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

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ABSTRACT

Oppdif is a Fortran program that computes the diffusion flame between two opposing nozzles. A similarity transformation reduces the two-dimensional axisymmetric flow field to a one-dimensional problem. Assuming that the radial component of velocity is linear in radius, the dependent variables become functions of the axial direction only. Oppdif solves for the temperature, species mass fractions, axial and radial velocity components, and radial pressure gradient, which is an eigenvalue in the problem. The Twopnt software solves the two-point boundary value problem for the steady-state form of the discretized equations. The Chemkin package evaluates chemical reaction rates and thermodynamic and transport properties.

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

INTRODUCTION

This report describes Oppdif: a Fortran computer program that computes the steady-state solution for axisymmetric diffusion flames between two opposing nozzles. The one-dimensional model predicts the species, temperature, and velocity profiles in the core flow between the nozzles (excluding edge effects). The model was originally developed by Kee *et al*[1] for premixed opposed flow flames; Oppdif extends the model to non-premixed flames.

The geometry consists of two concentric, circular nozzles directed towards each other, as in Fig. 1. This configuration produces an axisymmetric flow field with a stagnation plane between the nozzles. The location of the stagnation plane 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 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-dimensional flow is reduced to one dimension by assuming that the radial velocity varies linearly in the radial direction, which leads to a simplification in which the fluid properties are functions of the axial distance only.

The reduction of the two-dimensional stagnation flow is based upon similarity solutions advanced for incompressible flows by von Karman[2], which are more easily available in Schlichting.[3] Numerical solutions for diffusion flames in this geometry were produced by Hahn *et al.*[4,5] Solutions on the similar geometry of a counter-flow stagnating on a porous cylinder, originally studied by Tsuji,[6] were advanced by the GAMM workshop.[7] Miller *et al*[8] wrote a Tsuji-flame model to participate in the workshop, and much of the experience with solution techniques was gained during that effort.

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 does use the nozzle separation. The disadvantages are that an eigenvalue must be included in the solution of the equations, and the strain rate varies, so a characteristic strain rate must be defined from the velocity profile. Chapman and Bauer[9] used this more general formulation for numerical solution of an incompressible flow. Seshadri and Williams[10] used essentially this formulation in asymptotic studies. Hahn and Wendt[5] were the first to use this formulation in numerical solutions of compressible flames. Following the analysis of Evans and Grief[11], Kee *et al*[1] showed that this formulation allowed more accurate predictions of the extinction limits for premixed flames.

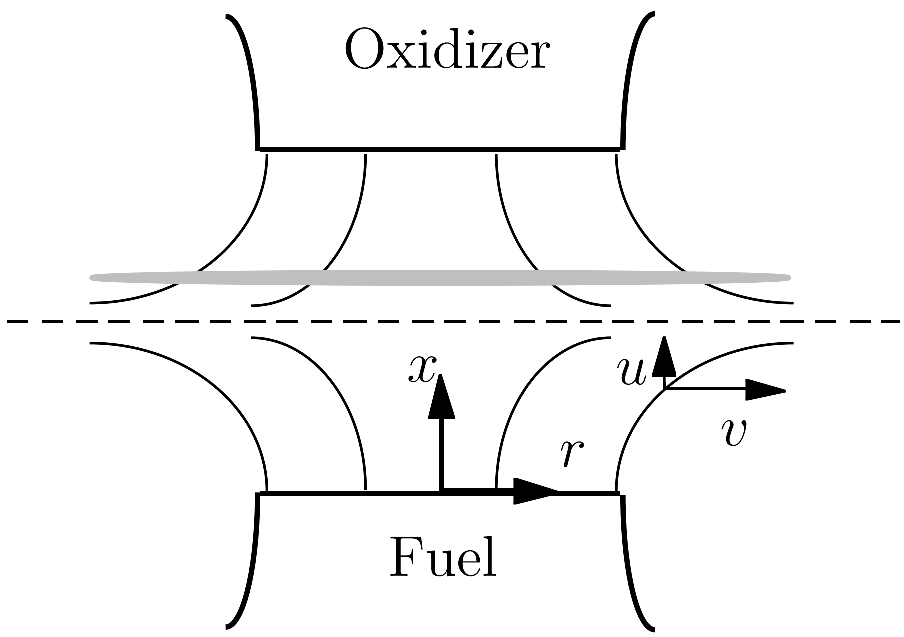

Figure 1. Geometry of the opposed-flow diffusion flame. The dashed line represents the stagnation plane; the dotted region suggests the flame.

As an example of an Oppdif solution, Fig. 2 shows the computed temperature profile of a methane-air diffusion flame examined by Puri *et al.*[12] The fuel and air velocities are 76.82 and 73.39 cm/s, separated by 1.49 cm. The plot compares the data (circles),[12] the single strain-rate solution (dashed curve),[12] and the Oppdif solution (solid curve). While there may be differences in the chemical mechanisms used in the two solutions, it does appear that the formulation in Oppdif provides a closer match of the flame location.

