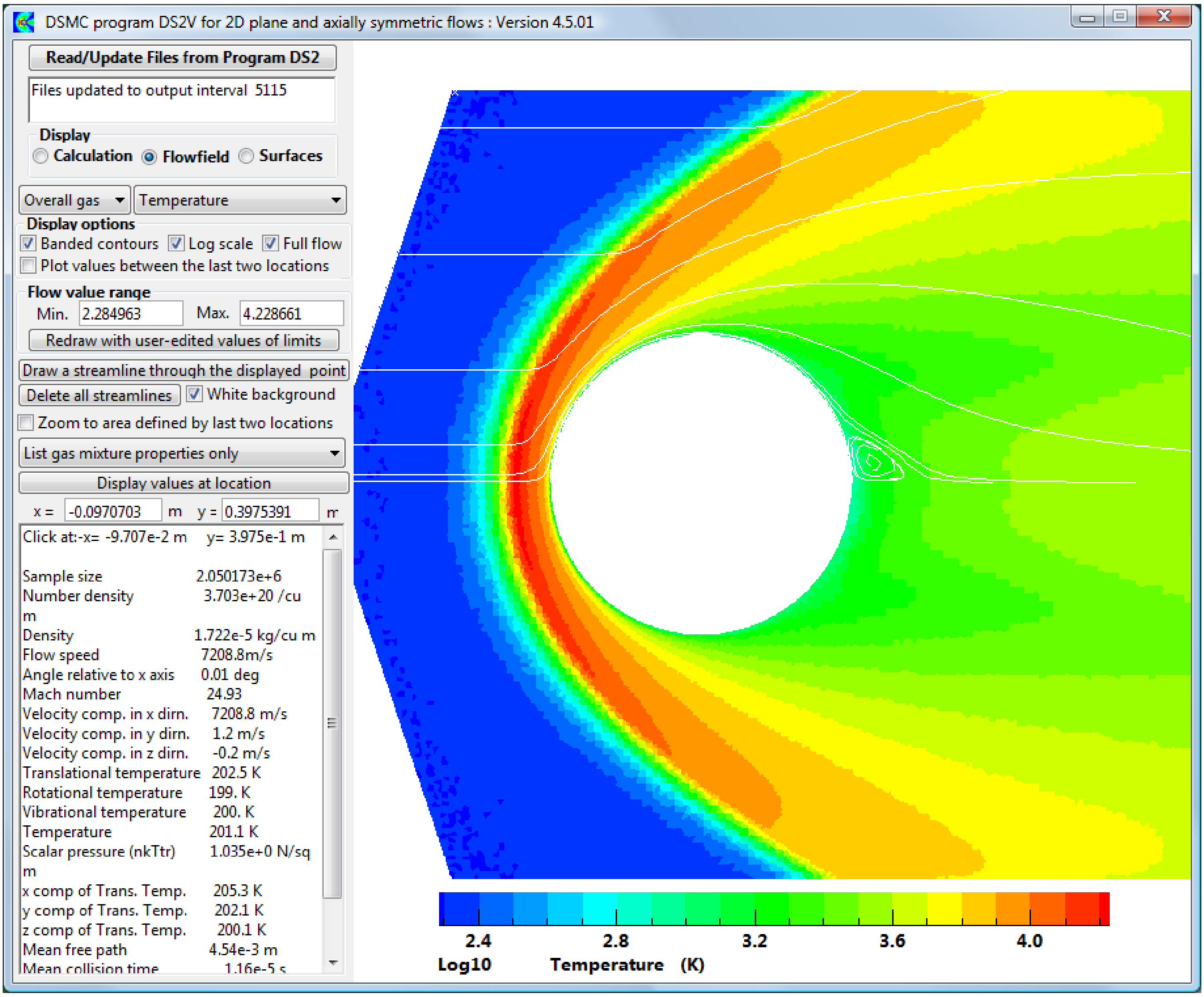
Mach 25 flow of nitrogen past a circular cylinder at a Knudsen number of 0.01



Files updated to output interval 5115

Display
○ Calculation ● Flowfield ○ Surfaces

Overall gas ▾ Temperature ▾

Display options
☑ Banded contours ☑ Log scale ☑ Full flow
☐ Plot values between the last two locations

