

CRESLAF

A PROGRAM FOR MODELING LAMINAR,
CHEMICALLY REACTING, BOUNDARY-LAYER
FLOW IN CYLINDRICAL OR PLANAR CHANNELS

Reaction Design

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Reaction Design cautions that some of the material in this manual may be out of date. Updates will be available periodically on Reaction Design's web site. In addition, on-line help is available on the program CD. Sample problem files can also be found on the CD and on our web site at www.ReactionDesign.com.

CRESLAF: A PROGRAM FOR MODELING LAMINAR, CHEMICALLY REACTING, BOUNDARY-LAYER FLOW IN CYLINDRICAL OR PLANAR CHANNELS

ABSTRACT

CRESLAF predicts the velocity, temperature, and species profiles in two-dimensional (planar or axisymmetric) channels. Applications of CRESLAF include chemical vapor deposition (CVD) reactors, heterogeneous catalysis on reactor walls, and corrosion processes. The program accounts for finite-rate gas-phase and surface chemical kinetics and molecular transport. The model employs the boundary-layer approximations for the fluid-flow equations, coupled to gas-phase and surface species continuity equations. The program employs the CHEMKIN, SURFACE CHEMKIN and TRANSPORT software packages for the gas-phase and surface chemical reaction mechanisms and for the transport properties. This manual presents the equations defining the model, the method of solution, the input parameters to the program, and a sample problem illustrating its use.

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NOMENCLATURE

		CGS Units
c_p	Mixture heat capacity	ergs / (g K)
c_{pk}	Specific heat capacity of k th species	ergs / (g K)
D_{kj}	Multicomponent diffusion coefficient	cm ² / sec
$D_{k,m}$	Mixture diffusion coefficient	cm ² / sec
D_k^T	Thermal diffusion coefficient	cm ² / sec
g	Acceleration of gravity	cm / sec ²
G_k	Linear growth rate for the k th bulk species	cm / sec
h_k	Specific enthalpy of k th species	ergs / g
K_g	Total number of gas-phase species	---
K_s	Total number of surface species	---
K_b	Total number of bulk species	---
$K_s^f(n)$	Index of the first surface species in surface phase n	---
$K_s^l(n)$	Index of the last surface species in surface phase n	---
$K_b^f(n)$	Index of the first bulk species	---
$K_b^l(n)$	Index of the last bulk species	---
M	Mass flux	g / (cm ^(1-α) sec)
M_l	Mass loss rate at the lower boundary	g / (cm ^(1-α) sec)
M_u	Mass loss rate at the upper boundary	g / (cm ^(1-α) sec)
M_0	Mass flux at the channel inlet	g / (cm ^(1-α) sec)
N_s	Number of surface site types (phases)	---
p	Thermodynamic pressure	dynes / cm ²
R	Universal gas constant	ergs / (mole K)
$\dot{s}_k$	Rate of production of k th species by surface reactions	mole / (cm ² sec)
T	Temperature	K
u	Fluid velocity in x direction	cm / sec
v	Fluid velocity in y direction	cm / sec
$V_{k,y}$	Diffusion velocity of k th species	cm / sec
x	Distance along principal flow direction	cm
X_k	Mole fraction of k th species	
y	Cross-stream coordinate	cm
$y_{\max}$	Maximum channel dimension	cm
Y_k	Mass fraction of the k th species	---
$\bar{W}$	Mixture mean molecular weight	g / mole

		<u>CGS Units</u>
W_k	Molecular weight of k th species	g / mole
$z_k(n)$	Site-fraction of k th surface species for surface phase n	
<u>GREEK</u>		
α	Coordinate index: 0 for planar, 1 for radial coordinates	---
λ	Mixture thermal conductivity	ergs / (cm K sec)
μ	Mixture viscosity	g / (cm sec)
ψ	Stream function	g / (cm ² sec)
ρ	Density	g / cm ³
ρ_i	Density at the reactor inlet	g / cm ³
ρ_k	Bulk density for the k th bulk species	g / cm ³
$\dot{\omega}_k$	Rate of production of k th species by gas-phase reactions	mole / (cm ³ sec)
ξ	Normalized stream function	---

1. INTRODUCTION

The CRESLAF (Chemically Reacting Shear-Layer Flow) program simulates the coupled hydrodynamics, gas-phase chemistry and surface chemistry in laminar-flow channels. Detailed mathematical formulation of the model and a demonstration of its application to chemistry in the chemical vapor deposition (CVD) of silicon from silane have been reported previously in the literature.^{2, 3} The model is general, in that it can be applied to many chemical systems for which gas-phase and surface kinetic mechanisms are known. It can also be applied to a wide variety of other chemically reacting flow situations. The model predicts gas-phase temperature and velocity fields, concentration fields for any number of chemical species, deposition or etching rates and surface-species coverage as a function of experimental conditions, such as surface temperature, flow rate, inlet partial pressure of the reactants, total pressure, and reactor dimensions. However, it is restricted to a two-dimensional geometry, using either planar or radial coordinates for 2-D Cartesian or 2-D axisymmetric flows, respectively.

The CRESLAF program employs the TRANSPORT software package for calculating thermal diffusion coefficients and for the rigorous calculation of ordinary multicomponent transport properties. CRESLAF includes the effects of thermal diffusion, which is the separation of species of differing size in a temperature gradient. Thermal diffusion can have an important effect on predicted concentration profiles.³ The boundary conditions describing chemical reactions at the surface are formulated using the SURFACE CHEMKIN Utility package, while the gas-phase kinetics calculations employ the CHEMKIN Gas-phase Utility software.

2. DESCRIPTION OF MODEL

2.1 Defining Equations

CRESLAF solves the boundary-layer equations for the fluid flow coupled with species equations. These equations describe chemical species production and destruction, and both convective and diffusive transport. Details of the formulation have been published by Coltrin, et al.^{2, 3} The applicability of the equations relies on the existence of a principal flow direction in which diffusive transport is negligible compared to convective transport. To simplify the numerical procedure somewhat, we recast the equations using the Von Mises transformation,⁴ in which the cross-stream coordinate is replaced by the stream function as an independent variable. We use an additional transformation of the stream function³ that accounts for possible mass loss (or gain) in the gas due to deposition (or etching) at the reacting surfaces.

The set of equations describing the CRESLAF model is as follows.

2.1.1 MOMENTUM:

$$\rho u \frac{\partial u}{\partial x} - \frac{\rho u}{M} \left(\xi \frac{dM}{dx} - \frac{dM_l}{dx} \right) \frac{\partial u}{\partial \xi} + \frac{dp}{dx} = \frac{\rho u}{M^2} \frac{\partial}{\partial \xi} \left(\rho u \mu y^{2\alpha} \frac{\partial u}{\partial \xi} \right) + g(\rho_i - \rho) \quad (1)$$

2.1.2 SPECIES:

$$\rho u \frac{\partial Y_k}{\partial x} - \frac{\rho u}{M} \left(\xi \frac{dM}{dx} - \frac{dM_l}{dx} \right) \frac{\partial Y_k}{\partial \xi} = \dot{\omega}_k W_k - \frac{\rho u}{M} \frac{\partial}{\partial \xi} \left(y^\alpha \rho Y_k V_{k,y} \right) \quad (k = 1, \dots, K_g) \quad (2)$$

2.1.3 ENERGY:

$$\begin{aligned} \rho u c_p \frac{\partial T}{\partial x} - \frac{\rho u c_p}{M} \left(\xi \frac{dM}{dx} - \frac{dM_l}{dx} \right) \frac{\partial T}{\partial \xi} &= \frac{\rho u}{M^2} \frac{\partial}{\partial \xi} \left(\rho u \lambda y^{2\alpha} \frac{\partial T}{\partial \xi} \right) - \sum_{k=1}^{K_g} \dot{\omega}_k W_k h_k \\ &\quad - \frac{\rho^2 u y^\alpha}{M} \sum_{k=1}^K Y_k V_{k,y} c_{pk} \frac{\partial T}{\partial \xi} \end{aligned} \quad (3)$$

2.1.4 STATE:

$$p = \frac{\rho RT}{\bar{W}}. \quad (4)$$

We provide the option of choosing from two different transport models. In these equations when multicomponent transport is used, the diffusion velocity $V_{k,y}$ is given by

$$V_{k,y} = \frac{\rho u y^\alpha}{X_k \bar{W} M} \sum_{j \neq k}^{K_g} W_j D_{kj} \frac{\partial X_k}{\partial \xi} - \frac{D_k^T}{\rho Y_k} \frac{\rho u y^\alpha}{TM} \frac{\partial T}{\partial \xi}, \quad (5)$$

or when mixture-averaged transport is used,

$$V_{k,y} = -\frac{D_{k,m}\rho uy^\alpha}{X_k M} \frac{\partial X_k}{\partial \xi} - \frac{D_k^T}{\rho Y_k} \frac{\rho uy^\alpha}{TM} \frac{\partial T}{\partial \xi}. \quad (6)$$

The equations represent either cylindrical or cartesian coordinates. For a flow in cylindrical coordinates, the parameter α is 1, and y represents the radius measured from the flow centerline. If α is zero then the equations are in planar coordinates for the flow between two infinitely wide plates, and y is the height above the lower wall. We also allow a third case of cartesian coordinates in which both walls are identical and there is a plane of symmetry. In this case y is the distance above the symmetry plane.

The independent variables x and ξ represent the axial coordinate and the normalized stream function, respectively. (All variables are defined in the Nomenclature section at the beginning of the manual.) The last term in the momentum equation, Eq. (1), can only be included when the gravity vector is along the principal flow direction, i.e., when the flow is either vertically upward or downward, rather than horizontal.

We define the stream function ψ as

$$\psi = \frac{1}{\alpha + 1} \int_0^y \rho u dy^{\alpha+1}. \quad (7)$$

The stream function is defined such that there is an equal mass flow rate between two lines of constant stream function value (between streamlines, when there is no mass loss). If there is no mass loss to the walls, the reactor walls themselves are streamlines, i.e., lines of constant streamfunction. The independent variable ψ then ranges from zero at one boundary to the total mass flux M at the other. If there is no mass loss at the surfaces, then the total mass flux is evaluated at the initial condition and is constant throughout the computation. In this case, the numerical method can use a mesh in which each mesh point has a specified value of stream function. However, if mass is lost from the gas then the total mass flux changes along the flow direction, and the independent variable changes at each mesh point (i.e., a moving coordinate system). In order to make a new independent variable whose total magnitude is fixed for the entire problem, we define a new stream function that is normalized by the local total mass flux

$$\xi = \frac{\psi}{M}, \quad (8)$$

where M is the *local value* of the total mass flux. Therefore, ξ ranges between 0 and 1, and is not dependent on the total mass previously lost (or gained) at the walls.

The relationships between the physical coordinates (y and x) and the transformed coordinates (ξ , ψ and x) are stated in the following equations that define the Von Mises transformation.

$$\left(\frac{\partial}{\partial x}\right)_y = \left(\frac{\partial}{\partial x}\right)_\psi - \rho v y^\alpha \left(\frac{\partial}{\partial \psi}\right)_x + \frac{dM_l}{dx} \left(\frac{\partial}{\partial \psi}\right)_x, \quad (9)$$

$$\left(\frac{\partial}{\partial x}\right)_y = \left[\left(\frac{\partial}{\partial x}\right)_\xi - \left(\frac{\xi}{M} \frac{dM}{dx} - \frac{1}{M} \frac{dM_l}{dx}\right) \left(\frac{\partial}{\partial \xi}\right)_x\right] - \rho v y^\alpha \frac{1}{M} \left(\frac{\partial}{\partial \xi}\right)_x, \quad (10)$$

$$\left(\frac{\partial}{\partial y}\right)_x = \rho u y^\alpha \left(\frac{\partial}{\partial \psi}\right)_x = \rho u y^\alpha \frac{1}{M} \left(\frac{\partial}{\partial \xi}\right)_x. \quad (11)$$

The total local mass flux M is computed from an equation that accounts for the mass deposited on each boundary

$$\frac{dM}{dx} = \frac{dM_l}{dx} + \frac{dM_u}{dx}. \quad (12)$$

The mass flux at the lower boundary (in the asymmetric planar case) is determined from the convective (Stefan) mass flux to the boundary,

$$\frac{dM_l}{dx} = \rho v|_{y=0}. \quad (\text{asymmetric, planar case only}) \quad (13)$$

(Calculation of the transverse velocity v at the boundary is discussed in Section 2.2) Note that Eq. (13) applies only in the asymmetric planar coordinate case (since in cylindrical coordinates or for a symmetric channel in planar coordinates the lower boundary is the centerline, and thus there is no mass change at that boundary). The rate of change of mass flux at the upper boundary (which is the upper wall in planar coordinates or the outer radius in cylindrical coordinates) is similarly defined by

$$\frac{dM_u}{dx} = -\rho v y^\alpha \Big|_{y=y_{\max}}. \quad (14)$$

The initial mass flux entering the channel is defined by

$$M_0 = \left(\int_0^{y_{\max}} \rho u y^\alpha dy \right)_0, \quad (15)$$

which serves as the initial condition for Eq. (12).

The system of equations is completed by an equation that relates the cross-stream coordinate y to the normalized stream function

$$\frac{1}{M} \frac{\partial y^{\alpha+1}}{\partial \xi} = \frac{\alpha+1}{\rho u}. \quad (16)$$

This equation comes from differentiating the definition of the streamfunction, Eq. (7).

In addition to including detailed gas-phase chemistry, we include detailed surface reaction chemistry through use of the SURFACE CHEMKIN package. Here we consider N_s different surface phases (or site-types), and at each axial position solve for the steady-state surface site fractions for each of the N_s surface phases. Thus, we solve additional equations, where K_s is the total number of surface species in the heterogeneous reaction mechanism. These equations are shown in Eqs. (17) and (18) below.

$$\dot{s}_k(n) = 0, \quad k = K_s^f(n), \dots, K_s^l(n) - 1; \quad n = 1, \dots, N_s \quad (17)$$

$$1 = \sum_{K_s^f(n)}^{K_s^l(n)} z_k(n), \quad n = 1, \dots, N_s \quad (18)$$

Here, $K_s^f(n)$ and $K_s^l(n)$ represent the first and last species for surface phase number n . This nomenclature is described in more detail in the SURFACE CHEMKIN manual. For one species in each surface phase, we do not solve the steady state condition given by Eq. (17), but instead use Eq. (18), which requires that the site fractions sum to unity in each phase.

To summarize the system of equations considered by CRESLAF, we solve Eqs. (1-4), (13), (14), and (6) at every gas-phase mesh point. In planar coordinates, we also solve Eqs. (17) and (18) at the upper and lower boundaries. In cylindrical coordinates (or for a symmetric channel in planar coordinates) we solve Eqs. (17) and (18) only at the upper boundary. This is a parabolic system of equations, where the dependent variables are: p , $y^{\alpha+1}$, u , T , M , M_w , and Y_k . The equations are subject to a set of algebraic constraints, which are the equations for the surface site fractions, z_k . This system of equations is solved using the method of lines. We treat the equations as a set of Differential / Algebraic Equations (DAE's),⁵ which we solve using the numerical software DASSL^{6, 7}

At the entrance to the reactor channel, the initial profiles of u , T , and Y_k , the pressure, and the surface site fractions z_k must be specified (see Section 2.3 on species concentration at boundaries). The velocity profile can be either a fully developed, parabolic profile or a flat velocity profile, with an optionally specified boundary-layer thickness. If the boundary-layer thickness is specified, then a parabolic profile is assumed only within the boundary layer. The initial gas temperature across the channel is usually set equal to the initial surface temperature. However, the user may also specify different gas and surface temperatures. As with the velocity profile, if a boundary-layer thickness is specified, the program linearly interpolates the gas-phase temperature between the surface temperature and the gas temperature over the boundary-layer thickness. The initial gas-phase species mass fractions Y_k are taken to be uniform across the channel, with the exception of the mass fractions at reactive walls. These are calculated by the procedure described in the Section 2.3 on species concentration at boundaries. From the initial profiles we compute the local mass flux M and the physical locations of all the mesh points, i.e., a profile of y^α .

