General Program for the Computation of

Two-Dimensional or Axially-Symmetric Flows by the

Direct Simulation Monte Carlo (DSMC) Method

The DS2G Program User's Guide

Version 3.2

June 1999

G.A.B. Consulting Pty Ltd
5 Fiddens Wharf Rd., Killara, N.S.W. 2071, Australia
Country code 61 City code 2 498 7809

gabird@compuserve.com
http://ourworld.compuserve.com/homepages/gabird

Table of Contents

1 INTRODUCTION

2 OPERATION OF THE PROGRAMS

3 DEMONSTRATION CASES

1 INTRODUCTION

1.1 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 coordinates 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 contrasts with the general philosophy of computational fluid dynamics which is 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 Knudsen number which is the ratio of the mean free path to a typical dimension of the flowfield. The Navier-Stokes equations are valid when the Knudsen number is very small in comparison with unity, and the limit as the Knudsen number tends 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 an "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 incorporates "local Knudsen numbers" which are the ratios of the local mean free paths to the scale lengths of 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 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. A steady flow 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 for 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 continuum equations is of no consequence.

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

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. This latter condition will dictate the cell size in high Knudsen number flows and, in practice, the cell size in low Knudsen number flows is set to about one third or one half the cell size. The time step is then set such that a typical molecule moves about one third of the cell dimension at each time step. This satisfies the above requirement for the size of time step in stationary low Knudsen number flows and is conservative for moving gases and/or high Knudsen numbers.

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. Primitive implementations of the DSMC method choose the collision partners from anywhere in the same cell. Later implementations, including Versions 1 and 2 of DS2G, employed fixed sub-cells to reduce the spacing of collision partners. Version 3 of DS2G introduces an adaptive transient rectangular background grid to one cell at a time within the collision routine. This yields nearest-neighbour collisions and is efficient with regard to both computation time and storage requirements. Version 3.1 adds output to the TECPLOT files that indicates whether the DSMC numerical criteria have been met. The ratio of the time step to the local mean collision time and the ratio of the mean separation between collision partners to the local mean free path should be well under unity over the whole of the flowfield.

The statistical consequences of the replacement of the extremely large number of real molecules by a very much smaller number of simulated molecules must always be kept in mind. The statistical scatter generally decreases as the square root of the sample size and, in order to attain a sufficiently small standard deviation, the programs employ either time averaging for steady flows or ensemble averaging for unsteady flows. The most serious statistical problem is when a significant effect in the real gas is a consequence of the few molecules towards the extremities of the distribution. A detailed exposition of the method is available in the reference which will be referred to as Bird (1994).

Reference

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

1.2 The Scope of the Program

1.2.1 Geometry

The DS2G program has a flexible system for the specification of the flow geometry. This enables the program to be applied to a wide variety of flows ranging from the flow past aerodynamic bodies and rocket plume flows through to internal flows in high vacuum equipment. The flow may be either a plane two-dimensional flow or an axially symmetric flow. There may be velocity components in the direction normal to the plane or, in the case of axially symmetric flows, circumferential velocity components. However, there must not be any flow gradients in these directions. The time-averaged flow properties may be sampled if the flow is such that it becomes steady at large times. Alternatively, an ensemble average may be made over multiple runs of an unsteady flow.

1.2.2 Gas Model

The program employs the physical gas models that have been described and validated in Bird (1994). The gas may be a mixture of VHS or VSS models and the cross-sections, the viscosity-temperature index (which determines the way in which the cross-section changes with the relative velocity), and the may VSS scattering parameter may be specified separately for every combination of 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.

1.2.3 Gas-Surface Interactions

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. The other "classical" model of specular reflection may be specified for the artificial case of complete slip and no energy transfer at the surface. Alternatively the CLL model may be employed, and this is capable of modelling realistic non-classical reflection cases. Version 3.2 adds a diffuse adiabatic reflection option and gives the recovery temperature distribution.

1.3 General Description of the DS2G Program

For the two-dimensional option, the flow is in the x-y plane. Alternatively in G2, the axis of an axially-symmetric flow lies along the x axis and the y coordinate is a radius from that axis.

The flowfield is divided into a number of four sided regions, the four sides being numbered from 1 to 4 in *clockwise* manner as shown in Fig. 1.

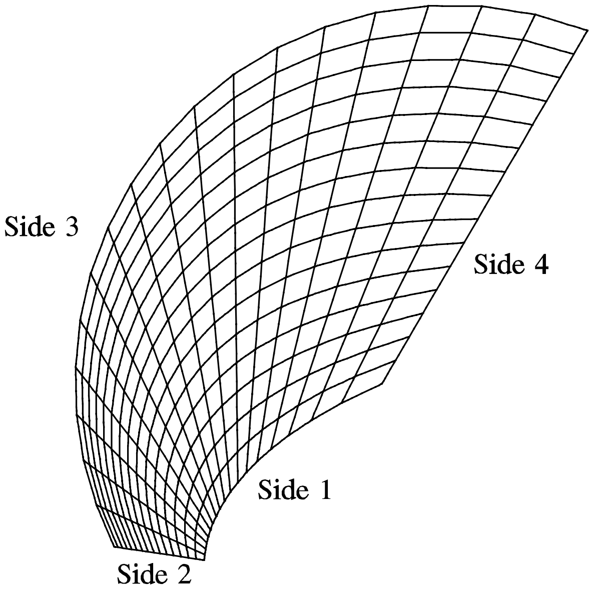

Fig. 1. A typical flow region.

Sides 1 and 3 of each region may be curved, but they must not be re-entrant. These sides are divided into a number of cell segments or elements and the number of elements on each side must be the same. The cell structure is defined by joining the corresponding points on each side by straight lines and then dividing each of these lines into the same number of cell elements. Sides 2 and 4 must therefore be straight. There are a number of options that relate to the way this geometry is defined, and the cells may be quite irregular, as long as none of the joining lines cross. The lines of cells in the direction of sides 1 and 3 are referred to as "rows" and lines in the direction of sides 2 and 4 as "columns". The numbering of cells is along successive rows, starting rom the cell at the intersection of sides 1 and 2. As noted earlier, the cells are used for the sampling of the flow information and the establishment of the collision rate.

Each side is one of the following:-

(1) On the axis of the flow. This would occur only for an axially-symmetric grid and no molecules would collide with such a side.

(2) A plane of symmetry. For an axially-symmetric flow, such a plane would have to be normal to the x axis. The flow velocity component normal to such a plane is zero and all flow gradients normal to the plane are zero. At the molecular level, the plane is equivalent to a specularly reflecting boundary.

(3) An interface with a specified uniform freestream flow. A set of molecules appropriate to those crossing the boundary into the region are generated at the side. Molecules crossing the side from the region are removed from the flow. The boundary is an exactly correct physical representation (even in subsonic or stationary flow) as long as the flow disturbance does not extend to the boundary.

(4) An interface with a non-uniform specified flow, the macroscopic properties of which can vary at each cell element. The flow gradients should be such that it can be regarded as effectively isentropic because the molecules are generated from the appropriate Maxwellian distribution.

(5) A solid surface. A specified fraction (which may vary with the molecular species) of the gas may be absorbed by the surface.

(6) A solid surface similar to the previous option, but which is outgassing at a specified rate.

(7) An interface with one or more sides of other regions.

(8) A boundary with a vacuum or a boundary with a molecule input file. This option is also suitable for an outflowing gas with a highly supersonic velocity component across such a boundary. This is because there are virtually no upstream moving molecules in a flow with Mach number or speed ratio greater than about three.

The whole of each side must be of the same type so that changes in boundaries, such as the end of a surface, can occur only at the corners of the regions.

The orientation of a region with respect to the x and y axes is quite arbitrary and any face of a region can interface with more than one other region. A typical set of regions is shown in Fig. 2.

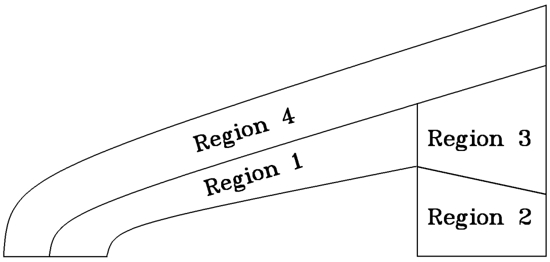

Fig. 2. Typical arrangement of regions.

If the regions in Fig. 2 were for the supersonic flow past a blunt cone with a flat base and, assuming that side 1 is the lowest side in each case, the specification of the sides is as follows:-

Region 1	Side 1	A surface (type 5).
	Side 2	On the axis (type 1).
	Side 3	An interface with side 1 of region 4 (type 7).
	Side 4	An interface with side 2 of region 3 (type 7).
Region 2	Side 1	On the axis (type 1).
	Side 2	A surface (type 5).
	Side 3	An interface with side 1 of region 3 (type 7).
	Side 4	A stream boundary (type 3)*.
Region 3	Side 1	An interface with side 3 of region 2 (type 7).
	Side 2	An interface with side 4 of region 1 (type 7).
	Side 3	An interface with side 1 of region 4 (type 7).
	Side 4	A stream boundary (type 3)*.
Region 4	Side 1	An interface with side 3 of region 1 and side 3 of region 3 (type 7).
	Side 2	On the axis (type 1).
	Side 3	A stream boundary (type 3).
	Side 4	A stream boundary (type 3)*.

* For high Mach numbers, type 8 boundaries would be preferable.

Side 3 of region 4 should be upstream of the disturbance. The boundary at the base is almost exact in the outer part of the flow as long as the x component of the velocity is well supersonic. Unless this boundary is very far downstream, there will be subsonic flow in the wake and some error in the flow. The magnitude of this could be determined by placing the downstream boundary at different locations. This system of flow boundaries has proved to be sufficiently flexible to cope with almost all flow problems that have been encountered.

When an interface between regions lies along curved sides, the cell elements will match exactly only if they are equal in number and identically distributed along the interface. Any mismatch will result in small "gaps" or "overlaps" at the interface. The program procedures are designed to cope with this eventuality, but it greatly increases the normally very small probability of simulated molecules going "astray". It is strongly recommended that the cell divisions be chosen such that curved interfaces are exactly matched. There are no problems with cell size discontinuities across straight interfaces as far as the flow calculations are concerned. However, if contour output is chosen, the contours will be continuous across the region boundaries only if the cells match exactly.

If the Knudsen number for the flow shown in Fig 2 was sufficiently small for the flow to be near-continuum, very thin cells would be necessary in the region of high vorticity near the surface. Should the desirable cell size lead to an excessively small number of simulated molecules in the cell, the problem can be overcome in a steady flow by calculating the boundary layer on a shorter time-scale. The number of molecules in the cell is increased by reducing the number of real molecules that are represented by each simulated molecule. If the time step is reduced by exactly the same fraction, the flux of molecules across the interfaces with the outer flow are exactly matched. This simultaneous change in DTM and FNUM is ideal for flows in the stagnation region where FNUM is reduced in order to increase the number of molecules in very thin cells near the surface. The reduction is DTM is also desirable because of the thin cells. However, for problems such a plume backflow, a reduction in FNUM is desirable because of the very low density, but the cells should be large and the reduction in DTM is most undesirable.

The above problem may be overcome by splitting separate calculations for the near and far plume. Up to three files of molecules G2MOFn.DAT (n=1 to 3) are generated at the low density boundary and these files may be renamed G2MIFn.DAT and used as the input files for the next section of the flow. This process may be repeated. If the normal component of the flow is well supersonic across the output/input boundary, so there is no upstream influence, the flow regions need not overlap. In the case of a wake flow or plume impingement problem where there is upstream influence, the output file may be generated *within* the flow. The next section of the flow may then be calculated with a much larger sample (because of its limited extent and the free choice of both FNUM and DTM which may be different from their values in the calculation that produced the file). Each molecule input side must be *coincident* with the side at which the molecule file was generated. The number of cells should be the same along curved sides, but may differ if the sides are straight. For axially-symmetric flows with radial weighting factors, the output files can either retain or remove these factors. If they are removed, the flow into which the molecules flow must not have radial weighting factors. The molecule entry side should be specified as a type 8 side because no molecules other than file molecules should *enter* the flow across this side, but molecules should be free to leave the flow across the file entry side. The inflow may be subsonic as long as the upstream moving molecules are allowed to leave the flow.

Note that the flow will be affected by the sample size of the input molecule file. The scatter in this sample will be transmitted as a systematic error to the flow generated from this file. The molecule input file should therefore be as large as possible. Note that only one record of this input file is in memory at any time.

A further application of the molecule file input/output feature is to allow a single upstream flow calculation to be used as the input to a number of downstream flows. In many cases, the upstream flow will be more dense and its re-use can save considerable re-calculation.

Program DS2G employs data and parameter files DS2GD.DAT and DS2GP.DAT. In general, these are generated by the "data screens" within DS2G and the user need not be aware of their existence. However, these are ASCII files and their content is specified in Appendix B. It is therefore possible to produce "front-end" programs as an alternative to the use of the data screens. (Only DS2GD.DAT need be generated externally because DS2GP.DAT is generated automatically when DS2GD.DAT is reviewed by cycling through the data screens.) These may allow graphical input from CAD programs or simplified data set-up for a restricted class of flow. There are a number of demonstration data files (DS2GD*n*.DAT where *n* ranges from 1 to 999) and these may be selected as one of the menu items when starting a new run. The initial menu also makes provision for the existing data file to be archived as DS2GA*n*.DAT, where *n* ranges from 1 to 999. The program automatically selects the smallest available value for *n* and an archive record file is opened under the DOS EDIT program so that a description of the archived file may be recorded.

