) =',F10.6,/,10X,'X(H2O) =',F10.6,/,10X, -
0042400      *'X(CO2) =',F10.6,/,10X,'TJ (K) =',F10.4,/)
0042500       WRITE(6,950)
0042600   950 FORMAT(/,T5,'RHOJ(G/CM**3)',T21,'UJ(CM/S)',T37,'ETAMIX(POISE)     -
0042700      C',T52,'LAMIX(CAL/CM/K/S)',T73,'CMIX(CAL/G/S)')
0042800       WRITE(6,951)RHOJ,UJ,ETAMIX,LAMIX,CMIX
0042900   951 FORMAT(4E16.6,4X,E16.6,//)
0043000       STOP
0043100       END
```

```
0043200 C
0043300 C*************************************************************************************
0043400 C
0043500       SUBROUTINE PARAM (J,EPSOVK,SIG2,M)
0043600 C
0043700 C  SUBROUTINE PARAM GIVES THE VALUES OF E/K,SIGMA AND MOLECULAR WEIGHT
0043800 C
0043900       REAL M
0044000       COMMON/VA/DATOS(3,5)
0044100       EPSOVK=DATOS(1,J)
0044200       SIG2=DATOS(2,J)
0044300       M=DATOS(3,J)
0044400       RETURN
0044500       END
0044600 C
0044700 C*************************************************************************************
0044800 C
0044900       SUBROUTINE CALESL(J,T,CJ)
0045000 C
0045100 C  THIS SUBROUTINE CALCULATES DIMENSIONLESS HEAT CAPACITY FROM A
0045200 C  CURVE FIT VALID FOR  300K < T < 1000K AND 1000K < T < 5000K
0045300 C
0045400       DIMENSION COEF1(5,4),COEF2(5,4)
0045500       DATA COEF1/ 0.28532899E+01 , 0.16022128E-02 ,-0.62936893E-06 ,    -
0045600      *            0.11441022E-09 ,-0.78057465E-14 ,                     -
0045700      *            0.36122139E+01 , 0.74853166E-03 ,-0.19820647E-06 ,    -
0045800      *            0.33749008E-10 ,-0.23907374E-14 ,                     -
0045900      *            0.26340654E+01 , 0.31121899E-02 ,-0.90278449E-06 ,    -
0046000      *            0.12673054E-09 ,-0.69164732E-14 ,                     -
0046100      *            0.44608041E+01 , 0.30981719E-02 ,-0.12392571E-05 ,    -
0046200      *            0.22741325E-09 ,-0.15525954E-13 /
0046300       DATA COEF2/ 0.37044177E+01 ,-0.14218753E-02 , 0.28670392E-05 ,    -
0046400      *           -0.12028885E-08 ,-0.13954677E-13 ,                     -
0046500      *            0.37837135E+01 ,-0.30233634E-02 , 0.99492751E-05 ,    -
0046600      *           -0.98189101E-08 , 0.33031825E-11 ,                     -
0046700      *            0.41675564E+01 ,-0.18106868E-02 , 0.59450878E-05 ,    -
0046800      *           -0.48670871E-08 , 0.15284144E-11 ,                     -
0046900      *            0.24007797E+01 , 0.87350957E-02 ,-0.66070878E-05 ,    -
0047000      *            0.20021861E-08 , 0.63274039E-15 /
0047100       IF(T.GT.1000.) GO TO 10
0047200       CJ=COEF2(5,J)*T**4+COEF2(4,J)*T**3+COEF2(3,J)*T**2+COEF2(2,J)*T   -
0047300      *+COEF2(1,J)
0047400       GO TO 20
0047500    10 CJ=COEF1(5,J)*T**4+COEF1(4,J)*T**3+COEF1(3,J)*T**2+COEF1(2,J)*T   -
0047600      *+COEF1(1,J)
0047700    20 RETURN
0047800       END
0047900 C
0048000 C*************************************************************************************
0048100 C
0048200       SUBROUTINE CALMIX(T,AM,CMIX)
0048300 C
0048400 C SUBROUTINE CALMIX PROVIDES MIXTURE HEAT CAPACITY IN CAL/(G*K)
0048500 C
```