2.2 Boundary Conditions

For the energy equation, either the temperature or a zero-heat-flux (adiabatic) condition is specified at the solid walls. In the transformed equations ξ is the independent variable and the physical coordinate y is a dependent variable. For the evaluation of y , then, we specify as boundary conditions that $y=0$ at the lower boundary and $y=y_{\max}$ at the upper boundary (the channel radius in the case of cylindrical coordinates). Notice that there is no explicit equation or boundary condition for the pressure p even though it is a dependent variable. Note also that a boundary value of y is specified at both boundaries even though

Eq. (16) is only a first-order equation. This apparent over-specification is resolved by the fact that there is no boundary condition for pressure.²

The boundary conditions for the species involve the heterogeneous reactions. The convective and diffusive mass fluxes of gas-phase species at the surface are balanced by the production (or depletion) rates of gas-phase species by surface reactions. This relationship is

$$\rho Y_k (V_{k,y} + v) = \dot{s}_k W_k, \quad (k = 1, \dots, K_g) \quad (19)$$

where the gas-phase diffusion velocities are given by Eqs. (5) or (6).

In nonreacting flows the fluid velocity normal and tangential to a solid wall is zero. However, if there are chemical reactions at the wall, then the normal velocity can be nonzero. This so-called Stefan flow velocity occurs when there is a net mass flux between the surface and the gas. The Stefan velocity is given by

$$v = \frac{1}{\rho} \sum_{k=1}^{K_g} \dot{s}_k W_k. \quad (20)$$

This expression is easily obtained from the interfacial mass balance, Eq. (19), by summing over all K_g gas-phase species and using the requirement that the mass fractions must sum to one, i.e.,

$$\sum_{k=1}^{K_g} Y_k = 1, \quad (21)$$

and that the sum of the diffusion fluxes must be zero.

The SURFACE CHEMKIN input includes the mass densities ρ_k for the K_b bulk species involved in a surface reaction mechanism. CRESLAF uses these densities to convert the surface reaction rate of production of a bulk species (in moles/cm²/sec) into a growth rate G_k (in cm/sec) for each bulk species. The relationship is given by:

$$G_k = \frac{\dot{s}_k W_k}{\rho_k}, \quad (k = K_b^f, \dots, K_b^l) \quad (22)$$

2.3 Initial Conditions on Species Concentrations at Boundaries

For an arbitrarily complex surface reaction mechanism, it can be difficult to provide an initial set of surface site fractions z_k and gas-phase mass fractions Y_k at the surface, which satisfies Eqs. (17), (18), (19) and (20) at $x=0$. This self-consistency is necessary because the equations for the surface site fractions and gas-phase mole fractions at the walls are actually algebraic equations, rather than ordinary differential equations. For the solution to begin smoothly, it is necessary to satisfy exactly the algebraic equations at $x=0$. To this end, CRESLAF first solves for the correct set of z_k and Y_k that satisfy these boundary condition equations at the channel inlet. This procedure employs the numerical software TWOPNT to solve for the self-consistent set of gas-phase and surface concentrations at each wall. The user can optionally give the

TWOPNT procedure initial guesses for the gas-phase and surface concentrations to aid in the convergence. The initial TWOPNT problem can also be bypassed altogether if the self-consistent values for the z_k and Y_k are supplied by the user.

2.4 Implementation of Multicomponent Transport

Although the mixture-averaged transport approximation is inadequate for some applications (for example, CVD at very low pressures, or when a carrier gas is not used), it has some properties that make it attractive for numerical computation. It is significantly less computationally intensive than the full-multicomponent transport formulation (see the TRANSPORT manual for more details of the transport options). Also, the mixture-averaged diffusion velocity of species k (Eq. 6) depends explicitly on the concentration gradient of species k , but the multicomponent diffusion velocity of Eq. (5) depends on the concentration gradients of all the remaining species. As a result, the Jacobian of the diffusion velocity has a strong diagonal term in the former case, but not in the latter case.

We find that solution of the set of differential/algebraic equations is aided by using a form for the multicomponent diffusion coefficient discussed by Coltrin, *et al.*,³ found by equating Eqs. (5) and (6) and solving for $D_{k,m}$,

$$D_{k,m} = \frac{\sum_{j \neq k}^{K_g} w_j D_{kj} (\partial X_j / \partial \xi)}{\bar{w} \sum_{j \neq k}^{K_g} (\partial X_j / \partial \xi)}. \quad (23)$$

The denominator in Eq. (23) is found by noting that

$$\frac{\partial X_k}{\partial \xi} = - \sum_{j \neq k}^{K_g} \frac{\partial X_j}{\partial \xi}. \quad (24)$$

In CRESLAF we implement multicomponent transport using the diffusion velocity of the form in Eq. (6), with $D_{k,m}$ calculated using Eq. (23).

Mass conservation requires that the diffusive mass fluxes sum to zero

$$\rho \sum_{k=1}^{K_g} Y_k V_k = 0. \quad (25)$$

However, a consequence of using the mixture-averaged transport formulation in Eq. (6) to define a diffusion velocity and using the mixture-averaged diffusion coefficients $D_{k,m}$ is that mass is not always conserved, i.e., the diffusive mass fluxes are not guaranteed to sum to zero. Therefore, at the mixture-averaged level of closure of the transport formulation some corrective measures must be taken. The user of CRESLAF has two options. One is to apply an ad-hoc correction velocity,⁸ defined as

$$V_c = - \sum_{k=1}^{K_g} Y_k V_k. \quad (26)$$

When this correction velocity (independent of species, k) is added to all the species diffusion velocities as computed from Eq. (6), diffusional mass conservation is assured. This option is specified by the keyword VCOR.

Another option to account for the deficiencies of the mixture-averaged closure of the transport problem and to assure mass conservation is to solve only $K_g - 1$ gas-phase species conservation equations and to determine the remaining mass fraction by requiring $\sum_{k=1}^{K_g-1} Y_k = 1$. (The mixture-averaged transport closure is asymptotically correct in the trace-species limit.) In cases where one species is present in large excess (such as a carrier gas), this is a reasonable option. The carrier-gas composition is conveniently determined as

$$Y_{K_g} = 1 - \sum_{k=1}^{K_g-1} Y_k. \quad (27)$$

If the user does not specify use of a correction velocity, CRESLAF assumes that the last-named species in the gas-phase CHEMKIN Interpreter input is the carrier gas and thus does not solve the corresponding conservation equation (Eq. 2) for that species, but applies Eq. (27).

2.5 Thermal Diffusion

Thermal diffusion is the separation of two species of differing size in the presence of a temperature gradient. Because there can be strong temperature gradients in a reactor, thermal diffusion can significantly influence deposition rates^{3, 9-11} as well as density profiles, as observed by *in situ* measurements.¹²⁻¹⁵ The effect of thermal diffusion is included in the diffusion velocity as the second term on the right side of Eqs. (5) or (6). Note that a full multicomponent model is used for the computation of thermal diffusion coefficients, regardless of whether the user has specified the mixture-averaged or the multicomponent option for the calculation of the diffusion velocity. See the TRANSPORT user manual for more details about this formulation.

2.6 Finite Difference Approximations

The governing conservation equations require discretization to allow numerical solution. CRESLAF uses finite difference approximations on a nonuniform grid with points numbered as $j=1$ at the lower boundary to $j=J$ at the upper boundary. Approximation of the spatial derivatives is accomplished by finite difference representations on a fixed grid in the normalized stream function.

In the momentum, species, and energy equations, we approximate the second derivatives with conventional central difference formulas as

$$\frac{\partial}{\partial \xi} \left(\alpha \frac{\partial f}{\partial \xi} \right) \approx \left(\frac{2}{\xi_{j+1} - \xi_{j-1}} \right) \left[\alpha_{j+1/2} \left(\frac{f_{j+1} - f_j}{\xi_{j+1} - \xi_j} \right) - \alpha_{j-1/2} \left(\frac{f_j - f_{j-1}}{\xi_j - \xi_{j-1}} \right) \right], \quad (28)$$

where the subscript j denotes the j th grid point. We approximate the first derivatives, as needed in Eq. (3), by central differences as

$$\frac{\partial T}{\partial \xi} \approx \frac{T_{j+1} - T_{j-1}}{\xi_{j+1} - \xi_{j-1}}. \quad (29)$$

We evaluate terms with no derivatives, such as the chemical production rate in Eq. (2), using the conditions existing at ξ_j . Likewise, the coefficients of derivatives, such as ρu in Eq. (1), are also evaluated at ξ_j .

First-order ODE's, such as Eq. (16), are differenced according to the trapezoidal rule as

$$\frac{1}{M} \left(\frac{y_j^{\alpha+1} - y_{j-1}^{\alpha+1}}{\xi_j - \xi_{j-1}} \right) = (\alpha + 1) \frac{2}{\rho_j u_j + \rho_{j-1} u_{j-1}}. \quad (30)$$

It is important to represent the integral equations as first-order differential equations and include the variables such as $y^{\alpha+1}$ in the dependent variable vector. The reason for this choice is associated with the structure of the Jacobian matrix, which is needed to solve the problem. When Eq. (30) is used, the number of dependent variables increases, but the Jacobian remains banded (a very desirable feature). On the other hand, if $y^{\alpha+1}$ were to be considered as a coefficient in the transport equations, as defined by the integral of the stream function, then the Jacobian loses its banded property and the required computer storage would increase enormously.

2.7 Non-Uniform Grid

In many reacting flow problems a thin reactive boundary layer forms near a surface. Many grid mesh points may be needed to resolve the important chemical species concentration profiles. However, further away from the surface there may be no need for such a finely resolved mesh. CRESLAF provides a means to produce a non-uniform grid, which will make the mesh fine near a surface and more widely spaced as distance from the surface increases. For cartesian coordinates, if the user has specified N mesh points (via the keyword NPTS), then the j th grid point will be placed at a distance $y(j)$ from the lower wall

$$y(j) = \frac{H}{(N-1)^s} (j-1)^s, \quad (31)$$

where H is the channel height. If $s = 1$, a uniform grid is produced. For $s > 1$, the grid is more tightly spaced at the lower boundary. In cylindrical coordinates the grid will be made finer at the outer boundary through use of an analogous formula.

2.8 Jacobian Matrix

The finite-difference representation of the defining equations forms a set of differential/algebraic equations (DAE's), which we solve numerically using the software package, DASSL.^{6, 7} The DAE's are written in the general form $g(y, y', t)=0$, where y and y' represent the components of the solution and their time derivatives, and t is time. As part of the solution to the equations, a numerical Jacobian is formed, i.e., the partial derivative of the residual g with respect to each component of the solution. A Jacobian is needed because DASSL employs an implicit time stepping method. Implicit methods are most efficient for solving the stiff equations usually found in chemical kinetics problems.

Calculating the Jacobian is expensive and the most computationally expensive aspect of evaluating it is calculation of the multicomponent transport properties. The computer time required to solve the set of DAE's can be reduced significantly by holding the transport properties fixed when calculating the numerical Jacobian. Although this introduces some error into the Jacobian, DASSL requires only an approximate Jacobian for the purpose of iterating to a converged solution.^{6, 7} No error is introduced into the solution by making this simplification in the Jacobian evaluation. However, the computer time required by the model can be decreased by a factor of ten or more.

2.9 Modified Version of DASSL

The CRESLAF program actually uses a slightly modified version of DASSL. One very minor modification enables us to hold the transport properties fixed during a Jacobian evaluation, as discussed in Section 2.8

We have also added options to DASSL for printing (sometimes copious amounts of) information when integration difficulties are encountered. A Keyword PRND controls these error diagnostics. The default level is 0, which results in no reporting. Levels 1 and 2 (the maximum) provide information on the step size, order of integration, time-step truncation error, and solution components that most significantly contributed to a convergence test failure. Level 1 prints this information only upon a convergence test failure. Level 2 prints this information at every time-step. This diagnostic information can be quite helpful, but requires thorough knowledge of DASSL's solution algorithm to be useful. The reader is referred to the DASSL citations for further documentation.^{6, 7}

3. PROGRAM STRUCTURE

The CHEMKIN Application User Interface runs the CRESLAF program automatically through a mouse-driven interface and then allows the user to directly launch visualization of solution results using the CHEMKIN Graphical Post-processor. The CRESLAF program has a modular structure with interfaces to the CHEMKIN Utility package for obtaining kinetic, thermodynamic, and transport parameters. In addition to input directly from the user, CRESLAF depends on data obtained from the CHEMKIN Gas-phase, SURFACE CHEMKIN and TRANSPORT packages. Therefore, to solve a reacting-flow problem the user must first execute the three preprocessor programs, “chem”, “tran” and “surf”, which have access to thermodynamic and transport-property databases. CRESLAF then reads input from the user (described in Chapter 4), defines the governing equations, solves the equations, and prints solutions for the reacting-flow problem. The CHEMKIN Graphical Post-processor can then be launched from the Application User Interface to plot solution data. Figure 1 shows the relationships between these components. For more information about the CHEMKIN Application User Interface or Graphical Post-processor, please see the CHEMKIN Getting Started manual.

The first step is to execute the CHEMKIN Interpreter, “chem”. The CHEMKIN Interpreter first reads user-supplied information about the species and chemical reactions for a particular reaction mechanism. It then extracts further information about the species’ thermodynamic properties from a database, “therm.dat”. The user may also optionally input thermodynamic property data directly in the input file to the CHEMKIN Interpreter to override or supplement the database information. The information from the user input and the thermodynamic properties is stored in the CHEMKIN Linking File, “chem.asc”; a file that is needed by the TRANSPORT property fitting program, “tran”, by the SURFACE CHEMKIN Interpreter, and later by the CHEMKIN subroutine library, which will be accessed by the CRESLAF program. The CHEMKIN Interpreter also writes text output (e.g. “chem.out”) that includes a formatted display of the user input and diagnostic messages from the Interpreter.

The next program to be executed is the TRANSPORT property-fitting program, “tran”. It needs input from a transport property database, “tran.dat” and from the CHEMKIN subroutine library. The user may also optionally input transport property data directly in a separate input file (e.g. “tran.inp”) to override or supplement the database information. The purpose of the TRANSPORT fitting program is to compute polynomial representations of the temperature-dependent parts of the individual species viscosities, thermal conductivities, and the binary diffusion coefficients. Like the CHEMKIN Interpreter, the TRANSPORT property-fitting program produces a Linking File, “tran.asc” that is later needed in the transport property library routines, which will evaluate mixture properties during the course of the CRESLAF computation.