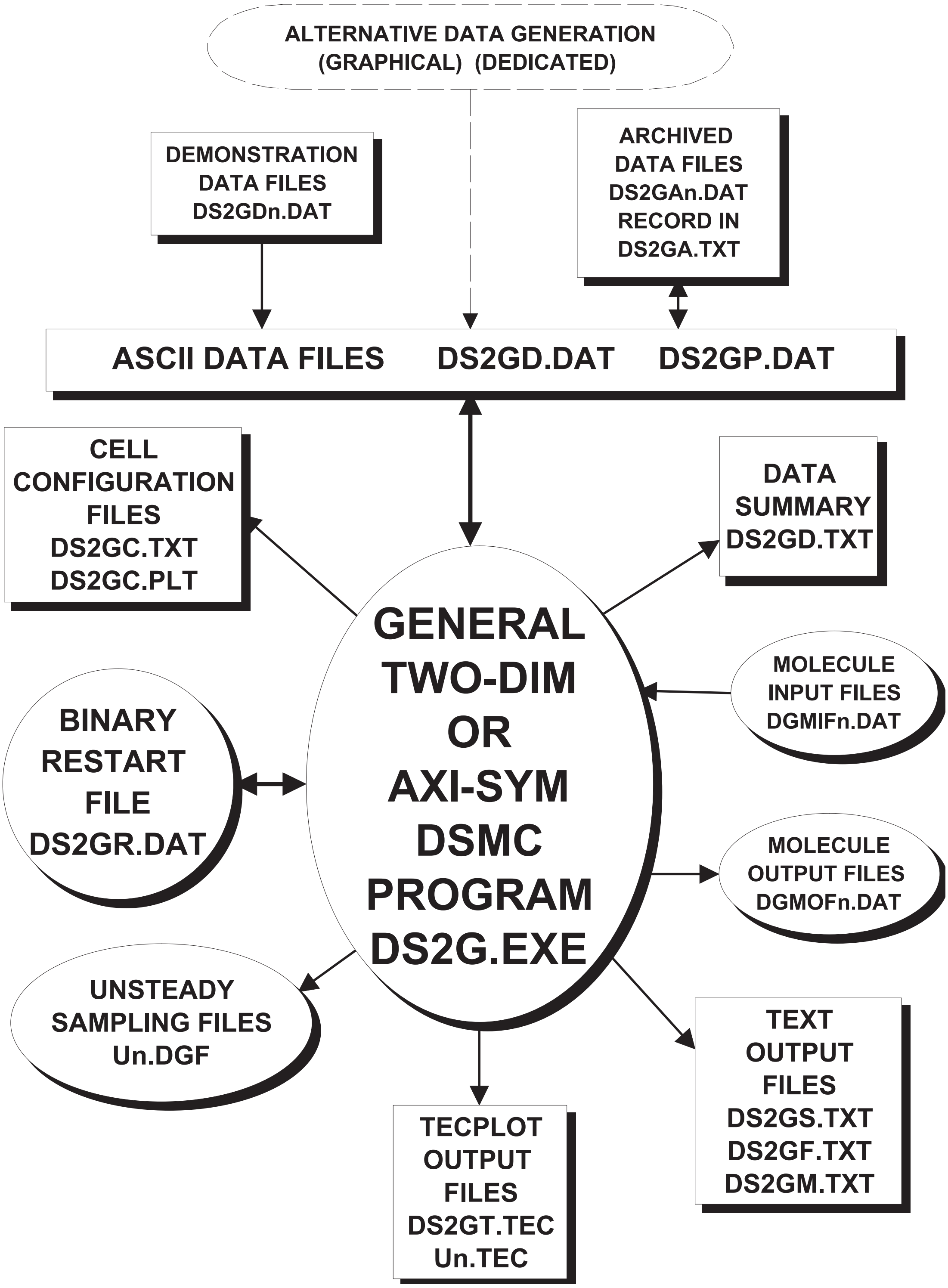

Fig. 3. The files associated with the DS2G program (ASCII files in rectangular shapes and binary files in rounded shapes).

2 OPERATION OF THE PROGRAM

The program is operated through succession of on-screen forms or menus. The appropriate option is chosen or numerical data entered into each "screen". The user progresses from screen to screen by pressing the "enter" key.

2.1 Program screens

2.1.1 Introductory Program Screen (Orange)

One of five options is chosen from this screen.

Generate and run a new case

The selection of this option causes the program to cycle through the data screens in order to generate a completely new set of data or to modify an existing data file. This choice is made through a subsidiary screen which presents a two-way choice. If the data file DS2GD.DAT is produced through the renaming of one of the DS2GDn.DAT files, or a similar file, it is necessary to choose the "modify" option and to cycle through the data screens even if there are to be no alterations to the data. This is to produce a matching DS2GP.DAT file. In the case of an ensemble-averaged unsteady flow, there is an option to either bypass or generate the cell report files DS2GC.TXT and DS2GC.PLT. There is a further screen with three options, to completely bypass the generation of the text output files, to generate text output for the surface properties only, or to generate the full output.

Continue an existing calculation

This should be chosen only when a run has proceeded to the point where a restart file DS2GR.DAT has been produced for a time-averaged flow or an unsteady sampling file has been produced for an unsteady flow. In the case of a steady flow, there is a subsidiary screen that provides a choice between the continuation of the existing time average or the commencement of a new average.

New run from existing data file

This starts a run from zero time and, in the case of an unsteady flow, removes any preceding runs from consideration in forming averages. It should only be chosen when a consistent DS2GP.DAT file exists.

Generate a TECPLOT file

In the case of a time-averaged flow, this generates the file DS2GT.TEC that is formatted according to the requirements of the TECPLOT post-processing program. For an unsteady flow a series of files U001.TEC, U002.TEC.... are generated, where the number corresponds to the print interval. These files may be used to generate a series of TECPLOT representations that may be captured within TECPLOT to produce a moving picture representation of the flow. This may be displayed through the FRAMER utility. The tecplot files are generated during the run when unsteady sampling is specified with a single run (no ensemble averaging).

The TECPLOT files deal only with the flowfield values. The surface values will generally be plotted as scatter or x-y plots and, if the descriptive text is edited out, the text data output in DS2GS.TXT is in a suitable form for TECPLOT. For unsteady flows, the word "ZONE" should be inserted between the records for the successive time intervals. The time interval may be included as the zone title.

The flow variables that are plotted in TECPLOT are distinguished by a code. The key to this is:-

X	*x* coordinate (m).
Y	*y* coordinate or, for axially symmetric flows, the radius (m).
Z	*z* coordinate (only for axi-sym flow and only if 3-D option is chosen).
N	number density (m^{-3}).
DN	density (kg m^{-3}).
U	velocity component in either the *x* or axial direction (m s^{-1}).
V	velocity component in either the *y* or radial direction (m s^{-1}).
W	velocity component in either the *z* or circumferential direction (m s^{-1}).
TT	translational temperature (K).
TR	rotational temperature (K).
TV	vibrational temperature (K).
T	overall temperature (K).
M	flow Mach number.
MC	the average number of simulated molecules per cell.
CTR	the ratio of the time step DTM to the local mean collision time
MFP	the local mean free path
CSR	the ratio of the mean separation between collision partners to the local mean free path
F1	fraction (by number) of species 1 in the flow *(mixture only).*
F2	fraction (by number) of species 2 in the flow.
..	... and so on ...(the code output assumes a maximum of 20 species).

Archive the current DS2GD.DAT file This causes the program to search for the lowest value of *n* that has not already been applied to an archived file DS2GA*n*.DAT. The current data file is copied as this file and the program then opens the archive record file DS2GA.TXT under the DOS text editor. This enables the details of the archived data file to be entered for future reference.

2.1.2 Subsidiary Screens (Green)

These appear after the Introductory Program Screen and the combination of screens depends on the choice that is made from the introductory screen.

Appears only for the "new case" option (choice of one of four options).

Create a completely new file The first option puts default values into all of the Data Screen items. The combination of default items does not lead to a valid data file and the desired data must be entered.

Modify the existing DS2GD.DAT file The second reads in the values from the existing DS2GD.DAT file. Any desired modifications may then be made as the data screens are cycled.

Re-run or modify an archived file This option leads to the selection of one of the archived data files DS2GA*n*.DAT files as the current data file.

Run a demonstration case

This selects one of the demonstration data files DS2GD*n*.DAT as the data file.

When either an archived or demonstration file is chosen, the data screens must be traversed by the "enter" key in order to generate a matching DS2GP.DAT file.

Appears only when an archived or demonstration file is to be selected.

Code number of the file

A integer less than equal to the number of available files is specified as the number *n* in the archive or demonstration file name. The help window displays the maximum integer that is available.

Appears only for the "continue" option with a time-averaged flow.

Extend an existing sample / Generate a new sample

The first option causes the existing sample for an assumed steady flow to be continued. The second option causes a new sample to be started and is useful if the number of print intervals to steady flow has been set in the data to an excessively small value. The screen has no effect if the flow has not reached the stage at which steady flow is assumed.

Appears only for the "TECPLOT" option with interfaces between regions.

Average across interfaces / Discontinuity at interfaces

The TECPLOT output file is divided into blocks that correspond to the flow regions. If the first option is chosen, the values in the two regions in either side of an interface between regions are averaged on the interface so that there will no discontinuities in the contours at the interface. The averaging requires extrapolation and this can sometimes cause problems that are avoided by the second option which bypasses the averaging.

Appears only for ensemble averaged (unsteady) flows.

Bypass cell report file / Generate cell report file

The cell report files can require significant time and this option allows them to be bypassed.

Appears only for ensemble averaged (unsteady) flows.

Bypass generation of text output
Text output for surface values only
Flowfield and surface text output

The output files DS2GF.TXT and DS2GM.TXT can be very large because they are generated at each print interval in an unsteady flow. Also, if many runs are made, the file need only generated after the final run.

The first of the three vertically listed choices bypasses the generation of the output file.

The second option provides output for the surface values only. As noted above, the TECPLOT output files are for flowfield values only, so that this will be a widely used option.

The third option leads to text output for both surface and flowfield properties.

2.2 Data Screens

The data screens are all blue in color. They are processed in a forward direction and the DS2GD.DAT file is modified progressively as "enter" is pressed for each screen. However, one can return to the first data screen by pressing the "F1" key. If one returns in this way, the changes that have already been made are preserved.

The program first copies DS2GD.DAT as DS2GD.OLD and, should the data generation process be abandoned by pressing the "esc" key, the original DS2GD.DAT file is restored through the renaming of DS2GD.OLD.

The altered or new values are confirmed in the new DS2GD.DAT file if the screens are progressed through to the end of the program by successive depression of the "enter" key.

All data is set in base SI units.

2.2.1 Introductory Data Screen

Flow geometry :

The space bar is used to toggle between the options of TWO-DIMENSIONAL in the *x-y* plane and AXIALLY SYMMETRIC about the *x* axis.

Steady or unsteady sampling

The flow is always unsteady but, with the STEADY option, the flow is assumed to be steady after a specified time and a time average of the flow properties is then accumulated. UNSTEADY averaging is employed when the unsteady flow is to be studied. If multiple runs are specified in the final screen, there is an ensemble average of the results over these runs.

Required only for axially symmetric flows.

Radial weighting factors :

These are used to increase the sample near the axis and decrease it at large radii. Molecules that are outside the reference radius and move towards the axis may be duplicated and those moving away from the axis may be removed. Molecule duplication can produce undesirable statistical effects, although a delay is imposed on duplication in steady flows. Radial weighting factors should be used with caution.

Required only for axially symmetric flows with weighting factors.

Reference radius for wt. factors (m) :

The weighting factors are all unity within this radius and are set equal to the ratio of the radius to the reference radius outside it. The molecular radius is used to define a molecule based weighting factor during the molecule move and output. For collisions, the weighting factor is based on the cell radius so that it does not vary from molecule to molecule within the cell.

Basic FNUM ratio :

This is the number of real molecules that are represented by each of the simulated molecules. If the number density was uniform, and in the absence of weighting factors, the number of simulated molecules would be equal to the product of the number density and the total volume of the flow divided by FNUM. When setting FNUM, account should be taken of the probable average number density, the presence of ant weighting factors (which will tend to reduce the required FNUM), and the fact that FNUM may vary with region in steady flows. A trial run will often be necessary to establish the value of FNUM that leads to the desired number of simulated molecules. In calculating the volume, a two-dimensional flow has a width of 1 m, while an axially symmetric flow occupies the full 2π azimuth angle.

Basic time step (s) : This is the time step or interval over which the molecular motion is uncoupled from the intermolecular collisions. This is normally set to a value such that the faster molecules move about one third of a cell width during a time step. It should be small in comparison with the local mean collision time. The time step may vary (along with FNUM) from region to region.

Type of gas : This chooses the gas species either as one of the eight preset cases or as a CUSTOM gas that requires the details to be entered in subsequent screens. Once a data file has been generated with a preset option, the CUSTOM option may be chosen in the modification of this file. The detailed gas screens then appear and the preset values for the gas may be modified.

If the preset gas is a mixture, it is necessary to know the species code numbers of the constituents. These are:

IDEAL AIR:- Oxygen is species 1 and nitrogen is species 2.

REAL AIR:- Oxygen is species 1, nitrogen is species 2, atomic oxygen is species 3, atomic nitrogen is species 4, and NO is species 5.

REAL NITROGEN:- Nitrogen is species 1 and atomic nitrogen is species 2.

ARGON-HELIUM:- Argon is species 1 and helium is species 2.

Number of regions : This sets the number of four-sided regions that will be set up by the data.

2.2.2 Introductory Gas Data Screen

This screen appears only when the CUSTOM gas option has been chosen.

Number of molecular species : Unity for a simple gas or the number of molecular species in a gas mixture.

Required only for gas mixtures.

Type of data for cross-collisions : The MEAN option causes the cross-sections, viscosity-temperature power laws, and VSS scattering parameters for collisions between unlike molecules (cross-collisions) to be set to the mean of the values for the separate species. The SEPARATE option leads to requests for values for all cross-collisions.

Required only for gas mixtures.

Number of species groups : Species groups may be employed to increase the efficiency of collision between particles with very different masses. Studies (Bird, 1994) have shown that, in general, this is worthwhile only when one of the species is an electron. The groups may also be used to implement species weighting factors (see next item). This item is generally set to unity.

Required only for gas mixtures and when there is more than one species group.