Flow value range
Min. 2.284963 Max. 4.228661

☑ White background
☐ Zoom to area defined by last two locations

List gas mixture properties only ▾

x = -0.0970703 m y = 0.3975391 m

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Click at:-x= -9.707e-2 m    y= 3.975e-1 m

Sample size                  2.050173e+6
Number density                3.703e+20 /cu
m
Density                      1.722e-5 kg/cu m
Flow speed                    7208.8m/s
Angle relative to x axis      0.01 deg
Mach number                    24.93
Velocity comp. in x dirn.       7208.8 m/s
Velocity comp. in y dirn.       1.2 m/s
Velocity comp. in z dirn.       -0.2 m/s
Translational temperature   202.5 K
Rotational temperature        199. K
Vibrational temperature        200. K
Temperature                   201.1 K
Scalar pressure (nkTtr)       1.035e+0 N/sq
m
x comp of Trans. Temp.         205.3 K
y comp of Trans. Temp.         202.1 K
z comp of Trans. Temp.          200.1 K
Mean free path                4.54e-3 m
Mean collision time             1.16e-5 s
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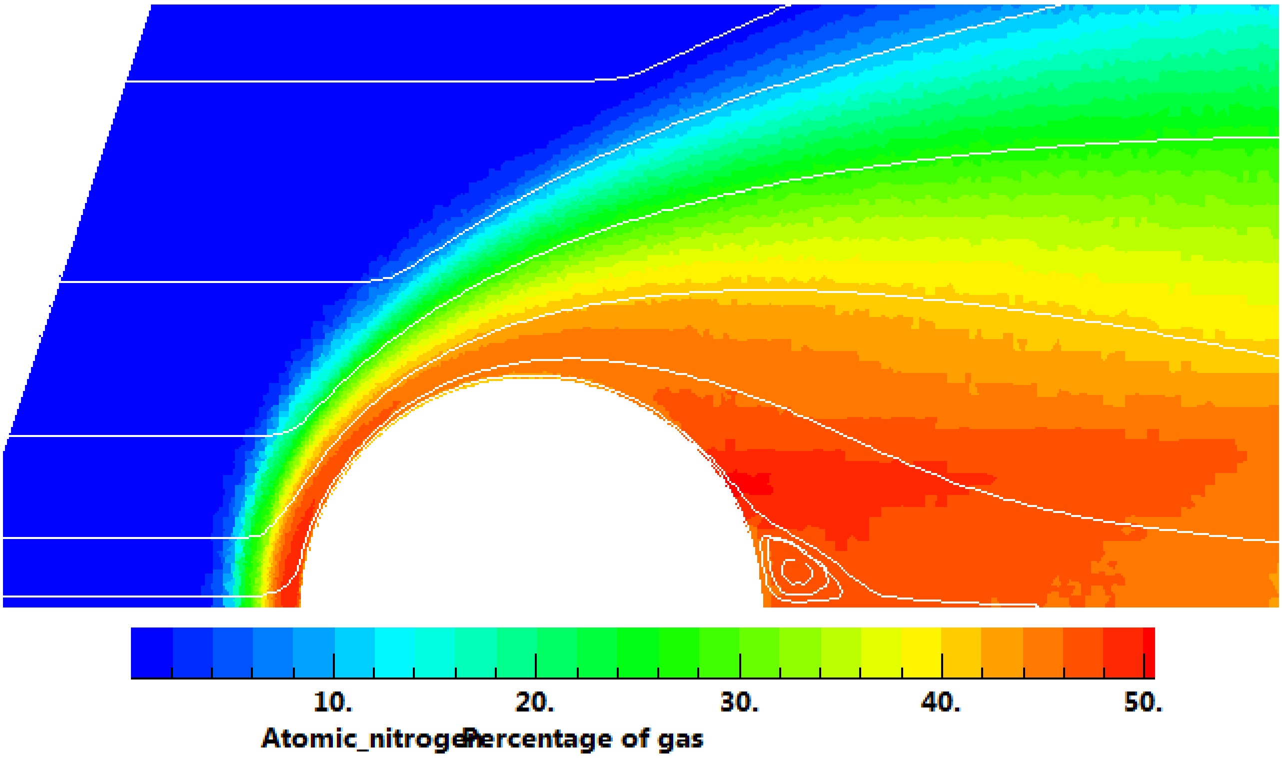
Version 4.5.01 of the DS2V program offers two options with regard to the chemistry model:

(i) The ***particle-based chemistry model*** in which the vibrational excitation rate depends on the "quantized collision temperature" based on the energies in each individual collision. Dissociation occurs naturally when the excitation is to the quantum level that corresponds to dissociation.