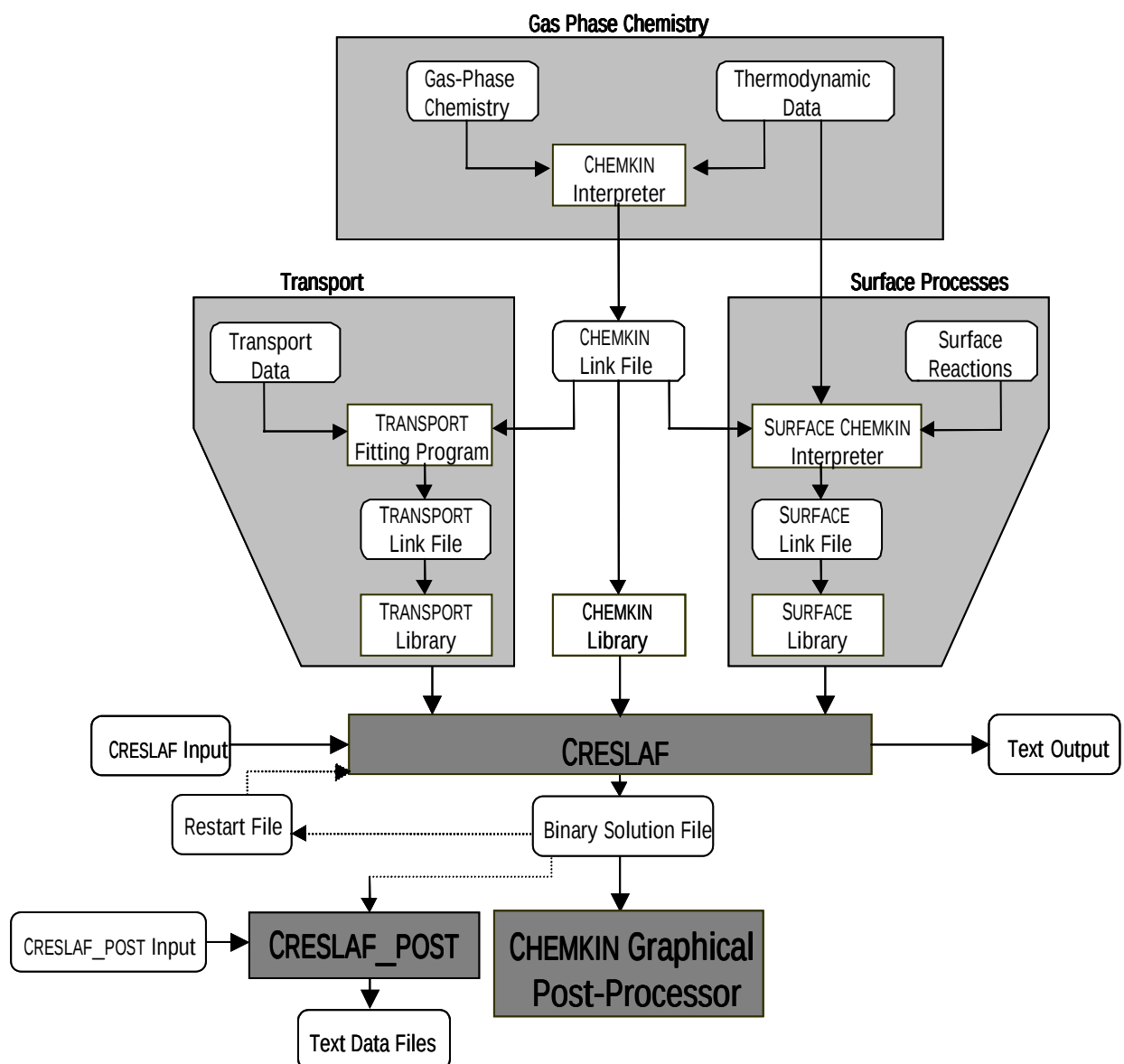


Figure 1. Relationship of CRESLAF to the CHEMKIN, SURFACE CHEMKIN, and TRANSPORT pre-processors, and the associated input and output files.

The SURFACE CHEMKIN Interpreter must also be executed after the CHEMKIN Interpreter has been run, because it relies on gas-phase species and element information in the CHEMKIN Linking file. The SURFACE CHEMKIN Interpreter reads user-supplied information (e.g., “surf.inp”) about surface and bulk species names, surface site types, surface reactions, and optional thermochemical information. This information is written to a SURFACE CHEMKIN Linking File (“surf.asc”), and later accessed by the SURFACE CHEMKIN subroutine library when called by the CRESLAF program. The SURFACE CHEMKIN Interpreter also generates a text file (e.g., “surf.out”) containing the input mechanism information and diagnostic messages.

Once the pre-processors have run successfully, the CRESLAF program can then be executed. Since the CHEMKIN, SURFACE CHEMKIN, and TRANSPORT subroutine libraries must be initialized before use, the CRESLAF program begins by making the appropriate initialization subroutine calls. The purpose of the initialization is to read the Linking Files and to set up the internal working and storage space required by all subroutines in the libraries.

CRESLAF then reads the user input that defines a particular reacting flow problem and the parameters needed to solve it. This input is read in Keyword format from the input file (e.g. “creslaf.inp”), described in Chapter 4. In addition to this input, there is a provision for the CRESLAF program to begin its solution from a previously computed solution. In this case the old solution is read from a binary Restart File, called “rest.bin”. The program produces printed output (e.g. “creslaf.out”) and it saves the solution in a binary Save File, “save.bin”. The Save File can be used to restart CRESLAF to the channel-flow simulation farther downstream. The Restart File is the same format as the Save File; a Restart File can therefore be created simply by copying a Save File, e.g. “save.bin” to the Restart File name, “rest.bin”.

3.1 Optional User Programming

In addition to using CRESLAF through the CHEMKIN Application User Interface, users have the flexibility to write their own interface to the reacting-flow model. To facilitate this, the CRESLAF program itself is written as a Fortran subroutine that may be called from a user-supplied driver routine. We provide examples of such driver routines as part of the CRESLAF software distribution, written in both C++ and Fortran. The driver routine performs the function of allocating total memory usage through definition of array sizes, as well as opening input and output files. CRESLAF checks internally to make sure that the allocated work arrays are sufficiently large to address the problem described by the input files. Programs can be linked to the CRESLAF subroutine by following the examples in the makefiles provided in the sample driver subdirectories (“drivers_f77” or “drivers_cpp”) of the standard distribution. Users taking advantage of this flexibility should be experienced with compiling and linking program files on their operating system and must have either a C++ or Fortran compiler installed.

3.2 The Save (or Restart) File

In addition to printed output, CRESLAF produces a binary solution file (“save.bin”) that contains the solution data. This file has two important uses. One use is when the program has terminated due to a time limit prior to reaching the requested channel distance. In this case, the file can be used to restart the computation where it left off. The second use for the binary solution file is for post-processing the solution, using the CHEMKIN Graphical Post-processor or an alternate program. Further information on this subject will be found in the post-processing discussion in Chapter 5.

3.3 Structure of the User-Supplied Initial-Profile File

Normally the user specifies the initial profile of gas-phase species concentrations, temperature, velocity, and surface site fractions via the keyword input described before. If more custom tailoring of the initial solution profile is desired, use of the PROF option will force CRESLAF to read a user-supplied solution profile. This solution profile will be used as the starting point for CRESLAF. The user has complete freedom in specifying a particular velocity profile, concentration profile, or grid-node placement (for example). A portion of FORTRAN code that will write the information needed on the profile file in the correct format is shown in Figure 2. Actual specification of the information in each array (for example, in the TEMPERATURE array), which would be up to the user, is not shown.

```
C      put components into the solution vector:
      DO 750 J = 1, JJ
        SOLUTION(1,J) = PRESSURE(J)
        IF (ICRD .EQ. 1) THEN
          radial coordinates
          SOLUTION(2,J) = HEIGHT(J)**2
        ELSE
          planar coordinates
          SOLUTION(2,J) = HEIGHT(J)
        ENDIF
        SOLUTION(3,J) = VELOCITY(J)
        SOLUTION(4,J) = TEMPERATURE(J)
        SOLUTION(5,J) = LOWERMASSLOSS(J)
        SOLUTION(6,J) = UPPERMASSLOSS(J)
        DO 500 K = 1, KKGAS
          SOLUTION(6+K,J) = MASSFRACTION(J,K)
500      CONTINUE
750    CONTINUE
C
      NATJ = KKGAS + 6
      WRITE (LPROF) ICRD, JJ, NATJ, KKGAS, KKSURF, KKBULK
C
      IF (ICRD .EQ. 0) THEN
        planar coordinates
        WRITE (LPROF) (SITELOW(K),K=1,KKSURF),
1          ((SOLUTION(N,J),N=1,NATJ),J=1,JJ),
2          (SITEHIGH(K),K=1,KKSURF),
3          (ACT(K),K=KK+KKSURF+1,KK+KKSURF+KKBULK)
        ELSE
C      radial coordinates or planar with symmetry axis
        WRITE (LPROF) ((SOLUTION(N,J),N=1,NATJ),J=1,JJ),
1          (SITEHIGH(K),K=1,KKSURF),
2          (ACT(K),K=KK+KKSURF+1,KK+KKSURF+KKBULK)
        ENDIF
```

Figure 2. Sample FORTRAN code segment for generating a user-supplied initial solution profile.

4. PROGRAM INPUT

4.1 Keyword Syntax and Rules

The CRESLAF program's input is in a Keyword format. On each input line an identifying keyword must appear first. For some keywords only the keyword itself is required, while for others additional information (such as a number) is required. Some keywords have default values associated with them and in such cases the keyword line is optional. The order of the keyword inputs is generally unimportant, except for some grouped lists that must be ordered. All keywords and associated modifiers are given in upper case. The rules governing the syntax of the keywords are listed below:

1. The first four columns of the line are reserved for the keyword, and it must begin in the first column.
2. Any further input associated with the keyword can appear anywhere in columns 5 through 80. The specific column in which the information begins is unimportant.
3. When more than one piece of information is required, the order in which the information appears is important.
4. When numbers are required as input, they may be stated in either integer, floating point, or E format. The program converts the numbers to the proper type. The double precision specification is not recognized; however, the double precision conversion is done internally as necessary.
5. When gas-phase species names are required as input, they must appear exactly as they were specified in the CHEMKIN input. When surface or bulk species names are required as input, they must appear exactly as they were specified in the SURFACE CHEMKIN input.
6. When more than one piece of information is required, the pieces are delimited by one or more blank spaces.
7. If more information is input than required, then the last read inputs are used. For example, if the same keyword is encountered twice or if conflicting keywords are given, the last one read is implemented.
8. A "comment" line can be inserted by placing either a period (.), a slash (/), or an exclamation point (!) in the first column. The program ignores such a line, but it is echoed back in the printed output.
9. The keyword END must be the last input line.

4.2 DASSL Numerical Solution Options

ATOL — Absolute error tolerance for DASSL. Typically ATOL should be smaller than the maximum mass fraction of any species of interest.

Units -- None

Default -- 1.E-8

Example -- ATOL 5.0E-6

RTOL — Relative error tolerance for DASSL. Typically RTOL should be in the range of 10^{-3} , which would provide roughly three significant digits to 10^{-6} , which would provide roughly six digits.

Units -- None

Default -- 1.E-4

Example -- RTOL 5.0E-4

IERW — Error tolerances specified for individual species, whether gas-phase or surface. This allows the flexibility to control the error species by species and overrides the values given by ATOL and RTOL for the species specified. The format is to include the keyword IERW, followed by the species name, followed by the desired ATOL and RTOL.

Units -- None

Default -- The values of ATOL and RTOL are used for every species.

Example -- IERW SI2 1.0E-8 1.0E-5

HO — Specifies the initial step size to be used by DASSL.

Units -- cm

Default -- None; chosen by DASSL

Example -- HO 1.0E-8

MORD — Maximum order of integration used by DASSL.

Units -- None

Default -- 5

Example -- MORD 3

PRND — Specifies level of output diagnostics reported by DASSL when integration difficulties are encountered. The default level is 0, which is no reporting. Levels 1 and 2 (the maximum) provide information on the step size, order of integration, time-step truncation error, and which solution components most significantly contributed to a failure in the convergence test. Level 1 prints this information only upon a convergence failure. Level 2 prints the information at every time-step.

Units -- None

Default -- 0

Example -- PRND 2

NOTP — Do not solve for the initial gas-phase and surface concentrations at the walls using the TWOPNT procedure.

Units -- None

Default -- Do the initial TWOPNT procedure.

Example -- NOTP

4.3 Twopnt Numerical Solution Options

(Note: TWOPNT is used to establish initial conditions for surface site fractions and gas mass fractions)

TWAB — Absolute error tolerance.

Name of parameter in TWOPNT manual -- SSABS

Units -- None

Default -- 1.0E-13

Example -- TWAB 1.0E-10

TWRE — Relative error tolerance.

Name of parameter in TWOPNT manual -- SSREL

Units -- None

Default -- 1.0E-14

Example -- TWRE 1.0E-10

TWTA — Absolute error tolerance if time-stepping required.

Name of parameter in TWOPNT manual -- TDABS

Units -- None

Default -- 1.0E-12

Example -- TWTA 1.0E-10

TWTR — Relative error tolerance if time-stepping required.

Name of parameter in TWOPNT manual -- TDREL

Units -- None

Default -- 1.0E-4

Example -- TWTR 1.0E-10

TWPR — Specifies print level.

Name of parameter in TWOPNT manual -- LEVELD, LEVELM

Units -- None

Default -- 22

Example -- TWPR 0

TWST — Number of time steps before trying another Newton step.

Name of parameter in TWOPNT manual -- STEPS1

Units -- None

Default -- 100

Example -- TWST 50

ISTP — Number of initial time steps before beginning initial Newton try.

Name of parameter in TWOPNT manual -- STEPS0

Units -- None

Default -- 0

Example -- ISTP 500

IRET — Minimum number of time steps before retiring this step size and trying a new one.

Name of parameter in TWOPNT manual -- STEPS2

Units -- None

Default -- 50

Example -- IRET 25

NJAC — Retirement age of Jacobian during Newton iteration.

Name of parameter in TWOPNT manual -- SSAGE

Units -- None

Default -- 20

Example -- NJAC 15

TJAC — Retirement age of Jacobian during time stepping.

Name of parameter in TWOPNT manual -- TDAGE

Units -- None

Default -- 20

Example -- TJAC 15

DTMX — Maximum time step size.

Name of parameter in TWOPNT manual -- TMAX

Units -- sec

Default -- 1.0E-4

Example -- DTMX 1.0E-6

DTMN — Minimum time step size.

Name of parameter in TWOPNT manual -- TMIN

Units -- sec

Default -- 1.0E-10

Example -- DTMN 1.0E-12

STP0 — Initial time step to be tried.

Name of parameter in TWOPNT manual -- STRID0

Units -- sec

Default -- 1.0E-6

Example -- STP0 1.0E-7

4.4 Grid Parameters

NPTS — The number of mesh points in the problem. The program will generate an equispaced mesh of NPTS points. The user can also specify a nonuniform mesh using the keyword STCH.

Units -- None

Default -- None; NPTS is a required input.

Example -- NPTS 50

STCH — Parameter to produce a non-uniform grid. For cartesian coordinates the initial grid location for a node J is $X(J)=A*(J-1)**STCH$, where $A=HITE/(NPTS-1)**STCH$, HITE is the reactor height, and NPTS is the total number of grid nodes. If STCH=1, a uniform grid is produced. For STCH > 1, the grid is more tightly spaced at the lower boundary (cartesian_coordinates) or at the outer boundary (cylindrical coordinates), and consequently the grid is more widely spaced at the other boundary.

Units -- None

Default -- 1.0

Example -- STCH 1.2

4.5 Reactor Description

PRES — The pressure.

Units -- atmospheres

Default -- None; PRES is a required input.

Example -- PRES 0.25

VEL — The maximum gas-phase velocity at the inlet. If the problem is in cartesian coordinates, then the average velocity equals two-thirds of the maximum velocity of the parabolic velocity profile. In cylindrical coordinates, the average velocity is half of the maximum velocity. If the keyword BLTK is given, a flat velocity profile will be used, i.e., everywhere the velocity will be set equal to VEL except within a distance BLTK of the walls.