Weighting factors for species groups

Species weighting factors may be used to increase the sample of a trace species. However, in collisions between molecules with different weighting factors, the velocity components of one of the molecules will sometimes not be altered. This means that momentum and energy are not exactly conserved and there will be a step of a random walk at every such collision. This can lead to serious errors and species weighting factors should only be used when absolutely necessary.

Required only for gas mixtures.

Number of reactions :

Set to the total number of chemical reactions in the gas. Set to zero in a non-reacting gas.

Required only for gas mixtures with reactions.

Number of third-body tables :

This is greater than zero only when there are recombination reactions in which the identity of the third-body molecule is not specified. Each table provides data on the relative efficiency of the species as third-bodies in one recombination.

2.2.3 Group Weighting Factor Screen

Appears only for CUSTOM gas mixtures with more than one group and when group weighting factors are employed. The screen is repeated for each group.

Weighting factor of group :

This weighting factor multiplies FNUM for this species. A value greater than unity decreases the relative prevalence of this group, and vice-versa.

2.2.4 Main Species Data Screen

Appears only for CUSTOM gases. It is the first screen in a loop over the molecular species and the code number of the species being set appears with the title at the top of the screen.

Reference diameter (m) :

The effective diameter of the molecule at the reference temperature.

Reference temperature (K) :

The reference temperature for the molecular diameter.

Viscosity temperature power law :

This controls the way in which the cross-section changes with relative velocity in collisions. It is 0.5 for hard sphere molecules, 1.0 for Maxwell molecules and of the order of 0.75 for real molecules.

Reciprocal of VSS scattering param.

Unity for the VHS model. The VSS

model is necessary only for gas mixtures when both the viscosity and diffusion coefficients are to be accurately modelled.

Molecular mass (Kg) :

Required only for gas mixtures.

Group in which the species lies :

Enter 1 if groups are not implemented, otherwise the group.

No. of rotational degrees of freedom

Zero for monatomic molecules, two for diatomic molecules, and generally three for polyatomic.

Required only for species with rotational degrees of freedom.

Temperature depend. of rotl. relax.

Choices are a CONSTANT value or a second order POLYNOMIAL in temperature.

Required only for mixtures and a species with internal degrees of freedom.

Partner dependence of relax. rates

Choices are to have relaxation rates that are COMMON to all collision partners, or rates that are DEPENDENT on the species of the collision partner. This applies to both the rotational and vibrational rates.

2.2.5 Rotational Mode Data Screen

Also in the loop over the molecular species of CUSTOM gases and is required only if the species has rotational degrees of freedom.

Should the rates in a mixture be species dependent (set as final item on previous screen), the values in this screen ate for collisions between like molecules.

Rotational relax. coll. number :

This is a the constant value of the rotational relaxation collision number if that option has been chosen in the second last item in the previous screen. If the option for a polynomial in the temperature had been chosen, it is the constant in the polynomial.

Required only if there is a polynomial for the rotational collision number.

Coefficient of temperature :

The coefficient of temperature in the second order polynomial.

Required only if there is a polynomial for the rotational collision number.

Coeff. of the square of temperature :

The coefficient of temperature squared in the second order polynomial.

The number of vibrational modes :

Set to zero if there are no vibrational modes or if these need not be taken into account. In the case of degenerate modes, the degeneracy should be added to the total.

2.2.6 Vibrational Mode Data Screen

Also in the loop over the species of CUSTOM gases and is required only if there are *vibrational modes. It is repeated in a loop over the number of vibrational modes.*

Should the rates in a mixture be species dependent, the values for like molecules are set in this screen.

The characteristic vibrational temp. Enter the value for this species in degrees K.

The constant C1 in eqn. (6.53) : The vibrational relaxation collision number is assumed to be either a constant or available in the form of eqn (6.53) of Bird (1994). This is

$$Z_v = (C_1/T^{\omega}) \exp(C_2 T^{-1/3})$$

where T is the temperature and ω is the temperature exponent of the coefficient of viscosity. Depending on the following item, either the constant value or the constant C_1 is entered here.

The constant C2 in eqn. (6.53) : Either -1. or the constant C_2 is entered here. The negative value indicates that the vibrational relaxation collision number is a constant equal to the preceding value. Both constants are in SI units.

2.2.7 Cross-collision Basic and Rotational Data Screen

Also in the loop over species.

Required only for gas mixtures in which the either the SEPARATE option has been chosen in the basic gas data screen or the DEPENDENT option has been chosen in the main species data screen.

The screen is repeated for all species other than that in the current loop and the combination of species is shown in the title of the screen.

First four items are required only for the SEPARATE option.

The reference diameter (m) : Based on the collision cross-section for this pair of species.

at the reference temperature (K) : The temperature on which the above cross-section is based.

Viscosity-temperature power law : Viscosity data is available for many combinations.

Reciprocal of VSS scatter parameter These can be quite different from the mean values.

Final three items are required only for species with rotational degrees of freedom and only if the DEPENDENT option was chosen in the main data screen for this species.

Constant, or const. in polynomial : Depends on the choice that was made in the main species data screen.

Final two items are required only if the POLYNOMIAL option was chosen in the main data screen for this species.

Coeff. of temperature in polynom. :

Coeff. of temp. squared in poly. :

2.2.8 Cross-collision Vibrational Screen

The final screen in the loop over species.

Required only for gas mixtures when the species has vibrational modes and when the DEPENDENT option has been chosen in the main species data screen.

The screen is repeated for all species other than that in the current loop and the combination of species is shown in the title of the screen.

The constant C1 in eqn. (6.53) : As for the like collisions.

The constant C2 in eqn. (6.53) : AS for the like collisions.

2.2.9 Basic Reaction Data Screen

This is required only for CUSTOM gases if there are chemical reactions and is repeated in a loop over the reactions.

The logic assumes that the reaction is one of:

> *A dissociation reaction in which one molecule in a binary collision splits into two separate molecules or atoms.*
>
> *An exchange reaction in which the two molecules or atoms in a binary reaction change their species.*
>
> *A recombination reaction which requires a ternary or three-body collision. Two of the atoms or molecules combine into a single molecule, while the third-body molecule does not change its identity.*

Species of first pre-coll. mol. : The pre-collision species code number of one of the molecules other than the third-body molecule in a recombination.

Species of second pre-coll. mol. : The pre-collision species code number of the second molecule other than the third-body molecule in a recombination.

First post-collision parameter : This varies with the type of the reaction and identifies the type of reaction. For a dissociation it is the code of the first post-collision species. It is set to zero for an exchange reaction or to -1 for a recombination.

Second post-collision parameter : The species code of the second post-collision species in a dissociation. The species code of the first post-collision species for an exchange reaction. The species code of the recombined molecule for a recombination.

Third post-collision parameter : The species code of the third post-collision species for a dissociation. The species code of the second post-collision species for an exchange reaction. In the case of a recombination it is the species code of the third-body molecule or, if this is not fixed, the negative of the code number of the third-body table.

Number of internal deg. of freedom : The logic converts the reaction rates into steric factors. This is based on eqn (6.10) of Bird (1994). This is an arbitrary parameter, but the temperature exponent in the Arrhenius equation cannot be more negative than the negative of the sum of this number and 3/2. Large negative values of this exponent are associated with reactions in which there is a large contribution from the internal degrees of freedom.

Activation energy (J) : The relative translational energy and contributing internal energy must exceed this energy for a reaction to be possible.

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 $molecule^{-1}s^{-1}$ for a binary reaction and $m^6molecule^{-1}s^{-1}$ for a ternary reaction.

The temperature exponent : The parameter η in the above equation.

The energy of the reaction (J) : This is positive for an exothermic reaction and negative for an endothermic reaction. In the latter case it is generally the negative of the activation energy.

2.2.10 Third-body Screen

This is only for CUSTOM gases. It is repeated for each table in a loop over the number set as the last item in the introductory gas screen.

It is repeated for each species and the screen title lists the table number and the species code.

Relative effectiveness of species : 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.

2.2.11 Stream Data Screen

Stream or initial gas :

There are two options. PRESENT if there is a stream or initial gas or ABSENT if there is not.

Number of molecule input files :

These generate input molecules along one side of one of the regions. There can be up to three files DGMIFn.DAT and they must have been produced by the renaming of molecule output files from other runs of DS2G.

Number of molecule output files :

Up to three files DGMOFn.DAT are generated from the molecules crossing the specified sides and regions.

The next four items are required only if the stream is PRESENT.

Stream temperature (K) :

The stream is in equilibrium at this temperature.

Stream number density ($/m^3$) :

Velocity component in x dirn. (m/s) :

Velocity comp. in the y dirn. (m/s) :

Initial state of the flowfield :

There are four options to indicate whether the flowfield is initially a uniform stream or a VACUUM, a STREAM (as specified above), is specified BY REGION through the next two screens, or is filled with molecules from the current RESTART FILE DS2GM.DAT. The last option is primarily to allow the calculation of a lower Knudsen number case to start from the fully developed steady flow in a higher Knudsen number case. This greatly reduces the time preceding the development of steady flow in very low Knudsen number case, particularly when the unsteady process largely depends on the diffusion of viscosity. The geometry of the flow must be the same in each case as far as the region boundaries are concerned, although the number and spacing of cells may be changed. Also, the FNUM ratio must be increased in direct proportion to the freestream density so that the total number of simulated molecules is the same in each case.

2.2.12 Stream Composition Screen

Required only if there is a stream and the gas is a mixture. It is then repeated for each of the species.

Fraction of species :

These are number fractions and their sum must be unity.

2.2.13 Region Dependent Initial Gas Screen

Required only if the BY REGION option was chosen for the initial state.

Initial state :

There are three options. VACUUM if there is initially no gas in this region, STREAM if it is initially set as stream, or AS BELOW if it is set to the conditions specified below. The STREAM option is valid only if a stream has been defined.

Region temperature (K) :

The gas is in equilibrium at this temperature.

Region number density (/m^3) :

Velocity component in x dirn. (m/s) :

Velocity comp. in the y dirn. (m/s) :

2.2.14 Initial Gas Composition Screen

Required only if the BY REGION option was chosen and the gas is a mixture. It is then repeated for each of the species.

Fraction of species :

These are number fractions and their sum must be unity.

2.2.15 Basic Region Data Screen

The first screen in a loop over the regions.

Ratio of FNUM and DTM :

FNUM is the number of real molecules represented by each simulated molecule (apart from the effects of radial and species weighting factors) and DTM is the time step over which the molecular motion and collisions are decoupled. The basic values of these quantities were specified in the introductory data screen and are multiplied by this factor in this region. Because both FNUM and DTM are altered by the same amount, the fluxes of the molecules between regions is not affected. This essentially allows the regions of steady flows to be calculated on different time scales. The unsteady phase in not then physically accurate and this ratio is unity for all regions in an ensemble-averaged unsteady flow. For unsteady flows, a positive value other than unity sets the number density in the region to this ratio times the standard number density, while a negative value similarly sets a temperature ratio. However, it is recommended that region dependent values be set explicitly through the Initial Gas Data screen which was introduced in Version 2.1.

Cell segments along sides 1 and 3 :

The cells are used for the sampling of the flow properties and for setting the collision rate. Sides 1 and 3 may be curved.

Cell segments along sides 2 and 4 :

Sides 2 and 4 are always straight.

The geometry specification of side 1

There are five choices for the specification of the geometry of side 1. "Point-by-point" requires the specification of every cell vertex along the side.

"Straight line" is the default choice and this requires only the coordinates of the intersection of side 1 with side 2 and those of the intersection of side 1 and side 4.
"Conic section" enables the side to be specified as a segment of a conic.
"Coincident" sets the side as being coincident with a previously defined side.
"Segmented" allows the side to be specified by a combination of the above four choices.

The geometry specification of side 3

The choices are the same as those for side 1.

The cell spacing along side 2 :

The straight side 2 may be divided in three ways to form the cell divisions.
"Equal elements" is the default choice.
"Arithmetic progression" leads to the elements being in an arithmetic progression.
"Arbitrary" requires the input of numbers proportional to the length of each cell element.

The cell spacing along side 4 :

The options are similar to those for side 2.

Weighting on 1-3 divisions :

The corresponding points on sides 1 and 3 are joined by straight lines. These lines are divided into intervals by the lines that define the cells. The intervals along sides 2 and 4 are defined in the above two items and the intervals along the intermediate lines are a weighted mean of these. This data defines the weighting for these mean values.

2.2.16 Side 1 Screen for "Point-by-Point" Option

This screen is repeated in a loop over the number of points on the side. The first point is at the intersection of sides 1 and 2, while the final point is at the intersection of sides 1 and 4. The points are at the cell vertices.

x coordinate (m)

The x coordinate of the point.

y coordinate (m)

The y coordinate of the point.

2.2.17 Side 1 Screen for "Straight Line" Option

x coordinate of startpoint (m) :

The startpoint is at the intersection with side 2.

y coordinate of startpoint (m) :

x coordinate of endpoint (m) :

The endpoint is at the intersection with side 4.

y coordinate of endpoint (m) :

Segment size ratio :

If this item is left at its default value of unity, the cell elements along side 1 are of equal length. If it is other than unity, the elements are in a arithmetic progression. Positive values define the ratio of the cell element adjacent to side 4 to that adjacent to side 2. The absolute value of a negative number defines the ratio of the size of the central element to that of the end elements.

2.2.18 Side 1 Screen for "Conic Section" Option

The side is a segment of the general conic section with the radial coordinate r and the angular (measured from the x axis which fixes the alignment of the conic) coordinate θ (both relative to the focus) given by

$$r = p\,/\,(\,1 - e\cos\theta\,)\,,$$

where p is the value of the radial coordinate when θ is $\pi/2$, and e is the eccentricity. The side is specified by the coordinates of the focus, the values of p and e, the angular coordinates of the endpoints of the side from the line through the focus parallel to the x axis, and the size ratio of the elements (these are in arithmetic progression based on the angle). Note that, when the eccentricity is zero, the side is an arc of the circle with its center at the focus and radius equal to p. The side is a portion of an ellipse if the eccentricity is less than unity, a parabola if it is equal to one, and a hyperbola if it is greater than one. Note that the major axes must be parallel to the x axis.

x coord. of focus of conic (m) :

y coordinate of focus (m) :

The parameter p (m) :

The eccentricity e :

Angle from x dirn. to startpoint (rad)

This is at the intersection with side 2.

