Visual DSMC Program for Three-Dimensional Flows

The DS3V Program User's Guide

Version 2.5

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1. The DS3V Implementation of the DSMC Method

The direct simulation Monte Carlo method is a technique for the computer modelling of a real gas by some thousands or millions of simulated molecules. The velocity components and position co-ordinates of these molecules are stored in the computer and are modified with time as the molecules are concurrently followed through representative collisions and boundary interactions in simulated physical space. This direct simulation of the physical processes is in contrast with conventional computational fluid dynamics which seeks to obtain solutions of the mathematical equations that model the processes. The computational task associated with the direct physical simulation becomes feasible when the gas density is sufficiently low. It also becomes necessary under these conditions because the Navier-Stokes equations do not provide a valid model for rarefied gases, and conventional CFD methods are unable to cope with the large number of independent variables that are involved in applications of the Boltzmann equation to realistic multi-dimensional problems.

The degree of rarefaction of a gas flow is generally expressed through the overall Knudsen number, which is the ratio of the mean free path in the undistured stream to a typical dimension of the flowfield. It is desirable to also define the local Knudsen number as the ratio of the local Knudsen number to the scale length of the gradient of a specified macroscopic (or continuum) flow property. The Navier-Stokes equations are valid only when the local Knudsen numbers based on flow speed, density, temperature and pressure are small in comparison with unity. The limit as the Knudsen numbers tend to zero may be identified with the inviscid limit that is modelled by the Euler equations. The opposite limit as the Knudsen number tends to infinity is the collisionless or free-molecule flow limit in which intermolecular collisions may be neglected. The flow regime between free-molecule and the limit of validity of the Navier-Stokes equations is generally referred to as the transition flow regime. A Knudsen number of 0.1 has traditionally been quoted as the boundary between the continuum and transition regimes, but the characteristic dimension of complex flow fields may be specified in many different ways and the use of the overall Knudsen number may be misleading.

The conservation equations of fluid mechanics are valid for all flow regimes, but the Navier-Stokes equations depend also on the Chapman-Enskog theory for the shear stresses, heat fluxes and diffusion velocities as linear functions of the velocity, temperature and concentration gradients. The Chapman-Enskog theory assumes that the velocity distribution is a small perturbation of the equilibrium or Maxwellian distribution. (In an isentropic flow for which the Euler equations are valid, the distribution function conforms everywhere to the Maxwellian). The formulation of the Chapman-Enskog distribution involves the local Knudsen numbers based on the velocity and temperature gradients. It has been found that errors become significant when these local Knudsen numbers exceed 0.1 and the continuum theory is hardly useable when they exceed 0.2. The transport property terms become zero in an isentropic flow and it might be thought that the Euler equation yield correct inviscid flow results at all Knudsen numbers. However, as the density decreases, the collision rate in the gas eventually becomes too low to maintain the isotropy of the pressure tensor. A breakdown parameter can then be defined as the ratio of the density scale time following the fluid element to the mean collision rate. For a steady flow, this parameter can be related to the local Knudsen number based on the density scale length.

Although it was shown many years ago that the Chapman-Enskog expansion for the distribution function is not uniformly valid, attempts are still being made to extend the range of validity of the Navier-Stokes equations to lower densities. However, the low density effects such as the development of an anisotropic pressure tensor are of a very basic nature and it is unlikely that much progress will be made for other than one-dimensional steady flows. In addition, effects such

as thermal and pressure diffusion become more prominent at low densities and these are not generally included in the Navier-Stokes formulations. It is certain that the necessary extensions (in the event that adequate ones can be developed) will add greatly to the difficulty of the continuum approach. On the other hand, once the density becomes sufficiently low for the DSMC solution to be computationally feasible, it is a much easier method to apply. The main reasons for this are:-

(i) The calculation is always unsteady with physical time as one of the principal variables in the simulation. If the flow becomes steady, it is obtained as the large time state of the unsteady flow. The method does not require an initial approximation to the flow field and there is no iterative procedure or convergence to the final solution. (In the case of a time averaged steady flow or an ensemble averaged unsteady flow, there will be a gradual decline in the statistical scatter as the sample increases, but "convergence" is not the appropriate description of this process.)

(ii) Additional effects, such as non-equilibrium chemistry, may be included simply by adding to the complexity of the molecular model and the fact that these may change the basic nature of the mathematical models is of no consequence.

(iii) Most importantly, there are no numerical instabilities!

While personal computers now readily permit DSMC calculations of two-dimensional and axially symmetric flows at overall Knudsen numbers well into the continuum regime, three-dimensional calculations can only just reach the continuum regime.

Note that the Reynolds number *(Re)* is related to the Knudsen number *(Kn)*, the Mach number *M,* and the specific heat ratio γ by

$$(Re) = \frac{16}{5} \left(\frac{\gamma}{2\pi} \right)^{\frac{1}{2}} \frac{M}{(Kn)}.$$

The total number of simulated molecules is limited and, in a three-dimensional calculation at normal and low densities, each simulated molecule must be regarded as representing an extremely large number of real molecules. The macroscopic or continuum flow properties are established through averages over the microscopic or molecular properties and are therefore subject to an unrealistic level of statistical scatter. However, the number of molecules in a cubic mean free path is inversely proportional to the square of the number density. The scatter in a typical DSMC calculation is, in fact, similar to the real scatter in a gas flow at a density of about five times normal or sea-level density. A flow with extremely small physical dimensions may therefore be calculated with a 1:1 correspondence between real and simulated molecules. The DSMC method may be modified to take account of the size of the molecules and the fluctuations in the simulation have then been shown to have the same physical characteristics as the real fluctuations. This has important philosophical consequences in that fluctuations are neglected in the formulation of the Boltzmann equation, so that the DSMC solution has a higher degree of physical realism than a (generally hypothetical) solution of the Boltzmann equation. Fluctuations are included in gas theory only at the level of the Fokker-Planck equations and are, of course, disregarded in the Navier-Stokes equations.

The uncoupling of the molecular motion and collisions over small time steps and the division of the flow field into small cells are the key computational assumptions associated with the DSMC method. The time step should be much less than the mean collision time and a typical cell dimension should be much less than the local mean free path. The cell

dimension should also be small compared with the distance over which there is a significant change in the flow properties. The DSMC method uses the cell system only for the sampling of the macroscopic properties and for the selection of possible collision partners, although the sampled density is used in the procedures for establishing the collision rate. This means that the cell geometry should be chosen to minimise the changes in the macroscopic properties across an individual cell.

A detailed exposition of the method is available in the reference that will be referred to as Bird (1994). However, the DS3V program takes advantage of several important developments in DSMC methodology that have occurred since that time.

Simple implementations of the DSMC method choose the collision partners from any location in the same cell. Later implementations, including those in Bird(1994), employed fixed sub-cells to reduce the spacing of collision partners. The condition relating to the cell size relative to the mean free path then applies to the sub-cell size, rather than to the cell size. The most recent programs, including the later versions of the DS2V program, employ separate cell systems for the sampling of flow properties and collisions. The first molecule for a potential collision is chosen at random from a collision cell. If the number of molecules in the cell is less than 30, the nearest molecule is chosen as the potential collision partner. For larger numbers, a transient rectangular background grid is generated and the molecules are indexed to this transient grid. The size of the background grid is such there is approximately one simulated molecule within each grid element. The transient sub-cell in which it lies is determined from the indexing and, if there is more than one molecule in the sub-cell, the collision partner is chosen from these. The ratio of the mean separation between collision partners to the local mean free path is output by the program and should be small (say 0.2) compared with unity over the flowfield. The nearest-neighbor procedures ensure that the lowest possible values of this ratio are achieved. Further reductions can be obtained only by an increase in the total number of simulated molecules.

A problem with nearest neighbour collisions is that, if the interval between collisions happens to be very small, a subsequent collision may involve the same collision pair. This is unphysical because molecules are always moving away from one-another after a collision. The program stores the code number of the immediately preceding collision partner for each molecule and this molecule is not allowed to be the next collision partner. It has been found that this avoids an error in the heat transfer and shear stress that can be as high as four or five percent.

The only computational parameter that must be set by the user in Version 2 is the initial number of megabytes to be used for storage. All other computational variables are set automatically by the program. However, there is an optional menu that allows experienced users to increase or decrease the default values of cell size, time step etc.

The traditional specification of a single value of this time step over the whole flowfield is computationally inefficient, particularly for supersonic and hypersonic flows. This is because a value that is small in comparison with the mean collision time in the stagnation region is extremely small in comparison with the collision time in the outer regions of the flow. This problem is avoided by new procedures that make the time step vary with every molecule as well as with every cell. To this end, separate time variables are associated with every molecule and every cell. The procedures keep all these variables concurrent with the overall time variable.

The overall time variable is advanced in very small time steps, but only a small fraction of the molecules are moved and collisions are calculated in only a small fraction of the cells at any one time step. The mean collision time is kept for each cell and collisions in a cell appropriate to a time interval of approximately one fifth the local mean collision time are calculated whenever the cell time variable falls one tenth of the local mean collision time behind the overall flow time.

Similarly, a molecule will generally be moved through a time interval of one fifth the mean collision time of its current cell when its time variable falls one tenth this local mean collision time behind the overall flow time. However, the logic can often be simplified if there is a molecule velocity dependent restriction that limits the distance that a molecule can move in a single step. The step set by the local collision time is then the maximum value of the time step.

Because of the very small overall time step and the small number of cells for which collisions are calculated at each step, the implementation of the traditional indexing routine at each step would involve a prohibitive computational effort. This problem has been solved through the introduction of "bi-directional" indexing. The traditional index array is comprised of the molecule numbers in order of the cells. If the address of the corresponding entry in this array is stored for each molecule, the indexing may be kept up to date continuously as molecules move from cell to cell. The index array must also be extended with sufficient free space between cells to cope with the fluctuations in the number of molecules in individual cells. Some general rearrangement takes place from time to time to allow for particularly large fluctuations or systematic changes in the distribution of molecules. In many other procedures, the ability to assign different times to molecules leads to a simplification of the program.

The new procedures are computationally faster than the traditional procedures but, because of the data structures necessitated by the continuous indexing, the number of simulated molecules that can be employed for a given amount of memory is reduced. Because of the automatic setting of the time step, it is no longer possible for this to be incorrectly specified. The nearest-neighbor minimize the errors that may be introduced by the incorrect setting of cell size. A poor calculation can be made if the total number of simulated molecule is too small. This may cause the mean separation of collision partners to exceed the local free path in significant areas of the flowfield, but the output enables this to be readily monitored.

Reference
BIRD, G.A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press, 1994.

2 The Scope of the DS3V Program

2.1 Geometry and Boundary Conditions

The flowfield limits are specified by the minimum and maximum values of the *x, y* and *z* co-ordinates. These six boundaries may be stream boundaries, planes of symmetry, vacuum boundaries or periodic boundaries. This basically rectangular flowfield may be modified by the definition of one or more separate "surfaces". Each of these must be either a closed surface or an open surface that starts and finishes on a boundary of the basic rectangular parallelepiped. Each surface is specified by a set of triangular elements in an externally generated surface definition file. As with the DS2V program, each of the surfaces may be a combination of solid surface triangles and specified flow input triangles. The surface definition triangles also form the sampling elements on solid surfaces. This means that many triangular elements are generally required even on a simple flat surface. **The production of this file generally requires a program separate to and in addition to the DS3V program.** Each surface may be set to move in its plane or, with some restrictions, normal to it.