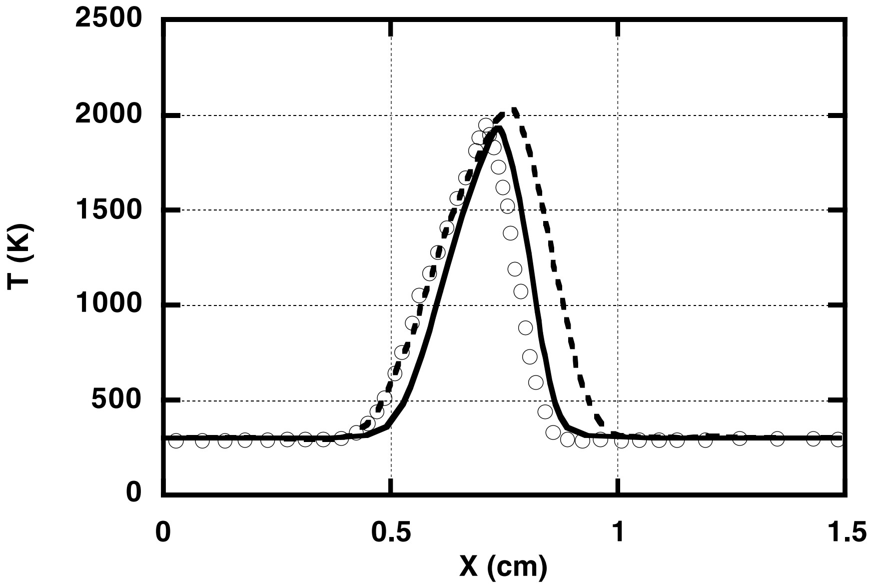

Figure 2. Temperature profile for CH_4-air flame. Symbols are measurements of Puri *et al.*[12] Dashed curve single strain-rate solution (also in Puri *et al*).

EQUATIONS

A derivation of the governing equations for the opposed-flow geometry is given in Kee *et al*,[1] so the derivation here is brief. The geometry and axes are sketched in Fig. 1.

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

$$\frac{\partial}{\partial x}(\rho u) + \frac{1}{r}\frac{\partial}{\partial r}(\rho v r) = 0$$

where u and v are the axial and radial velocity components and ρ is the mass density. Following von Karman,[2] who recognized that v/r and other variables should be functions of x only, we define

$$G(x) = -\frac{\rho v}{r} \qquad \text{and} \qquad F(x) = \frac{\rho u}{2}$$

for which continuity reduces to

$$G(x) = \frac{dF(x)}{dx} \tag{1}$$

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

The radial momentum equation is satisfied by the eigenvalue

$$H = \frac{1}{r}\frac{\partial p}{\partial r} = \text{constant} \tag{2}$$

The radial momentum equation is

$$H - 2\frac{d}{dx}\left(\frac{FG}{\rho}\right) + \frac{3G^2}{\rho} + \frac{d}{dx}\left[\mu\frac{d}{dx}\left(\frac{G}{\rho}\right)\right] = 0 \tag{3}$$

Energy and species conservation are

$$\rho u\frac{dT}{dx} - \frac{1}{c_p}\frac{d}{dx}\left(\lambda\frac{dT}{dx}\right) + \frac{\rho}{c_p}\sum_k c_{p_k} Y_k V_k \frac{dT}{dx} + \frac{1}{c_p}\sum_k h_k \dot{\omega}_k = 0 \tag{4}$$

$$\rho u\frac{dY_k}{dx} + \frac{d}{dx}\left(\rho Y_k V_k\right) - \dot{\omega}_k W_k = 0 \quad k = 1, K \tag{5}$$

where the diffusion velocities are given by either the multicomponent formulation

$$V_k = \frac{1}{X_k \bar{W}}\sum_{j=1}^{K} W_j D_{kj}\frac{dX_j}{dx} - \frac{D_k^T}{\rho Y_k}\frac{1}{T}\frac{dT}{dx} \tag{6}$$

or the mixture-averaged formulation

$$V_k = -\frac{1}{X_k}D_{km}\frac{dX_k}{dx} - \frac{D_k^T}{\rho Y_k}\frac{1}{T}\frac{dT}{dx} \qquad \text{where} \qquad D_{km} = \frac{1 - Y_k}{\sum_{j\neq k}^{K} X_j/\mathcal{D}_{jk}} \tag{7}$$

and D_{kj}, D_{km}, $\mathcal{D}_{jk}$ 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

$$\begin{aligned} x = 0: \quad & F = \frac{\rho_F u_F}{2}, \quad G = 0, \quad T = T_F, \quad \rho u Y_k + \rho Y_k V_k = (\rho u Y_k)_F \\ x = L: \quad & F = \frac{\rho_O u_O}{2}, \quad G = 0, \quad T = T_O, \quad \rho u Y_k + \rho Y_k V_k = (\rho u Y_k)_O \end{aligned} \tag{8}$$

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 (1) through (5) and boundary conditions (8) form a boundary value problem for the dependent variables (F, G, H, T, Y_k). The Chemkin[13] library of subroutines provides the reaction rates and thermodynamic properties. A Chemkin based package[14] evaluates the transport properties.

SOLUTION

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

$$\rho u \frac{dT}{dx} \approx \rho_j u_j \frac{T_j - T_{j-1}}{x_j - x_{j-1}}.$$

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 the coarse mesh. Alternatively, the convective terms can be central differenced using the keyword `CDIF`, but the default windward differencing is recommended.