Angle from the x-dirn. to endpoint

This is at the intersection with side 4.

Segment angular size ratio :

If this item is left at its default value of unity, the cell elements along side 1 are of equal angular extent. If it is other than unity, the elements are in an arithmetic progression. Positive values define the ratio of the cell element adjacent to side 4 to that adjacent to side 2. The absolute value of a negative number defines the ratio of the size of the central element to that of the end element.

2.2.19 Side 1 Screen for "Coincident" Option

The adjacent region number :

The region in which the identical side lies.

Number of the corresponding side : The code number of the side of that region. If the points are in reverse order, the negative of the side number is entered. The coordinates of all points along the sides must be coincident.

2.2.20 Side 1 Screen for "Segmented" Option

The number of type segments : This sets the number od "input type’ segments into which the side is divided.

2.2.21 Side 1 Segment Type Screen

This and the following "side segment" screens are repeated in a loop over the number that was set in the preceding screen.

The type of the segment : There are four choices for the specification of the geometry of each segment.
"Point-by-point" requires the specification of every cell vertex along the segment.
"Straight line" is the default choice and this requires only the coordinates of the startpoint (first segment only) and the endpoint.
"Conic section" enables the segment to be specified as a segment of a conic.
"Coincident" sets the segment as being coincident with a previously defined side.

Number of elem. along the segment : These are cell elements and the total over all segments must equal the number of cells along the side.

2.2.22 Side 1 Segment Screen for "Point-by-Point" Option

This screen is repeated in a loop over the number of points on the segment. The first point is that nearest the intersection of sides 1 and 2, while the final point is that nearest the intersection of sides 1 and 4.

x coordinate (m) The *x* coordinate of the point.

y coordinate (m) The *y* coordinate of the point.

2.2.23 Side 1 Segment Screen for "Straight Line" Option

The startpoint coordinates are required only for the first segment.

x coordinate of startpoint (m) : The startpoint is at the intersection with side 2.

y coordinate of startpoint (m) :

x coordinate of endpoint (m) : The endpoint is nearest the intersection with side 4.

y coordinate of endpoint (m) :

Segment size ratio :

If this item is left at its default value of unity, the cell elements along side 1 are of equal length. If it is other than unity, the elements are in an arithmetic progression. Positive values define the ratio of the cell element nearest to side 4 to that nearest to side 2. The absolute value of a negative number defines the ratio of the size of the central element to that of the end elements.

2.2.24 Side 1 Segment Screen for "Conic Section" Option

The conic section is as described for the full side.

x coord. of focus of conic (m) :

y coordinate of focus (m) :

The parameter p (m) :

The eccentricity e :

Required only for the first segment.

Angle from x dirn. to startpoint (rad)

This is at the intersection with side 2.

Angle from x-dirn. to endpoint (rad)

This is nearest the intersection with side 4.

Segment angular size ratio :

If this item is left at its default value of unity, the cell elements along the segment are of equal angular extent. If it is other than unity, the elements are in an arithmetic progression. Positive values define the ratio of the cell element nearest to side 4 to that nearest to side 2. The absolute value of a negative number defines the ratio of the size of the central element to that of the end elements.

2.2.25 Side 1 Segment Screen for "Coincident" Option

The adjacent region number :

The region in which the identical side lies.

Number of the corresponding side :

The code number of the side of that region. If the points are in reverse order, the negative of the side number is entered. The coordinates of all points along the segment and side must be coincident.

2.2.26 Side 3 Screen for "Point-by-Point" Option

This screen is repeated in a loop over the number of points on the side. The first point *is at the intersection of sides 3 and 2, while the final point is at the intersection of sides 3 and 4.*

x coordinate (m)

The *x* coordinate of the point.

y coordinate (m)

The *y* coordinate of the point.

2.2.27 Side 3 Screen for "Straight Line" Option

x coordinate of startpoint (m) :

The startpoint is at the intersection with side 2.

y coordinate of startpoint (m) :

x coordinate of endpoint (m) :

The endpoint is at the intersection with side 4.

y coordinate of endpoint (m) :

Segment size ratio :

If this item is left at its default value of unity, the cell elements along side 3 are of equal length. If it is other than unity, the elements are in an arithmetic progression. Positive values define the ratio of the cell element adjacent to side 4 to that adjacent to side 2. The absolute value of a negative number defines the ratio of the size of the central element to that of the end elements.

2.2.28 Side 3 Screen for "Conic Section" Option

The conic is similar to that described in § 2.2.18.

x coord. of focus of conic (m) :

y coordinate of focus (m) :

The parameter p (m) :

The eccentricity e :

Angle from x dirn. to startpoint (rad)

This is at the intersection with side 2.

Angle from x-dirn. to endpoint (rad)

This is at the intersection with side 4.

Segment angular size ratio :

If this item is left at its default value of unity, the cell elements along side 1 are of equal angular extent. If it is other than unity, the elements are in an arithmetic progression. Positive values define the ratio of the cell element adjacent to side 4 to that adjacent to side 2. The absolute value of a negative number defines the ratio of the size of the central element to that of the end element.

2.2.29 Side 3 Screen for "Coincident" Option

The adjacent region number :

The region in which the identical side lies.

Number of the corresponding side :

The code number of the side of that region. If the points are in reverse order, the negative of the side number is entered. The coordinates of all points along the sides must be coincident.

2.2.30 Side 3 Screen for "Segmented" Option

The number of type segments :

This sets the number od "input type’ segments into which the side is divided.

2.2.31 Side 3 Segment Type Screen

This and the following "side segment" screens are repeated in a loop over the number that was set in the preceding screen.

The type of the segment :

There are four choices for the specification of the geometry of each segment.
"Point-by-point" requires the specification of every cell vertex along the segment.
"Straight line" is the default choice and this requires only the coordinates of the startpoint (first segment only) and the endpoint.
"Conic section" enables the segment to be specified as a segment of a conic.
"Coincident" sets the segment as being coincident with a previously defined side.

Number of elem. along the segment :

These are cell elements and the total over all segments must equal the number of cells along the side.

2.2.32 Side 3 Segment Screen for "Point-by-Point" Option

This screen is repeated in a loop over the number of points on the segment. The first point is that nearest the intersection of sides 3 and 2, while the final point is that nearest the intersection of sides 3 and 4.

x coordinate (m)

The *x* coordinate of the point.

y coordinate (m)

The *y* coordinate of the point.

2.2.33 Side 3 Segment Screen for "Straight Line" Option

The startpoint coordinates are required only for the first segment.

x coordinate of startpoint (m) :

The startpoint is at the intersection with side 2.

y coordinate of startpoint (m) :

x coordinate of endpoint (m) :

The endpoint is nearest the intersection with side 4.

y coordinate of endpoint (m) :

Segment size ratio :

If this item is left at its default value of unity, the cell elements along side 1 are of equal length. If it is other than unity, the elements are in an arithmetic progression. Positive values define the ratio of the cell element nearest to side 4 to that nearest to side 2. The absolute value of a negative number defines the ratio of the size of the central element to that of the end elements.

2.2.34 Side 3 Segment Screen for "Conic Section" Option

The conic section is as described for side 1.

x coord. of focus of conic (m) :

y coordinate of focus (m) :

The parameter p (m) :

The eccentricity e :

Required only for the first segment.

Angle from x dirn. to startpoint (rad)

This is at the intersection with side 2.

Angle from x-dirn. to endpt. (rad)

This is nearest the intersection with side 4.

Segment angular size ratio :

If this item is left at its default value of unity, the cell elements along the segment are of equal angular extent. If it is other than unity, the elements are in an arithmetic progression. Positive values define the ratio of the cell element nearest to side 4 to that nearest to side 2. The absolute value of a negative number defines the ratio of the size of the central element to that of the end elements.

2.2.35 Side 3 Segment Screen for "Coincident" Option

The adjacent region number : The region in which the identical side lies.

Number of the corresponding side : The code number of the side of that region. If the points are in reverse order, the negative of the side number is entered. The coordinates of all points along the segment and side must be coincident.

2.2.36 Side 2 Screen for "Arithmetic Progression" Option

Size ratio from side 3 to 1 : If this number is positive, it is the cell element length ratio from side 3 to side 1. The magnitude of a negative number defines the ratio of the central element to the end elements.

2.2.37 Side 2 Screen for the "Arbitrary" Option

This screen is repeated for each cell element along side 2.

Number prop. to sub-cell segment : These numbers are summed and the element fractional lengths are equal to the number divided by the sum.

2.2.38 Side 4 Screen for "Arithmetic Progression" Option

Size ratio from side 3 to 1 : If this number is positive, it is the cell and cell element length ratio from side 3 to side 1. The magnitude of a negative number defines the ratio of the central element to the end elements.

2.2.39 Side 4 Screen for the "Arbitrary" Option

This screen is repeated for each cell element along side 4.

Number prop. to sub-cell segment : These numbers are summed and the element fractional lengths are equal to the number divided by the sum.

2.2.40 Side Specification Screen

The type of the side : There are eight options:-

"Axis"	This is valid only for axially symmetric flows and the side must lie on the *x* axis.
"Plane of symm."	This must be a straight side and, for axially symmetric flows, it must be normal to the axis. It is functionally equivalent to a specularly reflecting side with so sampling of surface properties.

"Stream bound."	An interface with the uniform stream.
"Specified flow"	A non-uniform entry flow is defined by the gas composition and flow properties at each element along the side.
"Solid surface"	This may have uniform or non_uniform properties and may have a velocity in its plane.
"Outgas surface"	A surface with superimposed outgassing.
"Interface"	A boundary with one or more sides of other regions.
"Vacuum or M.E."	Either an interface with a vacuum or a surface across which file entry molecules are introduced.

Applies only to specified flows or surfaces.

Distribution of properties :

There are three options:-

"Uniform"	This indicates that a single set of values applies to the whole side.
"Variable"	Requires the specification of the flow or surface properties at every cell element along the side.
"Power-Law"	The values at the ends of the side are specified and the other values follow a power-law distribution.

Applies only to the "Power-Law option

Index of power-law:

If the powerlaw is η, the value at distance s along a side of length l is

$$v = v_1 + (s/l)^{\eta}(v_2 - v_1).$$

Here, v_1 and v_2 are the values at the beginning and end of the side, respectively.

Applies only to interfaces.

The number of adjoining sides :

The number of sides of other regions that wholly or partially adjoin this side.

2.2.41 Specified Flow Property Screen

If the "uniform" option has been chosen, a single screen applies to the whole side (although this is titled "Element 1").

If the "variable" option has been chosen, the screen is repeated for each cell element.

If the power-law option has been chosen, a screen appears for each end of the line.

x velocity component (m/s) :

y velocity component (m/s) :

Temperature (K) :

Number density (/m3) :**

2.2.42 Specified Flow Composition Screen

This screen is required only for gas mixtures and is then repeated for each species.

If the "uniform" option has been chosen, a single screen applies to the whole side (although this is titled "Element 1").

If the "variable" option has been chosen, the screen is repeated for each cell element.

If the power-law option has been chosen, a screen appears for each end of the line.

Fraction of species :

2.2.43 Surface Screen

This screen is repeated for each species.

If the "uniform" option has been chosen, a single screen applies to the whole side.

If the "variable" option has been chosen, the screen is repeated for each cell element.

If the power-law option has been chosen, a screen appears for each end of the line.

Temperature of the element (K) : If this is set as a negative number, the surface is regarded as specularly reflecting for this species.

Indicates diffuse or CLL model : The default value is -1. and this leads to diffuse reflection with complete thermal accommodation. A value other than -1 specifies that the CLL (Cercignani-Lampis-Lord) model is to be used and, if the species has internal energy modes, this value is the accommodation coefficient for the internal modes of this species and must be between 0 and 1.

Applies only to CLL model.

Normal energy accomm. coeff. : The accommodation coefficient for the energy based on the normal component of the translational velocity of the incident molecule.

Applies only to CLL model.

Tangential mom. acc. coeff : Note that this coefficient is based on momentum while the previous one was based on energy. This avoids a singularity.

Fraction adsorbed at surface : This fraction of this species are simply removed from the calculation on striking the surface. This can simulate a cryogenic surface.

Applies only to outgassing surfaces.

The outgas mass flux (kg/m2/s) :**

This is the flux for this species and it is assumed that the molecules leaving the surface are completely accommodated to the surface temperature and effuse with a diffuse angular distribution.

Surface in-plane velocity (m/s) :

While the geometry is fixed, the surfaces may have a velocity that is parallel to the surface. This is the component of that velocity that lies in the plane of the flow.

If the flow is two-dimensional

Surf. cross-plane velocity (m/s) :

This is the component of the surface velocity that is normal to the plane of the flow.

or, for axially symmetric flows.

Surf. cross-plane vel. (m/s or rad/s) :

For positive values, this is the circumferential velocity component of the surface velocity. However, for negative values, it is an angular velocity.

Probability of catalytic recomb. :

A surface may act as a catalyst for the recombination of atoms to a molecule. It is assumed that the "residence time" of the atoms on the surface is such that "collisions" effectively occur at the surface. The data is the probability that a single atom striking the surface recombines. This fraction obviously cannot exceed 0.5 and will generally be very much smaller. The necessary physical data for the recombination is taken from the data for the corresponding gas phase recombination. A finite value for this fraction therefore requires that the data for this reaction be set.

2.2.44 Interface Screen

This screen is repeated for each of the sides that adjoin the side.

The adjacent side :

The code number of the adjacent side.

The region in which it lies :

The code number of the region.

Displacement in the x dirn:

The *x* coordinate of the molecule is altered by this amount in the transfer.

Displacement in the y dirn:

The *y* coordinate of the molecule is altered by this amount in the transfer.

The displacements are zero when transferring molecules between adjacent regions. Finite displacements can be used to set up periodic boundaries such that the molecules leaving a downstream boundary re-enter across the upstream boundary. For periodic boundaries, the 'adjacent side' may be another side in the same region.