Units -- cm/sec

Default -- None; VEL is required input.

Example -- VEL 15

BLTK — This keyword is used to specify a boundary-layer thickness. When BLTK is declared, a parabolic velocity profile is specified with a zero velocity at each wall increasing to the velocity specified by VEL at a distance of BLTK from the wall. A flat (constant) velocity profile is used for distances greater than BLTK from the wall. In addition, if the initial gas temperature differs from the initial surface temperature the program linearly interpolates the gas-phase temperature profile between the wall temperature and the bulk gas temperature over the distance BLTK.

Units -- cm

Default -- 0.

Example -- BLTK 0.05

HITE — The channel height (for cartesian coordinates), or the reactor radius (cylindrical coordinates), or distance between the channel wall and the symmetry line for a symmetric planar channel.

Units -- cm

Default -- None; HITE is a required input.

Example -- HITE 2.0

ICRD — Flag to specify coordinate system: planar coordinates (ICRD PLAN); or radial coordinates (ICRD RAD) or cartesian coordinates with symmetric channel walls (ICRD SYMC). Only one-half of the physical domain is used for the symmetric channel case, and the lower boundary is a symmetry line.

Units -- None

Default -- None; ICRD is a required input.

Example -- ICRD PLAN

XEND — The total length of the channel.

Units -- cm

Default -- None; XEND is a required input.

Example -- XEND 25.

DX — Print the solution every DX cm.

Units -- cm

Default -- 0.5

Example -- DX 0.25.

GRAV — The value of the acceleration of gravity. The buoyancy term can only be included in the boundary-layer equations if gravity acts parallel to the principal flow direction. Thus, GRAV 980 may be used to describe flow vertically upward, or GRAV -980 for flow downward. Omitting this keyword neglects the buoyancy term.

Units -- cm/sec²

Default -- 0.

Example -- GRAV -980

REAC — Mole fraction values of the reactants entering at the inlet. One of these REAC inputs must appear for each reactant species. The sum of all the reactant mole fractions should equal one. However, if they do not, a cautionary message will be printed and the mole fractions will be normalized so the sum does equal one.

Units -- None; mole fractions

Default -- None; required input for at least one gas species.

Example -- REAC SIH4 0.2

GASW— Mole fraction of the reactants estimated at the walls. The sum of all the GASW values should equal one. However, if they do not, a cautionary message will be printed and the mole fractions will be normalized so the sum does equal one. If GASW is not specified, then the values given by the REAC keyword will be used. The actual gas mole fractions at each wall at the initial condition of the boundary-layer calculation will be calculated via the TWOPNT procedure (unless the NOTP keyword appears).

Units -- None; mole fractions

Default -- Values given by the REAC keyword will be used.

Example -- GASW SIH2 1.0E-4

SURF — Surface site fraction values estimated for the surface species for each surface site-type (phase) on the surface. One of these SURF inputs should appear for each surface species in large concentration on the surface. The sum of the site fractions should equal one for each surface site type (surface phase). However, if they do not, a cautionary message will be printed and the site fractions for each surface site type will be normalized so the sum does equal one. The actual surface site fractions at each wall as the initial condition of the boundary-layer calculation will be calculated via the TWOPNT procedure (unless the NOTP keyword appears).

Units -- None; surface site fractions

Default -- None; required input for at least one surface species in each site phase.

Example -- SURF SIH2(S) 1.0E-3

ACT — Mole fraction values for the bulk species in each bulk mixture (phase). One of these ACT inputs should appear for each bulk species in a bulk phase. The sum of the bulk species fractions should equal one for each bulk mixture (bulk phase). However, if they do not, a cautionary message will be printed and the bulk species fractions for each bulk phase will be normalized so the sum does equal one.

Units -- None; bulk species mole fractions

Default -- None; required for at least one bulk species per bulk phase.

Example -- ACT SI(D) 1.0E-3

TSPL — This keyword allows an optional specification of the surface temperature profile as an (x,T) pair. There is a TSPL keyword line for each desired (x,T) pair. The x coordinates of each TSPL line must be given in ascending order.

Units -- cm, K

Default -- None; optional input.

Example -- TSPL 0.1 973

GTMP — Gas-phase temperature at the inlet.

Units -- K

Default -- None; GTMP is required input.

Example -- GTMP 298

STMP — Surface temperature.

Units -- K

Default -- None; STMP is required input, unless TSPL keyword is included.

Example -- STMP 973

XTMP — If STMP is used to specify the surface temperature, the program will set the surface temperature to GTMP at $x=0$ and smoothly ramp the temperature up to STMP at a distance of XTMP.

Units -- cm

Default -- 0.5

Example -- XTMP 0.25

FIXT — Keyword for temperature boundary condition on the upper wall (only used for cartesian coordinates). The upper wall is held at a fixed temperature of GTMP if FIXT is specified. A zero temperature gradient is enforced if FIXT is omitted (adiabatic wall).

Units -- None

Default -- Adiabatic top wall is used.

Example -- FIXT

SYMT — Keyword for temperature boundary condition on the upper wall (only used for cartesian coordinates). The upper wall temperature is set equal to the bottom wall temperature if SYMT is specified.

Units -- None

Default -- Top temperature is different than bottom.

Example -- SYMT

ADIA — Keyword that turns on the adiabatic wall condition for symmetric cases. For planar, non-symmetric cases, an adiabatic wall is the default, but for symmetric (planar or cylindrical) cases, the ADIA keyword is required for the adiabatic condition.

Units -- None

Default -- Specified (non-adiabatic) condition.

Example -- ADIA

4.6 Transport Property Options

MULT — Inclusion of this keyword causes the calculation to be run with a full multicomponent model for the transport coefficients and diffusion velocities.

Units -- None

Default -- Multicomponent transport is not used.

Example -- MULT

MIX — Inclusion of this keyword causes the calculation to be run using a mixture-average model for calculating the transport coefficients and diffusion velocities.

Units -- None

Default -- Mixture-averaged transport is used.

Example -- MIX

TDIF — Inclusion of this keyword causes the calculation to be run with thermal diffusion (Soret effect). The thermal diffusion coefficients are always calculated from the multicomponent model.

However, the keywords MULT or MIX still determine whether the diffusion coefficients and diffusion velocities are calculated with the multicomponent model.

Units -- None

Default -- Thermal diffusion is not used.

Example -- TDIF

VCOR — Inclusion of this keyword causes the calculation to be run using a correction velocity to ensure mass conservation, i.e., the sum of the diffusion fluxes is zero. See Eq. (26).

Units -- None

Default -- Correction velocity is not used.

Example -- VCOR

4.7 Miscellaneous Controls

IRST — Inclusion of this keyword causes the program to begin the calculation at the point where a previous solution ended. This previously-computed solution will be read from a binary solution file normally called “rest.bin”.

Units -- None

Default -- Solution started anew, not from a restart file.

Example -- IRST

PROF — Inclusion of this keyword causes the program to read an initial solution profile (gas-phase concentrations, temperatures, velocities, surface site fractions, etc.) from a user-supplied input file. This feature allows the user almost complete freedom in specifying customs of initial conditions (a flexibility not available from standard keyword input). This previously-computed profile will be read from a formatted ascii input file, normally called “cres.pro”. The format for this file is explained in Section 3.3.

Units -- None

Default -- User-supplied profile not used.

Example -- PROF

GFAC — Use of this keyword specifies that the rates of all gas-phase reactions will be multiplied (scaled) by the factor GFAC.

Units -- None

Default -- 1; actual values of the gas-phase reaction rates are used.

Example -- GFAC 0.1

SFAC — Use of this keyword specifies that the rates of all surface reactions will be multiplied (scaled) by the factor SFAC. SFAC cannot be set to zero; doing so would cause a singular Jacobian.

Units -- None

Default -- 1; actual values of the surface reaction rates are used.

Example -- SFAC 0.1

MOLF — Mole fractions of the gas-phase species will be used in the solution print out.

Units -- None

Default -- Mole fractions are printed.

Example -- MOLF

PARP — Partial-pressures of the gas-phase species will be used in the solution print out.

Units -- None

Default -- Mole fractions are printed, not partial pressures.

Example -- PARP

END — This line signifies the end of the input data.

5. POST PROCESSING

5.1 CHEMKIN Graphical Post-processor

The CHEMKIN Graphical Post-processor provides a means for quick visualization of results from CRESLAF. Launched from the CHEMKIN Application User Interface, the Graphical Post-processor will automatically read in the solution data from the “save.bin” file in the working directory. Alternatively, the post-processor may be launched independently and a solution file may be opened from within the Post-processor. The user may open one or more solution files in the Post-processor and may also import external data for comparisons with the simulation results. In addition, the Graphical Post-processor can be used to export all of the solution data into comma-, tab-, or space-delimited text for further analysis with other software packages. For more information on the Graphical Post-processor, please see the CHEMKIN Getting Started manual.

5.2 Configurable Command-line Post-processor

In addition to the CHEMKIN Graphical Post-processor representation of solution data, we provide the user with a FORTRAN post-processor called CRESLAF_POST. This program reads the binary solution file and prints selected data to text files, which can then be imported by many other graphics programs. The full source-code, `creslaf_post.f`, is provided in the CHEMKIN “post_processors” subdirectory. Also in this directory is a makefile script for re-building the CRESLAF_POST program, in case the user makes changes to the source code. In this way, the user may easily configure CRESLAF_POST for their own analysis needs.

To run CRESLAF_POST from the command-line, you will need to do the following:

1. Open a MS-DOS Prompt (PC) or shell (UNIX).
2. Change directories to your working directory, where your “save.bin” solution file resides.
3. Run CRESLAF_POST from the command-line, specifying the full path to the CHEMKIN “bin” directory where the “creslaf_post” executable resides, unless this is already in your environment “path” variable:

```
creslaf_post < creslaf_post.inp > creslaf_post.out
```

Here, “creslaf_post.inp” is an input file that contains keywords described below. The output “creslaf_post.out” will contain diagnostics and error messages for the CRESLAF_POST run. CRESLAF_POST will also create text files containing comma-separated values. The names for these files use a suffix (extension) of “.csv”.

CRESLAF_POST uses keyword input. The available keywords are printed as a banner when the program is invoked; they are also described briefly here:

- PREF** Requests the text file name be prefixed by a character string.
Default – “cres”
Example: PREF cres
- DIST** Requests a particular distance solution be selected from the binary solution file, or “ALL”.
Units – cm
Default – the final solution in the binary solution file.
Example: DIST 1.0.
- SPEC** Requests species fractions for a space-delimited list of species, or “ALL”.
Default - none.
Example: SPEC H2 O2 OH H2O HO2 H O
- MOLE** Print species as mole fractions.
Default - MOLE.
- MASS** Print species as mass fractions.
Default - MOLE.
- SMIN** Do not print species whose maximum fraction is less than SMIN.
Default – 0.0.
- HELP** Print a brief guide to keyword input.
- END** Begin post-processing.

6. SAMPLE PROBLEM: CHEMICAL VAPOR DEPOSITION IN SYMMETRIC CHANNEL

In this chapter we show solution of an example problem using the CRESLAF program. All sample input files and output files are listed in Sections 6.1 - 6.6. We have chosen as a sample the deposition of Si_3N_4 from SiF_4 and NH_3 . The gas-phase reaction mechanism contains a detailed description of NH_3 decomposition (about which there is much published information), two reactions describing SiF_4 decomposition, and three cross-reactions. At the low pressures we consider, the gas-phase decomposition of reactants is slow. The surface reaction mechanism contains six steps describing the overall conversion of 3 SiF_4 and 4 NH_3 molecules to 3 Si(d) and 4 N(d) and 12 HF . (Note that the surface reaction mechanism is from a preliminary analysis at one temperature, and thus we have not supplied any activation energies. As such, this mechanism should be considered only as illustrative and not as a source of kinetic data on the Si_3N_4 system.)

Section 6.1 shows the input file for the CHEMKIN Interpreter, which defines the gas-phase reaction mechanism. The output from the CHEMKIN Interpreter is shown next in Section 6.2. The input to and output from the SURFACE CHEMKIN Interpreter (Sections 6.3 and 6.4) show the surface species and surface reactions in the problem. More details on the CHEMKIN and SURFACE CHEMKIN Interpreters can be found in the user's manuals for each program.

The file containing the Keyword input to CRESLAF gives the specific run conditions for the problem and is listed in Section 6.5. The input specifies 15 grid points (NPTS), a computational domain that ends at 10 cm (XEND), and a pressure of 2.3684E-3 atmospheres (PRES). The reactor geometry is a radially symmetric channel (ICRD), with a radius of 2.0 cm (HITE). The reactant mole fractions at the inlet are given (REAC), as are the site fractions of the surface species (SURF), and the mole fractions of the bulk phase species (ACT). The rest of the Keywords specify numerical error tolerances, printing controls, etc.

The last file, shown in Section 6.6, is the output from the CRESLAF program. A series of banners are displayed showing the version numbers of CRESLAF and the CHEMKIN, SURFACE CHEMKIN, and TRANSPORT libraries being used. After giving statistics on the workspace requirements, the program echoes back the keyword inputs.

The CHEMKIN two-point boundary-value solver TWOPNT solves for the initial set of site fractions and gas-phase mass fractions, which satisfy Eqs. (17-20) at the boundary node. The results from the TWOPNT problem are shown next. The boundary values calculated are then used in solving the boundary-layer problem.

At a distance interval controlled by the keyword DX, CRESLAF prints the current value of the solution. At the top of each page it prints the distance and some statistics on the progress of the solution from DASSL, as well as the total mass in the flow and the pressure. For each gas-phase node the program prints the

value of the y coordinate, the velocity j , the temperature, and the mole fraction of each gas-phase species. The column labeled OMS contains the difference between the sum of the mass fractions and unity. Below each species name, the program also prints the flux of the species to the boundary (in $\text{g}/\text{cm}^2/\text{sec}$). This information is sometimes useful in identifying which species is most responsible for carrying mass to the surface in a deposition process.

The program then prints the values of surface site fractions at each wall (lower and upper for cartesian coordinates; outer wall only for cylindrical coordinates; top wall only for the symmetric planar channel). Finally, the program prints the deposition rate for each bulk-phase species. CRESLAF calculates the growth rate from the molar production rate and the value of the bulk density for each bulk species that was supplied to the SURFACE CHEMKIN Interpreter.

