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# OPPDIF

## A PROGRAM FOR COMPUTING OPPOSED-FLOW DIFFUSION FLAMES

Reaction Design

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This document is based on the Sandia National Laboratories Report SAND96-8243, authored by Andrew E. Lutz, Robert J. Kee, Joseph F. Grcar, and Fran M. Rupley.[1]

*Reaction Design cautions that some of the material in this manual may be out of date.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.*

# OPPDIF: A PROGRAM FOR COMPUTING OPPOSED-FLOW DIFFUSION FLAMES

## ABSTRACT

OPPDIF computes the diffusion flame between two opposing nozzles. A similarity transformation reduces the flow field to a one-dimensional problem, either for an axisymmetric flow or for a 2-dimensional planar case. For the radially axisymmetric case, the similarity solution assumes that the radial component of velocity is linear in radius and the dependent variables become functions of the axial direction only. For the planar case, the *y* velocity (perpendicular to the axis of the opposed flow) is linear with the distance in the *y* direction, and again the dependent variables become functions of the axial direction only. OPPDIF solves for the temperature, species mass fractions, axial and perpendicular (radial or *y*) velocity components, and perpendicular pressure gradient. The pressure gradient is an eigenvalue of the system of equations. OPPDIF employs the TWOPNT software to solve the two-point boundary value problem for the steady-state form of the discretized equations. CHEMKIN Utilities evaluate chemical reaction rates, as well thermodynamic and transport properties.

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# 1. INTRODUCTION

OPPDIF is a program that computes the steady-state solution for axisymmetric or planar diffusion flames between two opposing nozzles. The opposed-flow geometry makes an attractive experimental configuration, because the flames are flat, allowing for detailed study of the flame chemistry and structure. The two or three-dimensional flow is reduced mathematically to one dimension by assuming that the *y*- or radial velocity varies linearly in the *y*- or radial direction, which leads to a simplification in which the fluid properties are functions of the axial distance only. The one-dimensional model then predicts the species, temperature, and velocity profiles in the core flow between the nozzles (excluding edge effects). OPPDIF allows simulation of both premixed and non-premixed flames.

The axisymmetric geometry consists of two concentric, circular nozzles directed towards each other, as in Figure 1. This configuration produces an axisymmetric flow field with a stagnation plane between the nozzles. The planar geometry consists of two concentric linear nozzles directed towards each other as shown in Figure 2. This configuration produces a 2-D planar flowfield with a stagnation line between the two nozzles. The location of the stagnation plane (or line) depends on the momentum balance of the two streams. When the streams are premixed, two premixed flames exist, one on either side of the stagnation plane. When one stream contains fuel and the other oxidizer, a diffusion flame is established. Since most fuels require more air than fuel by mass, the diffusion flame usually sits on the oxidizer side of the stagnation plane; fuel diffuses through the stagnation plane to establish the flame in a stoichiometric mixture.

The OPPDIF program is based on a model that was originally developed by Kee *et al*[2] for premixed opposed flow flames. The reduction of the three-dimensional stagnation flow is based upon similarity solutions advanced for incompressible flows by von Karman[3], which are more easily available in Schlichting.[4] Hahn *et al.*[5, 6] developed numerical solutions for diffusion flames in this geometry. Solutions for the similar geometry of a counter-flow stagnating on a porous cylinder, originally studied by Tsuji,[7] were advanced by the GAMM workshop.[8, 9]. The formulation used as part of the GAMM workshop imposed an outer flow solution for the stagnation flow from a point source at infinity onto the solution for the compressible boundary layer. The point-source solution used a single strain rate, which sets both components of the velocity and pressure gradient. While the single strain rate is useful for parameterizing the solutions for use in flamelet models, the disadvantage is that there is no length scale for the problem. The point-source formulation cannot consider the finite distance between the nozzles in experiments.

In contrast, the more general formulation in OPPDIF is based on a finite domain, where the user specifies the nozzle separation. The disadvantages of this approach are that an eigenvalue must be included in the solution of the equations and the strain rate varies, such that a characteristic strain rate must be determined from the velocity profile. Chapman and Bauer[10] used this more general formulation for

numerical solution of an incompressible flow. Seshadri and Williams[11] used essentially this formulation in asymptotic studies. Hahn and Wendt[6] were the first to use this formulation in numerical solutions of compressible flames. Following the analysis of Evans and Grief,[12] Kee *et al*[2] showed that this formulation allowed more accurate predictions of the extinction limits for premixed flames.

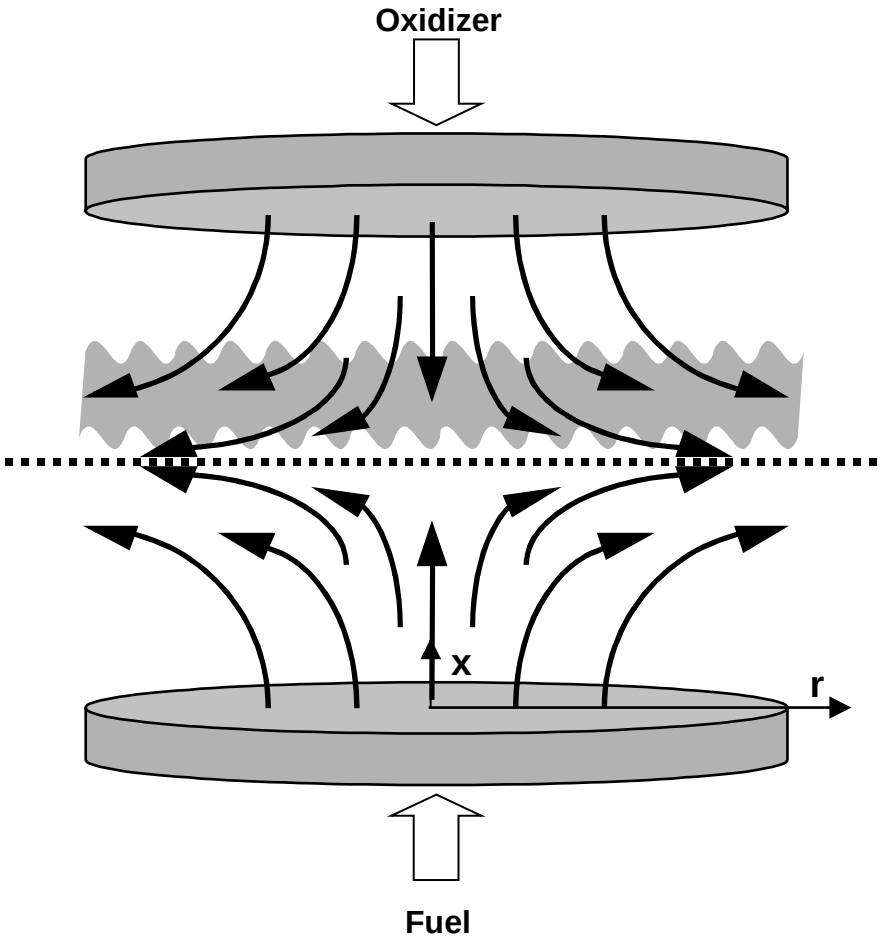


**Figure 1. Geometry of the axisymmetric opposed-flow diffusion flame. The dashed line represents the stagnation plane; the shaded region suggests the flame.**

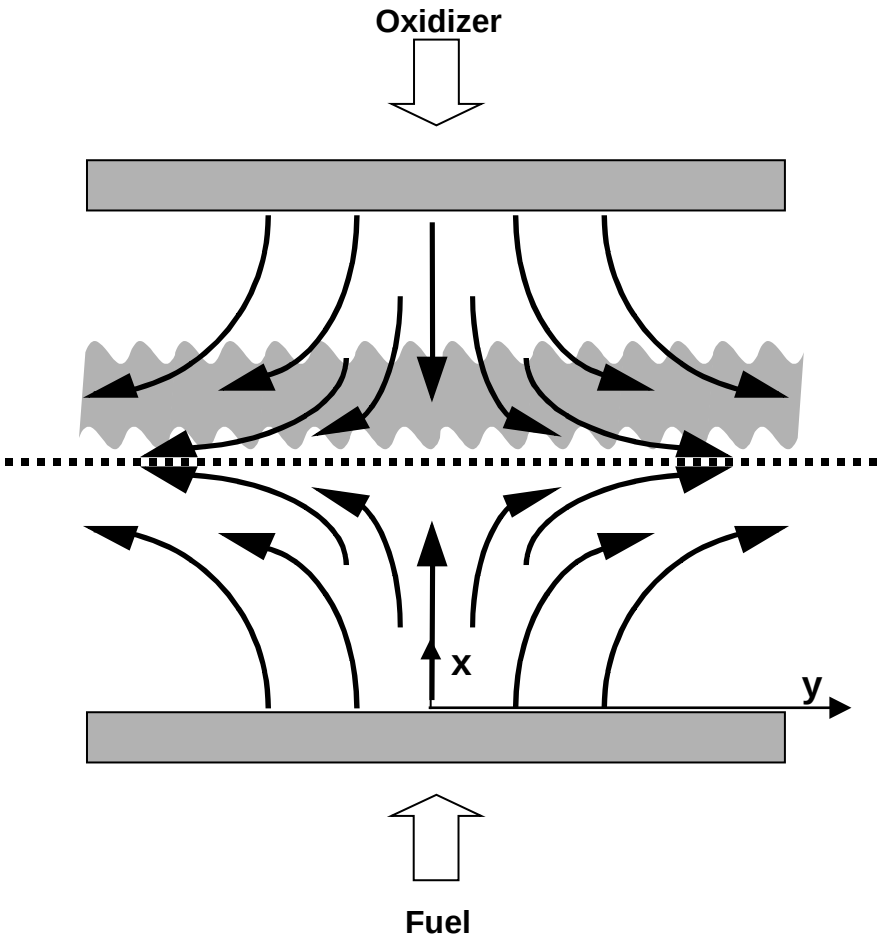


**Figure 2. Geometry of the planar opposed-flow diffusion flame. The dashed line represents the stagnation line; the shaded region suggests the flame.**