The flow input boundaries permit the study of a wide range of problems that involve jets and plumes. A secondary stream may be set to occupy part of the initial flowfield and this permits the

study of unsteady shock tube type flows and shear flows. Alternatively, shock waves may be generated by a moving "piston" type boundary for diffraction studies. Special "constant pressure" boundaries are available for the generation of steady internal flows that are unaffected by the boundary conditions. Periodic boundary conditions are also available. These features have been carried forward from the DS2V program and may need to be generalized to cover some 3-D flows.

The upstream region of a three-dimensional flow is frequently two-dimensional or axially symmetric. Starting with version 2.3 it is possible to combine DS2V and DS3V runs through molecule file output/input options. These procedures automatically allow for the width of the three-dimensional flow and differences in time-scale. It is possible for a number of copies of axially symmetric file molecules to enter a three-dimensional flow with various translations and rotations of the molecules. For example, a study may be made of the impact of multiple control jet plumes on a three-dimensional satellite model The molecule files can also connect two DS2V or two DS3V calculations. A molecule file may also be produce from the molecules crossing a specified plane in a DS3V calculation. The molecules from this file may be replayed into a separate DS3V calculation.

The flowfield grid consists of a background rectangular grid that is uniformly spaced in each of the three directions. Every "division" of this grid is divided into a finer grid of "elements", typically several hundred elements in each division. Solid surfaces must not be thinner than an element. The flowfield cells are defined by cell nodes that are initially set to the centers of the divisions and the points at the center of the surface definition triangles. The cell associated with a given node is comprised of the elements that are closer to that node than to any other. At any stage of the calculation, a new set of nodes may be adaped to the flow density and density gradients in order to set new cells with a specified number of simulated molecules in each cell.

2.2 Gas Specification and Model

The gas may be chosen from a menu that includes ideal air, real air with vibration and chemical reactions, nitrogen, argon and a hard sphere gas. Alternatively, a custom non-reacting or reacting gas may be specified.

The program employs the physical gas models that have been described and validated in Bird (1994). The gas is a mixture of the VHS models and the cross-sections, the viscosity-temperature index (which determines the way in which the cross-section changes with the relative velocity), are set separately for every molecular species. A classical Larsen-Borgnakke model is employed for the rotational degrees of freedom, while a quantum model is used for the vibrational modes. The chemical reaction model calculates reactive cross-sections that are consistent with the measured rate constants.

The classical diffuse reflection model with complete accommodation of the gas to the surface temperature is appropriate to "engineering surfaces" that have not been exposed for a long period to ultra-high vacuum. A set temperature distribution may be specified for the surface or it may be specified as an adiabatic surface with zero heat transfer. In the latter case, the temperature distribution on the surface is one of the output quantities. Alternatively, the other "classical" model of specular reflection may be specified for the artificial case of complete slip and no energy transfer at the surface. Partial accommodation may be modelled by a diffuse reflection with a specified fraction of specular reflection..

2.3 Parallel Operation

Starting with version 2.2, the program allows parallel operation on dual-core computers and this feature can be tested on a single core CPU. The process is largely transparent to the user who needs to set just one additional data item when parallel operation is selected. Domain decomposition is employed in a shared memory mode. The maximum number of domains will be increased to keep pace with the introduction of multi-core processors. Dual-core operation leads to an overall increase in computational speed of about 50% and it is hoped that, as the number of cores increase, the speed increase per core will be relatively higher. A surface triangle can spread over the domain boundary and the parallelization does not have to be taken into account in the DS3SD.DAT file.

3   Computer Requirements and Program Installation

(i)   The program requires Windows 98 or higher.

(ii)   A 2 GHz Pentium™ processor or higher is recommended.

(iii)   500+ MB RAM is required for the program to run efficiently.

(iv)   The program runs in an XGA (1024 x 768) window.

Windows 98 required "small fonts" to be specified in order for the DS2V windows to be sized and positioned correctly. With XP, it is essential that the "DPI setting" be set to "Normal size (96 DPI)". This is accessed through Control Panel -> Display -> Settings -> Advanced -> General.

The program is delivered as the compressed executable **DS3VZ.EXE**. This is run to produce the uncompressed executable **DS3V.EXE** of the main program and the program **DS3DG.EXE** for the generation of the surface data file. These files should be placed in separate directories. It also produces sample data files **DS3SD.DAT** and **DS3VD.DAT** that should be placed in the directory with DS3V.EXE and the sample triangle file **DS3TD.DAT** that should be placed in the directory with DS3DG.EXE.

4   The Geometry Definition File DS3SD.DAT

Version 2 introduces additional options but DS3SD.DAT files that were prepared for Version 1 remain valid if an additional line containing the integer 1 is added as the first line.

The first items in the file are now the version numbers and future programs will be backwardly compatible as far as the data files are concerned.

This file must be prepared independently of the DS3V program and must take into account the following conventions that relate to the DS3V geometry:-

(i) The coordinate system is such that with x to the right and y to the top of a sheet, z is up from the sheet

(ii) The order of the points that define each triangular element must be anticlockwise when looking from OUTSIDE the surface.

**(iii) Open surfaces must terminate on the faces of the bounding parallelepiped.
Faces 1,2 are at XMIN,XMAX; Faces 3,4 are at YMIN,YMAX; Faces 5,6 are at ZMIN,ZMAX**

The specification of the data file is as follows (comments are preceded by !) :-


```
!--NVERS the n in version n.m that creared the data file
!--MVERS the m in version n.m that creared the data file (only if NVERS > 1)
!
!--NSURF the number of unconnected surfaces
!----each surface must be either open or closed
!------every side of a closed surface must connect with just one side of another triangle
!------every side of an open surface must either connect with just one side of another
!    triangle or may terminate on a face of the computational region, in the latter case
!    the sides must form a closed line on the six faces the copmputational region
!
!--in a first loop (N) over NSURF
!----NPNT(N) the number of points that define surface N
!----NTRIS(N) the number of solid surface triangles on surface N
!----NTRIF(N) the number of flow entry triangles on surface N
!----NTRIC(N) the number of periodic boundary triangles on surface N        !added 1.2.02
!--end first loop over N
!--in a second loop (N) over NSURF
!----in a loop (M) over NPNT(N)
!------XS(M),YS(M),ZS(M) coordinates of point M
!----end of loop over points
!----in a loop M over the triangles (sum of NTRIS(N),NTRIF(N) and NTRIC(N))
!------ISEGI(1,M),ISEGI(2,M),ISEGI(3,M) the point numbers of the three vertices
!    the order must be anti-clockwise when viewed from the flow (outside)
!------ITYPS 0 if the triangle has the same properties as the preceding triangle
!        1 if the triangle is a solid surface with species independent properties
!        2 if it is a solid surface with species dependent properties
!          (an outgassing surface must be type 2)
!        3 if it is a gas entry boundary with specified properties
!        4 if it is a stream entry boundary
!        5 if it is a periodic boundary (such a boundary must be in a plane y=az)
!------if ITYPS = 1 (solid surface)
!--------TSURF if +ve, surface temperature for diffuse or CLL reflection
!        if -ve,diffuse or CLL adiabatic with the absolute value as the minimum temperature
!        if 0.0 generates the temperature of a perfectly (thermal) conducting surface that
!            extends over all triangles in the same (ITYPS=0) group
!    if diffuse adiabatic, (-ve or zero TSURF)
!    if the triangle is part of an adiabatic surface
!     if perfectly conducting
!------------TCAP thermal capacitance of the whole body defined by the surface
!     end if
!     EMISS  the surface emissivity
!    end if
!--------in a loop (K) over 1 for ITYPS=1 the number of species MSP for ITYPS=2
!     IRFM(K) 0,1 for diffuse, CLL model
!----------if IRFM(K) = 1
!------------EACN(K) the normal energy accommodation coefficient
!------------TMAC(K) the tangential momentum accommodation coefficient
```
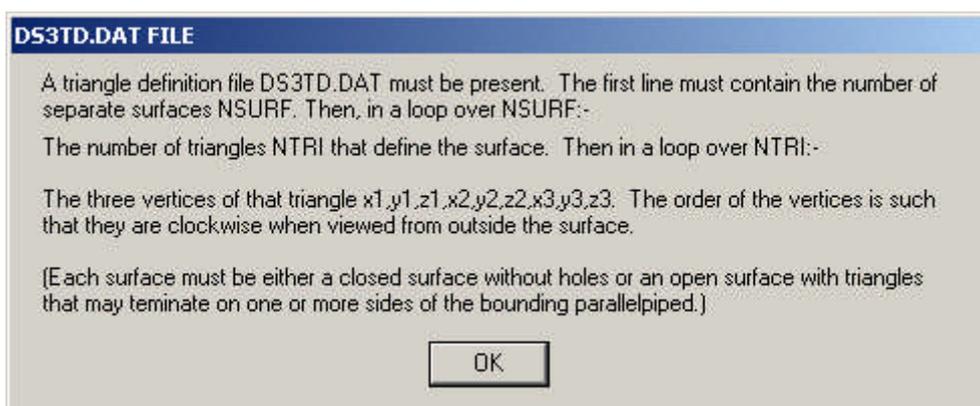
!----------end if
!----------ROTAC(K) rotational accommodation coefficient
!----------if MMVM > 0
!------------VIBAC(K) vibrational accommodation coefficient
!----------end if
!----------FRSPEC(K) fraction specular
!----------FRSORB(K) fraction adsorbed
!----------if ITYPS=2 OUTGMF(K) the outgas mass flux
!--------end of loop over 1 or MSP
!--------if MNSR > 0
!----------in a loop (K) over the number of surface reactions MNSR
!------------PROBSR(K) the probability of the surface reaction
!----------end of loop over MNSR
!--------end if
!--------the in-plane velocity component in direction 1   !--added 1.2.02
!--------the in-plane velocity component in direction 2   !--added 1.2.02
!------end if
!------if ITYPS = 3 (gas entry triangle)
!--------XVEL the velocity component in the x direction
!--------YVEL the velocity component in the y direction
!--------ZVEL the velocity component in the z direction
!--------EFTMP the flow temperature
!--------EFDEN the number density of the flow
!--------in a loop over the number of species L=1,MSP
!----------EFSP(L) the fraction of species L
!--------end of loop over species
!------end if
!------if ITYPS = 4 (periodic boundary)
!--------BANG the angle (about the x axis such that y=tan(BANG)*z of the plane
!--------TANG the similar angle of the matching plane
!------end if
!----end of the loop over the triangles
!--end of second loop over the surfaces

There is now a program DS3DG.EXE that employs menus similar to those in the DS2V and DS3V programs to convert a "raw triangle" file to this specification.

5   The Surface Data Generation Program DS3DG.EXE

The "raw triangle" format for a surface consists of a single line for each triangle. Each line contains nine floating point numbers that represent the x, y and z coordinates of the three vertices. The ordering of the vertices must be such that they are in *anticlockwise* order when viewed from *outside* the surface. This is one of the output options that are available in surface modeling programs such a Rhinoceros (www.rhino3d.com).