The Twopnt[15] (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.

RUNNING OPPDIF

Oppdif requires subroutines from the Chemkin,[13] transport,[14] and Twopnt[15] software packages. To solve a problem using Oppdif, the user must:

1. execute the Chemkin reaction interpreter, which reads the mechanism and the thermodynamic data base, and writes the Chemkin linking file;
2. execute the transport interpreter, which reads the Chemkin linking file and the transport data base, and writes the transport linking file;
3. compile and link Oppdif with the Chemkin, transport, and Twopnt libraries;
4. execute Oppdif, which reads the Chemkin and transport linking files, and a text input file, and writes both text and binary output files.

Figure 3 shows the relationships between the routines and files. Sharp-edged rectangles represent programs to be executed; rounded-edges denote files. Figure 3 contains default names for some of the files; files not labeled read or write to standard input or output.

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 data base. 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 the next section.

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.

<u>The Save File</u>

The binary file is written using the following Fortran statements. At the start of a run:

```
WRITE (LSAVE) 'CKLINK'
WRITE (LSAVE) ( ICKWRK(L), L = 1, LENI )
WRITE (LSAVE) ( RCKWRK(L), L = 1, LENR )
WRITE (LSAVE) ( CCKWRK(L), L = 1, LENC )
```

where `LENI`, `LENR`, and `LENC` can be obtained by a call to the Chemkin routine `CKPNT`.

```
WRITE (LSAVE) 'MCLINK'
WRITE (LSAVE) ( IMCWRK(L), L = 1, LENI)
WRITE (LSAVE) ( RMCWRK(L), L = 1, LENR)
```

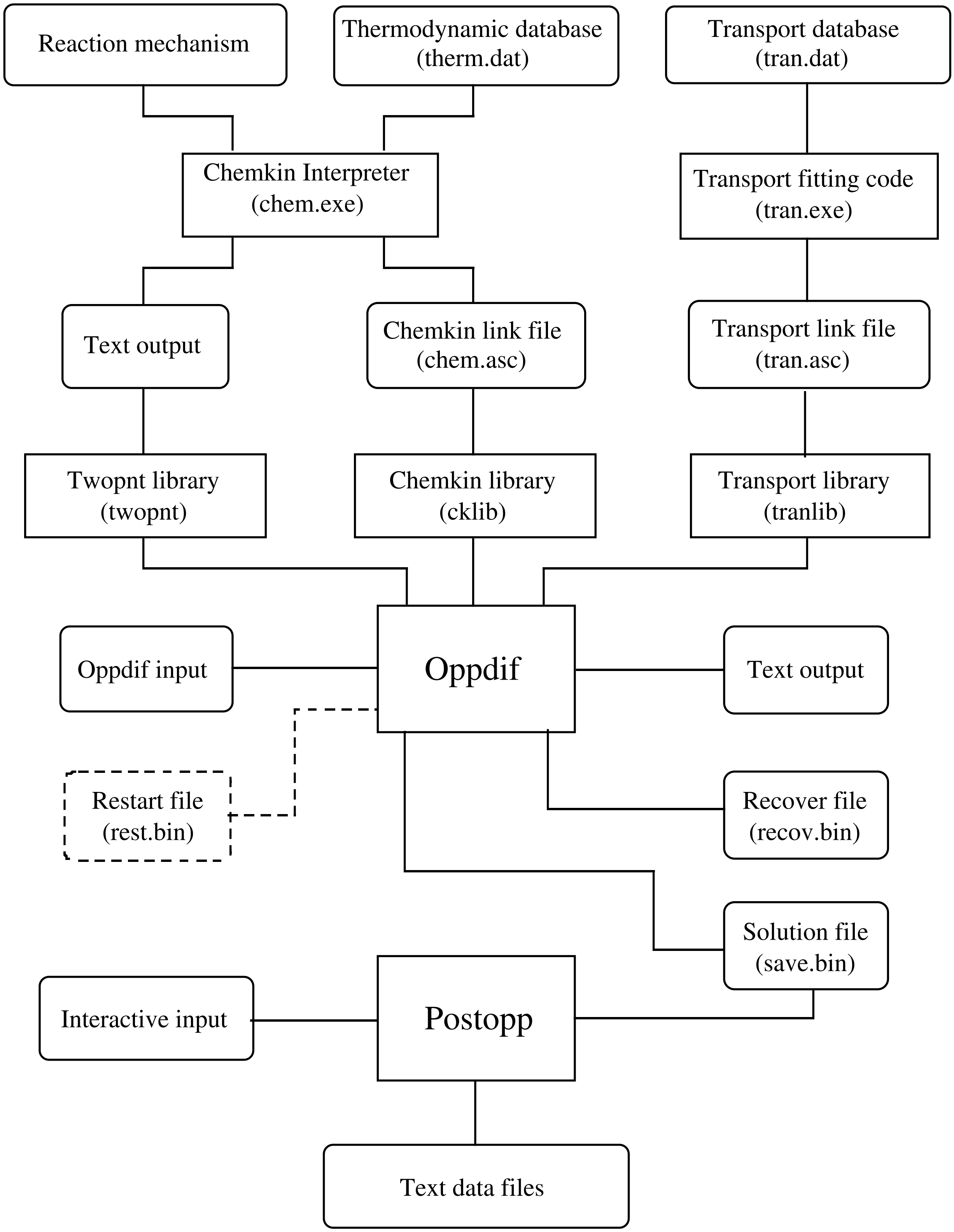

Figure 3. Diagram of Oppdif execution.

where here LENI and LENR can be obtained by a call to the routine MCPNT.