# 2. GOVERNING EQUATIONS

The geometry and axes for the axisymmetric and planar configurations are sketched in Figure 1 and Figure 2, respectively. In the following equations, $\xi$ represents either the radial direction $r$ for the axisymmetric case, or the perpendicular direction $y$ for the planar case. The coordinate parameter $n$ allows us to present one set of equations for both cases, with $n$=3 for the 3-D axisymmetric flow and $n$=2 for the 2-D planar case. A more detailed derivation of the governing equations for the opposed-flow geometry is provided by Kee, *et al.*[2]

At steady-state, conservation of mass in cylindrical or planar coordinates is

$$\frac{\partial(\rho u)}{\partial x}+\frac{1}{\xi^{n-2}}\frac{\partial\left(\rho v \xi^{n-2}\right)}{\partial \xi}=0 \tag{1}$$

where $u$ and $v$ are the axial and radial velocity components and $\rho$ is the mass density. Following von Karman,[3] who recognized that $v/\xi$ and other variables should be functions of $x$ only, we define

$$G(x)=-\frac{\rho v}{\xi} \qquad F(x)=\frac{\rho u}{(n-1)}$$

for which the continuity equation (1) reduces to

$$G(x)=\frac{dF(x)}{dx} \tag{2}$$

for the axial velocity $u$. Since $F$ and $G$ are functions of $x$ only, so are $\rho$, $u$, $T$ and $Y_k$.

The perpendicular momentum equation is satisfied by the eigenvalue

$$H=\frac{1}{\xi^{n-2}}\frac{\partial p}{\partial \xi}=\text{constant} \tag{3}$$

The perpendicular momentum equation is

$$H-(n-1)\frac{d}{dx}\left(\frac{FG}{\rho}\right)+\frac{nG^2}{\rho}+\frac{d}{dx}\left[\mu\frac{d}{dx}\left(\frac{G}{\rho}\right)\right]=0 \tag{4}$$

Energy and species conservation are

$$\rho u\frac{dT}{dx}-\frac{1}{c_p}\frac{d}{dx}\left(\lambda\frac{dT}{dx}\right)+\frac{\rho}{c_p}\sum_k c_{pk}Y_k V_k\frac{dT}{dx}+\frac{1}{c_p}\sum_k h_k\dot{\omega}_k=0 \tag{5}$$

$$\rho u \frac{dY_k}{dx} + \frac{d}{dx}\left(\rho Y_k V_k\right) - \dot{\omega}_k W_k = 0 \qquad k = 1, \ldots, K \tag{6}$$

where the diffusion velocities are given by either the multicomponent formulation

$$V_k = \frac{1}{X_k \overline{W}} \sum_{j \neq k}^{K} W_j D_{k,j} \frac{dX_j}{dx} - \frac{D_k^T}{\rho Y_k} \frac{1}{T} \frac{dT}{dx} \tag{7}$$

or the mixture-averaged formulation

$$V_k = -\frac{1}{X_k} D_{km} \frac{dX_k}{dx} - \frac{D_k^T}{\rho Y_k} \frac{1}{T} \frac{dT}{dx}, \quad \text{where} \quad D_{km} = \frac{1 - Y_k}{\sum_{j \neq k}^{K} \frac{X_j}{D_{jk}}}, \tag{8}$$

and $D_{k,j}$, $D_{km}$, $D_{jk}$ and $D_k^T$ are the multicomponent, mixture averaged, binary, and thermal diffusion coefficients, respectively.

The boundary conditions for the fuel ($F$) and oxidizer ($O$) streams at the nozzles are

$$\begin{aligned} x = 0: \quad & F = \frac{\rho_F u_F}{(n-1)}; \quad G = 0; \quad T = T_F; \quad \rho u Y_k + \rho Y_k V_k = (\rho u Y_k)_F \\ x = L: \quad & F = \frac{\rho_O u_O}{(n-1)}; \quad G = 0; \quad T = T_O; \quad \rho u Y_k + \rho Y_k V_k = (\rho u Y_k)_O \end{aligned} \tag{9}$$

The inflow boundary condition specifies the total mass flux, including diffusion and convection, rather than the species fraction ($Y_k = Y_{k,F}$). If gradients exist at the boundary, these conditions allow diffusion into the nozzle.

The differential equations (2) through (6) and boundary conditions (9) form a boundary value problem for the dependent variables ($F$, $G$, $H$, $T$, $Y_k$). The CHEMKIN Gas-Phase Subroutine Library provides the reaction rates and thermodynamic properties, while the TRANSPORT package evaluates the transport properties.

# 3. NUMERICAL SOLUTION METHOD

Discretization of the differential equations uses conventional finite differencing techniques for non-uniform mesh spacing. Diffusive terms use central differences, with truncation error that is second-order in the mesh spacing. For better convergence, convective terms use upwind differencing, which uses the sign of the velocity to choose which direction the spatial difference will go. If $u_j > 0$, for example, then the convective term in the energy equation is differenced as:

$$\rho u \frac{dT}{dx} \approx \rho_i u_j \frac{T_j - T_{j-1}}{x_j - x_{j-1}} \tag{10}$$

The truncation error of this approximation is first-order in the mesh spacing, leading to what is often called "artificial diffusion", but this form avoids unwanted oscillations during the solution on a coarse mesh. Alternatively, the convective terms can be centrally differenced using the keyword CDIF, but the default windward differencing is recommended.

The TWOPNT (for "two-point") boundary value solver solves the discretized equations. TWOPNT uses Newton's method to attempt solution of the steady-state equations, and resorts to time integration when the Newton iteration is not converging. After time integration evolves the solution toward the steady state, TWOPNT returns to Newton's method to rapidly converge on the steady solution. In computing the first solution of a new flame, TWOPNT may jump back and forth between time integration and Newton's method several times before converging. However, once one flame is solved, others can be solved much more efficiently by changing a boundary condition and re-starting from the previous solution. In order to speed convergence, experience shows that it is best to begin a new computation on a coarse mesh. Once the solution converges on the first mesh, TWOPNT refines the solution by adding new points into the regions of gradient or curvature in the solution. The degree of refinement is controlled by the GRAD and CURV parameters.

# 4. PROGRAM STRUCTURE

OPPDIF requires subroutines from the CHEMKIN, TRANSPORT, and TWOPNT Software Packages. To solve a problem using OPPDIF, the user must:

1. Execute the CHEMKIN Gas-Phase Interpreter, which reads the species information and the reaction mechanism, accesses the Thermodynamic database, and writes the CHEMKIN Linking File;
2. Execute the TRANSPORT Preprocessor, which reads the CHEMKIN Linking File, accesses the TRANSPORT database, and writes the TRANSPORT Linking File;
3. Execute OPPDIF, which reads the CHEMKIN and TRANSPORT Linking Files, initializes the CHEMKIN and TRANSPORT Subroutine Libraries, reads a text input file, computes a solution to the specified problem, and writes both text output and a binary solution file.

Figure 3 shows the relationships between the programs and files. Sharp-edged rectangles represent programs that are executed; rounded-edges denote files. The CHEMKIN Application User Interface runs the OPPDIF program and pre-processors through a mouse-driven interface and then allows the user to directly launch visualization of solution results using the CHEMKIN Graphical Post-processor.

The first step is to execute the CHEMKIN Interpreter, which reads user-supplied information about the species and chemical reactions for a particular reaction mechanism. It then extracts information about the species' thermodynamic properties from a database. All this information is stored in the CHEMKIN linking file, which is read by the CHEMKIN library when OPPDIF starts running. Refer to the CHEMKIN manual for more details.

The input that defines a particular problem and the parameters needed to solve it are read by OPPDIF, using a Keyword format described in Chapter 5.