```
0048600       COMMON/GFR/X(4)
0048700       C=0.
0048800       DO 8 J=1,4
0048900       CALL CALESL(J,T,CJ)
0049000       C=C+CJ*X(J)*1.9872
0049100     8 CONTINUE
0049200       CMIX=C/AM
0049300       RETURN
0049400       END
0049500 C
0049600 C*******************************************************************************************
0049700 C
0049800       SUBROUTINE COLINT(II,JJ,T,OVDT,ETA,CONDT,OMEDT)
0049900 C
0050000 C  THIS SUBROUTINE GIVES COLLISION INTEGRALS,VISCOSITY AND THERMAL
0050100 C  CONDUCTIVITY OF SPECIES USING CHAPMAN-ENSKOG THEORY
0050200 C
0050300       REAL M
0050400       DIMENSION OME(79),ALPA(79),OMED(79)
0050500       DATA ALPA/ 0.300 , 0.350 , 0.400 , 0.450 , 0.500 , 0.550 , 0.600 ,-
0050600      *           0.650 , 0.700 , 0.750 , 0.800 , 0.850 , 0.900 , 0.950 ,-
0050700      *           1.000 , 1.050 , 1.100 , 1.150 , 1.200 , 1.250 , 1.300 ,-
0050800      *           1.350 , 1.400 , 1.450 , 1.500 , 1.550 , 1.600 , 1.650 ,-
0050900      *           1.700 , 1.750 , 1.800 , 1.850 , 1.900 , 1.950 , 2.000 ,-
0051000      *           2.100 , 2.200 , 2.300 , 2.400 , 2.500 , 2.600 , 2.700 ,-
0051100      *           2.800 , 2.900 , 3.000 , 3.100 , 3.200 , 3.300 , 3.400 ,-
0051200      *           3.500 , 3.600 , 3.700 , 3.800 , 3.900 , 4.000 , 4.100 ,-
0051300      *           4.200 , 4.300 , 4.400 , 4.500 , 4.600 , 4.700 , 4.800 ,-
0051400      *           4.900 , 5.000 , 6.000 , 7.000 , 8.000 , 9.000 , 10.00 ,-
0051500      *           20.00 , 30.00 , 40.00 , 50.00 , 60.00 , 70.00 , 80.00 ,-
0051600      *           90.00 , 100.0 /
0051700       DATA OME/ 2.7850 , 2.6280 , 2.4920 , 2.3680 , 2.2570 , 2.1560 ,   -
0051800      *          2.0650 , 1.9820 , 1.9080 , 1.8410 , 1.7800 , 1.7250 ,   -
0051900      *          1.6750 , 1.6290 , 1.5870 , 1.5490 , 1.5140 , 1.4820 ,   -
0052000      *          1.4520 , 1.4240 , 1.3990 , 1.3750 , 1.3530 , 1.3330 ,   -
0052100      *          1.3140 , 1.2960 , 1.2790 , 1.2640 , 1.2480 , 1.2340 ,   -
0052200      *          1.2210 , 1.2090 , 1.1970 , 1.1860 , 1.1750 , 1.1560 ,   -
0052300      *          1.1380 , 1.1220 , 1.1070 , 1.0930 , 1.0810 , 1.0690 ,   -
0052400      *          1.0580 , 1.0480 , 1.0390 , 1.0300 , 1.0220 , 1.0140 ,   -
0052500      *          1.0070 , 0.9999 , 0.9932 , 0.9870 , 0.9811 , 0.9755 ,   -