2.2.45 Molecule Input File Screen

This is repeated for each of the (up to 3) files.

The region code : This is the region into which the molecules enter.

The side of this region : This side must have been specified as a "Vacuum or M.E." side.

Molecules per record : The entry file is divided into records that are read at random. Only one record is in the memory at any time and entry molecules are read from it at random.

Records on the file : The file is a renamed output file and these must correspond to the corresponding settings for the original output file.

2.2.46 Molecule Output File Screen

This is repeated for each of the (up to 3) files.

The region code :

The side of this region : This may be within the flow (e.g. an interface.

Molecules per record :

Records in the file :

Required only for an axially symmetric flows with radial weighting factors.

Weighting factor action : "REMOVE" writes the files as if weighting factors were not present. "RETAIN" preserves the weighting factors.

File completion action : The computation may either continue or stop when the output file has been completed. If there are other output files, the program will not stop until they have all been completed.

2.2.47 Computational Parameter Screen

The first five items are for time-averaged (steady) flows.

Time steps between sampling : The time step is usually chosen such that a typical molecule moves about one third of the way across a cell in one step. This number is usually in the range two to four.

Samples between prints : This sets the interval at which the restart file DS2GR.DAT and the output files DS2GS.TXT, DS2GF.TXT, and DS2GM.TXT are written.

Prints to assumes steady flow : The flowfield and surface sampling is reset at the start of each print interval less than value. The time average starts with this interval but, if the program is re-started, there is an opportunity to start a new average. This is useful if the original estimate of the steady flow time is too small.

Molecule multiplication factor : The unsteady phase of the flow may require an excessively long computation time. This enables the flow to be started with a small number of molecules and, at 80% of the steady flow time, the molecules are multiplied by this factor.

Number of prints to STOP : A run is usually stopped interactively by "Ctrl C" and this is usual set to a very large integer such that it would not be reached in any reasonable time. **The flow should not be stopped by "Ctrl C" while the restart file is being written because this may result in a defective file.**

For unsteady flows, the preceding items are replaced by the following five items.

Time steps between sample/print : This is the number of time steps between the generation of the unsteady sampling file U*n*.DGF and the updating of the text output file record.

Steps for short time average : A local average is taken over this number of time steps.

Number of prints in each run : This sets the length of the run.

Number of runs to STOP : The run is repeated this number of times unless stopped interactively. The number of runs should be set to one if the flow is not repeatable (e.g. in the study of flow instabilities. When it is set to unity, the TECPLOT files are generated during the run.

Maximum number of molecules : This is an estimate of the number of simulated molecules that will be generated and largely controls the memory requirement. The parameter FNUM is ideally chosen such that the number of simulated molecules grows to just under this value. Should it be exceeded, the DIMENSION’s are reallocated in order to increase it by 10%, as long as the additional memory is available!

3 DEMONSTRATION CASES

A set of data files DS2GDnnn.DAT serve as both tutorial examples for the application of the program and as a suite of test cases for its continuing validation as new features are added. In order to run one of these files, the "Generate and run a new case" option must be chosen from the first screen, followed by the "Run demonstration case" from the second screen. The "enter" key should then be used to step through the data file. This is necessary to generate the consistent DS2GP.DAT file, and also provides a tutorial overview of the data.

3.1 Steady supersonic flow of air past sphere (DS2GD001.DAT)

This calculates the flow of a 1,000 m/s stream of ideal air past a sphere of radius 0.1 m. The stream number density is 3×10^{20} /m^3 and there is diffuse reflection at the surface with complete accommodation to the surface temperature which is equal to the freestream static temperature of 300 K. The mean free path is about 1 twentieth of the sphere radius and the computational grid of Fig. 3 was adequate only because the transient sub-cells reduced the mean spacing of the collision pairs to a value well below the mean free path.

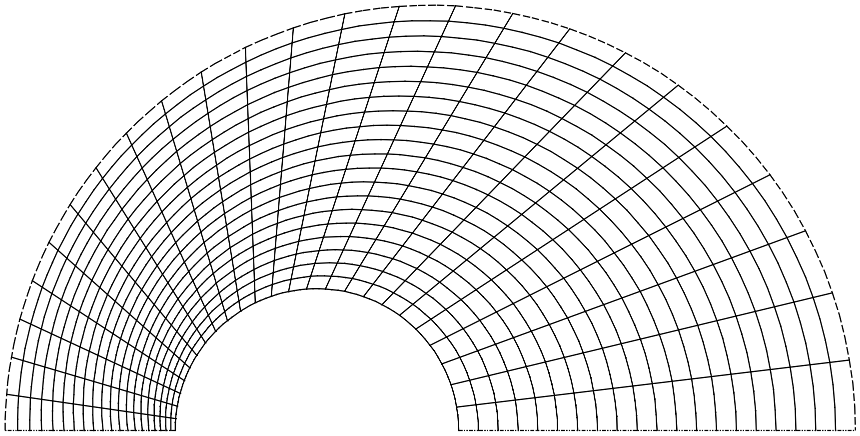

Fig. 4. Cell structure associated with DS2GD001.DAT.

There is just one region in the flow. Side 1 is the surface of the sphere, side 2 is the upstream portion of the axis, side 3 is a boundary with the stream, and side 4 is the downstream region of the axis. The stream boundary is exact for the upstream region of the undisturbed flow, but there will be some boundary interference to the disturbed region of the flow. The contours of constant Mach number are shown in Fig. 4 and these show that the Mach number based on the velocity component normal to the outer boundary would be supersonic over most of the downstream boundary. It is almost certain that the outer boundary is sufficiently far from the body for there to be no serious boundary interference, but the only way to prove this is to make matching calculations with the outer boundary in different locations.

The contours of Mach number and those for the overall temperature in Fig. 5 have been generated by the TECPLOT post-processing program using the file DS2GT.TEC that is generated by choosing the "TECPLOT" option in the menu for the initial options.

The quantity CTR in the TECPLOT file time step exceeds the mean collision time in the stagnation region and DTM should be reduced in the data.

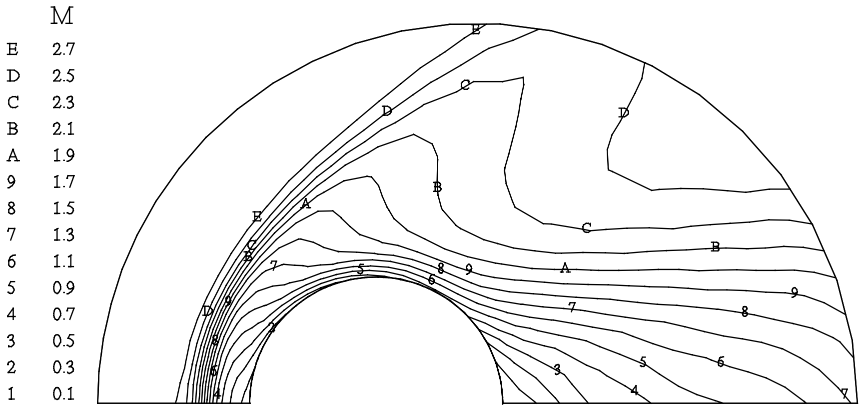

Fig. 5. Contours of constant Mach number for DS2GD001.PLT.

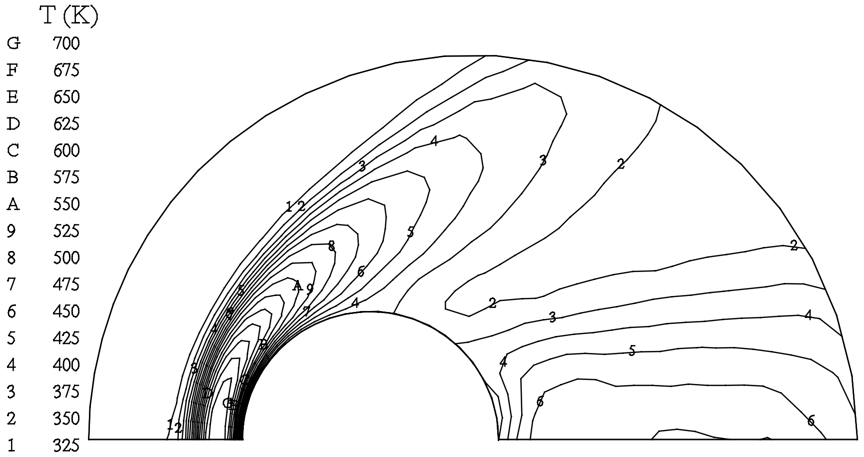

Fig. 6. Temperature contours for DS2GD001.DAT.

3.2 Steady 2-D internal expansion (DS2GD002.DAT)

This is the expansion of the stream from an infinite set if regular two-dimensional sonic slits. The upper and lower boundaries are, therefore, planes of symmetry. The flow is divided into two regions, as shown in Fig. 6. The lower region is bounded on the left by a diffusely reflecting surface and the upper region by the sonic inflow boundary. The right hand boundary is a vacuum and that between the regions is, of course, an interface. With the exception of those along the surface, the cell spacing is regular.

A representative set of streamlines are shown in Fig. 7, while the contours of constant Mach number are shown in Fig. 8. The expansion in the upper region of the flow is supersonic, but the lower region is largely subsonic. The vacuum boundary exerts a strong influence on the subsonic region and the sonic line very nearly intersects the downstream end of the lower plane of symmetry.

A vortex is formed downstream of the diffusely reflecting vertical surface. The magnitudes of the flow velocities in this vortex are small in comparison with the velocities in the bulk of the stream.

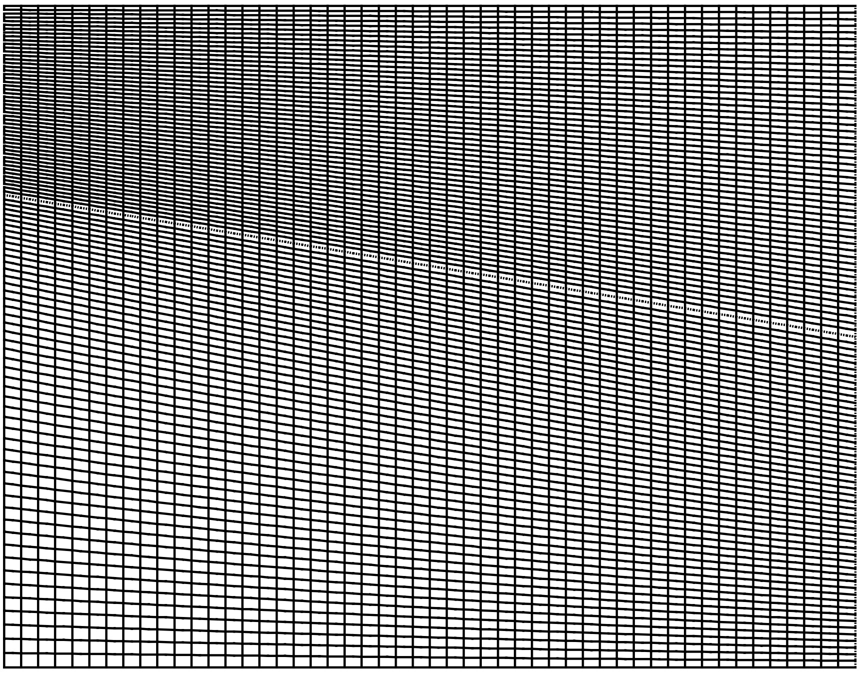

Fig. 7. Cell structure for test case DS2GD002.DAT.

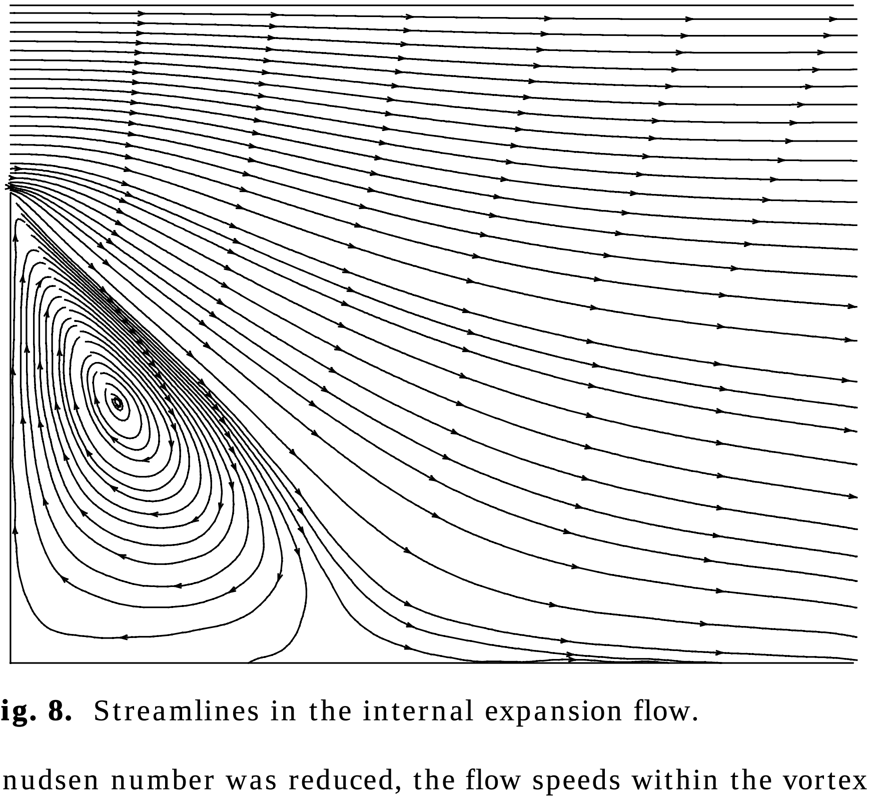

Fig. 8. Streamlines in the internal expansion flow.

If the Knudsen number was reduced, the flow speeds within the vortex would be expected to increase and, eventually, it would be desirable to double the size if the flowfield because the lower boundary would not necessarily be a plane of symmetry in a real flow. The separated region may become unsteady, but it would be a formidable task to study this case as an unsteady flow.