The solutions from Oppdif are then written in the form

```
WRITE (LSAVE) 'SOLUTION'
WRITE (LSAVE) NATJ, JJ, P, AFUEL, AOXID, VFUEL, VOXID
WRITE (LSAVE) ( X(J), J = 1, JJ )
WRITE (LSAVE) ( ( S(N,J), N = 1, NATJ ), J = 1, JJ )
```

The Recover File

The Recover file is the same as the Save file, without the Chemkin and transport linking data; the first record is 'SOLUTION'. The important difference between the Recover and Save files is that the Recover file is updated by Oppdif during time integration, whereas the Save file only receives converged steady-state solutions. If Oppdif should make some progress by time integration, but fail to converge to a steady solution, then you can copy the Recover file to the Restart file, and restart simply by including the RSRT keyword. Depending on why Twopnt quit in its attempt to compute a steady solution, it maybe useful to perform a Regrid when restarting from the Recover solution, as discussed below.

User-modifications

Some parts of the program, such as dimensions and file handling, depend on the machine or problem. To accomodate changes, the programs were written as subroutines to be called by a short "driver" program. Program compilation details are provided in a script or makefile with the software distribution.

Regrid Operation

Using the JJRG keyword invokes a Regrid operation that is useful for changing the number of gridpoints 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 gridpoint 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 where, 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, 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. The redistribution uses a transformation from the physical coordinate x to a new coordinate η,

$$\frac{dx}{d\eta} W(x,T) = C \tag{9}$$

with the weighting function,

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

Integration over the entire domain defines the constant.

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

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

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

The new grid locations x come by interpolation between the computed values of η defined using the old mesh, onto a uniform mesh in η-space. Since $d\eta$ is constant on this uniform mesh, the solution to Eqn. (9) states that $W(x,T) \cdot dx$ is constant, so the new values of x will be concentrated where the weighting function is large.