There may be more than one surface in a problem and the raw triangle files must be combined to produce the file DS3TD.DAT. The specification of this file is:-

!--NSURF the number of unconnected surfaces
(Each surface must be either open or closed. Every side of a closed surface must connect with just one side of another triangle. Every side of an open surface must either connect with just one side of another triangle or may terminate on a face of

the computational region. In the latter case, the sides must form a closed line on the six faces the computational region.)
!
!--in a loop (N) over NSURF
!----NTRI(N) the number of triangles on surface N
!
!----The "raw triangle" file for the surface i.e.
!
!----in a loop (M) over NTRI(N)
!
!------ISEGI(1,M),ISEGI(2,M),ISEGI(3,M) the point numbers of the three vertices
!   the order must be anti-clockwise when viewed from the flow (outside)
!
!----end loop over M
!
!--end loop over N

The first dialog that appears when the DS3DG.EXE file is run is an introductory dialog to remind the user that a DS3TD.DAT file must be present.

DS3TD.DAT FILE

A triangle definition file DS3TD.DAT must be present. The first line must contain the number of separate surfaces NSURF. Then, in a loop over NSURF:-

The number of triangles NTRI that define the surface. Then in a loop over NTRI:-

The three vertices of that triangle x1,y1,z1,x2,y2,z2,x3,y3,z3. The order of the vertices is such that they are clockwise when viewed from outside the surface.

(Each surface must be either a closed surface without holes or an open surface with triangles that may teminate on one or more sides of the bounding parallelpiped.)

OK

All the data (including that in the DS3TD.DAT file) must be in either SI or Engineering (US) units. If the latter, the values are automatically converted to the SI units that are mandatory for the DS3SD.DAT file.

Input Units

Units for Data Entry

Metric (SI)   Eng (US)

OK
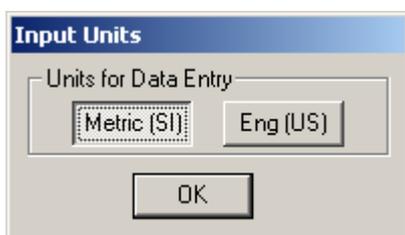
Some of the data may be species dependent, depend on whether any species have vibrational modes, or relate to optional surface reactions. The values in the following menu must be consistent with those in the DS3VD.EXE file,
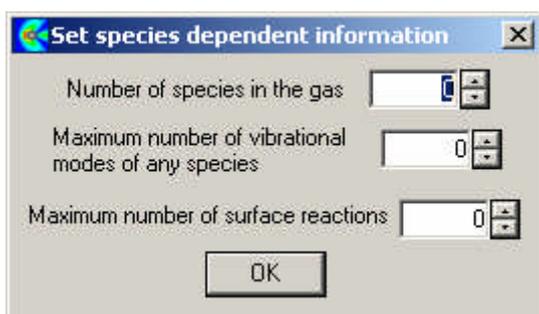
The program must be able to determine the number of distinct points that comprise the vertices of the triangles. The next dialog sets the number such that the points are distinct if they are separated by a distance that is greater than this number. Note that a typical dimension can vary by many orders of magnitude and that the coordinates in DS3DT.DAT may be single or double precision.
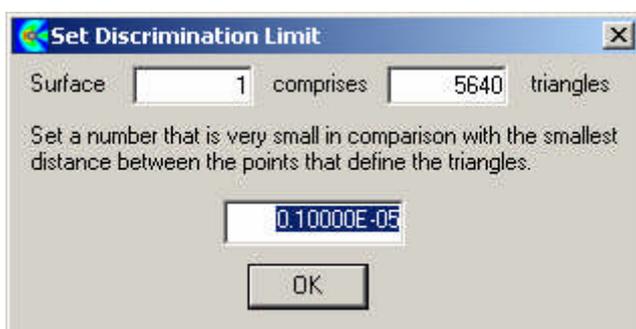
The program then determines the number of distinct points associated with the triangles, assigns numbers to the points and defines each triangle in terms of the point numbers of its vertices. The user is then asked to set the type of each triangle.

 There may be thousands of triangles on a surface and it is essential to take advantage of the fact that a given set of properties generally apply to more than one triangle on a surface and hopefully to all of them. The first menu for the setting of the surface properties allows the specification of the number of following (in numerical order) triangles that share the properties of the triangle that is being set.

Type of next Triangle or Group of Triangles

Triangle [1] of [5000] with Vertices at:-

-.4997500E-03	0.8000000E-04	0.1570500E-04
-.5000000E-03	0.8000000E-04	0.000000
-.5000000E-03	0.000000	0.000000

Solid surface triangle with species-independent properties (cannot be an outgassing surface)

Solid surface triangle with species-dependent properties

Stream Entry Triangle

Specified Flow Entry Triangle

Periodic Boundary Triangle

The number of additional (following) triangles that share these properties. [2]

OK

Solid surface intervals with species-independent properties
This choice brings up a menu to set the properties for this group.

Properties of Solid Surface Intervals

Reflection at a Uniform Set Temperature   Zero Heat Transfer (Adiabatic) Surface

Surface Temperature [300.00] K.

This is the minimum temperature in the case of an insulated adiabatic (zero heat transfer) surface. Set it to zero to generate the temperature of an adiabatic perfectly (thermal) conducting surface.

Emissivity - (Set only for an adiabatic surface) [0.0000]

Thermal Capacitance - (Assumes a perfectly conducting "adiabatic" body) (J/deg K) [0.0000]

A finite thermal capacitance should be set only for a closed surface that describes a nano-particle that is subject only to convective fluctuations with a one-to-one correspondence between real and simulated molecules.

The temperature history of the nano-particle is output in the file PTEMP.TXT.

In-plane velocity component in direction 1 (m/s) [0.0000]

In-plane velocity component in direction 2 (m/s) [0.0000]

Direction 1 is normal to the x axis or, if the triangle itself is normal to the x axis, in the y direction. Direction 2 is also in the plane of the surface and is normal to direction 1.

OK

Reflection at a Set Temperature
The molecules that are reflected according to the gas surface interaction to be specified later at the temperature that is specied below .

Zero Heat Transfer (Adiabatic) Surface
The incident heat transfer to the surface is calculated on a progressive basis and the surface temperature is adjusted such that there is net heat transfer to the surface. This is commonly referred to as an "adiabatic surface" and the adiabatic surface temperature appears as one of the options for the surface distribution output.

Surface Temperature
The surface temperature for molecular reflection or the minimum allowable surface temperature if the adiabatic option has been chosen and the surface is insulated (zero thermal conductivity). However, if this is set to zero, the surface is assumed to have infinite thermal conductivity such that the whole surface comes to a uniform temperature with no net heat transsfer to the surface as a whole.

Emissivity
This need be set only for adiabatic surfaces so that thermal radiation is taken into account in calculating the temperature for zero heat transfer.

Thermal Capacitance
This should be set only for the infinite conductivity case and is the heat reqired to raise the temperature of the body defined by the surface surface through one degree. Note that this option should be used only in the context of nanoparticles and a file of the nanoparticle temperature history is produced.

In-Plane Velocity in diretion 1
The surface moves in its own plane in a direction normal to the x axis or, if the triangle is normal to the x axis, in the y direction. This has effect only on the molecules are reflected diffusely.

In-Plane Velocity in diretion 2
The surface moves in its own plane in a direction normal to direction 1. This has effect only on the molecules are reflected diffusely

Diffuse Reflection
The classical diffuse reflection model is employed with full accommodation of the translational energy to the temperature that was defined earlier.

CLL reflection model
This model (see Reference) can provide a realistic model of the reflection processes that occur on extremely clean surfaces. It also employs the temperature that was defined earlier and requires the definition of the

Normal energy accommodation coefficient
and the
Tangential momentum accommodation coefficient
A major problem is that very little information is available on when this model should be used and the values of these coefficients that should be employed if it is used.

Rotational accommodation coefficient
Irrespective of the model that is used for the gas-surface interaction of the translational modes, the fraction accommodation of any rotational modes may be set.

Vibrational accommodation coefficient
Similarly for any vibrational modes.

Fraction of specular reflection

A combination of specified fractions of specular and diffuse reflection has often been used to provide an indication of non-diffuse effects. It is now recommended that the CLL model be used for this purpose. Full specular reflection can be used make a surface a plane of symmetry or to make an "inviscid" flow calculation.

Fraction adsorbed at surface

The specified fraction of molecules that strike the surface are removed from the calculation.

Outgas Mass Flux

This option should only be used when there is separate input for each molecular species.

The following dialog appears if any surface reactions have been defined.

Probability of surface reaction number

Up to 18 surface reactions were defined earlier. This is the probability when one of the incident molecules strikes the surface. If two are required, the other is removed later.

Solid surface intervals with species-dependent properties

This choice brings up similar menus to the species-independent choice, except that the dialog **Gas-surface interaction for this group** is repeated for each molecular species. Also, it is possible to set the

Outgas mass flux

This is set separately for each species.   The outgassed molecules are generated as if they were effusing from the surface at the temperature of the surface.

Stream entry intervals

The surface is a flow entry surface and is commonly used to cut off a region of flow that is undisturbed freestream flow.
No additional data is required.

Specified flow entry triangles

The items in this menu are self explanatory.

Molecule File Entry Triangle

This is a triangle at which molecules enter from the file DSMIF.DAT. The area defined by the triangles must be consistent with the geometry associated with the generation of the DS2MIF.DAT file that has been manually renamed DSMIF.DAT. The following dialog appears during the run when the flow is being set up.

Number of molecules in each record and
Number of records in the file
These much match the values when the DSMOF was generated in the DS2V program.

The two real variables set the location and extent of the tw0-dimensional or axially symmetric molecule file in the three-dimensional flow.

6   Running the DS3V Program

Running DS3V produces the **Run Type** window that contains six push button style radio buttons and an **OK** button to move on when the desired button has been selected.
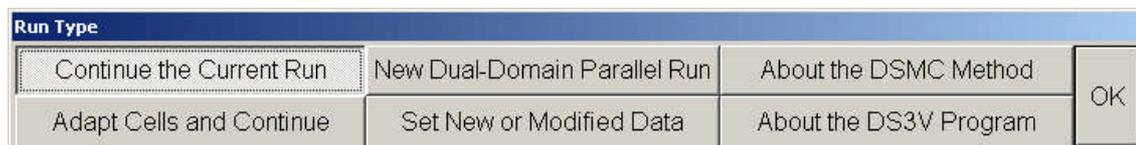
Continue the Current Run
This is the pre-selected button, but is valid only when a calculation has been stopped after it had reached the stage at which the flow and surface property displays are displayed. Restart files are written every time the "print-out" stage is reached. The selection of this option causes the last set of restart files to be read and re-starts the run from that flow time.
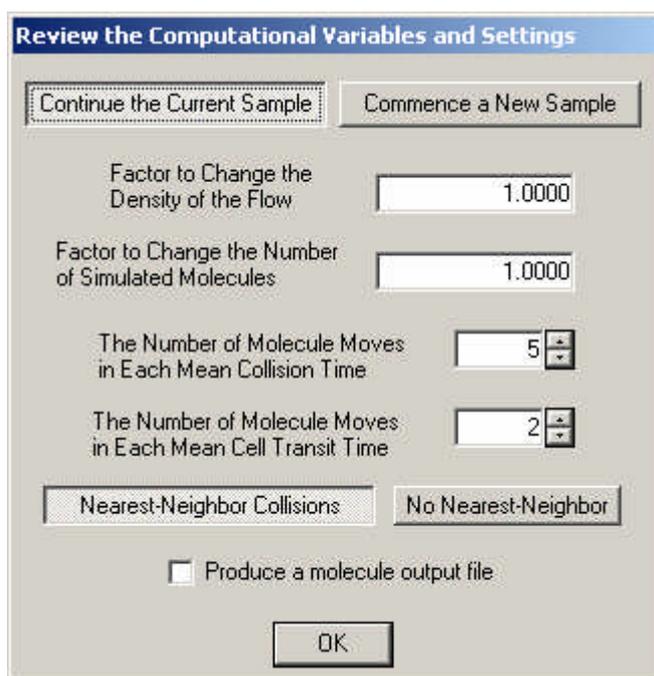
Continue the Current Sample
This and the following option is applicable only when the flow is assumed to become steady at large times and the specified time at which time averaging is to commence had been reached in the earlier calculation. This option continues the existing time average.