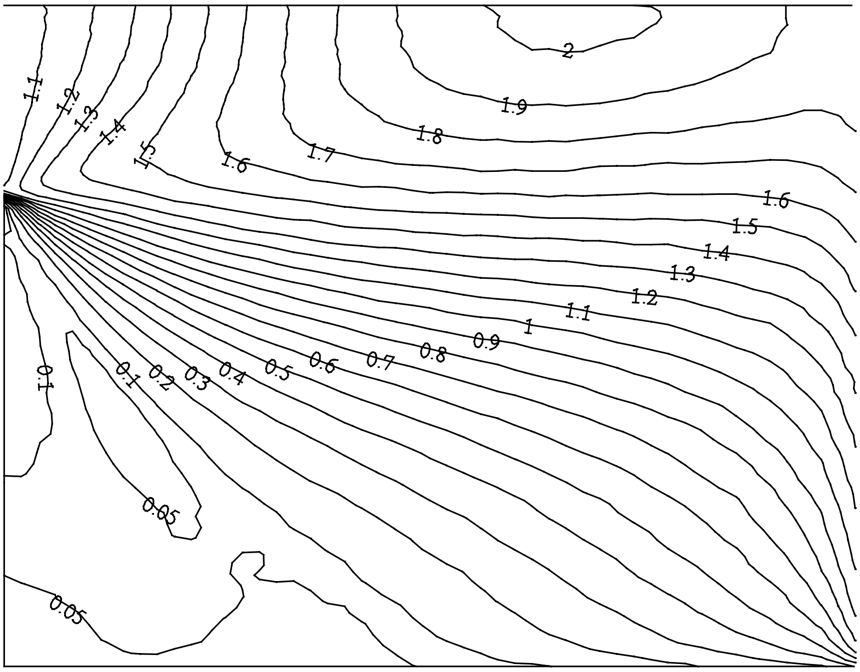

Fig. 9. Contours of constant Mach number.

3.3 Unsteady flow past a vertical flat plate (DS2GD003.DAT)

This case involves a vertical flat plate of height 0.2 m that is placed instantaneously into a uniform supersonic stream of argon at 1000 ms^{-1}. The undisturbed number density is 3×10^{20} m^{-3} and the temperature of both the stream and the surface is 300 K. The flow is symmetrical about the centreline of the plate and only the upper half is computed. There are three rectangular regions, the first extends 0.15 m directly upstream of the plate, the second directly downstream by an equal amount, and the third extends across the other two and has a height equal to the semi-height of the plate. The cell size is uniform across the regions.

The problem has been set up with "unsteady sampling" and ensemble averaging in order to study the establishment of steady flow about the plate. The most useful indicator of the establishment of steady flow is generally given by the total number of molecules in the flow. This is included in the on-screen information during the running of the program. In this case, the build-up in front of the plate is initially matched by the decline in the number of molecules behind the plate. There is then a systematic increase in the number with the steady flow value being attained before 1 ms.

The change in pressure on a vertical plate from the initial impulsive value to the steady flow value is comparatively small in a supersonic flow. This is illustrated, for this case, by the pressure distribution along the upstream face of the plate. This is shown for a number of time intervals in Fig. 9. This shows that the pressure effectively reaches the steady flow value by 0.6 ms. The number of molecules is still increasing at this time so that the total number of molecules is a conservative indicator as far as the surface values are concerned. The pressure is uniform at zero time but a gradient develops quickly.

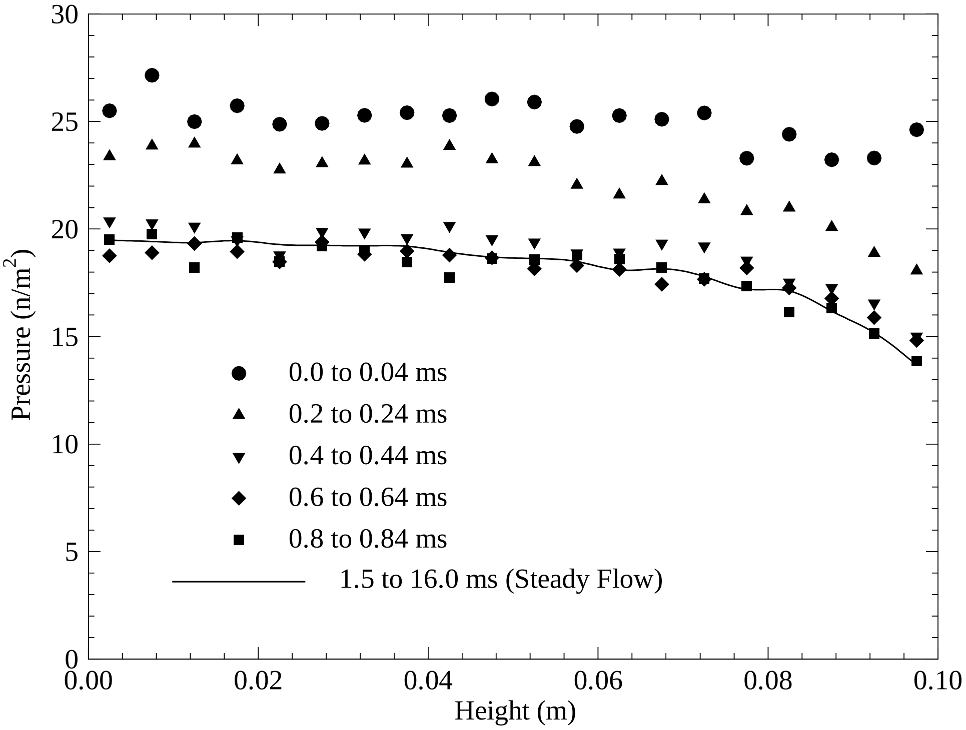

Fig. 10. The pressure distribution along the plate as a function of time.

3.4 Supersonic jet plume (DS2GD004.DAT)

The cell system for this flow involves five regions as shown in Fig. 11. The lip of the nozzle is at the boundary of the small cells with the large cells and the jet is in the horizontal direction in the lower left of the figure. The very small cells are in the boundary layer region of the flow within the nozzle.

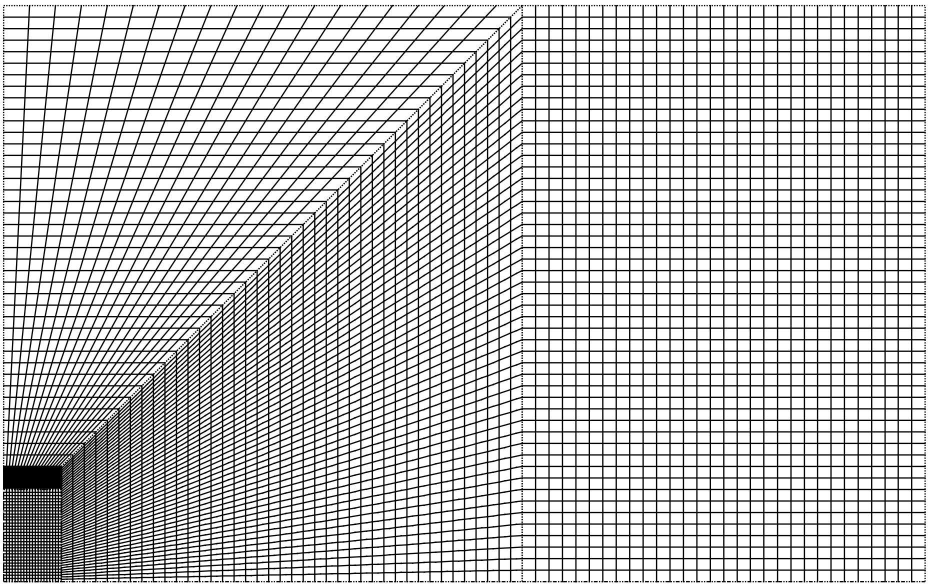

Fig. 11. The cell system for the jet plume problem.

The central portion of the jet is a uniform stream of 20% argon and 80% helium by number at a Mach number just under 2.5. The boundary layer inside the nozzle is represented by a specified stream at the left hand boundary of the small region with very small cells. The boundary layer velocity profile is assumed to be sinoidal with no slip at the wall. The Mach number contours are shown in Fig. 12. The two unlabelled contours are for M=0.5 and M=1.0. The subsonic flow accelerates and, as expected, the sonic line intersects the lip of the nozzle.

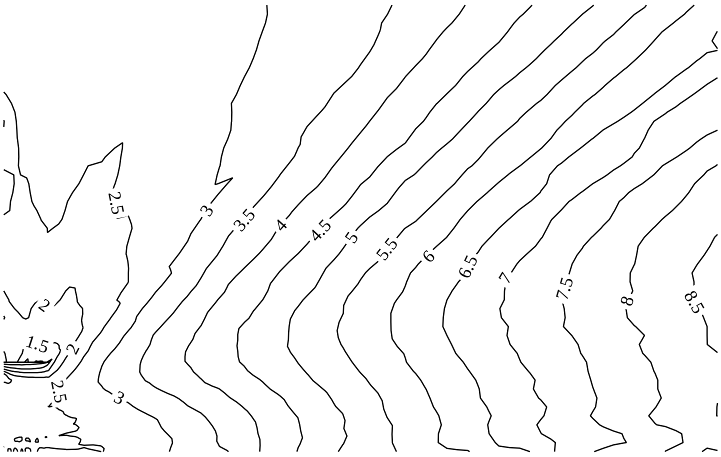

Fig. 12. Mach number contours in the plume.

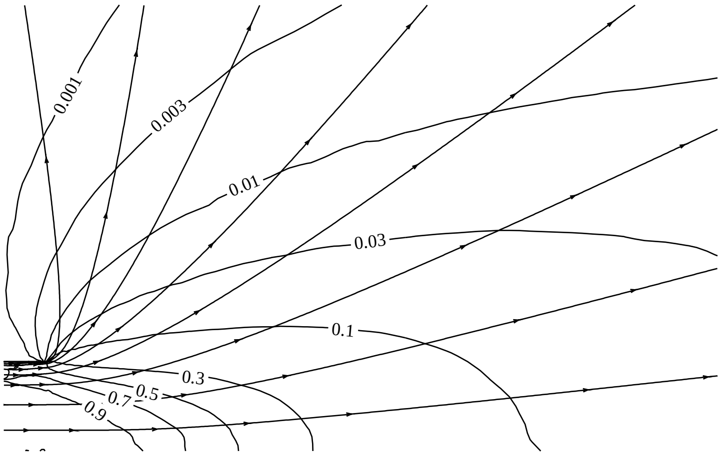

Fig. 13. Streamlines and number density ratio contours.

3.5 Plume backflow (DS2GD005.DAT)

A molecule output file DGMOF1.DAT was generated at the upstream boundary of the upper left region in the flow in §3.4. This was renamed DGMIF1.DAT and was used as the sole molecule input source for this case. There is a single region which matches region 5 along sides 3 and 4, but extends further in the backflow direction. The molecule entry boundary is side 4 and, as is required, this is coincident with (although the cells need not match) side 2 of region 4 of the previous calculation where the molecule file was generated. Both the number of molecules per cell and the time step were significantly larger than in the earlier calculation. The contours of number density ratio are shown in Fig. 14. The total number of molecules in the input file was only 250,000 (the current data file would produce 1,000,000). This was excessively small and was probably responsible for the higher density contours not being exactly matched with those from the preceding calculation.

Note that a surface could be placed in the backflow region and that, as long as the resulting disturbance did not reach the input boundary, the single input file could be used for a number of cases.

Fig. 14. Number density ratio in the backflow region.

3.6 Satellite contamination (DS2GD006.DAT)

This is concerned with the flow of atomic oxygen at 7,500 m/s and 1000 K past a vertical disk of radius 1 m. The number density of the stream is 3×10^{15} and the there is an outgas mass flux of 5×10^{-8} of a gas with molecular weight 500 from the disk. The disk is diffusely reflecting at a temperature of 300 K. There are no radial weighting factors and the flowfield extends 10 m upstream of the disk and to a radius of 5 m. There is a rectangular region upstream of the disk and another rectangular region outside the disk.

The number fraction of the outgassed molecules in the flowfield is shown in Fig. 15. The number of outgassed molecules is small compared with the stream molecules and a species weighting fraction of 20 was applied to the latter in order to equalize the samples. About 1 in 30 of the outgassed molecules return to the disk.

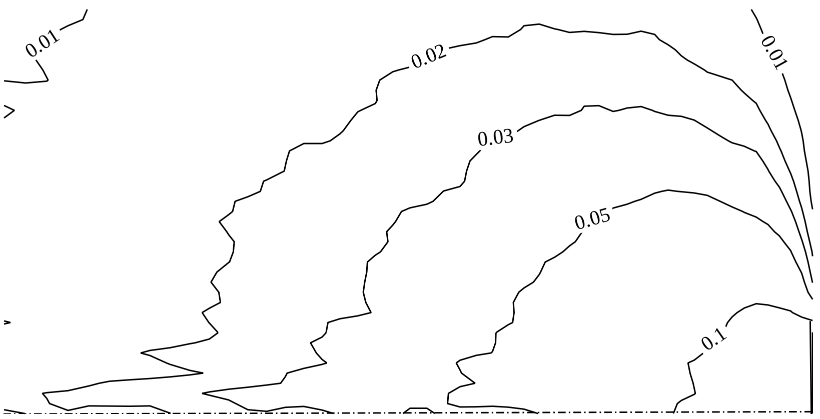

Fig. 15. The number fraction of outgassed molecules in the flow.

3.7 Hypersonic re-entry (DS2G007.DAT)

This considers the flow of real air at 200 K and 3×10^{19} m^{-3} past the spherically-nosed cone that is shown in Fig. 16. There are only two regions and the "segmented side" option has been used to have both a circle and straight line along the side 1 and 3 boundaries. The surface is diffusely reflecting at a temperature of 1000 K. There is almost a two order of magnitude increase in the density from the stream to the surface in such a flow and advantage is taken of the "variable DTM/FNUM" feature to set very thin cells in the region adjacent to the surface. It has been found that, while the pressure is insensitive to the cell height near the surface, the shear stress and the heat transfer are very sensitive to it. The gradients parallel to the surface are relatively small and the cell dimension in this direction may be larger than the local mean free path.