OPPDIF writes output in two forms: text and binary. Text output includes a summary of the initial solution guess, printouts of the partial solutions, and statistics that describe the progress of the computation. OPPDIF writes two separate binary files:

1. The Save file contains the last successful solution,
2. The Recover file contains the latest solution for restart purposes (in case a successful solution is not reached). The data sequences of these binary files are discussed below.

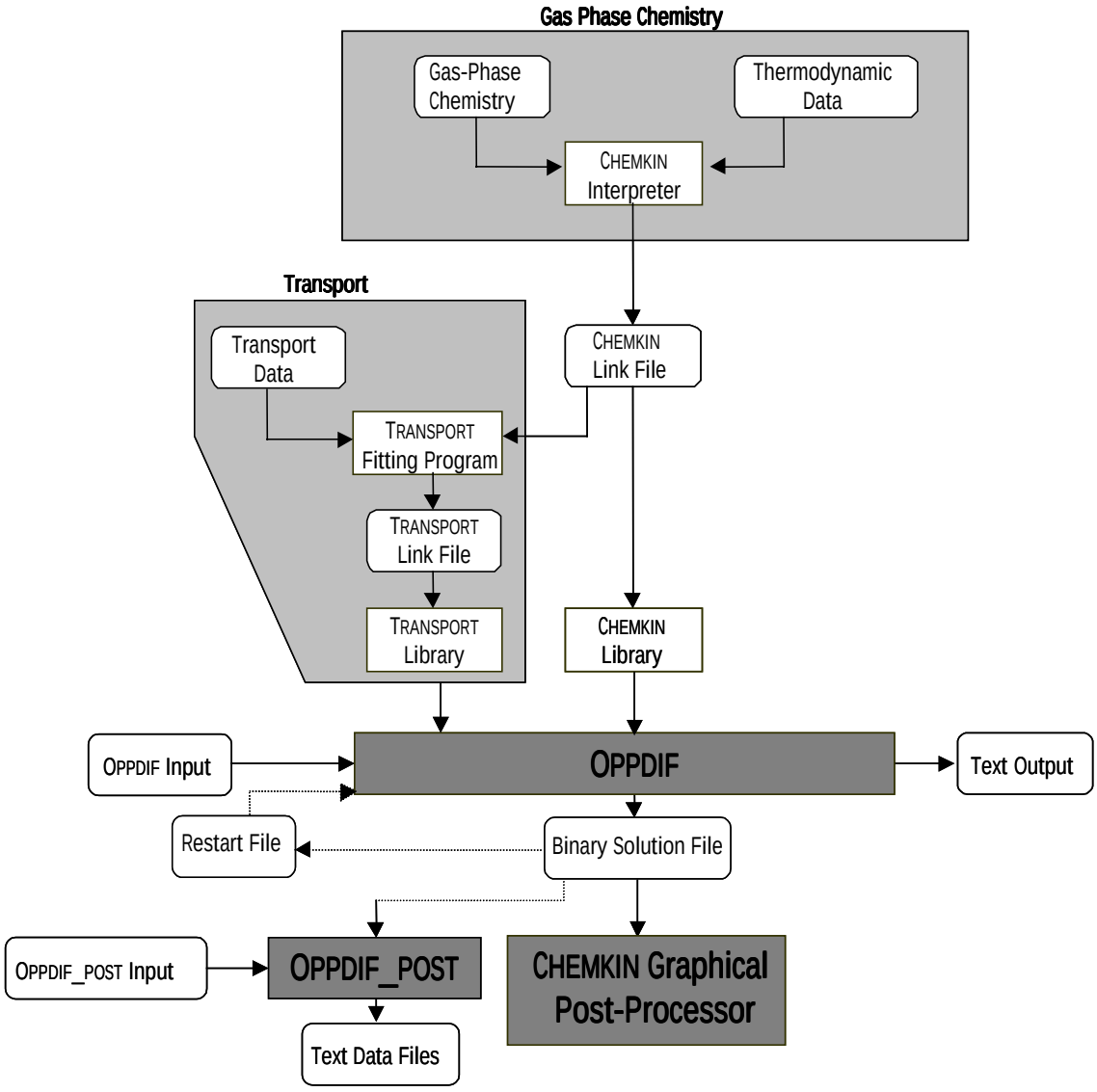


**Figure 3. Relationship of the OPPDIF program to the CHEMKIN, and TRANSPORT preprocessors and the associated input and output files**

## 4.1 Save, Restart, and Recover Files

In addition to printed output the program produces a binary Save File ("save.bin") that contains the solution and the first order sensitivity coefficients, if they were requested. This file has several uses. The solution in the file can be an initial estimate for a different calculation, through the restart option. It often saves computer time to begin a computation for a given set of conditions by starting with the solution of another set of conditions that are in some way related. In the case of a restart, the OPPDIF reads the input

keywords to specify some of the parameters, but the initial solution estimate will be read from the Restart file.

The binary solution Save File is written after the solution to a problem is complete. However, another file, the Recover File, is rewound and written after every successful return from a Newton iteration or a sequence of time steps. In the event that the program fails to complete a problem for some reason it may be possible to restart it from the Recover File. Starting from Recover File, but with different keyword inputs (for example a different time step) may be more efficient than restarting the problem from the beginning.

The binary solution file is also used to post-process the solution. Further information on this subject will be found in Chapter 7 of this document.

## 4.2 Optional User Programming

In addition to using OPPDIF through the CHEMKIN Application User Interface, users have the flexibility to write their own interface to the flame model. To facilitate this, the OPPDIF 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 OPPDIF 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. OPPDIF 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 OPPDIF 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.

## 4.3 Regrid Operation

Using the JJRG keyword invokes a Regrid operation that is useful for changing the number of grid points when restarting from one flame to another. Another use for Regrid is to revise the solution guess when a previous OPPDIF job made some progress towards a solution (by time integration, for example), but failed to converge to a steady solution.

TWOPNT's grid refinement adds points in regions where they are needed to resolve the first and second derivatives of the solution, using criteria controlled by the GRAD and CURV keywords. TWOPNT never moves or removes points. If it reaches a maximum number of points (internally defined by the dimensions), it simply prints a message and quits. Sometimes it may be necessary to reduce the number of points when starting a new solution. The Regrid operation redefines the solution guess on a specified number of mesh points; include the JJRG keyword, followed by the number of points.

The Regrid operation is different from the grid-point insertion operation performed by TWOPNT. Both operations attempt to resolve the gradient and curvature in the solution, except that TWOPNT considers all solution components, whereas Regrid only considers the temperature profile. TWOPNT only adds points, leaving the old points as they were, but Regrid alters the location and solution of all the points interior to the boundaries. Regrid computes new locations for the given number of points, and then interpolates the solution from the previous grid to obtain a new solution. Regrid does not conserve any properties of the solution; in fact, it tends to smooth the solution by the error inherent in the interpolation.

Regrid redistributes a weighting function of the first and second derivatives of the temperature. The profiles of the other dependent variables are ignored on the assumption that the temperature profile defines the flame location well enough for the purposes of realigning the mesh for an initial condition. The redistribution uses a transformation from the physical coordinate *x* to a new coordinate $\eta$

$$\frac{dx}{d\eta} W(x,T) = C \tag{11}$$

with the weighting function,

$$W(x,T) = 1 + b_1 \left| \frac{dT}{dx} \right| + b_2 \left| \frac{d^2T}{dx^2} \right| \tag{12}$$

Integration over the entire domain defines the constant.

$$C = \frac{1}{N-1} \int_O^L W(x,T)dx \tag{13}$$

Integrating over a portion of the domain gives an expression for the point locations in $\eta$-space.

$$\eta = 1 + \frac{1}{C} \int_0^x W(x,T)dx \tag{14}$$

The new grid locations *x* come by interpolation between the computed values of $\eta$ defined using the old mesh, onto a uniform mesh in $\eta$-space. Since $d\eta$ is constant on this uniform mesh, the solution to Eq. (11) states that *W(x,T)dx* is constant, so the new values of *x* will be concentrated where the weighting function is large.

Below is a sample set of Keywords that would direct OPPDIF to perform the Regrid operation at restart:

```
JJRG 20
PCAD 0.6
RGTC 1.0
```

This sequence will create a new solution guess on 20 points, devoting 60 percent of the points to resolving gradients, with equal weighting of gradient and curvature in the temperature profile. From experience, we recommend an RGTC value greater than or equal to 1. Depending on the resolution of the existing solution, PCAD should be in the neighborhood of 1/2. Note that PCAD equal to zero generates a uniform mesh.