To direct Oppdif to perform the Regrid operation at restart, include the keywords:

```
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 that `RGTC` be 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.

INPUT

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 card image 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 either integer, floating point, or E format. The program converts the numbers to the proper type, including conversion to double precision if the compiled version of the source code requests double precision.
5. Species names must appear exactly as they are specified in the Chemkin 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. Such a line is ignored by the code, but it is 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.

KEYWORDS

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 denoted by x, n, and c in the list.

Problem Type Keywords

`TGIV` – Energy equation is not included. User specifies a temperature profile using the `TEMP` keyword.

`ENRG` – Energy equation is included.

`NOFT` – Skip the fixed temperature problem and include the energy equation on the first attempt.

`LINE` – Linear profile used to set up initial solution.
Default – `PLAT`

`PLAT` – Plateau profile used to set up initial solution.
Default – `PLAT`

Method Option Keywords

`ATOL` x – Absolute convergence criteria for Newton iteration.
Default – 1.E-9

`RTOL` x – Relative convergence criteria for Newton iteration.
Default – 1.E-4

`ATIM` x – Absolute convergence criteria for time stepping.
Default – 1.E-9

`RTIM` x – Relative convergence criteria for time stepping.
Default – 1.E-4

`TIME` n x – Number of steps and time step for time stepping for the starting procedure.
Default – 50, 1.E-6

`TIM2` n x – Number of steps and time step for time stepping after adding the energy equation.
Default – 50, 1.E-6

`TRAN` n x – Perform timestepping only, without attempting Newton iteration for a steady solution.

`NDPR` x – Increment for output during time integration.
Default – 100 steps

`UFAC` x – Time step increase when time integration proceeds without changing the solution rapidly.
Default – 2.

`DFAC` x – Time step decrease when time integration experiences difficulties.
Default – 2.2

`DTMN` x – Minimum allowable time step.
Default – 1.E-10

`DTMX` x – Maximum allowable time step.
Default – 1.E-4

`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` x – Floor, or minimum, value for the species mass fractions.
Default – -1.E-4

`SPOS` x – Small positive value used to replace negative species upon restart or regridding.
Default – -1.E-10

`GFAC` x – Multiply all reaction rates by x.
Default – 1

`IRET` n – Retirement period for a given time step, or number of time steps prior to increasing the step size.
Default – 50

`ISTP` n – Directs Twopnt to take n time steps before attempting the Newton search for the steady-state solution.
Default – 0

`TJAC` n – Retirement age for the Jacobian during the time integration.
Default – 20

`KOUT` c – Species names for text output.
Default – All species printed

Grid Parameter Keywords

`NPTS` n – Number of initial mesh points. This specification gets overwritten by `GRID` input.
Default – 6

`GRID` x – Location of an initial mesh point.
Units – cm

`GRAD` x – Parameter that controls mesh adaptation on the first gradient in the solution.
Default – 0.1

`CURV` x – Parameter that controls mesh adaptation on the second gradient, or curvature, in the solution.
Default – 0.5

`NADP` n – Number of mesh points that Twopnt can add during each grid refinement.

Default – 10

`XEND` x – Physical length of the grid, or value of x at the end of the domain.
Units – cm

`XCEN` x – Center of the mixing region; used in defining the initial profile for the `LINE` or `PLAT` options.
Units – cm

`WMIX` x – Width of the mixing region; used in defining the initial profile for the `LINE` or `PLAT` options.
Units – cm

<u>Flame Definition Keywords</u>

`VFUE` x – Fuel inlet velocity (at $x = 0$).
Units – cm/s

`VOXI` x – Oxidizer inlet velocity (at $x =$`XEND`).
Units – cm/s

`AFUE` x – Radial gradient in fuel inlet velocity (at $x = 0$).
Units – 1/s
Default – 0.

`AOXI` x – Radial gradient in oxidizer inlet velocity (at $x =$`XEND`).
Units – 1/s
Default – 0.

`TFUE` x – Fuel inlet temperature (at $x = 0$).
Units – Kelvin
Default – 300.

`TOXI` x – Oxidizer inlet temperature (at $x =$`XEND`).
Units – Kelvin
Default – 300.

`TMAX` x – Maximum temperature for use with profiles defined by the `LINE` or `PLAT` options.
Units – Kelvin
Default – 2200.

`PRES` x – The initial pressure of the gas mixture.
Units – atmospheres
Default – 1.

`FUEL` c x – Species name, c, and moles of the 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.
Units – moles or mole fraction.
Default – None, species input is required.

`OXID` c x – Species name, c, and moles of the 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.
Units – moles or mole fraction.
Default – None, species input is required.

`PROD` c x – Species name, c, and moles of the species 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.
Units – moles or mole fraction.
Default – None, species input is required.

`TEMP` x x – Specifies a temperature profile in pairs of grid location and temperature, (x, T).

`USTG` – On a restart, use the given temperature profile, not the temperature solution from the restart file.

Transport Option Keywords

`MULT` – Use the multicomponent formula for diffusion velocities, equation (6).

`MIX` – Use the mixture-averaged formula for diffusion velocities, equation (7).

`TDIF` – Include thermal diffusion in the diffusion velocities.

Printing and Restarting Keywords

`PRNT` n – Integer controls the level of printing and diagnostics from Twopnt. n =0, 1, and 2 provide increasing amounts of output.

`RSTR` – Read a solution from the restart file.

`JJRG` n – Perform a regrid operation on the restart solution prior to attempting to solve the new problem. Use n points for the new mesh. The new grid is adapted to the temperature profile according to the weighting parameters `PCAD` and `RGTC`
Default – 40

`PCAD` x – Specifies the fraction of available mesh points to be used for adapting the mesh to the temperature profile in a regrid operation. Requires $0 \leq x < 1$. If x is zero, then a regrid will produce a uniform grid.
Default – 0.75

`RGTC` x – Specifies the ratio of weighting for adaption to first gradient to curvature (or second derivative) in the temperature profile. Theoretically, there is no limit on this ratio, but values $x \geq 1$ are recommended, because adaption to curvature is usually less important than gradient.
Default – 1.0

`END` – This keyword must appear at the end of the input data.

EXAMPLE

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.

Example 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-LW
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
```