These examples are to demonstrate and test the operation of the program and some further optimization (possibly involving the introduction of additional regions would be required in a serious engineering calculation. The build up in the number of simulated molecules is more than a factor of three and the memory required for the molecules increases automatically during the running of the program from the 50,000 that is set in the data to more than 80,000. The time to steady flow is large and this example could well use the molecule multiplication feature.

There is about 4% by number atomic oxygen in the stream and this represents degree of oxygen dissociation of 0.1. The increase in this degree of dissociation due to chemical reactions in the flowfield is shown in Fig.17. The maximum degree of dissociation is approximately 0.6. There is also considerable dissociation of nitrogen accompanied by the formation of a small fraction of NO. The surface is non-catalytic and, at there densities, no recombination reactions occur.

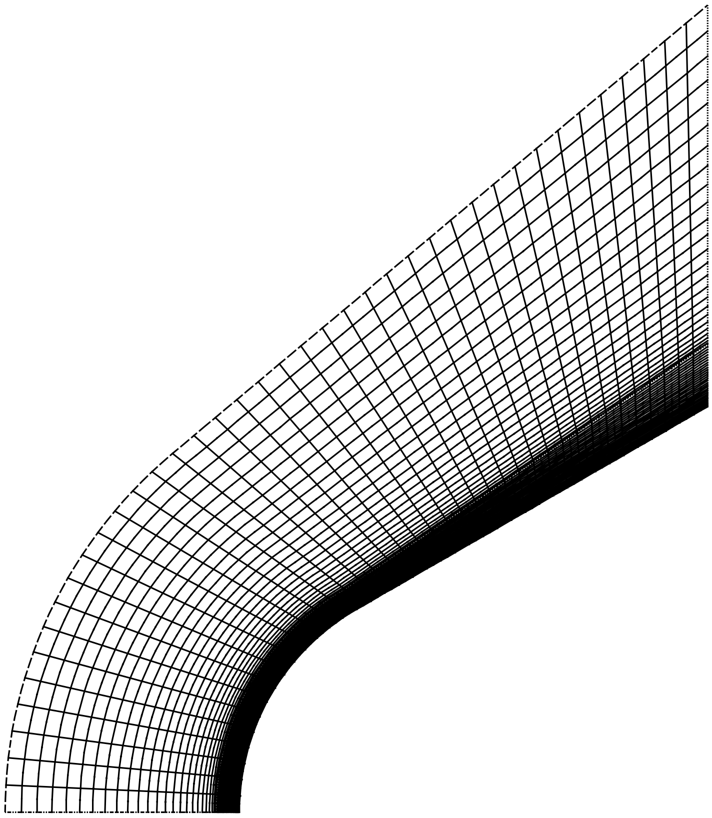

Fig. 16. The cells for the re-entry flow.

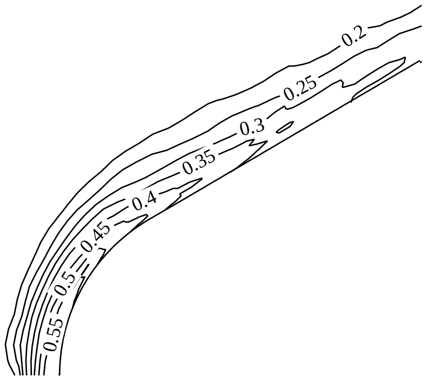

Fig. 17. Degree of dissociation of oxygen in the flowfield.

3.8 Flow past a curved plate (DS2G008.DAT)

This is the flow of argon at 300 K, 10^{20} m^{-3}, and 1000 ms^{-1} past a curved flat plate with its leading edge parallel to the flow. The plate is in the shape of one quadrant of a sine wave and the purpose of the test case is to check the "point input" option for region sides, surfaces with a variable temperature, and arbitrary cell spacing.

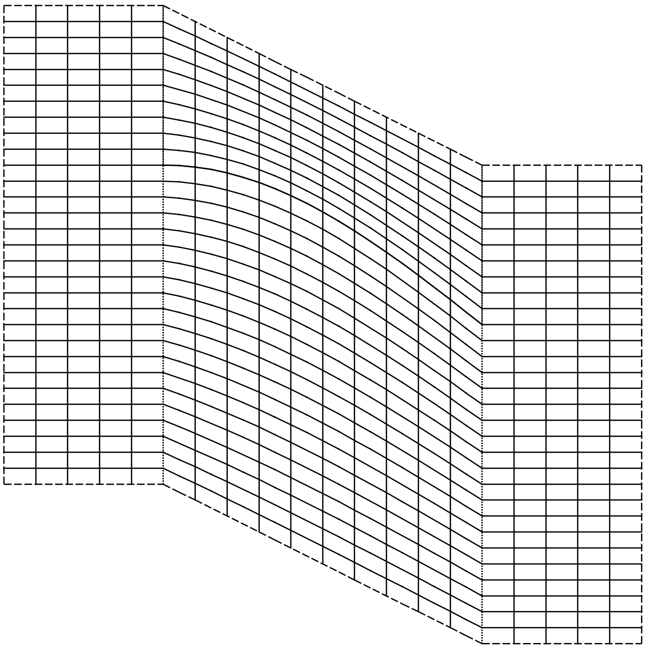

Fig. 18. The cell and region structure.

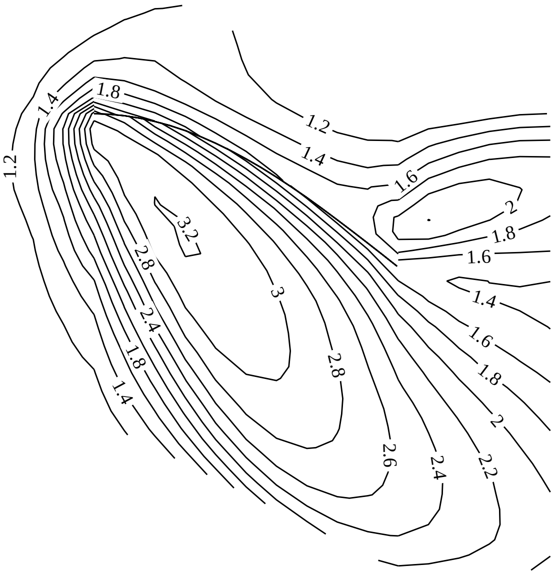

Fig. 19. Ratio of the temperature to the freestream value.

3.9 Taylor-Couette flow (DS2G009.DAT)

The Taylor-Couette flow is generated in the gap between two concentric cylinders when the outer cylinder is stationary and the inner cylinder rotates about the axis. This case is concerned with the case in which the radius of the outer cylinder is twice that of the inner cylinder and the region is defined by two planes of symmetry normal to the axis. The width of the flow is equal to the radius of the inner cylinder and the rotation commences at zero time.

The density of the monatomic hard sphere gas is such that there are initially 100 mean free paths between the inner and outer cylinder and the speed ratio of the circumferential velocity of the inner cylinder is 3.0.

This flow is a consequence od an instability and differs from the others in that it is not repeatable to within the statistical scatter. More than one vortex may be formed initially, their directions of rotation is not predictable, and the evolution to a single vortex may occur at different times.

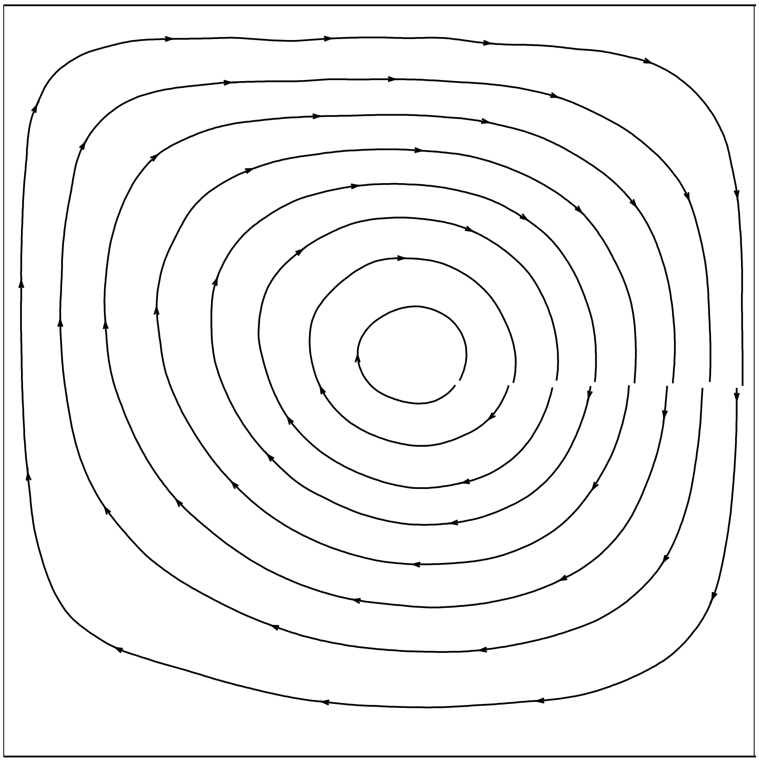

Fig. 20. Typical streamlines in the Taylor-Couette vortex.

3.10 Thermal creep flow (DS2G010.DAT)

This case demonstrates several of the features that were added to Version 2.3. They are the use of offsets on interfaces in order to set up periodic boundaries and the ability to set flow and surface conditions as power-law distributions. Thermal creep is a tendency for a transition regime flow to move towards a region od high temperature. It vanishes in the free molecule and continuum limits and is not present at the level of approximation that is provided by the Navier-Stokes equations.

This is an axially symmetric version of the ’One-way flow of a rarefied gas induced in a channel with a periodic temperature distribution’ of Sone, Waniguchi, and Aoki (Phys. Fluids **8**, 2227-2235, 1996). The results are shown in Fig. 21. This is a periodic flow and represents the maximum flow rate with no pressure change. The maximum surface temperature is at the ends of the flow and the creep velocities adjacent to the surfaces are towards the ends. A vortex forms in the enlarged section and there is a net flow to the right.

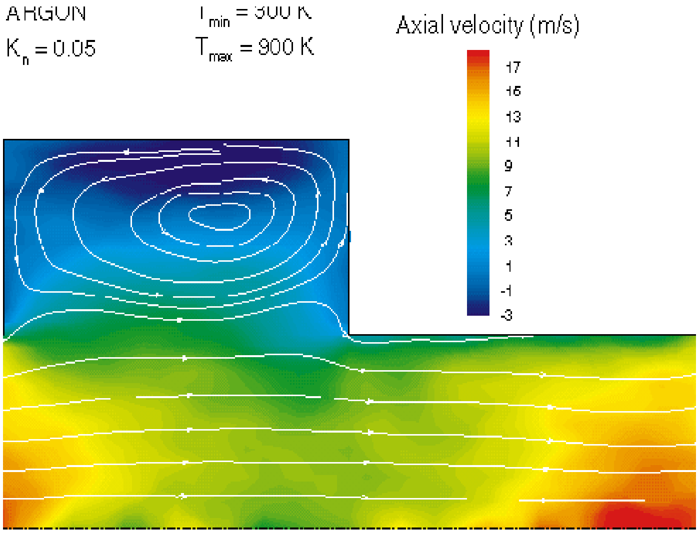

Fig. 21. Streamlines and axial velocity distribution.

APPENDIX A

Installation and run-time considerations

The program requires an "IBM compatible" computer with a 386DX, 486DX, or Pentium family processor (the mathematics co-processor is mandatory). While the program will run under DOS, it will generally be run in a Windows 95 environment. It is a 32 bit application and can use all the memory that is available. It can be run in a DOS window or by simply clicking on the executable.

The files on the distribution disc are the self-extracting compressed execution program DS2GZ.EXE and the set of demonstration data files DS2GD001.DAT, DS2GD002.DAT, and so on. A directory (say DSMC) should be created on the hard disk and the executable and all demonstration files on the distribution disc should be copied to it.

The execution of DS2GZ produces the executable file DS2G.EXE. This is the only file that is required for the operation of the program. Apart from the demonstration data files, all files in Fig. 3 (and additional self-deleting scratch files) are created during the execution of DS2G.

The general operation of the program is described in §2.1. The input of invalid data will lead to an error which may or may not lead to a diagnostic that identifies the error. The cell configuration file DS2GC.PLT may be useful in detecting inconsistent geometry input and should, in any case, be viewed in order to check the geometry. This is an HPGL file and may be viewed by importing it directly to a graphics or a wordprocessing program. This has been tested with both WordPerfect and Microsoft Word. In addition, the data summary file DS2GD.TXT may be studied and compared with its specification in Appendix B.

The geometry logic that is employed when moving the molecules traces their motion through all cells is sensitive to round-off error. If a molecule becomes "lost" during this process, it is discarded from the flow and produces a "removal error". These are indicated on the screen during the running of the program and the total number is listed in DS2GS.TXT. This number should be compared with the similar listing of the total number of molecules that enter the flow. The ratio of removed to entering molecules is normally about one in ten thousand. The total number of simulated molecules in the flow is preserved through the duplication of another molecule in the cell from which the molecule is removed.

The program has been compiled without the activation of array bounds checking or full floating point error detection. Should an isolated execution error occur, the restarting of the program will generally involve a different random number sequence and the problem should not recur.

Systematic errors will generally be a consequence of inconsistent data that leads to gaps between regions, time steps that are excessively large, and so on. Should problems persist with valid data, the problem should be reported to Graeme Bird on 100250.1101@compuserve.com. advice on new versions, together with instructions for the downloading of revised files is available at:

http://ourworld.compuserve.com/homepages/gabird

APPENDIX B

Specification of data file DS2GD.DAT

A data file may be generated externally to conform to these specifications.