0052600      *          0.9700 , 0.9649 , 0.9600 , 0.9553 , 0.9507 , 0.9464 ,   -
0052700      *          0.9422 , 0.9382 , 0.9343 , 0.9305 , 0.9269 , 0.8963 ,   -
0052800      *          0.8727 , 0.8538 , 0.8379 , 0.8242 , 0.7432 , 0.7005 ,   -
0052900      *          0.6718 , 0.6504 , 0.6335 , 0.6194 , 0.6076 , 0.5973 ,   -
0053000      *          0.5882 /
0053100       DATA OMED/ 2.6620 , 2.4760 , 2.3180 , 2.1840 , 2.0660 , 1.9660 ,   -
0053200      *           1.8770 , 1.7980 , 1.7290 , 1.6670 , 1.6120 , 1.5620 ,   -
0053300      *           1.5170 , 1.4760 , 1.4390 , 1.4060 , 1.3750 , 1.3460 ,   -
0053400      *           1.3200 , 1.2960 , 1.2730 , 1.2530 , 1.2330 , 1.2150 ,   -
0053500      *           1.1980 , 1.1820 , 1.1670 , 1.1530 , 1.1400 , 1.1280 ,   -
0053600      *           1.1160 , 1.1050 , 1.0940 , 1.0840 , 1.0750 , 1.0570 ,   -
0053700      *           1.0410 , 1.0260 , 1.0120 , 0.9996 , 0.9878 , 0.9770 ,   -
0053800      *           0.9672 , 0.9576 , 0.9490 , 0.9406 , 0.9328 , 0.9256 ,   -
0053900      *           0.9186 , 0.9120 , 0.9058 , 0.8998 , 0.8942 , 0.8888 ,   -
```

```
0054000      *           0.8836 , 0.8788 , 0.8740 , 0.8694 , 0.8652 , 0.8610 ,  -
0054100      *           0.8568 , 0.8530 , 0.8492 , 0.8456 , 0.8422 , 0.8124 ,  -
0054200      *           0.7896 , 0.7712 , 0.7556 , 0.7424 , 0.6640 , 0.6232 ,  -
0054300      *           0.5960 , 0.5756 , 0.5596 , 0.5464 , 0.5352 , 0.5256 ,  -
0054400      *           0.5170 /
0054500       IF(JJ.EQ.0)GO TO 67
0054600       CALL PARAM(JJ,EOKJ,SIGL,AJJ)
0054700       CALL PARAM(II,EOKI,SIGK,AII)
0054800       M=(AII+AJJ)/2.
0054900       SIG2=(SIGL+SIGK)/2.
0055000       EOVKIJ=SQRT(EOKJ*EOKI)
0055100       ADT=T/EOVKIJ
0055200       GO TO 68
0055300    67 CALL PARAM(II,EPSOVK,SIG2,M)
0055400       ADT=T/EPSOVK
0055500    68 J=3
0055600    69 IF(ADT-ALPA(J))112,111,110
0055700   110 J=J+1
0055800       IF(J.LE.79)GO TO 69
0055900       GO TO 204
0056000   111 OVDT=OME(J)
0056100       OMEDT=OMED(J)
0056200       GO TO 200
0056300   112 B=(ADT-ALPA(J-1))/(ALPA(J)-ALPA(J-1))
0056400       OVDT=B*(B-1.)*OME(J-2)/2.+(1.-B**2)*OME(J-1)+B*(B+1.)*OME(J)/2.
0056500       OMEDT=B*(B-1.)*OMED(J-2)/2.+(1.-B**2)*OMED(J-1)+B*(B+1.)*OMED(J)/2-
0056600      *.
0056700       GO TO 200
0056800   204 OVDT=0.5882*((ADT/100.)**(-0.17))