Example 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
```

Example Oppdif Output

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

 OPPDIF:  DOUBLE PRECISION VERSION 4.04 OF MARCH 1997


           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
             SANDIA NATIONAL LABORATORIES
             THERMAL & PLASMA PROCESSES DEPARTMENT 8345
             MS-9042
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          WITH THE ASSISTANCE OF:
             DR. JOSEPH F. GRCAR
             DR. ROBERT J. KEE
             MS. FRAN M. RUPLEY


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

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 OPPDIF:  THE WORK SPACE REQUIREMENTS ARE AS FOLLOWS.

                    CHARACTER    INTEGER    LOGICAL       REAL

             USED          22       2104        103     125065
           EXCESS         178      18396         97    2233935
```

```
    TOTAL        200      20500        200    2359000

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

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 3.27 OF FEBRUARY 1997 BY DR. JOSEPH F. GRCAR.

TWOPNT:  INITIAL GUESS:

 X(cm)      F        V(cm/s)        G          H           T(K)       RHO
 0.00  4.095E-03  1.000E+02 -3.135E-02 -1.000E+02  3.000E+02  8.189E-05
 0.05  2.527E-03  1.209E+02 -3.135E-02 -1.000E+02  7.200E+02  4.179E-05
 0.10  9.599E-04  5.638E+01 -3.135E-02 -1.000E+02  1.140E+03  3.405E-05
 0.25 -3.742E-03 -6.005E+01 -3.135E-02 -1.000E+02  2.400E+03  1.246E-04
 0.50 -1.158E-02 -1.858E+02 -3.135E-02 -1.000E+02  2.400E+03  1.246E-04
 0.75 -1.941E-02 -3.116E+02 -3.135E-02 -1.000E+02  2.400E+03  1.246E-04
 0.90 -2.412E-02 -3.870E+02 -3.135E-02 -1.000E+02  2.400E+03  1.246E-04
 1.00 -2.725E-02 -4.373E+02 -3.135E-02 -1.000E+02  2.400E+03  1.246E-04
 1.10 -3.039E-02 -4.876E+02 -3.135E-02 -1.000E+02  2.400E+03  1.246E-04
 1.25 -3.509E-02 -5.631E+02 -3.135E-02 -1.000E+02  2.400E+03  1.246E-04
 1.50 -4.292E-02 -6.888E+02 -3.135E-02 -1.000E+02  2.400E+03  1.246E-04
 1.75 -5.076E-02 -1.776E+02 -3.135E-02 -1.000E+02  6.000E+02  5.716E-04
 1.90 -5.546E-02 -1.338E+02 -3.135E-02 -1.000E+02  4.200E+02  8.288E-04
 1.95 -5.703E-02 -1.174E+02 -3.135E-02 -1.000E+02  3.600E+02  9.718E-04
 2.00 -5.860E-02 -1.000E+02 -3.135E-02 -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    -0.04    7.83   200 TIME STEPS, 1.0E-04 LAST STRIDE
           SEARCH    -2.45    7.68   6 SEARCH STEPS
```

```
TWOPNT:  FINAL SOLUTION:

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

 X(cm)   H2         O2         H2O
 0.00  9.951E-01  1.382E-09  2.177E-03
 0.05  9.836E-01  5.025E-09  7.456E-03
 0.10  9.581E-01  2.491E-08  1.793E-02
 0.25  7.722E-01  5.211E-07  7.976E-02
 0.50  2.841E-01  2.678E-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  9.027E-07  2.095E-01  5.326E-04
 1.25  6.371E-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 3.27 OF FEBRUARY 1997 BY DR. JOSEPH F. GRCAR.

TWOPNT:  INITIAL GUESS:

 X(cm)     F       V(cm/s)       G        H          T(K)       RHO
 0.00  2.634E-03  6.179E+01  0.000E+00 -3.143E+01  3.000E+02  8.525E-05
 0.05  2.366E-03  1.205E+02 -1.069E-02 -3.143E+01  7.200E+02  3.929E-05
 0.10  1.736E-03  1.150E+02 -1.453E-02 -3.143E+01  1.140E+03  3.018E-05
 0.25 -1.174E-03 -6.870E+01 -2.427E-02 -3.143E+01  2.400E+03  3.417E-05
 0.50 -9.208E-03 -2.079E+02 -4.001E-02 -3.143E+01  2.400E+03  8.860E-05
 0.75 -2.002E-02 -2.942E+02 -4.645E-02 -3.143E+01  2.400E+03  1.361E-04
 0.90 -2.675E-02 -3.696E+02 -4.328E-02 -3.143E+01  2.400E+03  1.447E-04
```

```
 1.00 -3.089E-02 -4.228E+02 -3.958E-02 -3.143E+01  2.400E+03  1.461E-04
 1.10 -3.464E-02 -4.732E+02 -3.552E-02 -3.143E+01  2.400E+03  1.464E-04
 1.25 -3.953E-02 -5.397E+02 -2.957E-02 -3.143E+01  2.400E+03  1.465E-04
 1.50 -4.574E-02 -6.244E+02 -2.013E-02 -3.143E+01  2.400E+03  1.465E-04
 1.75 -5.293E-02 -1.806E+02 -3.739E-02 -3.143E+01  6.000E+02  5.860E-04
 1.90 -5.739E-02 -1.371E+02 -2.217E-02 -3.143E+01  4.200E+02  8.371E-04
 1.95 -5.827E-02 -1.193E+02 -1.300E-02 -3.143E+01  3.600E+02  9.766E-04