Commence a New Sample
Resets the sampling variables so that a new time-averaged sample commences from the restart. This option is useful when the specified time to steady flow proves to be inadequate. In addition, it should be applied when the flow has settled down after a change in gas density or a change in the number of

simulated molecules. The program resets the sample automatically if the fluctuating number of simulated molecule changes by more than eight standard deviations.

Factor to Change the Density of the Flow

Most calculations start from an initially uniform flow and, at low Knudsen numbers, the computational time to steady flow may be very large. It is generally more efficient to establish steady flow at a higher Knudsen number and then increase the density of the flow. This option is particularly useful when a number of cases are to be calculated at gradually decreasing Knudsen numbers.

Factor to Change the Number of Molecules

Another strategy to decrease the computational effort for eventually steady flows is to employ a relatively small number of simulated molecules at the start of the calculation and to increase the number when steady flow is nearly attained. This option changes the number of real molecules that are represented by each simulated molecule. The initial number should not be so low that the criteria for a good DSMC calculation are violated by such large margins that the initial flow is unrepresentative of the real flow. In general, the increase will not be greater than a factor of about three. The option may also be used to reduce the number of simulated molecules if it appears that the eventual number will be beyond the memory capacity of the computer.

The Number of Molecule Moves in Each Mean Collision Time

One of the criteria for a good DSMC calculation is that the time step over which the molecule moves and collisions are uncoupled should be much smaller than the mean collision time. This can lead to prohibitive computation times for flows with large variations in the collision time if a fixed time step is used. The D3V program employs a variable time step that is a fixed fraction of the local mean collision time. Four or five moves in each mean collision time is usually adequate, although some systematic changes have been observed to a ratio of nine in some flows. The ratio is set in the data and this option provides an opportunity to vary it later in the calculation. The program logic sets internal limits on the time step and the actual ratio that appears in the output screen will generally be somewhat higher than the value set in the data.

The Number of Molecule Moves in a Cell Transit Time

If the Knudsen number is high, the time step set by the collision rate may be too large. This data item sets the maximum time step to a fraction of the time for a typical molecule to transit the cell. The recommended value of this parameter is two.

Nearest-Neighbor Collisions

This is the default option and should be accepted. The these procedures minimize the separation distances between the molecule pairs chosen as potential collision partners

No Nearest-Neighbor

The transient sub-cells may have been disabled to speed up a program or to investigate the effect of the sub cells. The program should normally be run with transient sub-cells and this option would rarely be chosen.

Produce a molecule output file

If this button is checked, a molecule output file DSMOF.DAT will be produced after the restart. The following menu then appears

The items to be set in this menu are similar to those for the generation of molecule files in DS2V. The program should not be stopped until the file is complete and, by checking the box, the program may be made to close automatically when the file is complete.

A DSMOF.DAT file that is generated by DS3V may be renamed DSMIF.DAT and read into a separate DS3V run. It cannot be read into a DS2V run.

New Dual-Domain Parallel Run

This option is intended for use on dual-core processors. It brings up the following sub-menu.
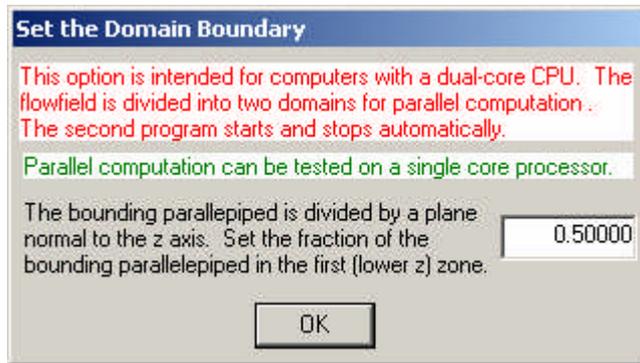
> The two domains are separated by a plane of constant z. The single data item sets the fraction of the bounding parallepiped that is in domain 1.
>
> Following this menu, the program transfers to **Set New or Modified Data**

About the DSMC method

This option brings up an information screen on the DSMC method and a "Frequently Asked Questions" screen on the method can be called from this. The program then returns to the **Initial Options** menu.

Adapt the Cells and Continue

Continues the current run with cells adapted to the density in the current flowfield sample. When selected, the user is asked to supply the desired number of simulated molecules in each of the new cells. Separate adaptions are made are made for the collision cells and sampling cells. The collision cells are adapted first and acceptance of the default eight molecules per collision cell is recommended.
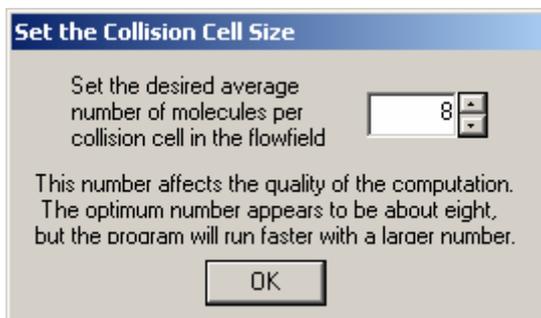
A plot of the new cells appears in a new window when the adaption is complete and the window should be closed for the computation to proceed. The sampling cell dialog then appears with a recommended number that depends on the magnitude of the calculation.
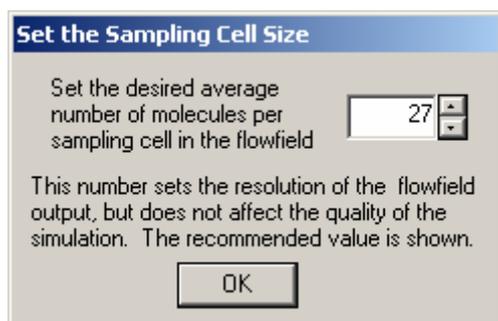
A plot again appears and this window should be closed for the calculation to proceed. An information dialog appears when the flow is ready to restart using the new cells.

In the case of flows that become steady, the option will normally be chosen after a substantial sample has been built up. However it can be selected any number of times and can be used for flows that remain unsteady.

IF THE PROGRAM STOPS WITH OR WITHOUT A DIAGNOSTIC WINDOW EXAMINE THE FILE DIAG.TXT FOR MESSAGES AND EXPLANATION.

A number of additional files are generated during the problem set-up phase. These are mainly for diagnostic purposes.

Set New or Modified Data
This option allows a new calculation to be specified. If there is no valid data file on the computer, it must be selected before a calculation can be made. The following dialog with three choices then appears:

Generate Completely New Data
Selection of this button asks for a choice of input units.
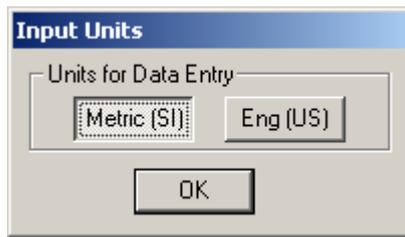
SI units are recommended. The program is rarely used with engineering units, so please report any errors. The program then moves straight to the data input dialogs of Section 5.

Modify the Existing Data Set
The user may choose to modify an existing **DS3VD.DAT** file. Should an "end of file" be encountered when modifying an existing file, the program automatically switches to the "new file" mode. The details of the input menu windows are described in Section 6.

New Run with Existing Data
There must, of course, be existing DS3VD.DAT and DS3SD.DAT files and this starts a new run from zero time.

About the DSMC method

This option brings up an information screen on the DS3V program and a "Frequently Asked Questions" screen on the program can be called from this. The program then returns to the **Initial Options** menu.

7. Data Input Dialogs

Initial Magnitude of the Computation

The computational variables will be set automatically by the program to values that are appropriate to the following number of megabytes.

[20] Mb

The number of simulated moleculesmay increase during the computation and the eventual memory requirements may be significantly higher than this value. If necessary, all available memory will be automatically allocated to the program.

OK

Flow Computation Region

The "bounding parallelepiped" of the flow must be defined. Each side of the parallelepiped may be a plane of symmetry, a stream boundary or interface, a vacuum interface, or may be partially or fully cut off by solid or stream surfaces.

Minimum x coordinate	-.500000	metres
Maximum x coordinate	0.500000	metres
Minimum y coordinate	-.500000	metres
Maximum y coordinate	0.500000	metres
Minimum z coordinate	-.500000	metres
Maximum z coordinate	0.500000	metres

The edges of open surfaces must lie on a boundary, but triangles cannot be coincident with a boundary. A closed surface must be entirely within the boundaries.

A significant fraction of the bounding parallelepiped may be cut off by solid and flow entry surfaces. An estimate of the fraction of the volume that is within the flow is useful in the automatic setting of the number of divisions .

Approximate fraction of the bounding parallelepiped that is within the flow.   [1.00000]

OK

Minimum x coordinate
Maximum x coordinate

Minimum y coordinate
Maximum y coordinate
Minimum z coordinate
Maximum z coordinate
These input variables set the limits on the basic rectangular parallelepiped flowfield. The effective shape of the flowfield may be changed through the definition of open surfaces and flow input lines that terminate on these boundaries

Approximate fraction of the bounding rectangle that is within the flow

The surfaces may be such that only a small fraction if the bounding rectangle is within the flow. The setting of this item to the approximate fraction assists with the automatic setting of the computational variables.

.

Retain Existing Composition
This option is available only when data is being modified and it retains the existing number and definitions of the gas species.

Custom Composition
Allows the detailed specification of the gas species and chemical reactions. Modified data files revert to custom composition unless the preceding option is chosen. The following dialogs appear under this option.
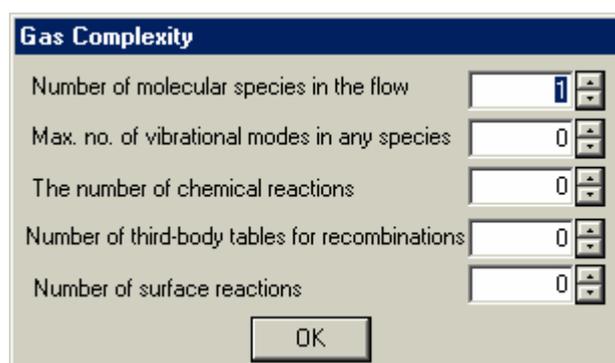
Number of molecular species in the flow
This is the total number that may appear in the stream, the secondary stream, or in the gas that enters the specified flow entry lines.

Max. no. of vibrational modes of any species
Vibrational modes need not be set unless the temperatures in the flow are sufficiently high for them to be activated to a significant extent.

The number of chemical reactions
This is the total number that will be specified.

Number of third-body tables for recombinations
These set the relative efficiencies of all the molecular species as third bodies in recombination of atoms and molecules.

Number of surface reactions
Molecules may recombine or dissociate as a result of collisions with solid surfaces.

The following dialog appears in a loop over the number of molecular species.

The physical properties of a number of common gases may be found in the Reference.