0056900       OMEDT=0.5170*((ADT/100.)**(-0.15))
0057000   200 ETA=26.693*SQRT(M*T)/((SIG2)**2*OVDT)*1.E-06
0057100       CALL CALESL(II,T,CR)
0057200       CONDT=(1.9872/M)*(15./4.+1.32*(CR-5./2.))*ETA
0057300       RETURN
0057400       END
0057500 C
0057600 C*******************************************************************************************
0057700 C
0057800       SUBROUTINE MIXPRO(T,ETAMIX,LAMIX)
0057900 C
0058000 C  THIS SUBROUTINE PROVIDES MIXTURE VISCOSITY AND THERMAL CONDUCTIVITY
0058100 C
0058200       REAL LAMP,LAMIX
0058300       DIMENSION VISC(4),LAMP(4)
0058400       COMMON/VA/DATOS(3,5)
0058500       COMMON/GFR/X(4)
0058600       ETAMIX=0.
0058700       LAMIX=0.
0058800       I1=0
0058900       DO 40 J=1,4
0059000       N=J
0059100       CALL COLINT(N,I1,T,OVDT,ETAMJ,CONDT,OMEDT)
0059200       VISC(J)=ETAMJ
0059300       LAMP(J)=CONDT
```

```
0059400     40 CONTINUE
0059500        DO 18 I=1,4
0059600        PROV=0.
0059700        DO 28 J=1,4
0059800        G=1./(2.*SQRT(2.))*((1.+DATOS(3,I)/DATOS(3,J))**(-0.5))*(1.       -
0059900       * +SQRT(VISC(I)/VISC(J))*SQRT(SQRT(DATOS(3,J)/DATOS(3,I))))**2
0060000        PROV=PROV+G*X(J)
0060100     28 CONTINUE
0060200        ETAMIX=ETAMIX+X(I)*VISC(I)/PROV
0060300        LAMIX=LAMIX+X(I)*LAMP(I)/PROV
0060400     18 CONTINUE
0060500        RETURN
0060600        END
0060700 C
0060800 C*************************************************************************************
0060900 C
0061000        SUBROUTINE COEDIF(T,P,I,J,D)
0061100 C
0061200 C  THIS SUBROUTINE CALCULATES BINARY DIFFUSION COEFFICIENT
0061300 C
0061400        CALL COLINT(I,J,T,OVDT,ETA,CONDT,OMEDT)
0061500        CALL PARAM(I,EPSOVK,SIGI,WI)
0061600        CALL PARAM(J,EPSOVK,SIGJ,WJ)
0061700        SIG=1./2.*(SIGI+SIGJ)
0061800        D=0.0018583*SQRT((T**3)*(1./WI+1./WJ))/(P*OMEDT*(SIG**2))
0061900        RETURN
0062000        END
0062100 C
0062200 C*************************************************************************************
0062300 C
0062400        SUBROUTINE DIF(T,P,DA)
0062500 C
0062600 C  SUBROUTINE DIF GIVES DIFFUSION COEFFICIENT OF TRACE SPECIES K
0062700 C  IN GAS MIXTURE
0062800 C
0062900        COMMON/GFR/X(4)
0063000        DEN=0.0
0063100        DO 101 J=1,4
0063200        K=5
0063300        CALL COEDIF(T,P,K,J,DIFF)
0063400        DEN=DEN+X(J)/DIFF
0063500   101 CONTINUE
0063600        DA=1./DEN
0063700        RETURN
0063800        END
0063900 C
0064000 C*************************************************************************************
0064100 C
0064200        SUBROUTINE TMDF(I,TW,TO,LEW,ALPHA,TAU,THERM)
0064300 C
0064400 C  SUBROUTINE TMDF CALCULATES THERMAL DIFFUSION EFFECT, F(SORET),
0064500 C  LABELLED AS 'THERM'.  IF FSORET IS FALSE, THERM=1.0 .
0064600 C
0064700        LOGICAL FSORET
```

```
0064800       COMMON FSORET
0064900       REAL LEW
0065000       DIMENSION ALPHA(7)
0065100       IF(FSORET) GO TO 10
0065200       THERM=1.0
0065300       TAU=0.0
0065400       GO TO 20
0065500    10 TAU=ALPHA(I)*LEW**0.4*(TO-TW)/TW
0065600       ET=EXP(-TAU)
0065700       THERM=TAU/(1.-ET)
0065800    20 RETURN
0065900       END
0066000 C
0066100 C*******************************************************************************