 2.00 -5.860E-02 -1.000E+02  0.000E+00 -3.143E+01  3.000E+02  1.172E-03

 X(cm)   H2         O2         H2O
 0.00  9.951E-01  1.382E-09  2.177E-03
 0.05  9.836E-01  5.025E-09  7.456E-03
 0.10  9.581E-01  2.491E-08  1.793E-02
 0.25  7.722E-01  5.211E-07  7.976E-02
 0.50  2.841E-01  2.678E-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  9.027E-07  2.095E-01  5.326E-04
 1.25  6.371E-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   -0.98   10.33   11 SEARCH STEPS

            REFINE    4.10           1.00 AND 1.00 RATIOS, 23 GRID POINTS
            SEARCH           11.22   GOING OUT OF BOUNDS
            EVOLVE    1.42    8.39   200 TIME STEPS, 1.0E-04 LAST STRIDE
            SEARCH   -1.44   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	V(cm/s)	G	H	T(K)	RHO
0.00	4.093E-03	9.997E+01	0.000E+00	-8.103E+00	3.000E+02	8.189E-05
0.05	3.997E-03	9.767E+01	-3.861E-03	-8.103E+00	3.002E+02	8.184E-05
0.08	3.876E-03	9.482E+01	-5.773E-03	-8.103E+00	3.005E+02	8.176E-05
0.10	3.709E-03	9.092E+01	-7.629E-03	-8.103E+00	3.013E+02	8.158E-05
0.14	3.374E-03	8.339E+01	-1.022E-02	-8.103E+00	3.045E+02	8.093E-05
0.17	2.947E-03	7.417E+01	-1.258E-02	-8.103E+00	3.136E+02	7.947E-05
0.21	2.437E-03	6.302E+01	-1.464E-02	-8.103E+00	3.374E+02	7.732E-05
0.25	1.850E-03	4.820E+01	-1.662E-02	-8.103E+00	3.906E+02	7.678E-05
0.31	6.877E-04	1.590E+01	-2.058E-02	-8.103E+00	5.795E+02	8.651E-05
0.38	-6.800E-04	-1.377E+01	-2.318E-02	-8.103E+00	8.878E+02	9.875E-05
0.44	-2.116E-03	-4.044E+01	-2.277E-02	-8.103E+00	1.259E+03	1.046E-04
0.50	-3.498E-03	-6.473E+01	-2.147E-02	-8.103E+00	1.631E+03	1.081E-04
0.56	-4.791E-03	-8.633E+01	-1.991E-02	-8.103E+00	1.964E+03	1.110E-04
0.62	-5.987E-03	-1.041E+02	-1.837E-02	-8.103E+00	2.221E+03	1.151E-04
0.66	-6.552E-03	-1.101E+02	-1.774E-02	-8.103E+00	2.290E+03	1.190E-04
0.69	-7.101E-03	-1.126E+02	-1.742E-02	-8.103E+00	2.283E+03	1.262E-04
0.70	-7.374E-03	-1.113E+02	-1.753E-02	-8.103E+00	2.233E+03	1.325E-04
0.72	-7.651E-03	-1.082E+02	-1.790E-02	-8.103E+00	2.146E+03	1.414E-04
0.73	-7.936E-03	-1.030E+02	-1.858E-02	-8.103E+00	2.019E+03	1.541E-04
0.75	-8.235E-03	-9.560E+01	-1.972E-02	-8.103E+00	1.850E+03	1.723E-04
0.77	-8.626E-03	-8.395E+01	-2.198E-02	-8.103E+00	1.592E+03	2.055E-04
0.79	-9.075E-03	-6.960E+01	-2.590E-02	-8.103E+00	1.283E+03	2.608E-04
0.80	-9.331E-03	-6.179E+01	-2.884E-02	-8.103E+00	1.118E+03	3.020E-04
0.81	-9.620E-03	-5.388E+01	-3.275E-02	-8.103E+00	9.540E+02	3.571E-04
0.81	-9.779E-03	-5.005E+01	-3.511E-02	-8.103E+00	8.751E+02	3.908E-04
0.82	-9.950E-03	-4.638E+01	-3.777E-02	-8.103E+00	8.000E+02	4.290E-04
0.82	-1.013E-02	-4.296E+01	-4.070E-02	-8.103E+00	7.298E+02	4.718E-04
0.82	-1.033E-02	-3.982E+01	-4.388E-02	-8.103E+00	6.655E+02	5.189E-04
0.83	-1.078E-02	-3.453E+01	-5.077E-02	-8.103E+00	5.561E+02	6.242E-04
0.84	-1.128E-02	-3.060E+01	-5.789E-02	-8.103E+00	4.725E+02	7.375E-04
0.86	-1.248E-02	-2.644E+01	-6.972E-02	-8.103E+00	3.709E+02	9.441E-04
0.88	-1.385E-02	-2.567E+01	-7.624E-02	-8.103E+00	3.254E+02	1.079E-03
0.90	-1.530E-02	-2.686E+01	-7.802E-02	-8.103E+00	3.085E+02	1.139E-03
0.93	-1.724E-02	-2.961E+01	-7.723E-02	-8.103E+00	3.019E+02	1.164E-03
0.95	-1.914E-02	-3.272E+01	-7.539E-02	-8.103E+00	3.004E+02	1.170E-03
0.97	-2.100E-02	-3.585E+01	-7.329E-02	-8.103E+00	3.001E+02	1.172E-03
1.00	-2.281E-02	-3.893E+01	-7.114E-02	-8.103E+00	3.000E+02	1.172E-03
1.05	-2.627E-02	-4.482E+01	-6.715E-02	-8.103E+00	3.000E+02	1.172E-03
1.10	-2.952E-02	-5.038E+01	-6.316E-02	-8.103E+00	3.000E+02	1.172E-03
1.18	-3.405E-02	-5.810E+01	-5.747E-02	-8.103E+00	3.000E+02	1.172E-03
1.25	-3.814E-02	-6.509E+01	-5.171E-02	-8.103E+00	3.000E+02	1.172E-03
1.50	-4.915E-02	-8.387E+01	-3.634E-02	-8.103E+00	3.000E+02	1.172E-03
1.75	-5.613E-02	-9.579E+01	-1.950E-02	-8.103E+00	3.000E+02	1.172E-03
1.90	-5.819E-02	-9.931E+01	-8.051E-03	-8.103E+00	3.000E+02	1.172E-03
1.95	-5.850E-02	-9.983E+01	-4.037E-03	-8.103E+00	3.000E+02	1.172E-03
2.00	-5.860E-02	-1.000E+02	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
0.62	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.
```