(ii) The ***continuum or temperature-based chemistry model*** in which the vibrational excitation rate depends on the local flow temperature. Dissociation is based on the conventional temperature dependent chemical rate equations. This model has been employed in almost all DSMC calculations and leads to agreement with the corresponding Navier-Stokes CFD results at low Knudsen number, but cannot be expected to provide realistic results for highly nonequilibrium flows. *All physical processes in a high temperature gas flow are a consequence of intermolecular collisions and the molecules in a collision have no knowledge of the overall gas temperature.*

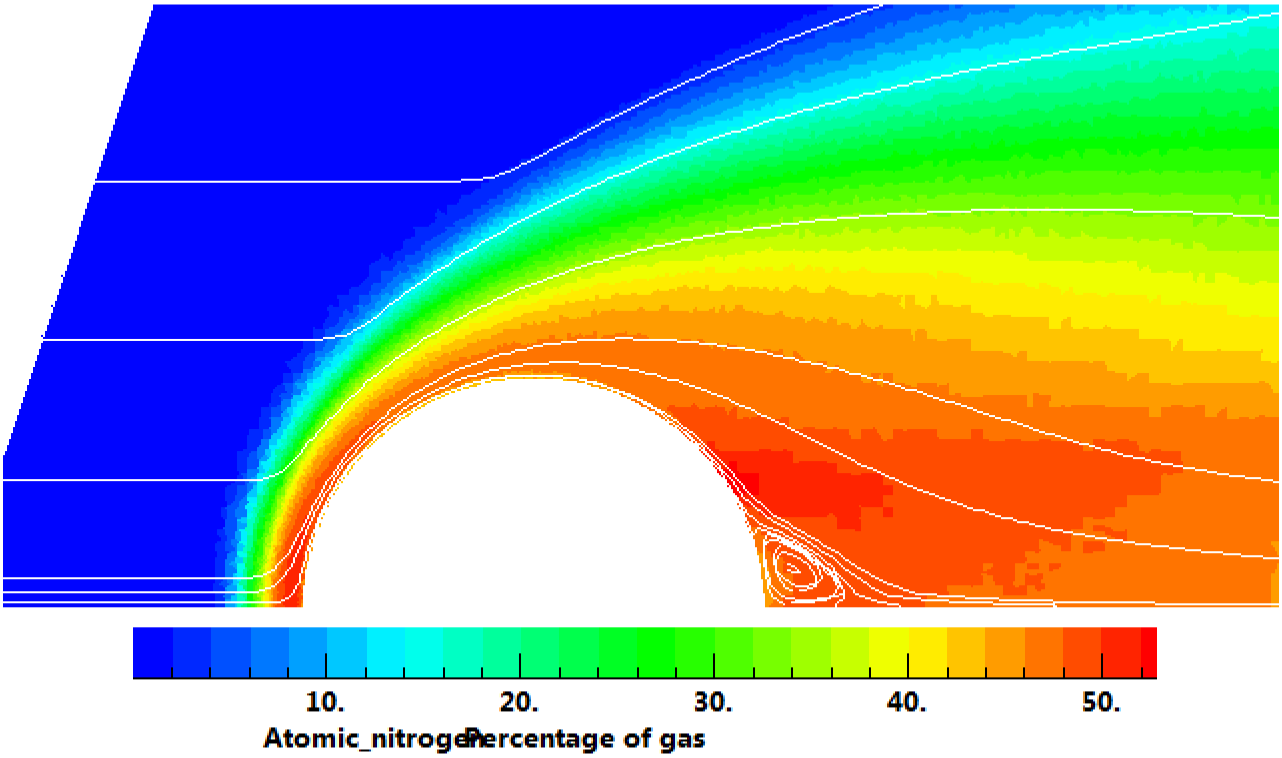
The chemistry model is a "CheckBox" selection and the above flow has been calculated with both options. The screen image is from the calculation based on the particle-based model, but there were no noticeable differences in this plot. Note that, if the shock wave thickness is based on the initial temperature rise, the shock wave thickness is many times larger than the shock-standoff distance that would be obtained for the limiting thin shock wave as the Knudsen number tends to zero. Navier-Stokes CFD calculations that employ captured shock waves will not provide an acceptable representation of this class of flow unless the overall Knudsen number is less than 0.001.