Diameter of the molecular model
The variable hard sphere and variable soft sphere molecular models employ the hard sphere (VHS) or modified hard sphere (VSS) scattering model but

have a diameter that varies with the collision energy. The energy for the specified diameter is characteristic of the temperature that is specified after:
at a reference temperature of

Inverse of the VSS scattering parameter.
This is set to unity if the VHS model is to be used or, for VSS molecules, to the value appropriate to the Schmidt number of the gas.

Viscosity-temperature power law
The variation in the VHS diameter is such as to produce a coefficient of viscosity that varies with temperature raised to this power. 0.5 is a hard sphere gas and 1.0 is effectively a Maxwell gas. These should be regarded as limiting values.

Molecular Mass
This is the mass of an individual molecule.

Number of rotational degrees of freedom
A monatomic molecule has no rotational degrees of freedom and a diatomic molecule or a linear triatomic molecule has two. Non-linear and complex polyatomic molecules have three rotational degrees of freedom.

Rotational relaxation collision number
This sets the rotational relaxation rate. It mat be made a constant (generally about five) or a second order polynomial in the temperature.

Fixed collision number or the constant in the polynomial

Coefficient of temperature in the polynomial
Required only if the polynomial option has been chosen.

Coefficient of temperature squared in the polynomial
Required only if the polynomial option has been chosen.

The number of vibrational modes
These do not become significantly excited until the temperature reaches values of the order of the characteristic vibrational temperature. For most gases, vibration may be neglected if the temperature is less than about 1000K.

The following dialog appears if there are vibrational modes in a loop over the number of modes.

Characteristic vibrational temperature
This is a basic physical property of the gas.

Vib. Collision number Zv, or constant C1 in eqn (6.53)
-1 for a constant Zv, or constant C2 in eqn (6.53)
If a constant vibrational collision number is to be used, the first value is set to that number and the second value to –1. However, vibrational relaxation is strongly temperature dependent and iit is preferable to use values correlated by the Millikan-White theory. The equation numbers refer to the supplementary theory in Bird(1994).

End of the loop over the number of molecular species.

Note that the molecules will be referred to in later data input items by a code number based on the order in which they were specified in this loop.

i.e. The first species to be input is regarded as species 1, the second as species 2, and so on....

The following dialog appears in a loop over the specified number of chemical reactions.

Chemical Reaction

Reaction 1

Pre-collision species code of first molecule   0
Pre-collision species code of seond molecule   0

[Dissociation]   [Recombination]   [Exchange Reaction]

Dissociation
Post-collision species code of first molecule   0
Post-collision species code of second mol.   0
Post-collision species code of third molecule   0

Recombination
Post-coll. species code of recombined mol.   0
The code of the third-body molecule, or
 if negative, the code of third-body table   0

Exchange Reaction
Post-collision species code of first molecule   0
Pre-collision species code of seond molecule   0

No. of internal d. of f. that contribute   0.0
Activation energy   0.0 J
1e10 x the pre-exponential parameter   0.0
Temperature exp. in the rate equation   0.0
Reaction energy input to gas   0.0 J

[OK]

Pre-collision species of the first molecule
Pre-collision species of the second molecule
The code numbers of the two pre-collision species. The identity of the third-body molecule in a recombination is specified later.

Choose one of **Dissociation**, **Recombination**, *and* **Exchange Reaction.**

If it is a dissociation.
> **Post-collision species code of the first molecule**
> **Post-collision species code of the second molecule**
> **Post-collision species code of the third molecule**
> A dissociation is a reactive collision that converts two molecules to three molecules.

If it is a recombination,
> **Post-collision species of the recombined molecule**
> A recombination leads to a single molecule and an unchanged third-body molecule.
>
> **The code of the third-body molecule or, if negative, the code of the third-body table**
> The first option is allows a reaction to be specified for a particular species as the third-body, while the second allows all species as third-bodies with the relative efficiencies given by the table with code number equal to the absolute value of the negative data variable.

If it is an exchange reaction
>   Post-collision species code of the first molecule
>   Post-collision species code of the second molecule
>   The number of molecules is unchanged in an exchange reaction.

The reaction model accepts data in the form of the continuum rate equations in the conventional Arrhenius form. The rate equation data is converted within the program to reactive cross-sections using the theory of Bird (1994). **Note that this is a quasi-equilibrium theory and, while it appears to work well for the reactions in hypersonic flows in air, large correction factors may be need in other reacting flows. For example, combustion reactions appear to be to slow and significant non-equilibrium effects may be present.**

No. of internal d. of. f. that contribute

The internal degrees of freedom of the reacting molecules may contribute to the activation energy that is required for the reaction to occur. The value of this data item will not affect the reaction rate but, if the temperature exponent in the rate equation is negative, the curve of reactive cross-section against collision energy may not have a physically reasonable shape unless the internal degrees of freedom contribute energy. The temperature exponent cannot be more negative than the negative of the sum of this number and 3/2.

Activation energy

The sum of relative translational energy and the contributing internal energy must exceed this energy for a reaction to be possible.

1.e10 × the pre-exponential factor

The reaction rate coefficient is assumed to be in the form

$$k(T) = \Lambda T^{\eta} \exp(-E_a / kT)$$

where E_a is the activation energy, Λ is the pre-exponential factor, and η is the temperature exponent. The units are such that the rate coefficient $k(T)$ is in m^3 molecule^{-1} sec^{-1} for a binary (dissociation or exchange) reaction and m^6 molecule^{-1} sec^{-1} for a ternary (dissociation) reaction. The input quantity is multiplied by ten orders of magnitude so that it does not become smaller than the minimum number that can be represented by a single precision variable.

Temperature exp. in the rate equation

The quantity η in the above equation.

Reaction energy input to the gas

This is positive for an exothermic reaction and negative for an endothermic reaction.
The following dialog appears in a double loop over the number of third-body tables and the number of molecular species.
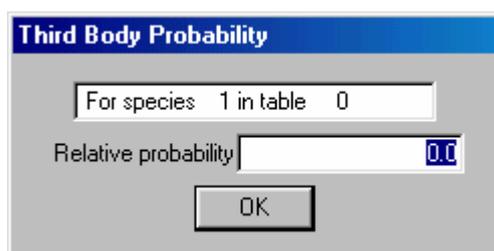
Relative probability
If this is set to unity, the rate coefficient is as set for the reaction. Otherwise, it is the factor by which the rate coefficient is multiplied.

The following dialog appears in a loop over the specified number of surface reactions.
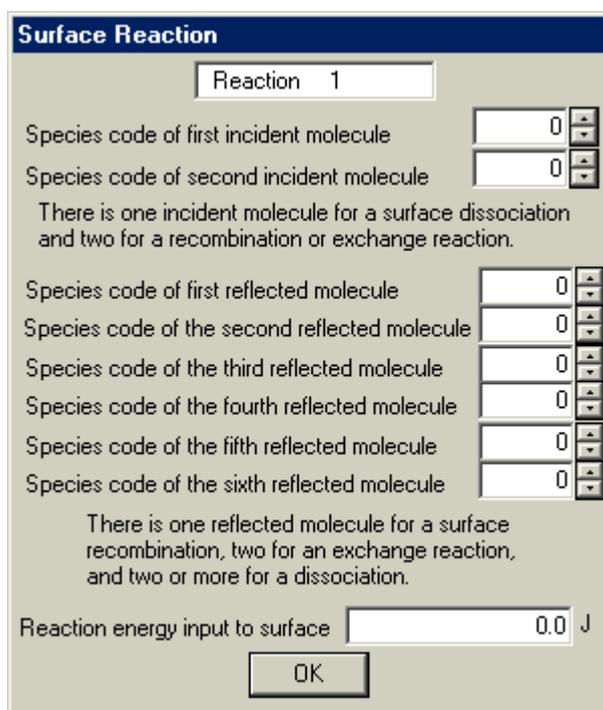
Species code of first incident molecule
Species code of second incident molecule
There is one incident molecule for a dissociation and two for recombination and exchange reactions

Species code of first reflected molecule
Species code of second reflected molecule
Species code of third reflected molecule
Species code of fourth reflected molecule
Species code of fifth reflected molecule
Species code of sixth reflected molecule
There is one reflected molecule in a recombination reaction, two in an exchange reaction, and at least two in a dissociation reaction.

Reaction energy input to the surface
This is the energy from a single event and will be negative when energy is required for the reaction.

The probabilities of the various surface reactions are set when the surface properties are specified.

Ideal air
This sets oxygen as species 1 and nitrogen as species 2. The vibrational modes are not active and there are no chemical reactions. It is useful for problems involving air at temperatures less than about a thousand degrees. The fractions of the two species are about 0.2 and 0.8 and are set in the stream property dialog.

Argon
Argon is set as a typical real monatomic gas.

Hard sphere gas
This employs a fixed molecular of 4×10^{-10} m and a molecular mass 10^{-25} kg.

Real air with reactions
This is a five species model with;
    oxygen as species 1,
    nitrogen as species 2,
    atomic oxygen as species 3,
    atomic nitrogen as species 4, and
    nitric oxide as species 5.
The vibrational modes are active and the data is set for 23 chemical reactions. The model has been extensively employed for atmospheric re-entry studies.

Martian atmosphere
This employs nine molecular species. The first five are as outlined for real air and
    atomic carbon is species 6,
    carbon monoxide is species 7,
    carbon dioxide is species 8, and
    argon is species 9.
The model is again intended for atmospheric entry problems and the vibrational modes are active. A typical Martian atmospheric composition is 95.6% carbon dioxide and 4.6% molecular nitrogen. Argon would have to be added as a trace species, but the other species are generated by the fifty nine chemical reactions that are included in the model.

x, y and z velocity components
Temperature and Number Density
Fraction of Species
A maximum of twelve molecular species may have been defined.
This sets the flow conditions for the gas that enters across the stream boundaries and which generally fills the flowfield at the start of the calculation. It is used for the normalization when the "non-dimensional" option is chosen during the run. It should therefore be set as a reference gas even when there are no stream boundaries and the flowfield is initially set as a vacuum.

The following screen appears in a loop over the six flow boundaries.
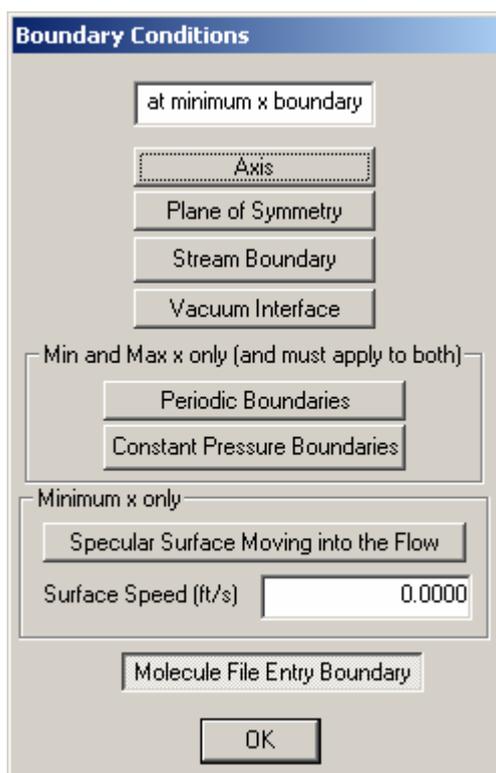
Axis
This choice is not valid for three-dimensional flows.

Plane of Symmetry
All molecules striking the boundary are specularly reflected. This is equivalent to setting the boundary as a plane of symmetry.

Stream Boundary
Molecules that are typical of the specified stream enter across the boundary. Molecules that strike stream boundaries are removed from the flow. This boundary conditions maintains a uniform flow in an empty flowfield, even for a subsonic or stationary stream.