# 5. PROGRAM INPUT

## 5.1 Keyword Syntax and Rules

OPPDIF reads input in a Keyword format. The Keyword must appear first on each input line. Some lines require only the keyword itself, while others need additional information. Keyword lines may be in any order. Syntax rules for the input file follow:

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.
3. When more than one piece of information is required, the order in which the information appears is important, and the pieces are delimited by one or more blank spaces.
4. Numbers may be stated in integer, floating-point, or E format. The program converts the numbers to the proper type, including conversion to double precision.
5. Species names must appear exactly as they are specified in the CHEMKIN Interpreter input.
6. If more information is input than required, then the last read inputs are used. For example, if contradictory keywords are encountered, the last one read is taken.
7. A comment line can be inserted by placing either a period (.), a slash (/), or a exclamation mark (!) in the first column. The program ignores comment lines, but the lines are echoed back in the printed output. In addition, on any keyword line, any input that follows the required input and is enclosed in parentheses is taken as a comment.
8. The keyword END must be the last line.

The keywords OPPDIF recognizes are listed with a description of their function and default values. Some keywords require real, integer, or character input, which are shown by example, in the list below.

## 5.2 Problem Type Keywords

**AXIS** — Radial axisymmetric coordinate system.
Default — Coordinate system is radial axisymmetric.

**PLAN** — Planar coordinate system.
Default — Coordinate system is radial axisymmetric.

**TGIV** — Energy equation is not included. User specifies a temperature profile using the TEMP keyword.
Default — None. Either TGIV or ENRG are required.

**ENRG**— Energy equation is included. A temperature profile specified by the TEMP keyword will be used as an initial guess in this case.
Default — None. Either TGIV or ENRG are required.

**NOFT** — Skip the fixed temperature problem and include the energy equation on the first attempt.
Default — Fixed temperature solution is obtained before adding the energy equation.

**LINE** — Linear profile used to set up initial solution estimates.
Default — PLAT

**PLAT** — Plateau profile used to set up initial solution estimates.
Default – PLAT

## 5.3 Method Option Keywords

**ATOL**— Absolute convergence criteria for Newton iteration.
Default — 1.E-9
Example: ATOL 1.E-8

**RTOL**— Relative convergence criteria for Newton iteration.
Default — 1.E-4
Example: RTOL 1.E-3

**ATIM**— Absolute convergence criteria for time stepping.
Default — 1.E-9
Example: ATIM 1.E-8

**RTIM**— Relative convergence criteria for time stepping.
Default — 1.E-4
Example: RTIM 1.E-3

**TIME**— Number of steps and time step value for time stepping for the starting procedure.
Units — none; seconds
Default — 50, 1.E-6
Example: TIME 100 5.E-7

**TIM2** — Number of steps and time step value for time stepping after adding the energy equation.
Units — none; seconds
Default — 50, 1.E-6
Example: TIM2 100 5.E-7

**TRAN**— Perform time-stepping only, without attempting Newton iteration for a steady solution. Specify the number of time steps to take and the initial time-step value.

Units — none; seconds

Default — A steady-state solution is attempted.

Example: TRAN 1000 1.E-6

**NDPR** — Frequency of output printing during time integration, given as the number of time-steps.

Default — 100

Example: NDPR 50

**UFAC** — Factor for increasing the time step when time integration proceeds without rapid changes to the solution.

Default — 2.

Example: UFAC 1.5

**DFAC** — Factor for decreasing the time step when time integration experiences difficulties.

Default — 2.2

Example: DFAC 1.5

**DTMN** — Minimum allowable time step.

Units — seconds

Default — 1.E-10

Example: DTMN 1.E-9

**DTMX** — Maximum allowable time step.

Units — seconds

Default — 1.E-4

Example: DTMX 1.E-3

**WDIF** — Use windward differencing on convective terms in the equations.

Default — Windward differencing.

**CDIF** — Use central differencing on convective terms in the equations.

Default — Windward differencing.

**SFLR** — Floor, or minimum, value for the species mass fractions.

Default — -1.E-4

Example: SFLR –1.E-5

**SPOS** — Small positive value used to replace negative species mass fractions upon restart or regridding.

Default — 1.E-10

Example: SPOS 1.E-14

**GFAC** — Multiplying factor used to modify all gas-phase reaction rates calculated using the CHEMKIN input reaction parameters.

Default – 1.0

Example: GFAC 1.1

**IRET** — Retirement period for a given time step, or number of time steps prior to increasing the step size.

Default – 50

Example: IRET 100

**ISTP**— Directs TWOPNT to take this number of initial time steps before attempting the Newton search for the steady-state solution.

Default – 0

Example: ISTP 100

**TJAC** — Retirement age for the Jacobian during the time integration.

Default – 20

Example: TJAC 50

**KOUT**— List of species names to be included in the text output.

Default — All species printed

Example: KOUT H2 O2 H2O H OH

## 5.4 Grid Parameter Keywords

**NPTS** — Number of initial mesh points. This specification will be ignored if GRID keywords are included.

Default – 6

Example: NPTS 11

**GRID** — Location of an initial mesh point. NOTE: GRID keyword lines must be in order of GRID location value.

Units – cm

Default — none; NPTS=6 assumed if no GRID keywords are included.

Example: GRID 0.0

**GRAD**— Parameter that controls the degree of mesh adaptation based on the first gradient in the solution.

Default — 0.1

Example: GRAD 0.5

**CURV**— Parameter that controls the degree of mesh adaptation based on the second gradient, or curvature, in the solution.

Default — 0.5

Example: CURV 0.7

**NTOT**— Maximum number of grid points allowed for this job.
Default—NTOT= maximum grid dimension set by OPPDIF driver program
Example: NTOT 200
Restart—cannot be changed on restart.

**NADP**— Number of mesh points that TWOPNT can add during each grid refinement.
Default – 10
Example: NADP 2

**XEND**— Physical length of the computational domain, or value of $x$ at the end of the domain. NOTE: The fuel inlet is assumed to be located at $x$=0.
Units – cm
Default – none; XEND keyword is required.
Example: XEND 10.0

**XCEN** — Center of the mixing region; used in defining the initial profile for the LINE or PLAT options.
Units – cm
Default – XEND * 0.35
Example: XCEN 3.0

**WMIX**— Width of the mixing region; used in defining the initial profile for the LINE or PLAT options.
Units – cm
Default – XEND * 0.5
Example: WMIX 2.0

## 5.5 Flame Definition Keywords

**VFUE**— Fuel inlet velocity (at $x$ = 0).
Units — cm / s
Default— none; VFUE must be specified.
Example: VFUE 100.

**VOXI**— Oxidizer inlet velocity (at $x$ = XEND).
Units — cm / s
Default— none; VOXI must be specified.
Example: VOXI 100.

**AFUE**— Radial gradient in fuel inlet velocity (at $x$ = 0).
Units — 1 / s
Default — 0.
Example: AFUE 5.0

**AOXI**— Radial gradient in oxidizer inlet velocity (at $x$ =XEND).
Units — 1/s
Default — 0.
Example: AOXI 5.0

**TFUE**— Fuel inlet temperature (at $x$ = 0).
Units — Kelvin
Default — none; TFUE must be specified.
Example: TFUE 300.

**TOXI**— Oxidizer inlet temperature (at $x$ =XEND).
Units — Kelvin
Default — none; TFUE must be specified.
Example: TOXI 300.

**TMAX**— Maximum temperature for use with profiles defined by the LINE or PLAT options.
Units — Kelvin
Default — 2200.
Example: TMAX 2500.

**PRES** — The initial pressure of the gas mixture.
Units — atmospheres
Default — 1.
Example: PRES 0.5

**FUEL**— Species name and the number of moles of that species in the fuel mixture. The mole fractions of the species will be normalized from the input mole quantities, so the absolute magnitudes of the input quantities are unimportant, as long as they are consistent for all FUEL entries
Units — moles or mole fraction.
Default — None, species input is required.
Example: FUEL H2 0.2

**OXID**— Species name and number of moles of that species in the oxidizer mixture. The mole fractions of the species will be normalized from the input mole quantities, so the absolute magnitudes of the input quantities are unimportant, as long as they are consistent for all OXID entries.
Units — moles or mole fraction.
Default — None, species input is required.
Example: OXID O2 0.3

**PROD**— Species name and number of moles of that species expected in the products of combustion of the fuel and oxidizer in stoichiometric proportions. The product mixture is used to define the initial profiles specified using the LINE or PLAT keywords. The mole fractions of the species will be normalized from the input mole quantities, so the absolute magnitudes of the input quantities are unimportant, as long as they are consistent for all PROD entries.

Units — moles or mole fraction.

Default — None, species input is required.

Example: PROD H2O 0.2

**TEMP** — Specifies an initial (for ENRG) or given (for TGIV) temperature profile in pairs of grid location and temperature, (*x; T*).

Units — cm; Kelvin.

Default— A linear temperature profile is assumed between the TOXI and TFUE values.

Example: TEMP 0.0 300.

**USTG** — On a restart, use the given temperature profile, not the temperature from the solution on the restart file.

Default — The temperature profile on the restart file will be used.