6.1 Input to CHEMKIN Interpreter for the Example

```

ELEMENTS H N SI F END
SPECIES H2 H N2 N NH NH2 NNH N2H2 N2H3 N2H4
        HF F SIF4 SIF3 SIHF3 SIF3NH2 NH3
END

THERMO
SI      J 3/67SI 100 0000 0000 00G 300.000 5000.000 1
0.26506014E 01-0.35763852E-03 0.29592293E-06-0.72804829E-10 0.57963329E-14 2
0.53437054E 05 0.52204057E 01 0.31793537E 01-0.27646992E-02 0.44784038E-05 3
-0.32833177E-08 0.91213631E-12 0.53339032E 05 0.27273204E 01 4
SIF2    41889SI 1F 2 0 0G 300.000 3000.000 1000.00 0 1
0.61424704E+01 0.78079745E-03-0.13393120E-06-0.62648393E-10 0.17251383E-13 2
-0.77440422E+05-0.47123275E+01 0.38453453E+01 0.60384651E-02-0.11677322E-05 3
-0.45795536E-08 0.26074143E-11-0.76816336E+05 0.72729836E+01 4
SIF     41889SI 1F 1 0 0G 300.000 3000.000 1000.00 0 1
0.41200666E+01 0.35488207E-03-0.72002223E-07-0.21904345E-10 0.67645906E-14 2
-0.75613784E+04 0.27842460E+01 0.31449478E+01 0.25885573E-02-0.57959124E-06 3
-0.18072788E-08 0.10411718E-11-0.72944390E+04 0.78767738E+01 4
SIF3NH2 41889SI 1N 1F 3H 2G 300.000 3000.000 1000.00 0 1
0.12109636E+02 0.43832823E-02-0.41422453E-06-0.39890902E-09 0.89589543E-13 2
-0.16417678E+06-0.30469284E+02 0.62294030E+01 0.17780151E-01-0.26123043E-05 3
-0.12672435E-07 0.70445559E-11-0.16258489E+06 0.20454407E+00 4
SIHF3   41889SI 1H 1F 3 0G 300.000 3000.000 1000.00 0 1
0.93635674E+01 0.29475559E-02-0.35776330E-06-0.28582245E-09 0.69157286E-13 2
-0.14860736E+06-0.21694529E+02 0.39180529E+01 0.14639172E-01-0.18560698E-05 3
-0.10582003E-07 0.56175433E-11-0.14704386E+06 0.70242615E+01 4
SIF3    41889SI 1F 3 0 0G 300.000 3000.000 1000.00 0 1
0.85247898E+01 0.13237924E-02-0.21042787E-06-0.11495040E-09 0.30553014E-13 2
-0.12235223E+06-0.15502343E+02 0.46628685E+01 0.10087878E-01-0.18055442E-05 3
-0.77692990E-08 0.43778518E-11-0.12129652E+06 0.46729660E+01 4
SIF4    J 6/76SI 1F 4 0 0G 300.000 5000.000 1
0.10478473E 02 0.28586756E-02-0.12646314E-05 0.24746863E-09-0.17824296E-13 2
-0.19790550E 06-0.27520641E 02 0.21893068E 01 0.33702007E-01-0.46723179E-04 3
0.31584638E-07-0.84506114E-11-0.19603289E 06 0.13287308E 02 4
HF      J 6/77H 1F 1 0 0G 300.000 5000.000 1
0.29919110E 01 0.71489475E-03-0.68630973E-07-0.11617130E-10 0.19412375E-14 2
-0.33621364E 05 0.38123288E 01 0.34379986E 01 0.53571598E-03-0.15229655E-05 3
0.17564491E-08-0.57869940E-12-0.33818972E 05 0.11930153E 01 4
F       J 9/65F 1 0 0 0G 300.000 5000.000 1
0.27004353E 01-0.22293182E-03 0.97941385E-07-0.19123038E-10 0.13768154E-14 2
0.87163617E 04 0.38067182E 01 0.28128740E 01-0.33023098E-05-0.12897310E-05 3
0.16837365E-08-0.64587833E-12 0.86604019E 04 0.30984198E 01 4
END

REACTIONS
H+H+M=H2+M 0.100E+19 -1.000 0.000 ! D-L
H2/0.0/
H+H+H2=H2+H2 0.920E+17 -0.600 0.000
NH+N=N2+H 0.300E+14 0.000 0.000 ! JAM
NH+H=N+H2 0.100E+15 0.000 0.000 ! NH3 CST
NH2+H=NH+H2 0.692E+14 0.000 3650.000
NH3+H=NH2+H2 0.636E+06 2.390 10171.000 ! MICHAEL
NNH=N2+H 0.100E+05 0.000 0.000 ! JAM
NNH+H=N2+H2 0.100E+15 0.000 0.000 ! JAM
NNH+NH2=N2+NH3 0.500E+14 0.000 0.000 ! JAM
NNH+NH=N2+NH2 0.500E+14 0.000 0.000 ! JAM
NH2+NH=N2H2+H 0.500E+14 0.000 0.000 ! NH3CST
NH+NH=N2+H+H 0.254E+14 0.000 0.000 ! NH3 CST
NH2+N=N2+H+H 0.720E+14 0.000 0.000 ! PG
N2H2+M=NNH+H+M 0.500E+17 0.000 50000.000 ! NH3 CST
N2/2/ H2/2/
N2H2+H=NNH+H2 0.500E+14 0.000 1000.000 ! NH3 CST
N2H2+NH=NNH+NH2 0.100E+14 0.000 1000.000 ! NH3 CST
N2H2+NH2=NH3+NNH 0.100E+14 0.000 1000.000 ! NH3 CST
NH2+NH2=N2H2+H2 0.500E+12 0.000 0.000 ! NH3 CST
NH3+M=NH2+H+M 0.140E+17 0.000 90600.000 ! MSGK
N2H3+H=NH2+NH2 1.60E+12 0.0 0.0 ! MSGK

```

N2H3+M=N2H2+H+M	3.50E+16	0.0	46000.0	! MSGK
N2H3+NH=NH2+N2H2	2.00E+13	0.0	0.0	! MSGK
NH2+NH2+M=N2H4+M	3.00E+20	-1.0	0.0	! MSGK
H+N2H4=H2+N2H3	1.30E+13	0.0	2500.0	! MSGK
NH2+N2H4=NH3+N2H3	3.90E+12	0.0	1500.0	! MSGK
NH+H+M=NH2+M	2.00E+16	-0.5	0.0	! MSGK
NH2+NH2=NH3+NH	5.00E+12	0.0	10000.0	! MSGK
F+NH3=NH2+HF	4.27E+11	0.5	800.0	! KONDRATIEV
SIF4=SIF3+F	3.00E+12	0.0	147170.0	! PHO&MEC
H+SIF4=HF+SIF3	1.00E+13	0.0	50000.0	! PHO&MEC
NH2+SIF4=SIF3NH2+F	1.00E+11	0.0	40950.0	! GUESS
NH3+SIF3=SIF3NH2+H	1.00E+11	0.0	5000.0	! GUESS
NH3+SIF3=SIHF3+NH2	1.00E+11	0.0	10000.0	! PHO&MEC
END				

6.2 Output from CHEMKIN Interpreter for the Example

CHEMKIN-III GAS-PHASE MECHANISM INTERPRETER:

DOUBLE PRECISION Vers. 6.24 2000/06/18

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		ELEMENTS CONSIDERED		ATOMIC WEIGHT						
		1. H		1.00797						
		2. N		14.0067						
		3. SI		28.0860						
		4. F		18.9984						
		C								
		P								
		H								
		A								
		R								
		S								
		G								
		E								
		E								
		MOLECULAR		TEMPERATURE						
		WEIGHT		LOW	HIGH					
		ELEMENT COUNT								
		H	N	SI	F					
1. H2		G	0	2.01594	300	5000	2	0	0	0
2. H		G	0	1.00797	300	5000	1	0	0	0
3. N2		G	0	28.01340	300	5000	0	2	0	0
4. N		G	0	14.00670	300	5000	0	1	0	0
5. NH		G	0	15.01467	300	5000	1	1	0	0
6. NH2		G	0	16.02264	300	5000	2	1	0	0
7. NNH		G	0	29.02137	250	4000	1	2	0	0
8. N2H2		G	0	30.02934	300	5000	2	2	0	0
9. N2H3		G	0	31.03731	300	5000	3	2	0	0
10. N2H4		G	0	32.04528	300	5000	4	2	0	0
11. HF		G	0	20.00637	300	5000	1	0	0	1
12. F		G	0	18.99840	300	5000	0	0	0	1
13. SIF4		G	0	104.07960	300	5000	0	0	1	4
14. SIF3		G	0	85.08120	300	3000	0	0	1	3
15. SIHF3		G	0	86.08917	300	3000	1	0	1	3
16. SIF3NH2		G	0	101.10384	300	3000	2	1	1	3
17. NH3		G	0	17.03061	300	5000	3	1	0	0

REACTIONS CONSIDERED			(k = A T**b exp(-E/RT))		
			A	b	E
1. H+H+M=H2+M			1.00E+18	-1.0	0.0
H2	Enhanced by	0.000E+00			
2. H+H+H2=H2+H2			9.20E+16	-0.6	0.0
3. NH+N=N2+H			3.00E+13	0.0	0.0
4. NH+H=N+H2			1.00E+14	0.0	0.0
5. NH2+H=NH+H2			6.92E+13	0.0	3650.0
6. NH3+H=NH2+H2			6.36E+05	2.4	10171.0
7. NNH=N2+H			1.00E+04	0.0	0.0
8. NNH+H=N2+H2			1.00E+14	0.0	0.0
9. NNH+NH2=N2+NH3			5.00E+13	0.0	0.0
10. NNH+NH=N2+NH2			5.00E+13	0.0	0.0
11. NH2+NH=N2H2+H			5.00E+13	0.0	0.0
12. NH+NH=N2+H+H			2.54E+13	0.0	0.0
13. NH2+N=N2+H+H			7.20E+13	0.0	0.0
14. N2H2+M=NNH+H+M			5.00E+16	0.0	50000.0
N2	Enhanced by	2.000E+00			
H2	Enhanced by	2.000E+00			
15. N2H2+H=NNH+H2			5.00E+13	0.0	1000.0
16. N2H2+NH=NNH+NH2			1.00E+13	0.0	1000.0

17. $\text{N}_2\text{H}_2 + \text{NH}_2 = \text{NH}_3 + \text{NNH}$	1.00E+13	0.0	1000.0
18. $\text{NH}_2 + \text{NH}_2 = \text{N}_2\text{H}_2 + \text{H}_2$	5.00E+11	0.0	0.0
19. $\text{NH}_3 + \text{M} = \text{NH}_2 + \text{H} + \text{M}$	1.40E+16	0.0	90600.0
20. $\text{N}_2\text{H}_3 + \text{H} = \text{NH}_2 + \text{NH}_2$	1.60E+12	0.0	0.0
21. $\text{N}_2\text{H}_3 + \text{M} = \text{N}_2\text{H}_2 + \text{H} + \text{M}$	3.50E+16	0.0	46000.0
22. $\text{N}_2\text{H}_3 + \text{NH} = \text{NH}_2 + \text{N}_2\text{H}_2$	2.00E+13	0.0	0.0
23. $\text{NH}_2 + \text{NH}_2 + \text{M} = \text{N}_2\text{H}_4 + \text{M}$	3.00E+20	-1.0	0.0
24. $\text{H} + \text{N}_2\text{H}_4 = \text{H}_2 + \text{N}_2\text{H}_3$	1.30E+13	0.0	2500.0
25. $\text{NH}_2 + \text{N}_2\text{H}_4 = \text{NH}_3 + \text{N}_2\text{H}_3$	3.90E+12	0.0	1500.0
26. $\text{NH} + \text{H} + \text{M} = \text{NH}_2 + \text{M}$	2.00E+16	-0.5	0.0
27. $\text{NH}_2 + \text{NH}_2 = \text{NH}_3 + \text{NH}$	5.00E+12	0.0	10000.0
28. $\text{F} + \text{NH}_3 = \text{NH}_2 + \text{HF}$	4.27E+11	0.5	800.0
29. $\text{SIF}_4 = \text{SIF}_3 + \text{F}$	3.00E+12	0.0	147170.0
30. $\text{H} + \text{SIF}_4 = \text{HF} + \text{SIF}_3$	1.00E+13	0.0	50000.0
31. $\text{NH}_2 + \text{SIF}_4 = \text{SIF}_3\text{NH}_2 + \text{F}$	1.00E+11	0.0	40950.0
32. $\text{NH}_3 + \text{SIF}_3 = \text{SIF}_3\text{NH}_2 + \text{H}$	1.00E+11	0.0	5000.0
33. $\text{NH}_3 + \text{SIF}_3 = \text{SIHF}_3 + \text{NH}_2$	1.00E+11	0.0	10000.0

NOTE: A units mole-cm-sec-K, E units cal/mole

NO ERRORS FOUND ON INPUT:
ASCII Vers. 1.1 CHEMKIN linkfile chem.asc written.

WORKING SPACE REQUIREMENTS ARE

INTEGER: 1086

REAL: 723

CHARACTER: 21

Total CPUtime (sec): 0.15625

6.3 Input to SURFACE CHEMKIN Interpreter for the Example

(Note: this mechanism is included for illustrative purposes only and should not be used as a source of kinetic data for the Si_3N_4 deposition system)

```
SITE/SI3N4/      SDEN/4.1683E-9/
  HN_SIF(S)/2/ F3SI_NH2(S)/2/ F2SINH(S)/2/
  H2NFSINH(S)/2/ HN(FSINH)2(S)/4/
  HN_NH2(S)/2/
END
BULK SI(D)/2.066/
BULK N(D) /1.374/
END
THERMO ALL
  300.      600.      1685.
HN_SIF(S)      J 3/67N  1H  1SI  1F  1S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
HN_NH2(S)      J 3/67N  2H  3SI  0F  0S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
F3SI_NH2(S)      J 3/67N  1H  2SI  1F  3S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
F2SINH(S)      J 3/67N  1H  1SI  1F  2S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
H2NFSINH(S)      J 3/67N  2H  3SI  1F  1S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
HN(FSINH)2(S)      J 3/67N  3H  3SI  2F  2S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
SI(D)      J 3/67SI  100  000  000  0S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
N(D)      J 3/67N  100  000  000  0S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
END

REACTIONS
  NH3      + HN_SIF(S) => HN_NH2(S)      + SI(D) + HF      7.562E08  0.5 0.0
  SIF4      + HN_NH2(S) => F3SI_NH2(S) + N(D) + HF      3.0967E8  0.5 0.0
  F3SI_NH2(S)      => F2SINH(S)      + HF      1.0E05  0.0 0.0
  NH3      + F2SINH(S) => H2NFSINH(S)      + HF      7.562E08  0.5 0.0
  H2NFSINH(S)      + F2SINH(S) => HN(FSINH)2(S)      + HF      1.0E15  0.0 0.0
  HN(FSINH)2(S)      + F2SINH(S) => 3HN_SIF(S) + N(D) + HF      1.0E15  0.0 0.0
END
```

6.4 Output from SURFACE CHEMKIN Interpreter for the Example

CHEMKIN-III SURFACE MECHANISM INTERPRETER:

DOUBLE PRECISION Vers. 7.20 2000/06/18

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CKLIB: CHEMKIN-III GAS-PHASE CHEMICAL KINETICS LIBRARY,

DOUBLE PRECISION Vers. 5.28 2000/08/05

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SPECIES CONSIDERED		MOLECULAR WEIGHT	Density	Nsites	ELEMENT COUNT			
					H	N	SI	F

Gas phase species:								
1.	H2	2.01594			2	0	0	0
2.	H	1.00797			1	0	0	0
3.	N2	28.01340			0	2	0	0
4.	N	14.00670			0	1	0	0
5.	NH	15.01467			1	1	0	0
6.	NH2	16.02264			2	1	0	0
7.	NNH	29.02137			1	2	0	0
8.	N2H2	30.02934			2	2	0	0
9.	N2H3	31.03731			3	2	0	0
10.	N2H4	32.04528			4	2	0	0
11.	HF	20.00637			1	0	0	1
12.	F	18.99840			0	0	0	1
13.	SIF4	104.07960			0	0	1	4
14.	SIF3	85.08120			0	0	1	3
15.	SIHF3	86.08917			1	0	1	3
16.	SIF3NH2	101.10384			2	1	1	3
17.	NH3	17.03061			3	1	0	0
SITE: SI3N4 0.417E-08 moles/cm**2								
18.	HN_SIF(S)	62.09907		2	1	1	1	1
19.	F3SI_NH2(S)	101.10384		2	2	1	1	3
20.	F2SINH(S)	81.09747		2	1	1	1	2
21.	H2NFSINH(S)	78.12171		2	3	2	1	1
22.	HN(FSINH)2(S)	139.21281		4	3	3	2	2
23.	HN_NH2(S)	31.03731		2	3	2	0	0
BULK: BULK1								
24.	SI(D)	28.08600	0.207E+01 g/cm**3		0	0	1	0
BULK: BULK2								
25.	N(D)	14.00670	0.137E+01 g/cm**3		0	1	0	0

SURFACE REACTIONS CONSIDERED				(k = A T**b exp(-E/RT))				
				A	b	E		
1.	NH3+HN_SIF(S)=>HN_NH2(S)+SI(D)+HF			7.56E+08	0.5	0.0		
2.	SIF4+HN_NH2(S)=>F3SI_NH2(S)+N(D)+HF			3.10E+08	0.5	0.0		
3.	F3SI_NH2(S)=>F2SINH(S)+HF			1.00E+05	0.0	0.0		
4.	NH3+F2SINH(S)=>H2NFSINH(S)+HF			7.56E+08	0.5	0.0		
5.	H2NFSINH(S)+F2SINH(S)			1.00E+15	0.0	0.0		

```

=>HN(FSINH)2(S)+HF
6. HN(FSINH)2(S)+F2SINH(S)          1.00E+15    0.0    0.0
=>3HN_SIF(S)+N(D)+HF

```

NOTE: A units mole-cm-sec-K, E units cal/mole

NO ERRORS FOUND ON INPUT:
ASCII Version 1.1 surface linkfile surf.asc written.