POSTOPP

Since graphics routines are not portable to all machines, Oppdif does not contain any graphical output. Instead, we provide the user with a text post-processor called Postopp that reads the raw solution and generates text files for plotting purposes. Postopp can read binary files in either the Save or Recover formats.

Postopp is intended to run interactively, using the same kind of keyword input. The specific keywords available for Postopp are printed as a banner when the program is invoked, and there is a help keyword that provides more information.

Postopp writes text files of data in columnar form. One file contains the species fractions requested by the interactive input. A second file contains other solution variables:

1) temperature, T
2) density, ρ
3) fuel mixture fraction: mass of fuel elements (C and H) per mass of mixture
4) velocities: axial, u and radial, v/r
5) strain rates: normal $\partial u/\partial x$ and shear $\partial(-v/r)/\partial x$

This file was used to generate the plots for the example solution shown on the next page.

A third file contains reaction rates, if requested, for a specific species of interest. Postopp 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.

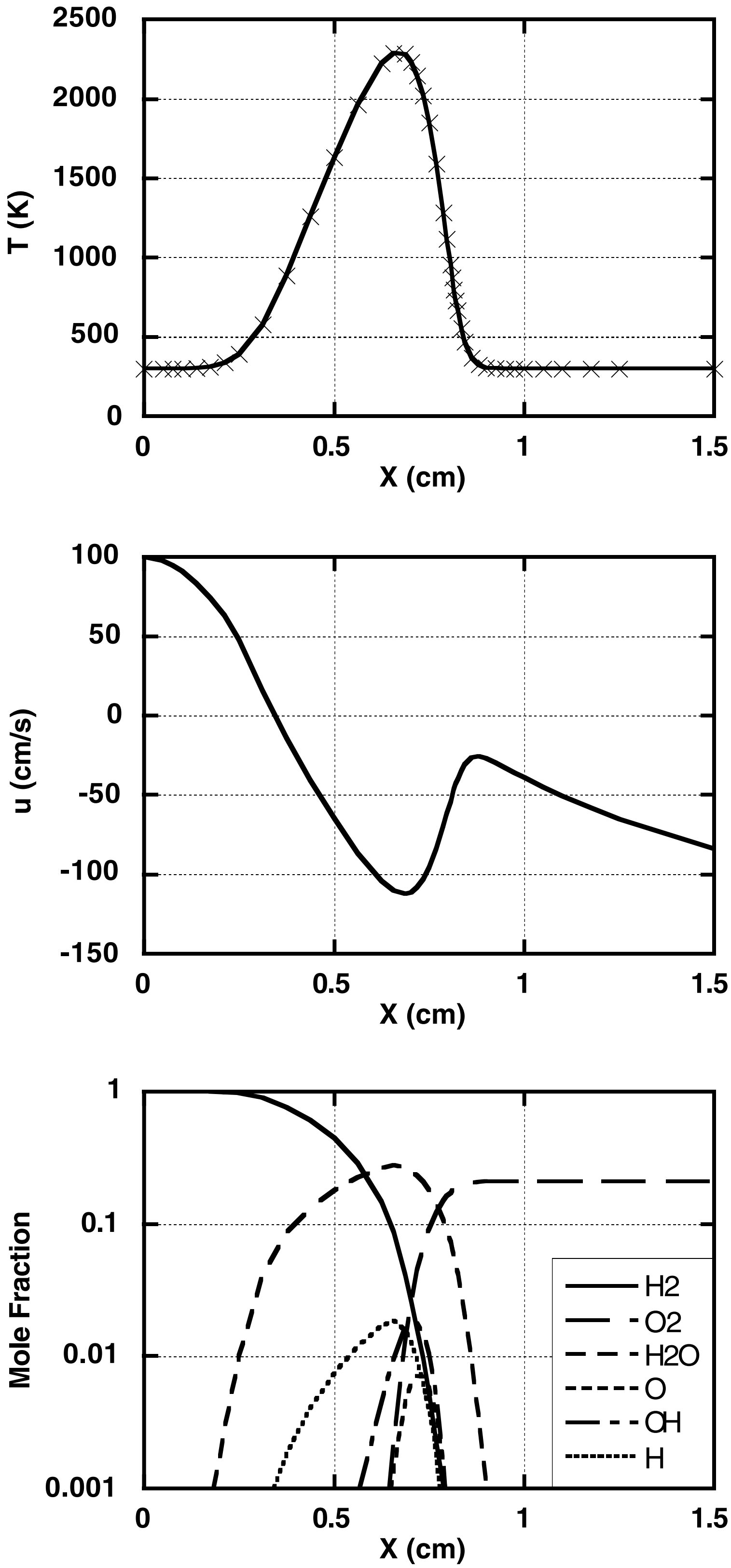

Figure 5. Temperature, velocity, and mole fraction profiles for example H_2-air flame computation. Symbols on the temperature curve denote gridpoint locations.

NUSTART

Nustart is a 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 Nustart:

1) Rename the solution file (`save.bin`) to `oldsave.bin`.
2) Re-run the Chemkin interpreter to create a new binary linking file (`chem.bin`).
3) Execute Nustart, which will create a new solution file: `newsave.bin`.
   Nustart allows you to specify species profiles for new species by reading them from unit 5 until it finds an `END`.
4) Rename the new solution file for Oppdif to use for restart: `rest.bin`

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