## 5.6 Transport Option Keywords

**MULT**— Use the multicomponent formula for diffusion velocities, Eq. (7).

Default —Use the mixture-averaged formula (MIX) .

**MIX** — Use the mixture-averaged formula for diffusion velocities, Eq. (8).

Default — Use the mixture-averaged formula.

**TDIF** — Include thermal diffusion in the calculation of diffusion velocities.

Default — Thermal diffusion is neglected.

## 5.7 Sensitivity Option Keywords

**ASEN**— Inclusion of this Keyword causes all the first-order sensitivity coefficients with respect to the rate constants to be determined.

Default—no sensitivities computed

Restart—can be changed.

**HSEN**— Inclusion of this Keyword causes all the first order sensitivity coefficients with respect to the species' heats of formation to be determined.

Default—no sensitivities computed

Restart—can be changed.

## 5.8 Printing and Restarting Keywords

**PRNT** — This integer value controls the level of printing and diagnostics from TWOPNT. A value of 0, 1, and 2 provide increasing amounts of text output.

Default — 1

Example: PRNT 2

**RSTR** — Read a solution from the restart file ("rest.bin").

Default — The program does not look for a restart file.

**JJRG** — Perform a regrid operation on the restart solution prior to attempting to solve the new problem. Use the specified number of points for the new mesh. The new grid is adapted to the temperature profile according to the weighting parameters PCAD and RGTC

Default — 40

Example: JJRG 40

**PCAD**— Specifies the fraction of available mesh points to be used for adapting the mesh to the temperature profile in a regrid operation. The value must be greater than zero and less than one. If the value is zero, then a regrid will produce a uniform grid.

Default — 0.75

Example: PCAD 0.5

**RGTC**— Specifies the ratio of weighting for adaptation of the grid by first gradient vs. curvature (or second derivative) in the temperature profile. Theoretically, there is no limit on this ratio, but values greater than or equal to one are recommended, because resolving to curvature is usually less important than gradient.

Default — 1.0

Example: RGTC 2.0

**END** — This keyword must appear on the last line of the input data.

# 6. SAMPLE PROBLEM

This section presents an example run for a hydrogen-air flame. You can use the example as a test case to prove you have OPPDIF running properly on your machine. In addition, the input file can serve as a template for your own specific input files.

The chemical reaction mechanism used for the hydrogen flame example follows.

## 6.1 Sample Input to CHEMKIN Interpreter

```
ELEMENTS
 H  O  N
END
SPECIES
 H2  H  O2  O  OH  HO2  H2O2  H2O   N2
END
REACTIONS
H+O2+M=HO2+M      3.61E17  -0.72       0.   !DIXON-LEWIS
  H2O/18.6/  H2/2.86/
H+H+M=H2+M        1.0E18   -1.0        0.   !D-L
H+H+H2=H2+H2      9.2E16   -0.6        0.
H+H+H2O=H2+H2O    6.0E19   -1.25       0.
H+OH+M=H2O+M      1.6E22   -2.0        0.   !D-L
  H2O/5/
H+O+M=OH+M        6.2E16   -0.6        0.   !D-L
  H2O/5/
O+O+M=O2+M        1.89E13   0.0    -1788.   !NBS
H2O2+M=OH+OH+M    1.3E17    0.0    45500.
H2+O2=2OH         1.7E13    0.0    47780.
OH+H2=H2O+H       1.17E9    1.3     3626.   !D-L$W
O+OH=O2+H         3.61E14  -0.5        0.   !JAM 1986
O+H2=OH+H         5.06E4    2.67    6290.   !KLEMM,ET AL 1986
OH+HO2=H2O+O2     7.5E12    0.0      0.0   !D-L
H+HO2=2OH         1.4E14    0.0     1073.   !D-L
O+HO2=O2+OH       1.4E13    0.0     1073.   !D-L
2OH=O+H2O         6.0E+8    1.3        0.   !COHEN-WEST.
H+HO2=H2+O2       1.25E13   0.0        0.   !D-L
HO2+HO2=H2O2+O2   2.0E12    0.0        0.
H2O2+H=HO2+H2     1.6E12    0.0     3800.
H2O2+OH=H2O+HO2   1.0E13    0.0     1800.
END
```

## 6.2 Sample OPPDIF Input

```
MIX
PCAD 0.7
RGTC 1.0
ENRG
PLAT
AFUE      0
AOXI      0
VFUE    100
VOXI    100
TFUE    300
TOXI    300
TMAX   2400
GRID   0.
GRID   0.05
GRID   0.1
GRID   0.25
GRID   0.5
GRID   0.75
GRID   0.9
GRID   1.0
GRID   1.1
GRID   1.25
GRID   1.5
GRID   1.75
GRID   1.9
GRID   1.95
GRID   2.0
XEND  2.0
XCEN  1.0
WMIX  1.5
PRES  1.0
IRET  20
UFAC  2.
SFLR  -1.E-4
PRNT   11
TIME 200 1.E-6
TIM2 200 1.E-6
GRAD 0.5
CURV 0.5
/
FUEL H2  1.0
/
OXID N2 0.79
OXID O2 0.21
/
PROD H2O   0.347
PROD N2    0.653
/
KOUT  H2 O2 H2O
/
RTOL  1.E-3
ATOL  1.E-6
ATIM  1.E-6
RTIM  1.E-3
END
```

## 6.3 Sample OPPDIF Output

```
         / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / /

 OPPDIF:  DOUBLE PRECISION VERSION 8.23 OF AUGUST 2000


          OOOOO  PPPPPP  PPPPPP  DDDDDD    III   FFFFFFF
         O     O P     P P     P D     D    I    F
         O     O P     P P     P D     D    I    F
         O     O PPPPPP  PPPPPP  D     D    I    FFFFF
         O     O P       P       D     D    I    F
         O     O P       P       D     D    I    F
          OOOOO  P       P       DDDDDD    III   F


         WRITTEN BY:

            DR. ANDREW E. LUTZ
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         WITH THE ASSISTANCE OF:
            DR. JOSEPH F. GRCAR
            DR. ROBERT J. KEE
            MS. FRAN M. RUPLEY



         / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / /

 OPPDIF:  THE WORK SPACE REQUIREMENTS ARE AS FOLLOWS.

                      CHARACTER    INTEGER    LOGICAL       REAL

                   USED         34       6209        328     433553
                  EXCESS          0          0          0          0
                   TOTAL         34       6209        328     433553

 CKLIB: CHEMKIN-III GAS-PHASE CHEMICAL KINETICS LIBRARY,
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 DOUBLE PRECISION Vers. 4.6 1999/06/03
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```

```
         / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / / /

 RDKEY:  READING THE KEYWORD INPUT.

         MIX
         PCAD 0.7
         RGTC 1.0
         ENRG
         PLAT
         AFUE      0
         AOXI      0
         VFUE    100
         VOXI    100
         TFUE    300
         TOXI    300
         TMAX   2400
         GRID   0.
         GRID   0.05
         GRID   0.1
         GRID   0.25
         GRID   0.5
         GRID   0.75
         GRID   0.9
         GRID   1.0
         GRID   1.1
         GRID   1.25
         GRID   1.5
         GRID   1.75
         GRID   1.9
         GRID   1.95
         GRID   2.0
         XEND  2.0
         XCEN  1.0
         WMIX  1.5
         PRES  1.0
         IRET  20
         UFAC  2.
         SFLR  -1.E-4
         PRNT   11
         TIME 200 1.E-6
         TIM2 200 1.E-6
         GRAD 0.5
         CURV 0.5
         /
         FUEL H2  1.0
         /
         OXID N2 0.79
         OXID O2 0.21
         /
         PROD H2O   0.347
         PROD N2    0.653
         /
         KOUT  H2 O2 H2O
         /
         RTOL  1.E-3
         ATOL  1.E-6
         ATIM  1.E-6
         RTIM  1.E-3
         END

 TWOPNT:  DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
         VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