WORKING SPACE REQUIREMENTS ARE

INTEGER: 481

REAL: 642

CHARACTER: 34

Total CPUTime (sec): 0.

6.5 Input to CRESLAF for the Example

```
PRES 2.3684E-3
REAC SIF4      0.14286
REAC NH3       0.85714
SURF HN_SIF(S) 5.368E-02
SURF F3SI_NH2(S) 4.067E-04
SURF F2SINH(S) 1.789E-02
SURF H2NFSINH(S) 3.636E-04
SURF HN(FSINH)2(S) 7.271E-04
SURF HN_NH2(S) 0.9269
ACT SI(D)      1.0
ACT N(D)       1.0
GRAV 980.
VEL 400.
STMP 1713.14
GTMP 573.15
XEND 10.
DX 2.5
HITE 2.0
NPTS 15
STCH 1.1
ATOL 1.E-6
RTOL 1.E-4
TDIF
MULT
ICRD RAD
IRST 0
MORD 5
END
```

6.6 Output from CRESLAF for the Example

CRESLAF: CHEMICALLY-REACTING SHEAR LAYER FLOW
(TWO-DIMENSIONAL BOUNDARY-LAYER MODEL)
(CHEMKIN-III Version 5.20, 2000/08/01)

DOUBLE PRECISION

	WORKING SPACE PROVIDED	REQUIREMENTS REQUIRED
LOGICAL	1	1
INTEGER	2073	1820
REAL	68899	28218
CHARACTER	84	84

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KEYWORD INPUT

PRES 2.3684E-3
REAC SIF4 0.14286
REAC NH3 0.85714
SURF HN_SIF(S) 5.368E-02
SURF F3SI_NH2(S) 4.067E-04
SURF F2SINH(S) 1.789E-02
SURF H2NFSINH(S) 3.636E-04
SURF HN(FSINH)2(S) 7.271E-04
SURF HN_NH2(S) 0.9269
ACT SI(D) 1.0
ACT N(D) 1.0
GRAV 980.
VEL 400.
STMP 1713.14
GTMP 573.15
XEND 10.
DX 2.5

```

HITE          2.0
NPTS          15
STCH          1.1
ATOL          1.E-6
RTOL          1.E-4
TDIF
MULT
ICRD  RAD
IRST          0
MORD          5
END

```

CAUTION...SURFACE FRACTIONS SUM TO 0.999967400000000

ERROR TOLERANCES TO BE USED:

(default values for all other species: ATOL = 0.1000E-05 RTOL = 0.1000E-03)

SPECIES	ATOL	RTOL
H2	0.1000E-05	0.1000E-03
H	0.1000E-05	0.1000E-03
N2	0.1000E-05	0.1000E-03
N	0.1000E-05	0.1000E-03
NH	0.1000E-05	0.1000E-03
NH2	0.1000E-05	0.1000E-03
NNH	0.1000E-05	0.1000E-03
N2H2	0.1000E-05	0.1000E-03
N2H3	0.1000E-05	0.1000E-03
N2H4	0.1000E-05	0.1000E-03
HF	0.1000E-05	0.1000E-03
F	0.1000E-05	0.1000E-03
SIF4	0.1000E-05	0.1000E-03
SIF3	0.1000E-05	0.1000E-03
SIHF3	0.1000E-05	0.1000E-03
SIF3NH2	0.1000E-05	0.1000E-03
NH3	0.1000E-05	0.1000E-03
HN_SIF(S)	0.1000E-05	0.1000E-03
F3SI_NH2(S)	0.1000E-05	0.1000E-03
F2SINH(S)	0.1000E-05	0.1000E-03
H2NFSINH(S)	0.1000E-05	0.1000E-03
HN(FSINH)2(S)	0.1000E-05	0.1000E-03
HN_NH2(S)	0.1000E-05	0.1000E-03
SI(D)	0.1000E-05	0.1000E-03
N(D)	0.1000E-05	0.1000E-03

WORKING SPACE REQUIREMENTS

	PROVIDED	REQUIRED
LOGICAL	1	1
INTEGER	2073	2073
REAL	68899	68899
CHARACTER	84	84

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,

VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

TWOPNT: INITIAL GUESS:

GAS PHASE SPECIES MASS FRACTIONS

Species_Name	Mass_frac(Wall)	Mass_frac(Gas)	Wdot	Residual	Bulk_Vel_Contrb	Dif_Vel_Cont	Surface_Mass_Rate
H2	0.00000E+00	0.00000E+00	0.00000E+00	- .10956E-26	0.00000E+00	- .10956E-26	0.00000E+00
H	0.00000E+00	0.00000E+00	0.00000E+00	0.12305E-26	0.00000E+00	0.12305E-26	0.00000E+00
N2	0.00000E+00	0.00000E+00	0.00000E+00	0.43779E-27	0.00000E+00	0.43779E-27	0.00000E+00
N	0.00000E+00	0.00000E+00	0.00000E+00	- .18696E-28	0.00000E+00	- .18696E-28	0.00000E+00
NH	0.00000E+00	0.00000E+00	0.00000E+00	0.12444E-27	0.00000E+00	0.12444E-27	0.00000E+00
NH2	0.00000E+00	0.00000E+00	0.00000E+00	0.71937E-27	0.00000E+00	0.71937E-27	0.00000E+00
NNH	0.00000E+00	0.00000E+00	0.00000E+00	- .12713E-26	0.00000E+00	- .12713E-26	0.00000E+00
N2H2	0.00000E+00	0.00000E+00	0.00000E+00	- .13233E-26	0.00000E+00	- .13233E-26	0.00000E+00
N2H3	0.00000E+00	0.00000E+00	0.00000E+00	0.31538E-28	0.00000E+00	0.31538E-28	0.00000E+00
N2H4	0.00000E+00	0.00000E+00	0.00000E+00	- .90510E-27	0.00000E+00	- .90510E-27	0.00000E+00
HF	0.00000E+00	0.00000E+00	0.36087E-06	- .72198E-05	0.00000E+00	0.35421E-27	0.72198E-05
F	0.00000E+00	0.00000E+00	0.00000E+00	0.18697E-26	0.00000E+00	0.18697E-26	0.00000E+00
SIF4	0.50460	0.50460	- .10304E-06	0.79540E-05	- .27699E-05	0.50391E-11	- .10724E-04
SIF3	0.00000E+00	0.00000E+00	0.00000E+00	0.13902E-27	0.00000E+00	0.13902E-27	0.00000E+00
SIHF3	0.00000E+00	0.00000E+00	0.00000E+00	- .54548E-27	0.00000E+00	- .54548E-27	0.00000E+00
SIF3NH2	0.00000E+00	0.00000E+00	0.00000E+00	- .88028E-27	0.00000E+00	- .88028E-27	0.00000E+00
NH3	0.49540	0.49540	- .11656E-06	- .73423E-06	- .27194E-05	- .50391E-11	- .19852E-05

Total Velocity into wall (positive indicates a net flux into wall) = 3.6993 cm/sec

Temperature at the wall = 573.150

Temperature in the gas = 573.150

SURFACE SPECIES SITE FRACTIONS

SITE 1: SI3N4	SITDOT
HN_SIF(S)	5.368E-02
F3SI_NH2(S)	4.067E-04
F2SINH(S)	1.789E-02
H2NFSINH(S)	3.636E-04
HN(FSINH)2(S)	7.271E-04
HN_NH2(S)	9.269E-01
	-2.669E-09
	1.827E-08
	-8.811E-10
	8.802E-10
	3.886E-12
	-1.561E-08

DEPOSITION RATE (MICRONS/MIN)

7 SI(D)	7.131E-01
8 N(D)	8.030E-01

RATE OF PROGRESS OF REACTIONS

1	NH3+HN_SIF(S)=>HN_NH2(S)+SI(D)+HF	8.743E-08
2	SIF4+HN_NH2(S)=>F3SI_NH2(S)+N(D)+HF	1.030E-07
3	F3SI_NH2(S)=>F2SINH(S)+HF	8.477E-08
4	NH3+F2SINH(S)=>H2NFSINH(S)+HF	2.914E-08
5	H2NFSINH(S)+F2SINH(S)=>HN(FSINH)2(S)+HF	2.826E-08
6	HN(FSINH)2(S)+F2SINH(S)=>3HN_SIF(S)+N(D)+HF	2.825E-08

TWOPNT: CALLING SEARCH TO SOLVE THE STEADY STATE PROBLEM.

SEARCH: SOLVE NONLINEAR, NONDIFFERENTIAL EQUATIONS.

SLTN NUMBER	LOG10				
	NORM F	COND J	NORM S	ABS AND REL	DELTA B AND D
0	0.64	7.86	-1.96	-1.96	-0.73
1	-0.95		-4.58	-4.58	-2.27
2	-1.77		-5.97	-5.97	-3.09
3	-2.58		-6.90	-6.90	-3.91
4	-3.40		-7.71	-7.71	-4.72
5	-4.21		-8.52	-8.52	-5.53
6	-5.02		-9.34	-9.34	-6.34
7	-5.84		-10.15	-10.15	-7.16
8	-6.65		-10.96	-10.96	-7.97
9	-7.46		-11.78	-11.78	-8.78
10	-8.28		-12.59	-12.59	-9.60
11	-9.09		-13.40	-13.40	ZERO

SEARCH: SUCCESS. THE SOLUTION:

GAS PHASE SPECIES MASS FRACTIONS

Species_Name	Mass_frac(Wall)	Mass_frac(Gas)	Wdot	Residual	Bulk_Vel_Contrb	Dif_Vel_Cont	Surface_Mass_Rate
H2	-.50222E-25	0.00000E+00	0.00000E+00	-.12204E-26	0.23636E-30	-.12206E-26	0.00000E+00
H	0.88494E-26	0.00000E+00	0.00000E+00	0.19009E-27	-.41648E-31	0.19014E-27	0.00000E+00
N2	0.81108E-25	0.00000E+00	0.00000E+00	-.35005E-26	-.38172E-30	-.35001E-26	0.00000E+00
N	0.35152E-25	0.00000E+00	0.00000E+00	-.41679E-27	-.16544E-30	-.41662E-27	0.00000E+00
NH	-.28395E-24	0.00000E+00	0.00000E+00	-.18775E-26	0.13363E-29	-.18788E-26	0.00000E+00
NH2	-.12558E-24	0.00000E+00	0.00000E+00	-.65151E-27	0.59102E-30	-.65210E-27	0.00000E+00
NNH	-.12251E-24	0.00000E+00	0.00000E+00	-.11729E-26	0.57658E-30	-.11734E-26	0.00000E+00
N2H2	0.18871E-24	0.00000E+00	0.00000E+00	0.23908E-26	-.88812E-30	0.23917E-26	0.00000E+00
N2H3	0.64420E-25	0.00000E+00	0.00000E+00	-.13237E-28	-.30318E-30	-.12934E-28	0.00000E+00
N2H4	-.14538E-24	0.00000E+00	0.00000E+00	-.10091E-26	0.68421E-30	-.10098E-26	0.00000E+00
HF	0.23264E-02	0.00000E+00	0.40258E-06	-.44340E-16	-.10949E-07	0.80651E-05	0.80541E-05
F	0.44516E-25	0.00000E+00	0.00000E+00	0.11742E-26	-.20950E-30	0.11744E-26	0.00000E+00
SIF4	0.50110	0.50460	-.10064E-06	0.21411E-16	-.23583E-05	-.81167E-05	-.10475E-04
SIF3	0.37011E-24	0.00000E+00	0.00000E+00	-.39094E-27	-.17418E-29	-.38920E-27	0.00000E+00
SIHF3	0.80743E-26	0.00000E+00	0.00000E+00	-.25435E-27	-.38000E-31	-.25431E-27	0.00000E+00
SIF3NH2	0.21378E-24	0.00000E+00	0.00000E+00	-.57366E-27	-.10061E-29	-.57266E-27	0.00000E+00
NH3	0.49657	0.49540	-.13419E-06	0.22912E-16	-.23370E-05	0.51644E-07	-.22854E-05

=====

Total Velocity into wall (positive indicates a net flux into wall) = 3.1787 cm/sec

Temperature at the wall = 573.150

Temperature in the gas = 573.150

SURFACE SPECIES SITE FRACTIONS

SITE 1: SI3N4		SITDOT
HN_SIF(S)	6.193E-02	3.388E-18
F3SI_NH2(S)	4.829E-04	3.176E-22
F2SINH(S)	2.064E-02	-2.254E-18
H2NFSINH(S)	3.742E-04	-1.124E-18
HN(FSINH)2(S)	7.483E-04	-4.970E-21
HN_NH2(S)	9.158E-01	-2.515E-22

DEPOSITION RATE (MICRONS/MIN)

7 SI(D)	8.209E-01
8 N(D)	8.208E-01

RATE OF PROGRESS OF REACTIONS

1 NH3+HN_SIF(S)=>HN_NH2(S)+SI(D)+HF	1.006E-07
2 SIF4+HN_NH2(S)=>F3SI_NH2(S)+N(D)+HF	1.006E-07
3 F3SI_NH2(S)=>F2SINH(S)+HF	1.006E-07
4 NH3+F2SINH(S)=>H2NFSINH(S)+HF	3.355E-08
5 H2NFSINH(S)+F2SINH(S)=>HN(FSINH)2(S)+HF	3.355E-08
6 HN(FSINH)2(S)+F2SINH(S)=>3HN_SIF(S)+N(D)+HF	3.355E-08

TWOPNT: SEARCH FOUND THE STEADY STATE.

TWOPNT: SUCCESS. PROBLEM SOLVED.