0066200 C
0066300       SUBROUTINE NUM(TW,TO,RE,SC,NU)
0066400 C
0066500 C  SUBROUTINE NUM CALCULATES PERIMETER AVERAGED NUSSELT NUMBER
0066600 C  INCLUDING EFFECTS OF MACH NUMBER AND VARIABLE PROPERTIES
0066700 C
0066800       REAL NU
0066900       NU=(0.40*SQRT(RE)+0.06*RE**(2./3.))*(SC**0.4)*                    -
0067000      1(TO/TW)**(-0.04)
0067100       RETURN
0067200       END
0067300 C
0067400 C*******************************************************************************
0067500 C
0067600       SUBROUTINE TURBL(RE,TURB,TURIN,TURL,DIAW)
0067700 C
0067800 C  SUBROUTINE TURBL CALCULATES EFFECT OF MAINSTREAM TURBULENCE
0067900 C
0068000       REAL LOD
0068100       IF(TURIN.NE.0.0) GO TO 5
0068200       IF(TURB.EQ.0.0) GO TO 10
0068300       GO TO 30
0068400     5 LOD=TURL/DIAW
0068500       IF(LOD.GT.2.0) PSI=0.124*(LOD-11.0)**2.+2.
0068600       IF(LOD.LE.2.0) PSI=-4.0*(LOD-1.75)**2.+12.25
0068700       PSI=PSI/1000.
0068800       XI=TURIN*RE/100.
0068900       IF(XI-100.)1,2,2
0069000     1 PHI=12.375*(1.-(1.-XI/100.)**1.5)
0069100       GO TO 20
0069200     2 PHI=9.0+0.03375*XI
0069300    20 TURB=1.+PSI*PHI
0069400       GO TO 30
0069500    10 TURB=1.0
0069600    30 RETURN
0069700       END
0069800 C
0069900 C********************************* END OF PROGRAM *********************************
```

## REFERENCES


1. Rosner, Daniel E.; and et al.: Chemically Frozen Multicomponent Boundary Layer Theory of Salt/Ash Deposition Rates from Combustion Gases. Combust. Sci. Technol., vol. 20, no. 3-4, 1979, pp. 87-106.
2. Helt, James E.: Evaluation of Alkali Metal Sulfate Dew Point Measurement for Detection of Hot Corrosion Conditions in PFBC Flue Gas. ANL/CEN/FE-80-12, Argonne National Laboratory, 1980.
3. Santoro, Gilbert J.; Kohl, Fred J.; Stearns, Carl A.; Gökoğlu, Süleyman A.; and Rosner, Daniel E.: Experimental and Theoretical Deposition Rates from Salt-Seeded Combustion Gases of a Mach 0.3 Burner Rig. NASA TP-2225, 1984.
4. Gordon, Sanford; and McBride, Bonnie J.: Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouget Detonations. NASA SP-273, 1971.
5. Rosner, Daniel E.; and Nagarajan, Ramamurthy: Transport Induced Shifts in Condensate Dew Point and Identity in High Temperature Multicomponent Systems with Chemical Reaction, Chem. Eng. Sci. (In press, 1984.)
6. Seshadri, K.; and Rosner, Daniel E.: Optical Methods of Dew Point and Deposition Rate Measurements in Salt/Ash-Containing Combustion Gases--1. $B_2O_3(l)$ Deposition Rates by the Interference Method and Comparison with Theory, AIChE J. Vol. 30, No. 2, pp. 187-196, 1984.
7. Rosner, Daniel E.: Thermal (Soret) Diffusion Effects on Interfacial Mass Transport Rates. PCH PhysicoChemical Hydrodynamics, vol. 1, no. 2-3, 1980, pp. 159-185.
8. Svehla, Roger A.: Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures. NASA TR-R-132, 1962.
9. Bird, Robert B.; Stewart, Warren E.; and Lightfood, Edwin N.: Transport Phenomena. John Wiley, 1960.
10. Whitaker, Stephen: Forced Convection Heat Transfer Correlations for Flow in Pipes, Past Flat Plates, Single Cylinders, Single Spheres, and for Flow in Packed Beds and Tube Bundles, AIChE J., vol. 18, no. 2, Mar. 1972, pp. 361-371.