 TWOPNT:  INITIAL GUESS:
```

```
 X(cm)     F       U(cm/s)       G      V/R(1/s)       H          T(K)       RHO
 0.00  4.095E-03  1.000E+02 -3.135E-02  3.828E+02 -1.000E+02  3.000E+02  8.189E-05
 0.05  2.527E-03  1.209E+02 -3.135E-02  7.500E+02 -1.000E+02  7.200E+02  4.179E-05
 0.10  9.599E-04  5.638E+01 -3.135E-02  9.205E+02 -1.000E+02  1.140E+03  3.405E-05
 0.25 -3.742E-03 -6.005E+01 -3.135E-02  2.515E+02 -1.000E+02  2.400E+03  1.246E-04
 0.50 -1.158E-02 -1.858E+02 -3.135E-02  2.515E+02 -1.000E+02  2.400E+03  1.246E-04
 0.75 -1.941E-02 -3.116E+02 -3.135E-02  2.515E+02 -1.000E+02  2.400E+03  1.246E-04
 0.90 -2.412E-02 -3.870E+02 -3.135E-02  2.515E+02 -1.000E+02  2.400E+03  1.246E-04
 1.00 -2.725E-02 -4.373E+02 -3.135E-02  2.515E+02 -1.000E+02  2.400E+03  1.246E-04
 1.10 -3.039E-02 -4.876E+02 -3.135E-02  2.515E+02 -1.000E+02  2.400E+03  1.246E-04
 1.25 -3.509E-02 -5.631E+02 -3.135E-02  2.515E+02 -1.000E+02  2.400E+03  1.246E-04
 1.50 -4.292E-02 -6.888E+02 -3.135E-02  2.515E+02 -1.000E+02  2.400E+03  1.246E-04
 1.75 -5.076E-02 -1.776E+02 -3.135E-02  5.483E+01 -1.000E+02  6.000E+02  5.716E-04
 1.90 -5.546E-02 -1.338E+02 -3.135E-02  3.782E+01 -1.000E+02  4.200E+02  8.288E-04
 1.95 -5.703E-02 -1.174E+02 -3.135E-02  3.226E+01 -1.000E+02  3.600E+02  9.718E-04
 2.00 -5.860E-02 -1.000E+02 -3.135E-02  2.675E+01 -1.000E+02  3.000E+02  1.172E-03

 X(cm)   H2          O2          H2O
 0.00  1.000E+00  0.000E+00  0.000E+00
 0.05  9.799E-01  0.000E+00  6.982E-03
 0.10  9.481E-01  0.000E+00  1.801E-02
 0.25  0.000E+00  0.000E+00  3.470E-01
 0.50  0.000E+00  0.000E+00  3.470E-01
 0.75  0.000E+00  0.000E+00  3.470E-01
 0.90  0.000E+00  0.000E+00  3.470E-01
 1.00  0.000E+00  0.000E+00  3.470E-01
 1.10  0.000E+00  0.000E+00  3.470E-01
 1.25  0.000E+00  0.000E+00  3.470E-01
 1.50  0.000E+00  0.000E+00  3.470E-01
 1.75  0.000E+00  1.756E-01  5.684E-02
 1.90  0.000E+00  1.960E-01  2.308E-02
 1.95  0.000E+00  2.030E-01  1.160E-02
 2.00  0.000E+00  2.100E-01  0.000E+00

TWOPNT:  SOLVE THE PROBLEM.

                  LOG10   LOG10
            TASK  NORM F  COND J   REMARK

           START     2.01
          SEARCH              7.82   GOING OUT OF BOUNDS
          EVOLVE    -0.01     7.81   200 TIME STEPS, 1.0E-04 LAST STRIDE
          SEARCH    -2.52     7.68   6 SEARCH STEPS

TWOPNT:  FINAL SOLUTION:

 X(cm)     F       U(cm/s)       G      V/R(1/s)       H          T(K)       RHO
 0.00  2.634E-03  6.179E+01  0.000E+00  0.000E+00 -3.143E+01  3.000E+02  8.525E-05
 0.05  2.366E-03  1.205E+02 -1.069E-02  2.721E+02 -3.143E+01  7.200E+02  3.929E-05
 0.10  1.736E-03  1.150E+02 -1.453E-02  4.814E+02 -3.143E+01  1.140E+03  3.018E-05
 0.25 -1.174E-03 -6.870E+01 -2.427E-02  7.101E+02 -3.143E+01  2.400E+03  3.417E-05
 0.50 -9.208E-03 -2.079E+02 -4.001E-02  4.516E+02 -3.143E+01  2.400E+03  8.860E-05
 0.75 -2.002E-02 -2.942E+02 -4.645E-02  3.413E+02 -3.143E+01  2.400E+03  1.361E-04
 0.90 -2.675E-02 -3.696E+02 -4.328E-02  2.990E+02 -3.143E+01  2.400E+03  1.447E-04
 1.00 -3.089E-02 -4.228E+02 -3.958E-02  2.709E+02 -3.143E+01  2.400E+03  1.461E-04
 1.10 -3.464E-02 -4.732E+02 -3.552E-02  2.426E+02 -3.143E+01  2.400E+03  1.464E-04
 1.25 -3.953E-02 -5.397E+02 -2.957E-02  2.019E+02 -3.143E+01  2.400E+03  1.465E-04
 1.50 -4.574E-02 -6.244E+02 -2.013E-02  1.374E+02 -3.143E+01  2.400E+03  1.465E-04
 1.75 -5.293E-02 -1.806E+02 -3.739E-02  6.380E+01 -3.143E+01  6.000E+02  5.860E-04
 1.90 -5.739E-02 -1.371E+02 -2.217E-02  2.648E+01 -3.143E+01  4.200E+02  8.371E-04
 1.95 -5.827E-02 -1.193E+02 -1.300E-02  1.331E+01 -3.143E+01  3.600E+02  9.766E-04
 2.00 -5.860E-02 -1.000E+02  0.000E+00  0.000E+00 -3.143E+01  3.000E+02  1.172E-03
```

```
 X(cm)   H2         O2         H2O
 0.00  9.951E-01  1.386E-09  2.177E-03
 0.05  9.836E-01  5.039E-09  7.456E-03
 0.10  9.581E-01  2.497E-08  1.793E-02
 0.25  7.722E-01  5.212E-07  7.976E-02
 0.50  2.841E-01  2.680E-04  2.196E-01
 0.75  5.259E-03  1.244E-01  9.994E-02
 0.90  2.032E-04  1.960E-01  1.445E-02
 1.00  1.257E-05  2.072E-01  2.784E-03
 1.10  9.026E-07  2.095E-01  5.326E-04
 1.25  6.370E-08  2.099E-01  6.418E-05
 1.50  4.777E-09  2.100E-01  3.368E-06
 1.75  3.428E-10  2.100E-01  9.186E-08
 1.90  1.414E-11  2.100E-01  1.171E-09
 1.95  2.325E-12  2.100E-01  6.495E-11
 2.00  3.693E-13  2.100E-01  3.369E-12

TWOPNT:  SUCCESS.  PROBLEM SOLVED.

FLDRIV:  FINISHED FIXED TEMPERATURE CASE, ADDING THE ENERGY EQUATION.

TWOPNT:  DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
         VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

TWOPNT:  INITIAL GUESS:

 X(cm)     F        U(cm/s)       G       V/R(1/s)       H          T(K)       RHO
 0.00  2.634E-03  6.179E+01  0.000E+00  0.000E+00 -3.143E+01  3.000E+02  8.525E-05
 0.05  2.366E-03  1.205E+02 -1.069E-02  2.721E+02 -3.143E+01  7.200E+02  3.929E-05
 0.10  1.736E-03  1.150E+02 -1.453E-02  4.814E+02 -3.143E+01  1.140E+03  3.018E-05
 0.25 -1.174E-03 -6.870E+01 -2.427E-02  7.101E+02 -3.143E+01  2.400E+03  3.417E-05
 0.50 -9.208E-03 -2.079E+02 -4.001E-02  4.516E+02 -3.143E+01  2.400E+03  8.860E-05
 0.75 -2.002E-02 -2.942E+02 -4.645E-02  3.413E+02 -3.143E+01  2.400E+03  1.361E-04
 0.90 -2.675E-02 -3.696E+02 -4.328E-02  2.990E+02 -3.143E+01  2.400E+03  1.447E-04
 1.00 -3.089E-02 -4.228E+02 -3.958E-02  2.709E+02 -3.143E+01  2.400E+03  1.461E-04
 1.10 -3.464E-02 -4.732E+02 -3.552E-02  2.426E+02 -3.143E+01  2.400E+03  1.464E-04
 1.25 -3.953E-02 -5.397E+02 -2.957E-02  2.019E+02 -3.143E+01  2.400E+03  1.465E-04
 1.50 -4.574E-02 -6.244E+02 -2.013E-02  1.374E+02 -3.143E+01  2.400E+03  1.465E-04
 1.75 -5.293E-02 -1.806E+02 -3.739E-02  6.380E+01 -3.143E+01  6.000E+02  5.860E-04
 1.90 -5.739E-02 -1.371E+02 -2.217E-02  2.648E+01 -3.143E+01  4.200E+02  8.371E-04
 1.95 -5.827E-02 -1.193E+02 -1.300E-02  1.331E+01 -3.143E+01  3.600E+02  9.766E-04
 2.00 -5.860E-02 -1.000E+02  0.000E+00  0.000E+00 -3.143E+01  3.000E+02  1.172E-03