1

DISTANCE= 0.000E+00 LAST STEP SIZE= 0.000E+00 NUMBER OF STEPS= 0
 ORDER OF INTEGRATION= 0 NUMBER OF FUNCTION CALLS = 0 JACOBIAN EVALUATIONS= 0
 ERROR TEST FAILURES = 0 CONVERGENCE TEST FAILURES= 0
 MASS IN THE FLOW= 0.373E-02 P(TORR)= 0.180E+01

	Y(CM)	U	T	OMS	H2	H	N2	N	NH	NH2	NNH
		DEPOSITION RATE--	UPPER WALL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
15	0.200E+01	0.000E+00	0.573E+03	0.000E+00	-0.731E-24	0.258E-24	0.849E-25	0.736E-25	-0.555E-24	-0.230E-24	-0.124E-24
14	0.189E+01	0.427E+02	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
13	0.176E+01	0.885E+02	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
12	0.163E+01	0.133E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
11	0.150E+01	0.176E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
10	0.136E+01	0.216E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
9	0.121E+01	0.253E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
8	0.107E+01	0.286E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
7	0.919E+00	0.315E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
6	0.770E+00	0.341E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
5	0.619E+00	0.362E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4	0.466E+00	0.378E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
3	0.312E+00	0.390E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	0.157E+00	0.398E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	0.222E-15	0.398E+03	0.573E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

	Y(CM)	N2H2	N2H3	N2H4	HF	F	SIF4	SIF3	SIHF3	SIF3NH2	NH3
	UPPER WALL	0.000E+00	0.000E+00	0.000E+00	0.157E-04	0.000E+00	-0.204E-04	0.000E+00	0.000E+00	0.000E+00	-0.445E-05
15	0.200E+01	0.184E-24	0.609E-25	-0.133E-24	0.341E-02	0.687E-25	0.141E+00	0.128E-24	0.275E-26	0.620E-25	0.855E+00
14	0.189E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
13	0.176E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
12	0.163E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
11	0.150E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
10	0.136E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
9	0.121E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
8	0.107E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
7	0.919E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
6	0.770E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
5	0.619E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
4	0.466E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
3	0.312E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
2	0.157E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00
1	0.222E-15	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.143E+00	0.000E+00	0.000E+00	0.000E+00	0.857E+00

SURFACE SPECIES SITE FRACTIONS

SITE 1: SI3N4 OUTER WALL
 HN_SIF(S) 6.193E-02
 F3SI_NH2(S) 4.829E-04
 F2SINH(S) 2.064E-02
 H2NFSINH(S) 3.742E-04
 HN(FSINH)2(S) 7.483E-04
 HN_NH2(S) 9.158E-01

DEPOSITION RATE (MICRON/MIN)

1 SI(D) 8.209E-01
 2 N(D) 8.208E-01

DISTANCE= 0.250E+01 LAST STEP SIZE= 0.161E+00 NUMBER OF STEPS= 84
ORDER OF INTEGRATION= 5 NUMBER OF FUNCTION CALLS = 175 JACOBIAN EVALUATIONS= 14
ERROR TEST FAILURES = 2 CONVERGENCE TEST FAILURES= 0
MASS IN THE FLOW= 0.372E-02 P(TORR)= 0.180E+01

	Y(CM)	U	T	OMS	H2	H	N2	N	NH	NH2	NNH
		DEPOSITION RATE--	UPPER WALL		0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
15	0.200E+01	0.000E+00	0.171E+04	0.411E-13	0.102E-05	0.222E-07	0.460E-11	0.144E-14	0.308E-10	0.211E-05	0.768E-12
14	0.189E+01	0.134E+03	0.171E+04	-0.320E-13	0.102E-05	0.222E-07	0.460E-11	0.151E-14	0.308E-10	0.211E-05	0.768E-12
13	0.176E+01	0.277E+03	0.171E+04	0.488E-14	0.102E-05	0.222E-07	0.454E-11	0.135E-14	0.306E-10	0.211E-05	0.753E-12
12	0.163E+01	0.417E+03	0.171E+04	-0.155E-13	0.102E-05	0.222E-07	0.445E-11	0.126E-14	0.304E-10	0.210E-05	0.739E-12
11	0.150E+01	0.550E+03	0.171E+04	-0.520E-13	0.102E-05	0.222E-07	0.431E-11	0.157E-14	0.300E-10	0.208E-05	0.721E-12
10	0.136E+01	0.674E+03	0.171E+04	-0.189E-13	0.101E-05	0.221E-07	0.414E-11	0.146E-14	0.295E-10	0.207E-05	0.697E-12
9	0.121E+01	0.788E+03	0.171E+04	-0.195E-13	0.101E-05	0.221E-07	0.396E-11	0.607E-15	0.290E-10	0.205E-05	0.674E-12
8	0.107E+01	0.890E+03	0.171E+04	0.921E-14	0.101E-05	0.220E-07	0.378E-11	0.889E-16	0.285E-10	0.203E-05	0.648E-12
7	0.920E+00	0.980E+03	0.171E+04	0.152E-12	0.100E-05	0.220E-07	0.360E-11	-0.867E-16	0.279E-10	0.202E-05	0.622E-12
6	0.770E+00	0.106E+04	0.171E+04	-0.879E-13	0.998E-06	0.220E-07	0.344E-11	-0.509E-16	0.274E-10	0.200E-05	0.600E-12
5	0.619E+00	0.112E+04	0.171E+04	-0.205E-12	0.995E-06	0.219E-07	0.329E-11	0.250E-16	0.270E-10	0.198E-05	0.579E-12
4	0.467E+00	0.117E+04	0.171E+04	0.351E-13	0.992E-06	0.219E-07	0.318E-11	0.166E-15	0.266E-10	0.197E-05	0.562E-12
3	0.313E+00	0.120E+04	0.171E+04	-0.244E-14	0.990E-06	0.219E-07	0.309E-11	0.354E-15	0.264E-10	0.196E-05	0.549E-12
2	0.157E+00	0.122E+04	0.171E+04	0.142E-13	0.989E-06	0.219E-07	0.304E-11	0.492E-15	0.262E-10	0.196E-05	0.543E-12
1	0.222E-15	0.122E+04	0.171E+04	0.142E-13	0.989E-06	0.219E-07	0.304E-11	0.492E-15	0.262E-10	0.196E-05	0.543E-12

	Y(CM)	N2H2	N2H3	N2H4	HF	F	SIF4	SIF3	SIHF3	SIF3NH2	NH3
	UPPER WALL	0.000E+00	0.000E+00	0.000E+00	0.799E-05	0.000E+00	-0.104E-04	0.000E+00	0.000E+00	0.000E+00	-0.227E-05
15	0.200E+01	0.246E-10	0.110E-11	0.127E-12	0.577E-01	0.653E-11	0.124E+00	0.781E-10	0.729E-11	0.358E-10	0.819E+00
14	0.189E+01	0.246E-10	0.110E-11	0.127E-12	0.570E-01	0.653E-11	0.124E+00	0.781E-10	0.729E-11	0.358E-10	0.819E+00
13	0.176E+01	0.244E-10	0.109E-11	0.125E-12	0.562E-01	0.645E-11	0.124E+00	0.777E-10	0.724E-11	0.355E-10	0.819E+00
12	0.163E+01	0.240E-10	0.107E-11	0.114E-12	0.554E-01	0.633E-11	0.125E+00	0.770E-10	0.710E-11	0.348E-10	0.820E+00
11	0.150E+01	0.234E-10	0.106E-11	0.914E-13	0.545E-01	0.620E-11	0.125E+00	0.760E-10	0.693E-11	0.338E-10	0.820E+00
10	0.136E+01	0.227E-10	0.105E-11	-0.521E-13	0.536E-01	0.604E-11	0.126E+00	0.747E-10	0.671E-11	0.327E-10	0.821E+00
9	0.121E+01	0.220E-10	0.102E-11	-0.895E-13	0.527E-01	0.589E-11	0.126E+00	0.732E-10	0.646E-11	0.314E-10	0.821E+00
8	0.107E+01	0.213E-10	0.986E-12	-0.633E-13	0.519E-01	0.574E-11	0.127E+00	0.717E-10	0.621E-11	0.300E-10	0.821E+00
7	0.920E+00	0.205E-10	0.950E-12	-0.782E-13	0.511E-01	0.560E-11	0.127E+00	0.701E-10	0.596E-11	0.287E-10	0.822E+00
6	0.770E+00	0.199E-10	0.918E-12	-0.825E-13	0.504E-01	0.548E-11	0.128E+00	0.686E-10	0.573E-11	0.275E-10	0.822E+00
5	0.619E+00	0.193E-10	0.888E-12	-0.787E-13	0.498E-01	0.537E-11	0.128E+00	0.673E-10	0.553E-11	0.265E-10	0.822E+00
4	0.467E+00	0.188E-10	0.868E-12	-0.704E-13	0.494E-01	0.528E-11	0.128E+00	0.661E-10	0.537E-11	0.256E-10	0.822E+00
3	0.313E+00	0.184E-10	0.848E-12	-0.568E-13	0.490E-01	0.522E-11	0.128E+00	0.653E-10	0.524E-11	0.249E-10	0.823E+00
2	0.157E+00	0.182E-10	0.835E-12	-0.498E-13	0.488E-01	0.518E-11	0.128E+00	0.648E-10	0.517E-11	0.246E-10	0.823E+00
1	0.222E-15	0.182E-10	0.835E-12	-0.498E-13	0.488E-01	0.518E-11	0.128E+00	0.648E-10	0.517E-11	0.246E-10	0.823E+00

SURFACE SPECIES SITE FRACTIONS

SITE 1: SI3N4 OUTER WALL
HN_SIF(S) 5.708E-02
F3SI_NH2(S) 2.462E-04
F2SINH(S) 1.903E-02
H2NFSINH(S) 2.070E-04
HN(FSINH)2(S) 4.140E-04
HN_NH2(S) 9.230E-01

DEPOSITION RATE (MICRON/MIN)

1 SI(D) 4.186E-01
2 N(D) 4.185E-01

DISTANCE= 0.500E+01 LAST STEP SIZE= 0.644E+00 NUMBER OF STEPS= 92
 ORDER OF INTEGRATION= 3 NUMBER OF FUNCTION CALLS = 191 JACOBIAN EVALUATIONS= 16
 ERROR TEST FAILURES = 2 CONVERGENCE TEST FAILURES= 0
 MASS IN THE FLOW= 0.371E-02 P(TORR)= 0.180E+01

	Y(CM)	U	T	OMS	H2	H	N2	N	NH	NH2	NNH
		DEPOSITION RATE--	UPPER WALL		0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
15	0.200E+01	0.000E+00	0.171E+04	0.833E-13	0.295E-05	0.225E-07	0.213E-09	0.279E-13	0.368E-09	0.596E-05	0.133E-10
14	0.189E+01	0.139E+03	0.171E+04	0.354E-13	0.295E-05	0.225E-07	0.213E-09	0.264E-13	0.367E-09	0.596E-05	0.134E-10
13	0.177E+01	0.287E+03	0.171E+04	-0.910E-14	0.295E-05	0.225E-07	0.212E-09	0.261E-13	0.367E-09	0.596E-05	0.133E-10
12	0.163E+01	0.432E+03	0.171E+04	-0.262E-13	0.295E-05	0.225E-07	0.211E-09	0.255E-13	0.366E-09	0.595E-05	0.132E-10
11	0.150E+01	0.570E+03	0.171E+04	0.577E-13	0.295E-05	0.225E-07	0.208E-09	0.249E-13	0.364E-09	0.594E-05	0.131E-10
10	0.136E+01	0.699E+03	0.171E+04	0.250E-12	0.294E-05	0.227E-07	0.205E-09	0.234E-13	0.362E-09	0.593E-05	0.130E-10
9	0.121E+01	0.817E+03	0.171E+04	-0.444E-13	0.294E-05	0.227E-07	0.202E-09	0.226E-13	0.359E-09	0.591E-05	0.128E-10
8	0.107E+01	0.923E+03	0.171E+04	-0.121E-12	0.294E-05	0.227E-07	0.199E-09	0.221E-13	0.357E-09	0.589E-05	0.127E-10
7	0.920E+00	0.102E+04	0.171E+04	0.736E-13	0.293E-05	0.227E-07	0.195E-09	0.216E-13	0.355E-09	0.588E-05	0.125E-10
6	0.771E+00	0.110E+04	0.171E+04	-0.149E-13	0.293E-05	0.227E-07	0.192E-09	0.213E-13	0.352E-09	0.586E-05	0.124E-10
5	0.619E+00	0.116E+04	0.171E+04	0.488E-14	0.293E-05	0.227E-07	0.189E-09	0.212E-13	0.350E-09	0.585E-05	0.122E-10
4	0.467E+00	0.121E+04	0.171E+04	-0.733E-14	0.292E-05	0.227E-07	0.187E-09	0.212E-13	0.349E-09	0.584E-05	0.121E-10
3	0.313E+00	0.125E+04	0.171E+04	-0.190E-12	0.292E-05	0.227E-07	0.185E-09	0.214E-13	0.347E-09	0.583E-05	0.121E-10
2	0.157E+00	0.127E+04	0.171E+04	0.244E-13	0.292E-05	0.227E-07	0.184E-09	0.214E-13	0.347E-09	0.582E-05	0.120E-10
1	0.222E-15	0.127E+04	0.171E+04	0.245E-13	0.292E-05	0.227E-07	0.184E-09	0.214E-13	0.347E-09	0.582E-05	0.120E-10

	Y(CM)	N2H2	N2H3	N2H4	HF	F	SIF4	SIF3	SIHF3	SIF3NH2	NH3
	UPPER WALL	0.000E+00	0.000E+00	0.000E+00	0.718E-05	0.000E+00	-0.934E-05	0.000E+00	0.000E+00	0.000E+00	-0.204E-05
15	0.200E+01	0.396E-09	0.145E-10	0.594E-12	0.101E+00	0.324E-10	0.111E+00	0.134E-09	0.378E-10	0.187E-09	0.789E+00
14	0.189E+01	0.396E-09	0.145E-10	0.588E-12	0.100E+00	0.324E-10	0.111E+00	0.135E-09	0.378E-10	0.187E-09	0.789E+00
13	0.177E+01	0.395E-09	0.145E-10	0.594E-12	0.993E-01	0.323E-10	0.111E+00	0.134E-09	0.377E-10	0.187E-09	0.789E+00
12	0.163E+01	0.392E-09	0.144E-10	0.593E-12	0.986E-01	0.320E-10	0.112E+00	0.134E-09	0.375E-10	0.186E-09	0.790E+00
11	0.150E+01	0.389E-09	0.143E-10	0.590E-12	0.978E-01	0.317E-10	0.112E+00	0.134E-09	0.372E-10	0.184E-09	0.790E+00
10	0.136E+01	0.385E-09	0.141E-10	0.589E-12	0.970E-01	0.314E-10	0.112E+00	0.134E-09	0.368E-10	0.182E-09	0.791E+00
9	0.121E+01	0.381E-09	0.139E-10	0.586E-12	0.962E-01	0.310E-10	0.113E+00	0.134E-09	0.364E-10	0.179E-09	0.791E+00
8	0.107E+01	0.376E-09	0.137E-10	0.585E-12	0.955E-01	0.307E-10	0.113E+00	0.133E-09	0.360E-10	0.177E-09	0.791E+00
7	0.920E+00	0.372E-09	0.135E-10	0.587E-12	0.948E-01	0.304E-10	0.114E+00	0.133E-09	0.356E-10	0.175E-09	0.792E+00
6	0.771E+00	0.367E-09	0.134E-10	0.590E-12	0.942E-01	0.301E-10	0.114E+00	0.133E-09	0.352E-10	0.173E-09	0.792E+00
5	0.619E+00	0.364E-09	0.132E-10	0.595E-12	0.937E-01	0.299E-10	0.114E+00	0.133E-09	0.349E-10	0.171E-09	0.792E+00
4	0.467E+00	0.361E-09	0.133E-10	0.601E-12	0.933E-01	0.297E-10	0.114E+00	0.133E-09	0.346E-10	0.169E-09	0.792E+00
3	0.313E+00	0.358E-09	0.143E-10	0.607E-12	0.930E-01	0.295E-10	0.115E+00	0.133E-09	0.344E-10	0.168E-09	0.792E+00
2	0.157E+00	0.357E-09	0.146E-10	0.610E-12	0.928E-01	0.294E-10	0.115E+00	0.132E-09	0.342E-10	0.167E-09	0.793E+00
1	0.222E-15	0.357E-09	0.146E-10	0.610E-12	0.928E-01	0.294E-10	0.115E+00	0.132E-09	0.342E-10	0.167E-09	0.793E+00