The atomic oxygen percentage contours in the above figure depend only on the reference vibrational collision number $Z_{ref} = 10000$ at $T_{ref} = 5000$ K. At the quantized collision temperature T,

$$Z_v = \left(\frac{\Theta_d}{T}\right)^{\omega} \left[Z_{ref} \left(\frac{\Theta_d}{T_{ref}}\right)^{-\omega}\right]^{\left[\left(\frac{\Theta_d}{T}\right)^{1/3} - 1\right] \Big/ \left[\left(\frac{\Theta_d}{T_{ref}}\right)^{1/3} - 1\right]} \tag{1}$$

where Θ_d is the dissociation temperature and ω is the viscosity-temperature index. Equation (1) preserves the Millikan-White inverse one third power temperature dependence, but sets the vibrational collision number to unity at the dissociation temperature. This is essentially a more precise version of the so-called “Park correction factor” for the vibrational excitation rate in high temperature gas flows.



The second set of contours employs the “continuum data” option. The vibrational collision rate was again based on Equation (1), but with T given by the overall flow temperature. The total collision energy model was applied to the following rate coefficients in SI units.

For $2N_2 \rightarrow N_2 + 2N$, $k(T) = 7.968 \times 10^{-13}\, T^{-1/2} \exp(-113500/T)$,and
for $N_2 + N \rightarrow 3N$, $k(T) = 6.9 \times 10^{-8}\, T^{-3/2} \exp(-113500/T)$.

There are some differences in the contours and, after the establishment of steady flow, the total number of molecules in the second calculation was 0.8% higher than that in the first. However, these differences are much smaller than the uncertainties associated with the data. Chemical rate equations for dissociations now appear to be redundant data for DSMC calculations.

Calculations that linked vibrational rate data with dissociations in DSMC had been made on a number of occasions over the past twenty years, but were not pursued because equipartition was not achieved for the vibrational modes when the rates were based on the collision energy rather than the overall temperature. This problem disappeared when the collision temperature for the vibrational redistribution to a particular mode was also quantized in accordance with the levels in that mode. The DS2V data set currently allows only a single rate for each mode but, because Equation (1) requires just a single value for Zv at a reference temperature, the rate can easily be made to depend on the species of the colliding molecule. Species-dependent data for vibrational excitation is available for some gas mixtures.

It appears that the rates for the forward (endothermic) exchange reactions can be matched by a simple probability that is applied when the selected vibrational level of the diatomic molecule matches the activation energy of the reaction. The probabilities of all reverse (exothermic) reactions can be based on the law of mass action, but the calculation of the partition functions in the equilibrium constant must be based on the collision energies rather than on the flow temperature. A successful implementation of these extensions would enable calculations for Earth orbit re-entry to be made without any need for reaction rate equations.

The challenge will then be to develop procedures for the electronic modes that are similar to the procedures for vibration related phenomena. The advantages of particle-based data over continuum or temperature-based data are overwhelming for escape velocity re-entry problems. For example, with rotation also quantized, bound-bound radiation can be modelled precisely. In addition, the absorption of radiation poses no special problems in DSMC calculations.

The DS2V program employs the “sophisticated DSMC” procedures that permit engineering calculations to be made with computation times comparable to those for Navier-Stokes CFD. The above calculations were made concurrently on an Intel Core 2 Quad processor in about twelve hours. The samples are larger than would generally be required and reasonably good results were available in about two hours. The steady flow number of simulated molecule was about 430,000.

Version 4.5.01 of DS2V was posted on gab.com.au for free download on 27th August. The data file for this flow was also posted as CYL2501.DAT and should be renamed to DS2VD.DAT in order to reproduce these calculations for closer study.

Studies of the sensitivity of the flowfield to changes in both the particle based and continuum based data sets would be particularly instructive.