Vacuum Interface
No molecules enter the flow and all molecules striking the boundary are removed from the flow.

Periodic Boundaries
This applies only to the minimum and maximum x boundaries and must be applied to both. Molecules that leave across the minimum x boundary enter across the maximum x boundary, and vice-versa.

Constant Pressure Boundaries
These boundary conditions require the definition of a secondary stream and an initial flow separation boundary at a specified x location. The minimum x boundary is a stream boundary, but the number of molecules that enter is

made equal to the number that crosses the initial flow separation line in the positive direction. The maximum x boundary is a similar boundary for the secondary stream and the number of molecules that enter is equal to the number that cross the flow separation line in the negative direction. This boundary is intended for use in calculations involving steady subsonic flow through channels and tubes.

Specular Surface Moving into the Flow
This boundary can be set only at the minimum x boundary and causes a specular piston to move into the flow at a constant speed given by the specified

Surface Speed
This produces a shock wave ahead of the piston. Steady flow sampling should not be employed with this option.

Molecule File Entry Boundary

There must be a file DSMIFn.DAT file, where n may be 1 to 4. that is a renamed DSMOF.DAT file that was generated by the DS2V program.
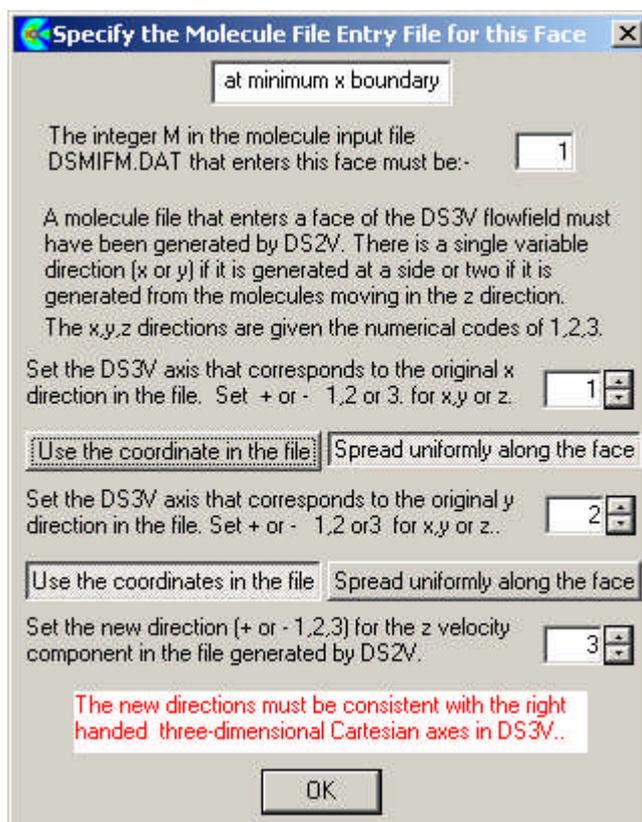
The first item sets the name of the molecule input file for this boundary. The setting of the other items in this menu is more demanding than is the case with the other menus. The DS2V flow

is necessarily in the *x-y* plane so that it is necessary to make provision to reassign the axes. The files generated from molecules leaving across one of the DS2V boundaries are necessarily moving in either the x or y directions and, when replayed into DS3V

The following menu comes up for each input file after the cells have been set.

End of the loop over the boundaries

There are three options with regard to the separation boundary and secondary stream.

No Separation Boundary
There is no separation boundary and no secondary stream.
Boundary at line of constant x
A secondary stream must be set and applies at x coordinates greater than this value.
Boundary at line of constant y
A secondary stream must be set and applies at y coordinates greater than this value.

Coordinate of the Boundary
The x or y coordinate of the separation boundary (if one is set).

One of the following options must be chosen.

Set Initial Flow to Stream or Ref. Gas
The initial (zero time) state of the gas is set to the stream definition. If a separation boundary has been set the gas beyond this boundary is set to the secondary stream.

Set Initial Flow to a Vacuum
There are no molecules in the flow at zero time.

(Note that these options have been carried over from the DS2V program and will be extended appropriately for the three-dimensional environment when this is required for a particular application. Any queries or problems should be referred to GAB Consulting)

If there is a secondary stream, it is set by the above dialog that is identical to that for the stream and for the specified stream elements.

The total number M of separate molecule input files DSMIF1.DAT ……..DSMIFM.DAT.

This number includes the boundary input files that have already been set for each boundary and the files that supply the molecules for the file entry sources within the flow. Note that a single file can be employed at a number of locations.

This number cannot exceed four.

The Number of Molecule File Entry Sources

This is a molecule file entry process is distinct from that involving file entry surface triangles. If entry triangles have been set, this number MUST be set to zero. Although there can be only one DSMIF.DAT file, the molecules from this can be translated and rotated to multiple locations. The following menu is repeated for instance of molecule entry.

As with the file entry triangles, the following menu comes up during the early stages of the run

It provides information on the structure of the molecule file and, if it was generated by DS2V rather than DS3V, it specifies the way in which it is to be converted from a two dimensions to three dimensions.

Either steady or unsteady sampling must be chosen.

Assumed Steady Flow at Large Times

This is chosen when the boundary conditions are such the flow becomes steady at large times and a long time average will be required to produce a large sample. The

sample is automatically reset whenever the total number of simulated molecules changes by seven or eight standard deviations. For most problems, this automatically causes a time sample to be made over the eventual steady flow. However, in some cases , the unsteady phase of the flow does not involve much (or even any) change in the number of molecules. The user must then stop the program after the flow has become steady and select the **Commence a New Sample** option when re-starting it. A large time-averaged sample may then be accumulated.

Continued Unsteady Flow

The flow is not assumed to become steady at any time. This option requires a very large number of molecules. The flow is time-averaged over an interval at the end of each output interval.

Employ Standard Options

The computation is made with the standard or default options that are adequate for most problems.

Set Custom Options

This brings up the following dialog that can be used to modify the standard options.

The data file DS3VD has now been generated. The program may be run with this data or it can be recycled for corrections and/or alterations
.
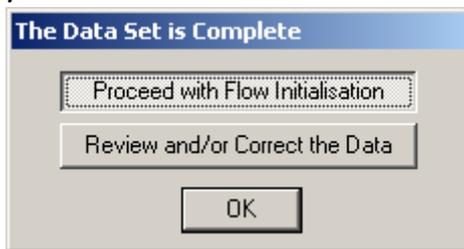
8 DS3V Tutorial/Demonstration Case

The DS3VD.DAT and DS3SD.DAT files that are produced when the DS3VZ.EXE file is run are for the supersonic flow past a delta wing. Note that the surface definition file was produced for Version 1 and does not conform to the specification in Section 4. As noted earlier, DS3SD files for Version 1 are accepted by Version 2 if a line containing 1 is added as a new first line.

The first window to appear provides a check of the geometry that has been defined. The graphical representation of the axes, bounding rectangle, and surfaces can be rotated in three dimensions by mouse movements with the left button depressed. Mouse movements with the right button depressed resize the image, which can also be moved by the arrow keys.
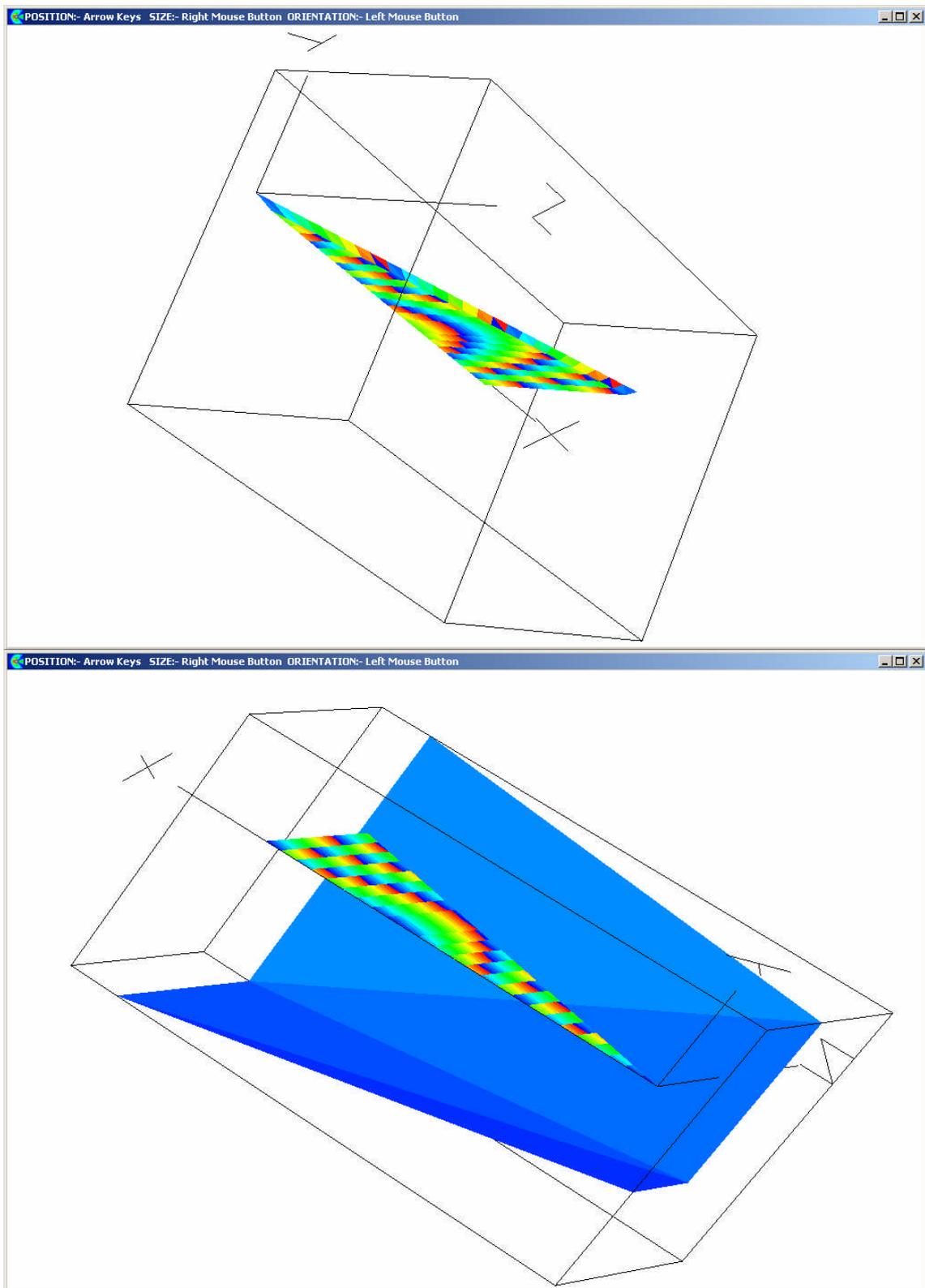
The mouse should be moved around until the geometry of the flow becomes clear.

The minimum z face is a plane of symmetry and the other faces are stream boundaries. The solid surfaces that define the delta wing are coloured triangle by triangle. The flow entry surfaces that cut off regions of uniform flow in the corners of

the parallelepiped are also shown. These are much larger and all appear as blue in this case. The surface images are transparent if they are viewed from behind. The program is paused while any of the flow establishment windows are displayed and the window must be closed in order for the calculation to continue.