11. Kays, William M.; and Crawford, Michael E.: Convective Heat and Mass Transfer. Second ed. McGraw Hill, 1980.
12. Gökoğlu, Süleyman A. and Rosner, Daniel E., "Engineering Correlations of Variable-Property Effects on Laminar Forced Convection Mass Transfer for Dilute Vapor Species and Small Particles in Air," NASA CR-168322 (1984).
13. Kays, William M.; and Bjorklund, I. S.: Heat Transfer from a Rotating Cylinder with and without Crossflow. Trans. ASME., vol. 80, 1958, pp. 70-78.
14. Gökoğlu, Süleyman A.; and Rosner, Daniel E.: Correlation of Thermophoretically-Modified Small Particle Deposition Rates in Forced Convection Systems with Variable Properties, Transpiration Cooling and/or Viscous Dissipation, Int. J. Heat Mass Transfer. Vol. 27, No. 5, pp. 639-645, 1984.
15. Srivastava, R.; and Rosner, Daniel E.: A New Approach to the Correlation of Boundary Layer Mass Transfer Rates with Thermal Diffusion and/or Variable Properties. Int. J. Heat and Mass Transfer, vol. 22, Sept. 1979, pp. 1281-1294.
16. Rosner, Daniel E.; Gökoğlu, Süleyman A.; and Israel, Rajasingh: Rational Engineering Correlations of Diffusional and Inertial Particle Deposition Behavior in Non-Isothermal Forced Convection Environments. Fouling of Heat Exchange Surfaces, Engineering Foundation Inc., 1983, pp. 235-256.

17. Gökoğlu, Süleyman A.: Thermophoretically Enhanced Deposition of Particulate Matter Across Nonisothermal Boundary Layers. Ph.D. Dissertation, Yale Univer., 1982.
18. Morgan, V. T.: The Overall Convective Heat Transfer from Smooth Circular Cylinders. Adv. Heat Transfer, vol. 11, 1975, pp. 199-264.
19. Kestin, J.: The Effect of Free-Stream Turbulence on Heat Transfer Rates. Adv. Heat Transfer, vol. 3, 1966, pp. 1-32.
20. Van der Hegge Zijnen, B. G.: Heat Transfer from Horizontal Cylinders to a Turbulent Air Flow. Appl. Sci. Res., Sect. A, vol. 7, 1958, pp. 205-223.

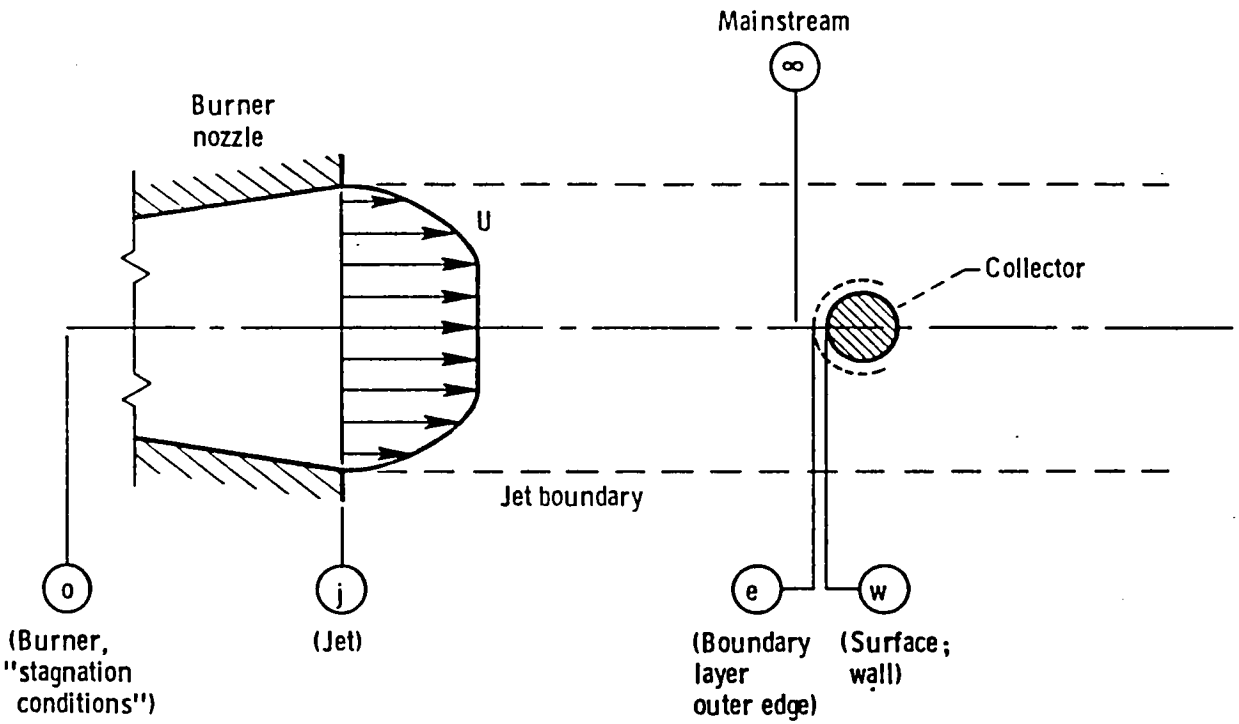



Figure 1. - Station nomenclature.

| 1. Report No. | 2. Government Accession No. | 3. Recipient's Catalog No. |
|---|---|---|
| NASA CR-168329 | | |

**4. Title and Subtitle**
Computer Program for the Calculation of Multicomponent Convective Diffusion Deposition Rates from Chemically Frozen Boundary Layer Theory