 X(cm)   H2         O2         H2O
 0.00  9.951E-01  1.386E-09  2.177E-03
 0.05  9.836E-01  5.039E-09  7.456E-03
 0.10  9.581E-01  2.497E-08  1.793E-02
 0.25  7.722E-01  5.212E-07  7.976E-02
 0.50  2.841E-01  2.680E-04  2.196E-01
 0.75  5.259E-03  1.244E-01  9.994E-02
 0.90  2.032E-04  1.960E-01  1.445E-02
 1.00  1.257E-05  2.072E-01  2.784E-03
 1.10  9.026E-07  2.095E-01  5.326E-04
 1.25  6.370E-08  2.099E-01  6.418E-05
 1.50  4.777E-09  2.100E-01  3.368E-06
 1.75  3.428E-10  2.100E-01  9.186E-08
 1.90  1.414E-11  2.100E-01  1.171E-09
 1.95  2.325E-12  2.100E-01  6.495E-11
 2.00  3.693E-13  2.100E-01  3.369E-12

TWOPNT:  SOLVE THE PROBLEM.
                     LOG10   LOG10
             TASK   NORM F  COND J   REMARK
```

```
 START     2.83           15 GRID POINTS
SEARCH             11.22   GOING OUT OF BOUNDS
EVOLVE     1.46     8.31   200 TIME STEPS, 1.0E-04 LAST STRIDE
SEARCH    -1.94    11.15   14 SEARCH STEPS

REFINE     4.10           1.00 AND 1.00 RATIOS, 23 GRID POINTS
SEARCH             11.21   GOING OUT OF BOUNDS
EVOLVE     1.43     8.38   200 TIME STEPS, 1.0E-04 LAST STRIDE
SEARCH    -1.53    10.74   13 SEARCH STEPS

REFINE     3.58           0.96 AND 1.00 RATIOS, 33 GRID POINTS
SEARCH    -1.15    11.47   23 SEARCH STEPS

REFINE     3.46           0.85 AND 0.94 RATIOS, 39 GRID POINTS
SEARCH    -0.22    11.26   20 SEARCH STEPS

REFINE     2.55           0.53 AND 0.91 RATIOS, 44 GRID POINTS
SEARCH    -0.85    11.42   7 SEARCH STEPS

REFINE     2.14           0.47 AND 0.54 RATIOS, 46 GRID POINTS
SEARCH    -1.43    11.49   5 SEARCH STEPS

REFINE                    0.47 AND 0.46 RATIOS
```

TWOPNT: FINAL SOLUTION:

| X(cm) | F | U(cm/s) | G | V/R(1/s) | H | T(K) | RHO |
|---|---|---|---|---|---|---|---|
| 0.00 | 4.093E-03 | 9.997E+01 | 0.000E+00 | 0.000E+00 | -8.103E+00 | 3.000E+02 | 8.189E-05 |
| 0.05 | 3.997E-03 | 9.767E+01 | -3.861E-03 | 4.718E+01 | -8.103E+00 | 3.002E+02 | 8.184E-05 |
| 0.08 | 3.876E-03 | 9.482E+01 | -5.773E-03 | 7.060E+01 | -8.103E+00 | 3.005E+02 | 8.176E-05 |
| 0.10 | 3.709E-03 | 9.092E+01 | -7.629E-03 | 9.351E+01 | -8.103E+00 | 3.013E+02 | 8.158E-05 |
| 0.14 | 3.374E-03 | 8.339E+01 | -1.022E-02 | 1.262E+02 | -8.103E+00 | 3.045E+02 | 8.093E-05 |
| 0.17 | 2.947E-03 | 7.417E+01 | -1.258E-02 | 1.583E+02 | -8.103E+00 | 3.136E+02 | 7.947E-05 |
| 0.21 | 2.437E-03 | 6.302E+01 | -1.464E-02 | 1.893E+02 | -8.103E+00 | 3.374E+02 | 7.732E-05 |
| 0.25 | 1.850E-03 | 4.820E+01 | -1.662E-02 | 2.165E+02 | -8.103E+00 | 3.906E+02 | 7.678E-05 |
| 0.31 | 6.877E-04 | 1.590E+01 | -2.058E-02 | 2.379E+02 | -8.103E+00 | 5.795E+02 | 8.651E-05 |
| 0.38 | -6.800E-04 | -1.377E+01 | -2.318E-02 | 2.348E+02 | -8.103E+00 | 8.878E+02 | 9.875E-05 |
| 0.44 | -2.116E-03 | -4.044E+01 | -2.277E-02 | 2.175E+02 | -8.103E+00 | 1.259E+03 | 1.046E-04 |
| 0.50 | -3.498E-03 | -6.473E+01 | -2.147E-02 | 1.986E+02 | -8.103E+00 | 1.631E+03 | 1.081E-04 |
| 0.56 | -4.791E-03 | -8.633E+01 | -1.991E-02 | 1.793E+02 | -8.103E+00 | 1.964E+03 | 1.110E-04 |
| 0.63 | -5.987E-03 | -1.041E+02 | -1.837E-02 | 1.596E+02 | -8.103E+00 | 2.221E+03 | 1.151E-04 |
| 0.66 | -6.552E-03 | -1.101E+02 | -1.774E-02 | 1.490E+02 | -8.103E+00 | 2.290E+03 | 1.190E-04 |
| 0.69 | -7.101E-03 | -1.126E+02 | -1.742E-02 | 1.381E+02 | -8.103E+00 | 2.283E+03 | 1.262E-04 |
| 0.70 | -7.374E-03 | -1.113E+02 | -1.753E-02 | 1.324E+02 | -8.103E+00 | 2.233E+03 | 1.325E-04 |
| 0.72 | -7.651E-03 | -1.082E+02 | -1.790E-02 | 1.265E+02 | -8.103E+00 | 2.146E+03 | 1.414E-04 |
| 0.73 | -7.936E-03 | -1.030E+02 | -1.858E-02 | 1.206E+02 | -8.103E+00 | 2.019E+03 | 1.541E-04 |
| 0.75 | -8.235E-03 | -9.560E+01 | -1.972E-02 | 1.145E+02 | -8.103E+00 | 1.850E+03 | 1.723E-04 |
| 0.77 | -8.626E-03 | -8.395E+01 | -2.198E-02 | 1.070E+02 | -8.103E+00 | 1.592E+03 | 2.055E-04 |
| 0.79 | -9.075E-03 | -6.960E+01 | -2.590E-02 | 9.931E+01 | -8.103E+00 | 1.283E+03 | 2.608E-04 |
| 0.80 | -9.331E-03 | -6.179E+01 | -2.884E-02 | 9.549E+01 | -8.103E+00 | 1.118E+03 | 3.020E-04 |
| 0.81 | -9.620E-03 | -5.388E+01 | -3.275E-02 | 9.171E+01 | -8.103E+00 | 9.540E+02 | 3.571E-04 |
| 0.81 | -9.779E-03 | -5.005E+01 | -3.511E-02 | 8.985E+01 | -8.103E+00 | 8.751E+02 | 3.908E-04 |
| 0.82 | -9.950E-03 | -4.638E+01 | -3.777E-02 | 8.803E+01 | -8.103E+00 | 8.000E+02 | 4.290E-04 |
| 0.82 | -1.013E-02 | -4.296E+01 | -4.070E-02 | 8.626E+01 | -8.103E+00 | 7.298E+02 | 4.718E-04 |
| 0.82 | -1.033E-02 | -3.982E+01 | -4.388E-02 | 8.456E+01 | -8.103E+00 | 6.655E+02 | 5.189E-04 |
| 0.83 | -1.078E-02 | -3.453E+01 | -5.077E-02 | 8.135E+01 | -8.103E+00 | 5.561E+02 | 6.242E-04 |
| 0.84 | -1.128E-02 | -3.060E+01 | -5.789E-02 | 7.849E+01 | -8.103E+00 | 4.725E+02 | 7.375E-04 |
| 0.86 | -1.248E-02 | -2.644E+01 | -6.972E-02 | 7.384E+01 | -8.103E+00 | 3.709E+02 | 9.441E-04 |
| 0.88 | -1.385E-02 | -2.567E+01 | -7.624E-02 | 7.066E+01 | -8.103E+00 | 3.254E+02 | 1.079E-03 |
| 0.90 | -1.530E-02 | -2.686E+01 | -7.802E-02 | 6.850E+01 | -8.103E+00 | 3.085E+02 | 1.139E-03 |
| 0.93 | -1.724E-02 | -2.961E+01 | -7.723E-02 | 6.634E+01 | -8.103E+00 | 3.019E+02 | 1.164E-03 |
| 0.95 | -1.914E-02 | -3.272E+01 | -7.539E-02 | 6.442E+01 | -8.103E+00 | 3.004E+02 | 1.170E-03 |
| 0.97 | -2.100E-02 | -3.585E+01 | -7.329E-02 | 6.256E+01 | -8.103E+00 | 3.001E+02 | 1.172E-03 |
| 1.00 | -2.281E-02 | -3.893E+01 | -7.114E-02 | 6.070E+01 | -8.103E+00 | 3.000E+02 | 1.172E-03 |