All dimensioned quantities are in base SI units.

n in version number *n.m*

m in version number *n.m*

(The following specification is for n=3 and m=0, i.e. Version 3.0)

0,1 for two-dimensional, axially symmetric flows, respectively.

0,1 for steady time averaged, unsteady averaged sampling.

Required only for axially symmetric flows.

> 0,1 for no weighting factors, or factors proportional to radius.

Required only for axially symmetric flows with weighting factors.

> Reference radius below which the weighting factors are unity.

The basic value for the number of real molecules that are represented by each simulated molecule.

The basic time step for uncoupling movement and collisions.

Gas menu code.

Number of regions.

Number of molecular species in the flow.

Required only for gas mixtures.

> 0 if the diameter, viscosity exponent, and VSS scattering parameter for the cross collisions are to be set to the mean values, or 1 if these quantities are to be set as data
>
> Number of species groups.
>
> *Required only if the number of species groups is greater than one.*
>
> > 0,1 for group weighting factors not implemented, implemented.

Number of chemical reactions.

Required only if there are chemical reactions.

> Number of third-body probability tables for recombinations.

Required only if there are more than one species group and is repeated for each group.

> Weighting factor of species group L.

The following data is repeated for each species.

> Reference diameter.
>
> Reference temperature.
>
> Viscosity temperature power law.
>
> Reciprocal of the VSS scattering parameter (1. for VHS).
>
> Molecular mass.
>
> *Required only for gas mixtures.*
>
> > Species group in which the molecule lies.
>
> Number of rotational degrees of freedom.
>
> *Required only if there are rotational degrees of freedom.*
>
> > 0, 1 for constant, polynomial rotational relaxation number.
> >
> > *Required only for gas mixtures.*
> >
> > > 0, 1 for common or collision partner species dependent rotational and vibrational relaxation rate.

The constant value, or constant in the polynomial for Zr (either the common or the like collision value).

Required only if there is a polynomial for Zr.

Coefficient of temperature in the polynomial.

Coefficient of temperature squared in the polynomial.

Number of vibrational modes of this species.

Required only if there are vibrational modes in a loop over the modes.

Characteristic temperature of the mode.

Constant C1 in eqn (6.53) for the relaxation collision number or, if C2 is negative, the relaxation collision number (either the common or like collision value at this stage).

Constant C2 in eqn (6.53), or -1 to indicate a constant Zv

Required only for a gas mixture in a loop over species, but only for collisions between molecules of different species and when the cross-collision values are to be set as data rather than through mean values.

Reference diameter for the cross-collisions.

Reference temperature for the cross-collisions.

Viscosity temperature power law for the cross-collisions.

Reciprocal of the VSS scattering parameter for the cross-collisions.

Required only for rotational degrees of freedom and collision partner dependent relaxation rates.

Constant value, or constant in the polynomial for Zr in the cross-collision.

Required only for polynomial rotational relaxation rate.

Coefficient of temperature in the polynomial.

Coefficient of temperature squared in the polynomial.

Required only for specie with vibration in a loop over the modes.

Constant C1 in eqn (6.53) for the relaxation collision number or, if C2 is negative, the constant value of the relaxation collision number.

Constant C2 in eqn (6.53), or -1 to indicate a const. Zv.

Required only when there are chemical reactions in a loop over the reactions.

Species code of the first molecule.

Species code of the second molecule.

If it is a dissociation.

First post-reaction species code.

Second post-reaction species code.

Third post-reaction species code.

If it is a recombination.

-1.

Species code of the recombined molecule.

Species code of the third body or, if negative, the code of the third-body table.

If it is an exchange reaction.

0.

First post-reaction species code.

Second post-reaction species code.

Number of internal degrees of freedom that contribute energy to the reaction.

Activation energy for the reaction.

1.E10 times the pre-exponential parameter in the Arrhenius rate equation.

Temperature exponent in the rate equation.

Energy of the reaction.

Required only when there are third-body probability tables in a loop over the tables.

In a loop over the species.

The relative efficiency of the species in recombinations.

0,1 for stream or initial gas, no stream or initial gas.

Number of molecule input files.

Number of molecule output files.

Required only if there is a stream.

Stream temperature.

Stream number density.

Stream velocity in the x direction (along the axis for axially symmetric flows).

Stream velocity in the y direction

(The following item was required only for a stream in versions below 2.1)

0,1,2,3 if the flowfield is initially a vacuum, uniform stream, specified by region, or from the restart file.

Required only if there is a stream and a gas mixture in a loop over the species.

Fraction (by number) of the species in the initial stream

Required only if the initial gas is set for each region in a loop over the regions.

(These items were introduced in version 2.1)

0,1,2 if the region is initially a vacuum, a stream, or is specified below.

Required only if the gas is specified for the region.

Initial temperature for the region.

Initial number density for the region.

Initial velocity in the x direction.

Initial velocity in the y direction.

Required only for a mixture in a loop over all the species.

Initial fraction of the species in the region.

In a loop over the regions.

For a steady flow.

The ratio of FNUM and DTM to basic values.

For an unsteady flow.

If positive, a density ratio to basic value or, if negative, a temperature ratio (0. for a vacuum).

Number of cell elements along sides 1 and 3.

Number of cell elements along sides 2 and 4.

Either 1,2,3,4,5 to indicate type of side 1:-

1 if the co-ordinates of the points are read individually, or

2 if the side is straight, the endpoints are specified and the spacing is an arithmetic progression, or

3 if the side is a segment of a conic section, or

4 if the points are identical with another side, or

5 if the side is defined by more than one segment.

Either 1 to 5 as defined above, but for side 3.

Either 1, 2, or 3 to indicate the type of input for side 2:-

1 if the segments are of equal length, or

2 if the segments are in a arithmetic progression, or

3 if the segment lengths are arbitrarily distributed.

Either 1, 2, or 3 as above, but for side 4.

Weighting (<1 towards side 2 or >1 towards side 4) when dividing the intermediate lines joining sides 1 and 3.

If side 1 is type 1 in a loop over the number of (cell) points on the side.

- x coordinate of the point.
- y coordinate of the point.

If side 1 is type 2.

- x coord of intersection with side 2.
- y coord of intersection with side 2.
- x coord of intersection with side 4.
- y coord of intersection with side 4.
- Size ratio (if positive) of cell at side 4 to that at side 2, or (if negative) of the center to the end elements.

If side 1 is type 3.

- x coord of the focus of the conic section.
- y coord of the focus of the conic section.
- Parameter p for the conic section.
- Eccentricity of the conic section.
- Angle (rads) from x dirn. to the int. of sides 1 and 2.
- Angle (rads) from x dirn. to the int. of sides 1 and 4.
- Size ratio defined as for type 2 but applied to angular elements.

If side 1 is type 4.

- Number of the region with an identical side.
- Number of the side (-ve for points in reverse order).

If side 1 is type 5.

- Number of type segments along the side.
- *In a loop over the segments (starting at side 2).*
    - Either 1, 2, 3, or 4 for the type of the segment.
    - The number of cell segments along the type segment.
    - *If the segment is type 1 in a loop over the number of points on the segment.*
        - x coordinate of the point.
        - y coordinate of the point.
    - *If the segment is type 2.*
        - x coord of the first point (first segment only).
        - y coord of the first point (first segment only).
        - x coord of the final point.
        - y coord of the final point.
        - Size ratio of the segment defined as for the side.
    - *If the segment is type 3.*
        - x coord of the focus.
        - y coord of the focus.
        - Parameter p for the conic.
        - Eccentricity of the conic.
        - Angle from x direction to first point (first segment only).
        - Angle (rad) from x dirn. to last point on segment.
        - Size ratio defined as for the side.
    - *If the segment is type 4.*

- Number of the region with an identical side.
- Number of corres. side (-ve for points in reverse order)

- *If side 3 is type 1 in a loop over the number of points on the side.*
  - x coordinate of the point.
  - y coordinate of the point.
- *If side 3 is type 2.*
  - x coord of intersection with side 2.
  - y coord of intersection with side 2.
  - x coord of intersection with side 4.
  - y coord of intersection with side 4.
  - Size ratio (if positive) of cell at side 4 to that at side 2, or (if negative) of the center to the end segments.
- *If side 3 is type 3.*
  - x coord of the focus of the conic section.
  - y coord of the focus of the conic section.
  - Parameter p for the conic section.
  - Eccentricity of the conic section.
  - Angle (rads) from x dirn. to the int. of sides 1 and 2.
  - Angle (rads) from x dirn. to the int. of sides 1 and 4.
  - Size ratio defined as for type 2 but applied to angular segments.
- *If side 3 is type 4.*
  - Number of the region with an identical side.
  - Number of the side (-ve for points in reverse order).
- *If side 3 is type 5.*
  - Number of type segments along the side.
  - *In a loop over the segments (starting at side 2).*
    - Either 1, 2, 3, or 4 for the type of the segment.
    - The number of cell segments along the type segment.
    - *If the segment is type 1 in a loop over the number of points on the segment.*
      - x coordinate of the point.
      - y coordinate of the point.
    - *If the segment is type 2.*
      - x coord of the first point (first segment only).
      - y coord of the first point (first segment only).
      - x coord of the final point.
      - y coord of the final point.
      - Size ratio of the segment defined as for the side.
    - *If the segment is type 3.*
      - x coord of the focus.
      - y coord of the focus.
      - Parameter p for the conic.
      - Eccentricity of the conic.
      - Angle from x direction to first point (first segment only).
      - Angle (rad) from x dirn. to last point on segment.
      - Size ratio defined as for the side.
    - *If the segment is type 4.*
      - Number of the region with an identical side.

Number of corres. side (-ve for points in reverse order)

If side 2 is type 2.

Ratio of cell size (if positive) at side 3 to that at side 1, or (if negative) at centre segment to the end segments.

If side 2 is type 3 in a loop over the cell segments.

Number proportional to segment length (side 1 to side 3)

If side 4 is type 2.

Ratio of cell size (if positive) at side 3 to that at side 1, or (if negative) at centre segment to the end segments.

If side 4 is type 3 in a loop over the cell segments.

Number proportional to segment length (side 1 to side 3).

In a loop over the four sides of the region.

Either 1, 2, 3, 4, 5, 6, 7, or 8 for the type code for the side:-

1 for an axis of symmetry, or
2 for a plane of symmetry, or
3 for a stream boundary, or
4 for a specified flow boundary, or
5 for a surface, or
6 for an outgassing surface, or
7 an interface with another side or sides, or
8 the side is a vacuum or molecule entry file boundary.

If the side is type 4, 5, or 6.

0,1 for constant, variable input along the side.

If the side is type 7.

Number of sides that adjoin this side.

If the side is type 4 input a single value for constant input, or in a loop over the cell segments for variable input.

Velocity component in the x or axial direction.

Velocity component in the y direction.

Temperature of the stream.

Number density.

Required only for a mixture in a loop over the species.

Fraction of the species in the stream.

If the side is type 5 or 6 input a single value for constant input, or in a loop over the cell segments for variable input and in a loop over the species.

Temperature (if -1, the reflection is specular or if -2, the reflection follows the diffuse adiabatic model with zero heat transfer).

For other than specular or diffuse adiabatic reflection.

-1, for full diffuse reflection, or between 0 and 1 for internal energy accommodation coefficient.

For other than diffuse reflection.

Normal energy accommodation coefficient.

Tangential momentum accommodation coefficient.

Fraction of molecules adsorbed at the surface.

If the side is type 6.

Outgas mass flux.

The tangential velocity component of the surface in the plane of the flow.

The tangential velocity component of the surface in the plane normal to the flow.

The following item was introduced in Version 1.1.

The probability of catalytic recombination at the surface for this species.

If the side is type 7 in a loop over the adjacent sides.

Code (1 to 4) of the adjoining side.

Code number of the region in which side NSD lies.

If there are molecule input files in a loop over the files.

Region into which the molecules enter.

Side of this region at which they enter.

Number of molecules in each record of the entry file.

Number of records in the molecule entry file.

If molecule input files are to be generated in a loop over the files.

Required only for axially symmetric flows with radial weighting factors.

0, 1 if weighting factors are to be removed, kept.

0,1 if program continues,stops when file is completed

Region containing the output side.

Code of the output side.

Number of molecules in each record.

Number of records in the output file.

Number of DTM time steps between sampling.

Number of samples between prints.

Number of prints to the assumed start of steady flow, or the number of prints in one run of the unsteady flow.

Required only for a steady flow.

The factor for the molecule multiplication at 80% of the steady flow time.

Number of prints to STOP in a steady flow, or the total number of runs in an unsteady flow.

The maximum number of simulated molecules.

Specification of parameter file DS2GP.DAT

If externally generated data in DS2GD.DAT is selected through the "Generate and run a new case" option in the Introductory Program Screen followed by "Modify the existing DS2GD.DAT" in the subsidiary screen, the DS2GP.DAT file is generated automatically as the data screens are cycled. However, if it is selected through the "New run from an existing data file" in the Introductory Program Screen, a consistent DS2GP.DAT file must also have been generated externally.

Maximum number of simulated molecules.

Maximum number of molecules in the duplication buffer.

Number of molecular species.

3 for all monatomic species, or 4 if some species have internal modes.

2 for a simple gas, or 3 for a gas mixture.

Number of species groups.

Number of reactions.

Number of third-body tables.

Number of regions.

Number of cells.

Number of cell corner points.

Number of boundary elements.
Max number of specification type segments on any side.
Number of surface (cell) elements.
Number of molecule entry elements.
Number of interface elements.
Maximum number of adjacent sides.
Maximum number of adjacent elements (specified).
Maximum number of points along 1,3 sides in any one region.
Maximum number of points along 2,4 sides in any one region.
Maximum number of points on any side.
Maximum number of vibrational modes of any species.
Number of molecule input files.
Number of molecules in one record (repeated for each molecule input file).
Number of molecule output files.
Number of molecules in one record (repeated for each molecule output file).
0,1 if weighting factors are removed, retained (repeated for each output file).
Number of prints to assumed steady flow or total number of runs in unsteady flow.
0,1 for steady, unsteady flow.