**5. Report Date**
January 1984

**6. Performing Organization Code**

**7. Author(s)**
Süleyman A. Gökoğlu, Bor-Kuan Chen* and Daniel E. Rosner

**8. Performing Organization Report No.**
None

**10. Work Unit No.**

**9. Performing Organization Name and Address**
Analex Corporation and Yale University
21000 Brookpark Rd. Chemical Engineering Dept.
Cleveland, Ohio New Haven, Connecticut
44135 06520

**11. Contract or Grant No.**
NAS3-23293 and NAG3-201

**13. Type of Report and Period Covered**
Contractor Report

**12. Sponsoring Agency Name and Address**
National Aeronautics and Space Administration
Washington, D.C. 20546

**14. Sponsoring Agency Code**
533-04-1A (E-1971)

**15. Supplementary Notes**
Final report. Project Manager, Carl A. Stearns, Materials Division, NASA Lewis Research Center, Cleveland, Ohio 44135. *Present address: E.I. du Pont de Nemours & Co., Biochemicals Dept. E335, Wilmington, Delaware 19898.

**16. Abstract**
The computer program developed based on multicomponent chemically frozen boundary layer (CFBL) theory for calculating vapor and/or small particle deposition rates is documented. A specific application to perimter-averaged $Na_2SO_4$ deposition rate calculations on a cylinderical collector is demonstrated. The manual includes a typical program input and output for users.

**17. Key Words (Suggested by Author(s))**
Deposition; CVD; Corrosion; Heat and mass transfer; Boundary layer; Computer program

**18. Distribution Statement**
Unclassified - unlimited
STAR Category 34

| 19. Security Classif. (of this report) | 20. Security Classif. (of this page) | 21. No. of pages | 22. Price* |
|---|---|---|---|
| Unclassified | Unclassified | | |

*For sale by the National Technical Information Service, Springfield, Virginia 22161

National Aeronautics and
Space Administration

Washington, D.C.
20546

Official Business
Penalty for Private Use, $300

SPECIAL FOURTH CLASS MAIL
BOOK


Postage and Fees Paid
National Aeronautics and
Space Administration
NASA-451

NASA

POSTMASTER: If Undeliverable (Section 158
Postal Manual) Do Not Return