The next window shows the elements that are intersected by surface triangles as black and those inside the solid surfaces or beyond the flow entry surfaces as white. The elements within the flow are coloured according to the distance from a surface of the division in which they lie. The colours show the "level" of the division relative to the surfaces. This is used within the logic of the program to determine whether possible surface interactions need be considered when moving the molecules.

The main purpose of this window is to allow the user to determine whether the elements have been correctly marked as being within or outside the flow. Round-off error occasionally causes an element near a surface to be incorrectly marked. Should an inside element be marked as outside, the problem is obvious because the incorrect marking propagates throughout the region. An inside element marked as outside is less obvious because it produces an isolated white element surrounded by coloured elements.

Note that the plane of the plot can be changed to be normal to any of the three axes. The plane may then be moved along this axis by setting the division and the element within that division.

Should an incorrectly marked element be found, the program should be stopped. A small change in the data items that set the number of divisions, and possibly elements, generally fixes the problem. Any data and geometry files that lead to persistent problems should be reported.

The next window shows the initial cells. Again this plot may be normal to any of the three axes and may be moved along the axis. Initially, the sampling cell nodes are the centres of the divisions that are entirely within the flow and the centres of the surface triangles. The smaller collision cells are generated next and are shown on the following page. Note that the whole of the elements that are partly within the flow are coloured in these plots.

The cells are near uniform in size and the apparent size irregularity is an artefact of the three-dimensionality of the cells an that a two-dimensional cut intersects only a small cross-section of some cells. Each cell is assigned a random colour out of a palette of 190 colours and adjacent cells will occasionally have the same colour
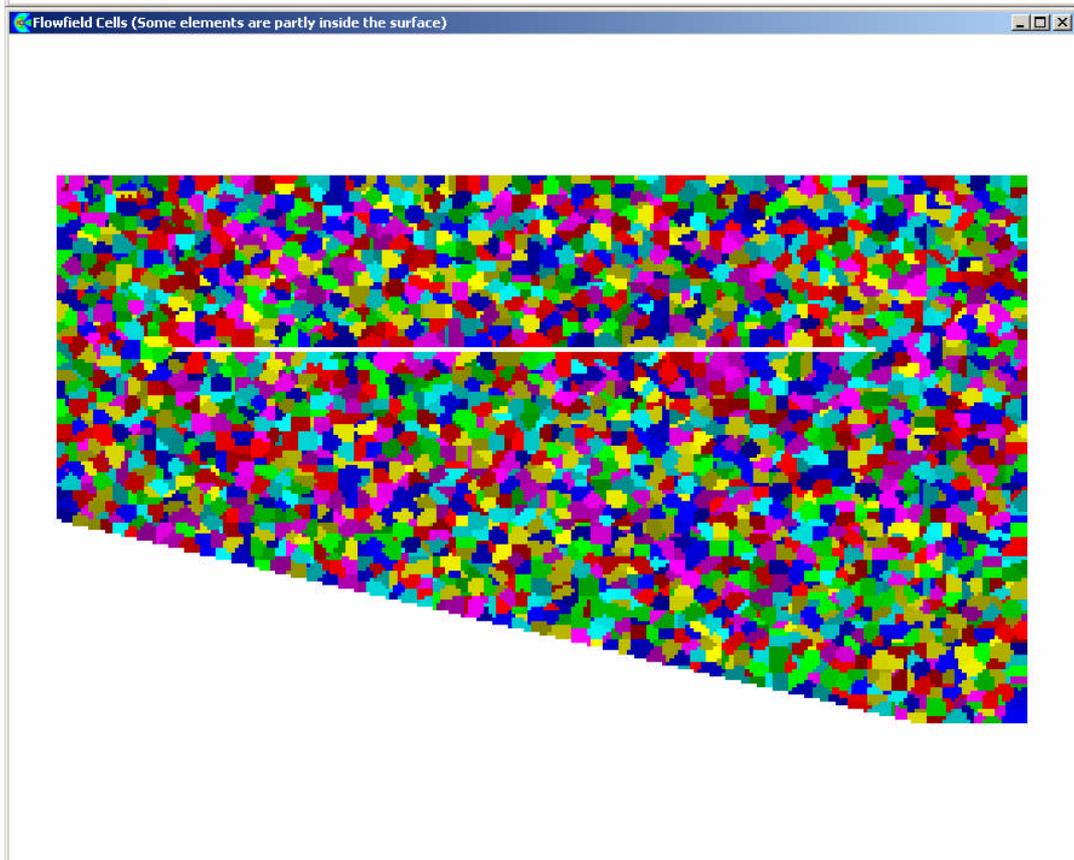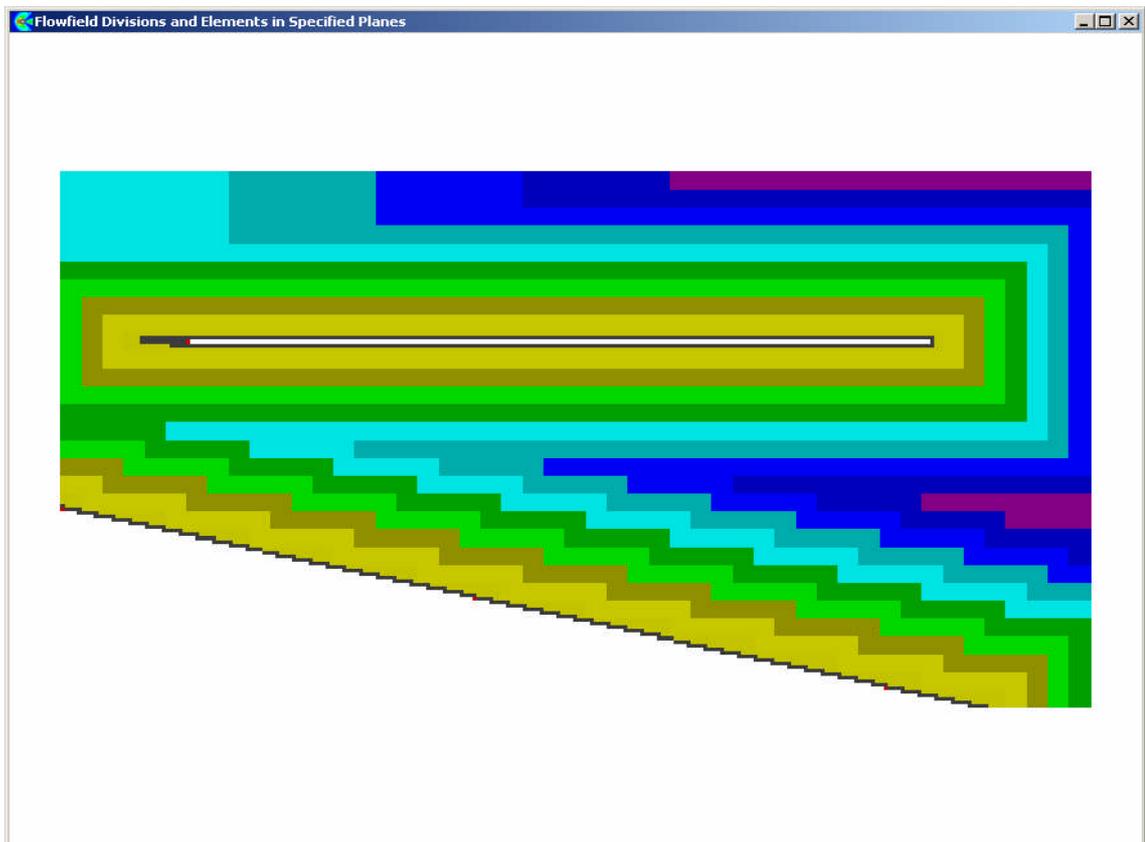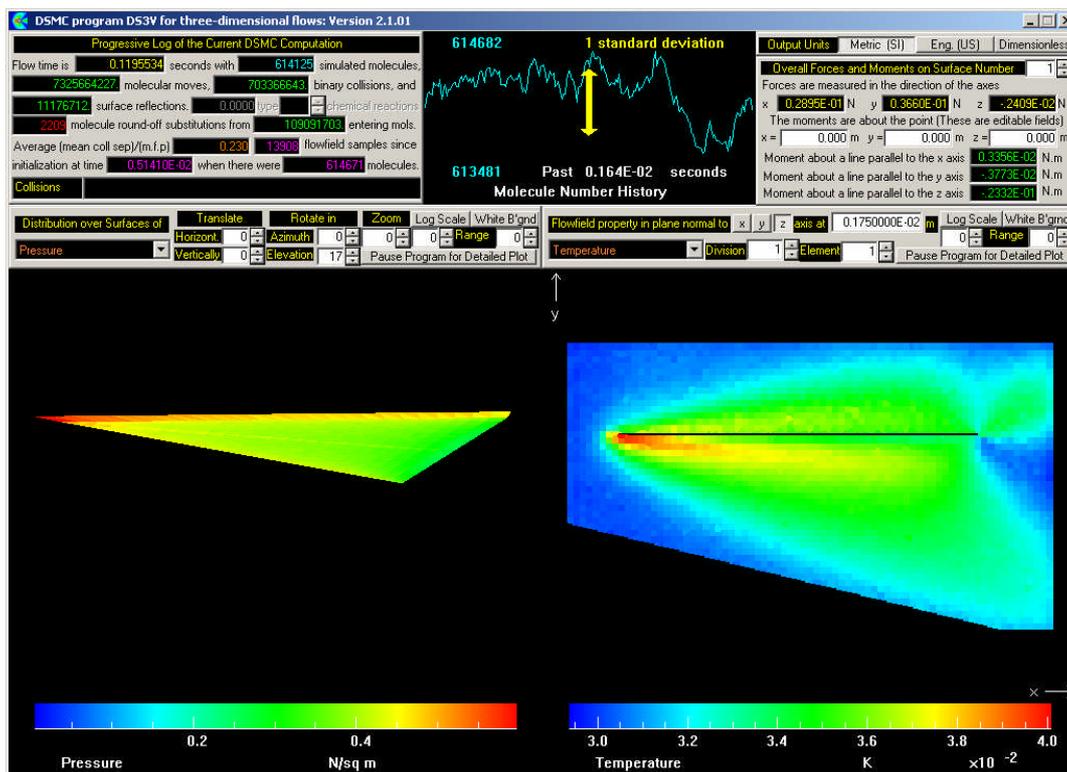
This main window is visible throughout the running of the calculation. It contains graphics areas that show the surface distributions and the flowfield properties. The amount of detail in these is limited and subsidiary screens may be selected by the "Pause Program for Detailed Plot" buttons.

The windows are largely self-explanatory but some comment and clarification is useful for some of the contents.

(i)   The **Flow time** is the time in seconds since the surfaces were instantaneously inserted into the uniform stream. The flow time advances in steps equal to the set fraction of the smallest value of the sampled mean collision time in any of the cells. The flow properties are sampled at set time intervals. With the eventual steady flow option, until the flow becomes steady the samples are reset each time the restart files are written. The flow and surface property displays are therefore time-averaged over time intervals that are small in comparison with the steady flow time and give a realistic picture of the unsteady flow development process. Steady flow time averaging builds up a large sample. Ensemble averaging will eventually be added, but the unsteady sampling option in the current version essentially continues the unsteady phase indefinitely. However the short time averaging may be confined to the specified fraction of the output interval.