```
 1.05 -2.627E-02 -4.482E+01 -6.715E-02  5.730E+01 -8.103E+00  3.000E+02  1.172E-03
 1.10 -2.952E-02 -5.038E+01 -6.316E-02  5.389E+01 -8.103E+00  3.000E+02  1.172E-03
 1.18 -3.405E-02 -5.810E+01 -5.747E-02  4.904E+01 -8.103E+00  3.000E+02  1.172E-03
 1.25 -3.814E-02 -6.509E+01 -5.171E-02  4.413E+01 -8.103E+00  3.000E+02  1.172E-03
 1.50 -4.915E-02 -8.387E+01 -3.634E-02  3.101E+01 -8.103E+00  3.000E+02  1.172E-03
 1.75 -5.613E-02 -9.579E+01 -1.950E-02  1.664E+01 -8.103E+00  3.000E+02  1.172E-03
 1.90 -5.819E-02 -9.931E+01 -8.051E-03  6.870E+00 -8.103E+00  3.000E+02  1.172E-03
 1.95 -5.850E-02 -9.983E+01 -4.037E-03  3.445E+00 -8.103E+00  3.000E+02  1.172E-03
 2.00 -5.860E-02 -1.000E+02  0.000E+00  0.000E+00 -8.103E+00  3.000E+02  1.172E-03

 X(cm)   H2         O2         H2O
 0.00  1.000E+00  4.284E-15  3.497E-07
 0.05  1.000E+00  3.021E-14  2.385E-06
 0.08  1.000E+00  1.011E-13  7.737E-06
 0.10  9.999E-01  3.770E-13  2.780E-05
 0.14  9.997E-01  2.230E-12  1.561E-04
 0.17  9.986E-01  1.145E-11  7.332E-04
 0.21  9.940E-01  5.582E-11  2.985E-03
 0.25  9.788E-01  2.677E-10  1.005E-02
 0.31  9.028E-01  2.327E-09  4.123E-02
 0.38  7.658E-01  1.786E-08  8.609E-02
 0.44  6.062E-01  1.021E-07  1.330E-01
 0.50  4.438E-01  9.100E-07  1.805E-01
 0.56  2.894E-01  1.505E-05  2.266E-01
 0.63  1.484E-01  3.216E-04  2.668E-01
 0.66  8.701E-02  2.216E-03  2.781E-01
 0.69  4.105E-02  1.321E-02  2.690E-01
 0.70  2.646E-02  2.637E-02  2.536E-01
 0.72  1.640E-02  4.486E-02  2.326E-01
 0.73  9.642E-03  6.737E-02  2.078E-01
 0.75  5.259E-03  9.220E-02  1.805E-01
 0.77  2.275E-03  1.226E-01  1.451E-01
 0.79  1.069E-03  1.510E-01  1.081E-01
 0.80  8.310E-04  1.633E-01  8.985E-02
 0.81  7.086E-04  1.742E-01  7.238E-02
 0.81  6.620E-04  1.790E-01  6.414E-02
 0.82  6.206E-04  1.834E-01  5.633E-02
 0.82  5.819E-04  1.874E-01  4.901E-02
 0.82  5.447E-04  1.909E-01  4.223E-02
 0.83  4.732E-04  1.968E-01  3.043E-02
 0.84  4.041E-04  2.012E-01  2.106E-02
 0.86  2.795E-04  2.065E-01  9.044E-03
 0.88  1.811E-04  2.088E-01  3.336E-03
 0.90  1.123E-04  2.096E-01  1.141E-03
 0.93  5.708E-05  2.099E-01  2.671E-04
 0.95  2.793E-05  2.100E-01  5.765E-05
 0.97  1.345E-05  2.100E-01  1.197E-05
 1.00  6.601E-06  2.100E-01  2.735E-06
 1.05  1.745E-06  2.100E-01  2.523E-07
 1.10  4.652E-07  2.100E-01  2.420E-08
 1.18  7.538E-08  2.100E-01  1.217E-09
 1.25  1.478E-08  2.100E-01  8.038E-11
 1.50  5.377E-10  2.100E-01  8.567E-13
 1.75  1.302E-11  2.100E-01  6.016E-15
 1.90  3.659E-13  2.100E-01  4.644E-17
 1.95  5.065E-14  2.100E-01  2.018E-18
 2.00  7.003E-15  2.100E-01  8.752E-20
TWOPNT:  SUCCESS.  PROBLEM SOLVED.
```

# 7. POST PROCESSING

## 7.1 CHEMKIN Graphical Post-processor

The CHEMKIN Graphical Post-processor provides a means for quick visualization of results from OPPDIF. Launched from the CHEMKIN Application User Interface, the Graphical Post-processor will automatically read in the solution date 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.

## 7.2 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 OPPDIF_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, oppdif_post.f, is provided in the CHEMKIN "post_processors" subdirectory. Also in this directory is a makefile script for re-building the OPPDIF_POST program, in case the user makes changes to the source code. In this way, the user may easily configure OPPDIF_POST for their own analysis needs.

To run OPPDIF_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 OPPDIF_POST from the command-line, specifying the full path to the CHEMKIN "bin" directory where the "oppdif_post" executable resides, unless this is already in your environment "path" variable:

```
oppdif_post < oppdif_post.inp > oppdif_post.out
```

Here, "oppdif_post.inp" is an input file that contains keywords described at the end of this section. The output "oppdif_post.out" will contain diagnostics and error messages for the OPPDIF_POST run. OPPDIF_POST will also create text files containing comma-separated values. The names for these files use a suffix (extension) of ".csv". One file contains the species fractions as requested by the input keywords. A second file contains other solution variables:

1. Temperature, $T$
2. Density, $\rho$
3. Fuel mixture fraction: mass of fuel elements (C and H) per mass of mixture
4. Velocities: axial, $u$ and radial, $v/\xi$
5. Strain rates: normal $\partial u / \partial \xi$ and shear $\partial(-v/\xi)/\partial x$

Additional files contain reaction rates or sensitivity coefficients, if requested, for a species. OPPDIF_POST compares the peak rates for individual reactions to the total rate to filter out unimportant reactions. The printed rate is scaled by $\dot{\omega}_k W_k / \rho$ with units of inverse seconds.

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

**PREF** — A character-string prefix used to name output files.
Default — "Opp".

**SPEC** — List of the names of species for which fractions are output.
Default — No species fractions will be printed.
Example: SPEC H2 O2 H2O H O OH

**MASS**— Print species fractions as mass fractions
Default — Mole fractions are printed.

**MOLE**— Print species fractions as mole fractions
Default — Mole fractions are printed.

**EINO** — Include emission indices in output. NOTE: this keyword must be followed by the FUEL keyword on the next line.
Default — Emission indices are not printed.

**FUEL** — Specification of fuel species name
Default — None; this is required input if EINO keyword is included.
Example: FUEL H2

**SMIN** — Minimum species fraction quantity of interest.
Default —0.0, all species fractions listed.
Example: SMIN 1.0E-3

**RATE** — List of the names of species for which production rates are listed.
Default — No species production rates will be printed.
Example: PROD H2 O2 H2O H O OH

**SENS** — List of the names of species for which reaction rate sensitivity coefficients are listed.
Default — No species reaction rate sensitivity coefficients will be printed.
Example: SENS H2 O2 H2O H O OH

**HSEN** — List of the names of species for which formation enthalpy sensitivity coefficients are listed.
Default — No species formation enthalpy sensitivity coefficients will be printed.
Example: HSEN H2 O2 H2O H O OH

**DROP** — Filter out lowest reaction rates and sensitivity coefficients, by percent.
Default — 10., lowest 10% of reaction rates and sensitivity coefficients are not printed.
Example: DROP 15

**HELP** — List descriptions of the keywords available.

**END** — Must be the last keyword in the input

## 7.3 OPPDIF Restart Utility – OPPDIF_NUSTART

OPPDIF_NUSTART is a command-line post-processing routine that converts the binary solution file into a restart file for a different chemical mechanism than the original solution used. Since the solution file contains a list of the species, any change in the mechanism that adds a new species would require starting a new OPPDIF computation from an original job. Original jobs almost always require more computational effort than restart jobs, so there is an advantage in being able to revise the solution file for restart. For example, users with large mechanisms may save computation time by running their first flame with a smaller mechanism, then converting the solution file to the full mechanism and restarting.

To run OPPPDIF_NUSTART:

1. Rename the solution file ("save.bin") to "oldsave.bin."
2. Re-run the CHEMKIN interpreter to create a new Linking File ("chem.asc").
3. Execute OPPDIF_NUSTART, which will create a new solution file: "newsave.bin". OPPDIF_NUSTART allows you to specify species profiles for new species by reading them from standard input until it finds an END keyword.
4. Rename the new solution file ("newsave.bin") for OPPDIF to use for restart: "rest.bin"

# 8. REFERENCES


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