SURFACE SPECIES SITE FRACTIONS

SITE 1: SI3N4		OUTER WALL
HN_SIF(S)		5.327E-02
F3SI_NH2(S)		2.213E-04
F2SINH(S)		1.776E-02
H2NFSINH(S)		1.993E-04
HN(FSINH)2(S)		3.986E-04
HN_NH2(S)		9.282E-01
DEPOSITION RATE (MICRON/MIN)		
1 SI(D)		3.761E-01
2 N(D)		3.761E-01

DISTANCE= 0.750E+01 LAST STEP SIZE= 0.129E+01 NUMBER OF STEPS= 95
 ORDER OF INTEGRATION= 3 NUMBER OF FUNCTION CALLS = 197 JACOBIAN EVALUATIONS= 17
 ERROR TEST FAILURES = 2 CONVERGENCE TEST FAILURES= 0
 MASS IN THE FLOW= 0.370E-02 P(TORR)= 0.180E+01

	Y(CM)	U	T	OMS	H2	H	N2	N	NH	NH2	NNH
		DEPOSITION RATE--	UPPER WALL		0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
15	0.200E+01	0.000E+00	0.171E+04	0.676E-12	0.473E-05	0.226E-07	0.122E-08	0.126E-12	0.119E-08	0.951E-05	0.456E-10
14	0.189E+01	0.143E+03	0.171E+04	0.120E-12	0.473E-05	0.226E-07	0.122E-08	0.125E-12	0.119E-08	0.951E-05	0.456E-10
13	0.177E+01	0.296E+03	0.171E+04	0.134E-12	0.473E-05	0.226E-07	0.122E-08	0.122E-12	0.118E-08	0.951E-05	0.455E-10
12	0.163E+01	0.446E+03	0.171E+04	0.135E-12	0.473E-05	0.226E-07	0.121E-08	0.124E-12	0.118E-08	0.950E-05	0.454E-10
11	0.150E+01	0.589E+03	0.171E+04	0.101E-12	0.473E-05	0.226E-07	0.121E-08	0.126E-12	0.118E-08	0.949E-05	0.451E-10
10	0.136E+01	0.722E+03	0.171E+04	0.120E-12	0.473E-05	0.226E-07	0.120E-08	0.125E-12	0.118E-08	0.948E-05	0.448E-10
9	0.121E+01	0.843E+03	0.171E+04	0.154E-12	0.472E-05	0.226E-07	0.118E-08	0.126E-12	0.117E-08	0.947E-05	0.445E-10
8	0.107E+01	0.953E+03	0.171E+04	-0.137E-11	0.472E-05	0.226E-07	0.117E-08	0.126E-12	0.117E-08	0.945E-05	0.442E-10
7	0.920E+00	0.105E+04	0.171E+04	0.893E-13	0.472E-05	0.226E-07	0.116E-08	0.123E-12	0.116E-08	0.943E-05	0.439E-10
6	0.771E+00	0.113E+04	0.171E+04	-0.305E-12	0.471E-05	0.226E-07	0.115E-08	0.127E-12	0.116E-08	0.942E-05	0.436E-10
5	0.620E+00	0.120E+04	0.171E+04	-0.271E-12	0.471E-05	0.226E-07	0.114E-08	0.103E-12	0.115E-08	0.941E-05	0.433E-10
4	0.467E+00	0.125E+04	0.171E+04	-0.135E-12	0.471E-05	0.226E-07	0.113E-08	0.989E-13	0.115E-08	0.940E-05	0.431E-10
3	0.313E+00	0.129E+04	0.171E+04	-0.250E-12	0.471E-05	0.226E-07	0.113E-08	0.998E-13	0.115E-08	0.939E-05	0.430E-10
2	0.157E+00	0.131E+04	0.171E+04	-0.276E-12	0.471E-05	0.226E-07	0.112E-08	0.109E-12	0.115E-08	0.938E-05	0.429E-10
1	0.222E-15	0.131E+04	0.171E+04	-0.276E-12	0.471E-05	0.226E-07	0.112E-08	0.109E-12	0.115E-08	0.938E-05	0.429E-10

	Y(CM)	N2H2	N2H3	N2H4	HF	F	SIF4	SIF3	SIHF3	SIF3NH2	NH3
	UPPER WALL	0.000E+00	0.000E+00	0.000E+00	0.647E-05	0.000E+00	-0.842E-05	0.000E+00	0.000E+00	0.000E+00	-0.184E-05
15	0.200E+01	0.133E-08	0.431E-10	0.148E-11	0.137E+00	0.729E-10	0.993E-01	0.140E-09	0.722E-10	0.366E-09	0.763E+00
14	0.189E+01	0.133E-08	0.431E-10	0.147E-11	0.137E+00	0.729E-10	0.996E-01	0.140E-09	0.722E-10	0.366E-09	0.764E+00
13	0.177E+01	0.132E-08	0.431E-10	0.149E-11	0.136E+00	0.727E-10	0.999E-01	0.140E-09	0.721E-10	0.365E-09	0.764E+00
12	0.163E+01	0.132E-08	0.429E-10	0.150E-11	0.136E+00	0.721E-10	0.100E+00	0.140E-09	0.718E-10	0.364E-09	0.764E+00
11	0.150E+01	0.131E-08	0.427E-10	0.150E-11	0.135E+00	0.717E-10	0.101E+00	0.140E-09	0.716E-10	0.362E-09	0.765E+00
10	0.136E+01	0.131E-08	0.425E-10	0.152E-11	0.134E+00	0.713E-10	0.101E+00	0.140E-09	0.712E-10	0.360E-09	0.765E+00
9	0.121E+01	0.130E-08	0.422E-10	0.152E-11	0.133E+00	0.708E-10	0.101E+00	0.140E-09	0.708E-10	0.358E-09	0.765E+00
8	0.107E+01	0.129E-08	0.419E-10	0.152E-11	0.133E+00	0.703E-10	0.102E+00	0.140E-09	0.704E-10	0.355E-09	0.766E+00
7	0.920E+00	0.128E-08	0.416E-10	0.154E-11	0.132E+00	0.698E-10	0.102E+00	0.140E-09	0.700E-10	0.353E-09	0.766E+00
6	0.771E+00	0.127E-08	0.413E-10	0.155E-11	0.132E+00	0.694E-10	0.102E+00	0.138E-09	0.695E-10	0.351E-09	0.766E+00
5	0.620E+00	0.126E-08	0.410E-10	0.159E-11	0.131E+00	0.690E-10	0.102E+00	0.138E-09	0.691E-10	0.348E-09	0.766E+00
4	0.467E+00	0.126E-08	0.407E-10	0.625E-12	0.131E+00	0.687E-10	0.103E+00	0.138E-09	0.689E-10	0.347E-09	0.766E+00
3	0.313E+00	0.125E-08	0.403E-10	0.702E-12	0.131E+00	0.687E-10	0.103E+00	0.138E-09	0.687E-10	0.345E-09	0.767E+00
2	0.157E+00	0.125E-08	0.401E-10	0.738E-12	0.130E+00	0.685E-10	0.103E+00	0.138E-09	0.686E-10	0.345E-09	0.767E+00
1	0.222E-15	0.125E-08	0.401E-10	0.738E-12	0.130E+00	0.685E-10	0.103E+00	0.138E-09	0.686E-10	0.345E-09	0.767E+00

SURFACE SPECIES SITE FRACTIONS

SITE 1: SI3N4	OUTER WALL
HN_SIF(S)	4.969E-02
F3SI_NH2(S)	1.996E-04
F2SINH(S)	1.656E-02
H2NFSINH(S)	1.927E-04
HN(FSINH)2(S)	3.854E-04
HN_NH2(S)	9.330E-01
DEPOSITION RATE (MICRON/MIN)	
1 SI(D)	3.393E-01
2 N(D)	3.392E-01

DISTANCE= 0.100E+02 LAST STEP SIZE= 0.257E+01 NUMBER OF STEPS= 97
 ORDER OF INTEGRATION= 3 NUMBER OF FUNCTION CALLS = 201 JACOBIAN EVALUATIONS= 18
 ERROR TEST FAILURES = 2 CONVERGENCE TEST FAILURES= 0
 MASS IN THE FLOW= 0.369E-02 P(TORR)= 0.179E+01

	Y(CM)	U	T	OMS	H2	H	N2	N	NH	NH2	NNH
		DEPOSITION RATE--	UPPER WALL		0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
15	0.200E+01	0.000E+00	0.171E+04	0.682E-13	0.639E-05	0.227E-07	0.365E-08	0.354E-12	0.251E-08	0.128E-04	0.964E-10
14	0.189E+01	0.147E+03	0.171E+04	0.437E-13	0.639E-05	0.227E-07	0.365E-08	0.353E-12	0.251E-08	0.128E-04	0.964E-10
13	0.177E+01	0.305E+03	0.171E+04	0.795E-13	0.639E-05	0.227E-07	0.365E-08	0.351E-12	0.251E-08	0.128E-04	0.963E-10
12	0.163E+01	0.459E+03	0.171E+04	-0.664E-13	0.639E-05	0.227E-07	0.363E-08	0.351E-12	0.250E-08	0.128E-04	0.961E-10
11	0.150E+01	0.605E+03	0.171E+04	-0.142E-13	0.639E-05	0.227E-07	0.362E-08	0.350E-12	0.250E-08	0.128E-04	0.956E-10
10	0.136E+01	0.742E+03	0.171E+04	-0.111E-14	0.639E-05	0.227E-07	0.360E-08	0.349E-12	0.249E-08	0.128E-04	0.953E-10
9	0.121E+01	0.868E+03	0.171E+04	-0.109E-13	0.638E-05	0.227E-07	0.357E-08	0.347E-12	0.249E-08	0.128E-04	0.948E-10
8	0.107E+01	0.980E+03	0.171E+04	-0.786E-13	0.638E-05	0.227E-07	0.355E-08	0.346E-12	0.248E-08	0.127E-04	0.944E-10
7	0.920E+00	0.108E+04	0.171E+04	-0.266E-14	0.638E-05	0.227E-07	0.352E-08	0.344E-12	0.247E-08	0.127E-04	0.940E-10
6	0.771E+00	0.116E+04	0.171E+04	-0.167E-13	0.637E-05	0.227E-07	0.350E-08	0.343E-12	0.247E-08	0.127E-04	0.935E-10
5	0.620E+00	0.123E+04	0.171E+04	-0.866E-14	0.637E-05	0.227E-07	0.348E-08	0.341E-12	0.246E-08	0.127E-04	0.932E-10
4	0.467E+00	0.129E+04	0.171E+04	-0.264E-13	0.637E-05	0.227E-07	0.347E-08	0.341E-12	0.245E-08	0.127E-04	0.929E-10
3	0.313E+00	0.133E+04	0.171E+04	-0.138E-13	0.637E-05	0.227E-07	0.345E-08	0.340E-12	0.245E-08	0.127E-04	0.926E-10
2	0.157E+00	0.135E+04	0.171E+04	-0.153E-13	0.637E-05	0.227E-07	0.345E-08	0.340E-12	0.245E-08	0.127E-04	0.925E-10
1	0.222E-15	0.135E+04	0.171E+04	-0.155E-13	0.637E-05	0.227E-07	0.345E-08	0.340E-12	0.245E-08	0.127E-04	0.925E-10

	Y(CM)	N2H2	N2H3	N2H4	HF	F	SIF4	SIF3	SIHF3	SIF3NH2	NH3
	UPPER WALL	0.000E+00	0.000E+00	0.000E+00	0.586E-05	0.000E+00	-0.762E-05	0.000E+00	0.000E+00	0.000E+00	-0.166E-05
15	0.200E+01	0.278E-08	0.835E-10	0.272E-11	0.169E+00	0.124E-09	0.895E-01	0.133E-09	0.103E-09	0.539E-09	0.741E+00
14	0.189E+01	0.278E-08	0.835E-10	0.272E-11	0.169E+00	0.124E-09	0.898E-01	0.133E-09	0.103E-09	0.539E-09	0.742E+00
13	0.177E+01	0.278E-08	0.834E-10	0.271E-11	0.168E+00	0.124E-09	0.901E-01	0.133E-09	0.103E-09	0.538E-09	0.742E+00
12	0.163E+01	0.277E-08	0.832E-10	0.272E-11	0.168E+00	0.124E-09	0.904E-01	0.133E-09	0.103E-09	0.537E-09	0.742E+00
11	0.150E+01	0.276E-08	0.829E-10	0.271E-11	0.167E+00	0.123E-09	0.907E-01	0.134E-09	0.103E-09	0.535E-09	0.742E+00
10	0.136E+01	0.275E-08	0.826E-10	0.268E-11	0.166E+00	0.122E-09	0.910E-01	0.134E-09	0.103E-09	0.533E-09	0.743E+00
9	0.121E+01	0.274E-08	0.823E-10	0.267E-11	0.166E+00	0.122E-09	0.913E-01	0.134E-09	0.102E-09	0.531E-09	0.743E+00
8	0.107E+01	0.273E-08	0.819E-10	0.266E-11	0.165E+00	0.121E-09	0.916E-01	0.134E-09	0.102E-09	0.529E-09	0.743E+00
7	0.920E+00	0.271E-08	0.815E-10	0.265E-11	0.165E+00	0.121E-09	0.919E-01	0.134E-09	0.101E-09	0.526E-09	0.744E+00
6	0.771E+00	0.270E-08	0.812E-10	0.264E-11	0.164E+00	0.120E-09	0.922E-01	0.134E-09	0.101E-09	0.524E-09	0.744E+00
5	0.620E+00	0.269E-08	0.809E-10	0.263E-11	0.164E+00	0.120E-09	0.924E-01	0.134E-09	0.101E-09	0.522E-09	0.744E+00
4	0.467E+00	0.268E-08	0.806E-10	0.266E-11	0.163E+00	0.119E-09	0.926E-01	0.135E-09	0.100E-09	0.520E-09	0.744E+00
3	0.313E+00	0.268E-08	0.804E-10	0.265E-11	0.163E+00	0.119E-09	0.927E-01	0.135E-09	0.100E-09	0.519E-09	0.744E+00
2	0.157E+00	0.267E-08	0.803E-10	0.265E-11	0.163E+00	0.119E-09	0.928E-01	0.135E-09	0.100E-09	0.518E-09	0.744E+00
1	0.222E-15	0.267E-08	0.803E-10	0.265E-11	0.163E+00	0.119E-09	0.928E-01	0.135E-09	0.100E-09	0.518E-09	0.744E+00

SURFACE SPECIES SITE FRACTIONS

SITE 1: SI3N4	OUTER WALL
HN_SIF(S)	4.637E-02
F3SI_NH2(S)	1.807E-04
F2SINH(S)	1.546E-02
H2NFSINH(S)	1.870E-04
HN(FSINH)2(S)	3.740E-04
HN_NH2(S)	9.374E-01
DEPOSITION RATE (MICRON/MIN)	
1 SI(D)	3.072E-01
2 N(D)	3.071E-01

DISTANCE=	0.121E+02	LAST STEP SIZE=	0.257E+01	NUMBER OF STEPS=	97
ORDER OF INTEGRATION=	3	NUMBER OF FUNCTION CALLS =	201	JACOBIAN EVALUATIONS=	18
ERROR TEST FAILURES =	2	CONVERGENCE TEST FAILURES=	0		

Total CPUtime (sec): 6.59375

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