(ii) The **Molecule Number History** window plots the number of simulated molecules over a time interval immediately preceding the current flow time. There is usually an increase in the number of simulated molecules during the unsteady phase of a flow but, when a flow has become steady, the fluctuations should be characteristic of the statistical fluctuations. These have a standard deviation of approximately the

inverse square root of the number of simulated molecules. The magnitude of the standard deviation is indicated by the length of the double-ended yellow arrow at the center of the window. The scatter in a steady two-dimensional flow shows the expected characteristics. With an assumed steady flow, should the number of molecules depart by more than about seven standard deviations from the value at the start of the sampling interval, the sample is reset. Should a flow become periodic rather than steady, it should be clear from the behaviour of the total molecule number in this screen.

(iii) The log of the computation in the top left hand corner of the screen shows the number of **molecule round-off substitutions** that have been made during the calculation. A molecule is removed from the flow and is replaced by randomly selected molecule from the same cell if the computer is unable to fix its position within the flow. This problem arises from the six or seven significant digit limitation of 32 bit arithmetic..

(iv) The units are quoted when one of the dimensioned output options are chosen.. The **dimensionless** output option requires specific definitions for some of the output quantities.

The flow quantities are expressed as their ratios to selected undisturbed stream quantities. The non-dimensional positions are the x and y co-ordinates divided, respectively, by either the length or height of the working section. The speeds and velocity components are normalized by the speed U_∞ of the undisturbed flow. The overall temperatures and the separate components of the temperatures are normalized by the overall temperature of the stream. The pressure is normalized by the pressure p_∞ in the stream. The densities and number densities are normalized by the stream density ρ_∞ and number density n_∞.

A number flux coefficient is $\dot{N}/(n_\infty U_\infty)$.

A surface pressure coefficient is $(p - p_\infty)/(\frac{1}{2}\rho_\infty U_\infty^2)$.

A shear stress coefficient is $\tau/(\frac{1}{2}\rho_\infty U_\infty^2)$.

A heat flux coefficient is $h/(\frac{1}{2}\rho_\infty U_\infty^3)$.

A characteristic length or area is required for the normalization of the surface forces and moments. The input of this parameter is through a pop-up menu that appears the first time that non-dimensional output option is selected. The force coefficients are the force divided by the product of $\frac{1}{2}\rho_\infty U_\infty^2$ and a characteristic area

(v) For gases with active vibrational modes, there is an apparent anomaly in that the vibrational temperature is usually output as zero in a low temperature stream. This is a result of the quantum model that is employed in the program. The minimum vibrational energy of any molecule is the Boltzman constant times the characteristic vibrational temperature. The characteristic vibrational temperatures in air are of the order of two or three thousand degrees Kelvin and, at temperatures

of the order of one or two hundred degrees, only about one in a million molecules would be in the first vibrational level. This means that there is likely to be no vibrational energy in the number of molecules that are involved in a typical DSMC sample. The amount of vibrational energy at the low temperatures is so small that the zero values are of no consequence. To balance the zero vibrational temperatures in most samples in a low temperature gas, a small sample that happened to include one molecule at the first vibrational level would be assigned an extremely high vibrational temperature. These would appear even more anomalous to the casual user and they have been suppressed in the output. The calculation contains the correct average amount of vibrational energy despite the exaggerated scatter in the vibrational temperature at low overall temperatures.

(vi) The ratio of the local mean separation of the collision partners to the local mean free path is the key verification parameter for the calculation. The largest, and therefore the worst, value in any cell is output in the flow log. There could be some error in the calculation unless this is small compared with unity. On the other hand, higher values might be tolerated in a small region of the flowfield and the largest value might be an extreme fluctuation in one of the very small cells at the boundary of the surface cell region and the rectangular cells. Therefore, if the largest value is undesirably large, the **Coll. Sep. / m.f.p** option for the property in the flow display should be selected. The distribution of the ratio can then be studied and a judgement made about the quality of the calculation. The ratio can be reduced only by the use of a larger number of simulated molecules in the calculation.

(vii) The average number of simulated molecules in the cells may also be selected for the flow property display. This is a computational parameter and, unlike the flow properties, aspects of the cell structure are apparent in the display. The smallest numbers will generally be associated with the small cells that are remnants of the rectangular cells that are not quite cut out when the surface cells are superimposed on the background grid. Small cells are also occur adjacent to sharp corners in the surface cell regions, while the outermost cells in the corner regions are larger than normal. The total sample in the cell is obtained by multiplying the average number of molecules by the total number of samples that is shown in the flow log.

There is a button marked **Pause Program for Detailed Plot** for both the flowfield and surface properties.
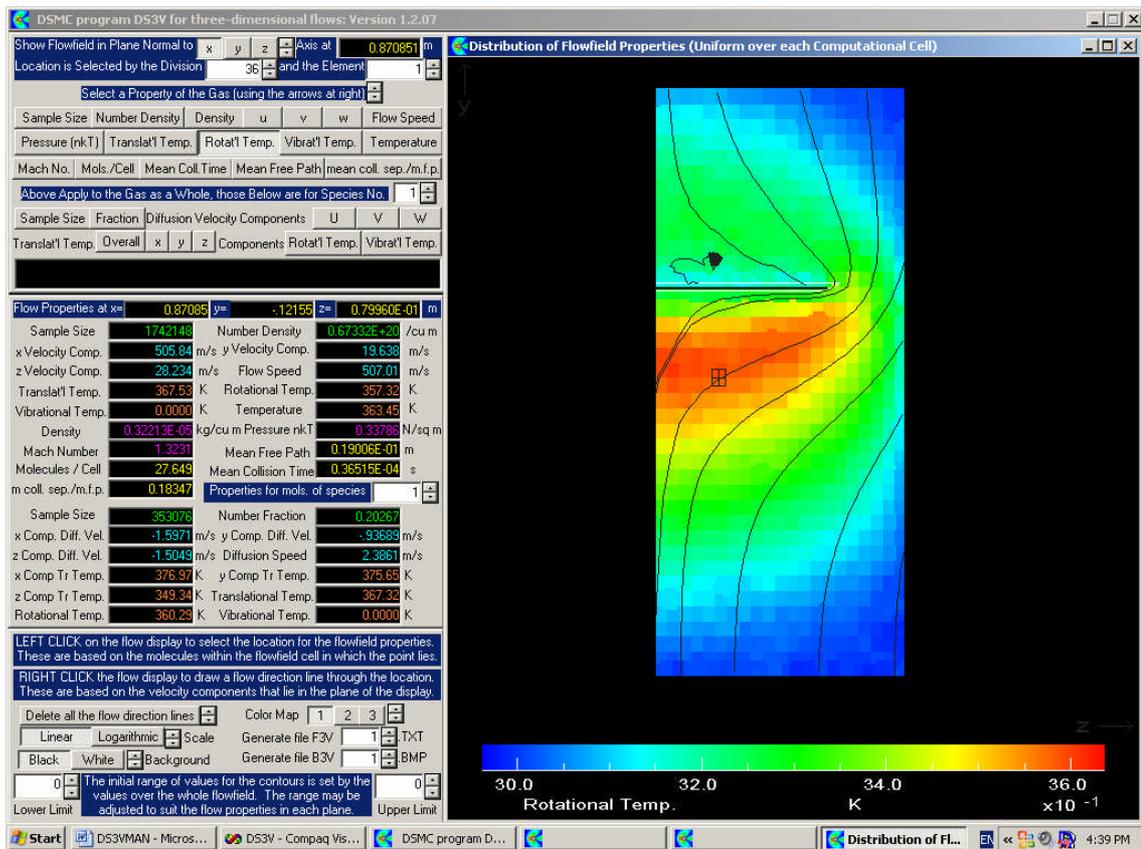
The flowfield may be viewed in planes normal to any of the three axes. **Note that the planes and the properties to be viewed in the plane must be selected by the arrow controls and not through clicking on the buttons.** The flow properties at any point are selected by left clicking on the location and a right click produces the path line in the plane.
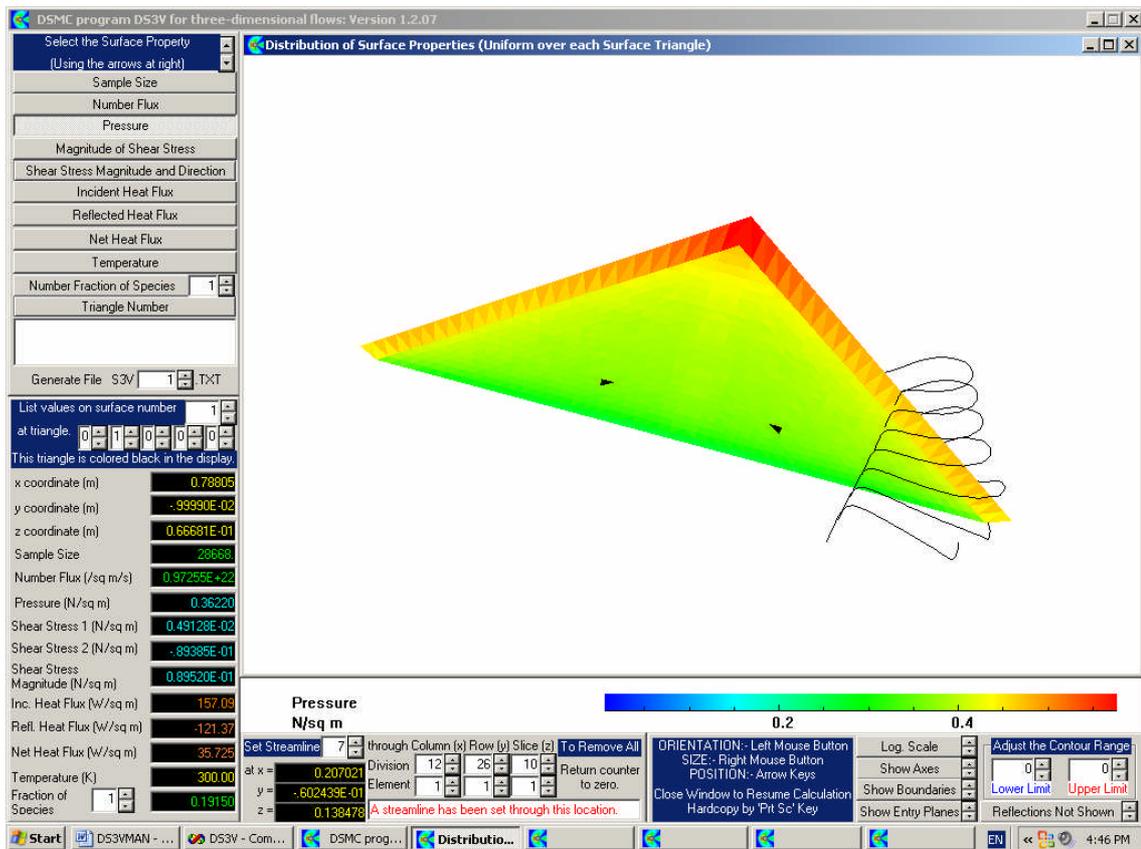
The surface properties at any location are displayed when the triangle number is selected. The selected triangle then becomes black in the display. Three-dimensional streamlines may be drawn through the center of any division in the flow.

9 The DS3DG Tutorial/Demonstration Case

The DS3DG.EXE file should be in a directory with the sample triangle file DS3TD.DAT. The sample triangle file for a sphere of unit radius was generated by the Rhinoceros program and was exported as "raw triangle" file with the coordinates of the triangles in double precision. Two lines were added at the beginning of the file for the number of surfaces and the number of triangles on that surface. The DS3DG file may be run to produce a DS3SD.DAT file.