Chapter 6

Numerical results

We present in this chapter some of the main results we have achieved by applying the numerical methods introduced in Chapter 5 to the aerothermodynamic physical models described in 4. Wherever possible, we make direct validation against experimental data and/or reference solutions available in literature.

6.1 RTO Task Group 43 Topic No. 2

Starting from June 2007, the Von Karman Institute has been involved in a RTO task group dealing with the Assessment of Aerothermodynamic Flight Prediction Tools Through Ground and Flight Experimentation together with US leading institutions like NASA Ames, NASA Langley, US Air Force Research Laboratory (AFRL), Calspan University of Buffalo Research Center (CUBRC), University of Minnesota and DLR, ESA and EPFL on the European side. In particular, the topic No. 2 focuses on a further assessment of CFD for the specific issue of shock interactions and control surfaces in nonequilibrium flows. A set of three configurations with growing level of complexity has been adopted for the evaluation of CFD methods. Only contributors who have shown ability to solve the first two entry testcases, namely a 3D cylinder configuration from DLR (blind testcase) and an axisymmetric double cone geometry from CUBRC, are allowed to participate to the third case, the FRESH Fx prototype proposed by the AFRL. On the side of VKI, the author was responsible for handling the simulations and the corresponding testcases will be presented in this section, together with the numerical results obtained with COOLFluiD and the validation with the available experimental data.
6.1.1 Double Cone (CUBRC)

The experimental studies have been conducted in the LENS I shock tunnel at CUBRC to obtain detailed surface and flow characteristics over an axisymmetric double cone configuration with semi angles of $25^\circ$ and $55^\circ$ and a base diameter of 10.3 inches, as shown in Fig. 6.1.

![Double Cone Geometry](image)

**Figure 6.1:** Double cone geometry (lengths are given in inches).

Measurements were made in both air and nitrogen for total enthalpy conditions of 5 and 10 MJ/kg, but only numerical simulations of nitrogen flows were required for the first contributors’ selection. As extensively explained in [42, 105], this kind of simulations is extremely challenging from a computational point of view, mainly due to the complexity of the shock-shock and shock-boundary layer interactions and to the difficulty of the numerical schemes to approach convergence, because of the unsteadiness associated to the large separation region developing on the cone-cone juncture. Double cone flows are therefore ideal candidates for the purpose of CFD validation of aerothermodynamic solvers.

A sketch of a typical hypersonic flowfield around a double cone is depicted in Fig. 6.2 ([105]). The oblique shock generated by the first cone strongly interacts with the detached bow shock created by the second one and the resulting transmitted shock impinges on the surface downstream of the cone-
cone juncture. Here, the adverse pressure gradient forces the boundary layer to separate. The separated region on the corner generates its own shock, which interacts with the bow shock and causes a shift of the interaction point and this in turns alters the separation zone. This process feeds back on itself until the flow reaches a steady state, if such a state exists. Moreover, a supersonic jet forms along the surface of the second cone, downstream the impingement point, and it undergoes a series of compressions and expansions. An accurate prediction of the aerodynamic field and related quantities (heat flux) for hypersonic double cone flows requires thermo-chemical non equilibrium effects to be taken into account, as demonstrated for instance in [93, 107, 108]. To this end, all our simulations have accounted for those effects with the conventional 2-temperature model for thermo-chemical nonequilibrium described in Sec. 4.3.

![Figure 6.2: Schematic of double-cone flowfield at high enthalpy nitrogen free-stream conditions (run 42).](image)

**6.1.1.1 Double cone: run 35**

This double cone configuration, whose conditions are listed in Table 6.1, was not part of the RTO task, but we report it here because it is a very well documented testcase in literature [42, 108] and has given us the opportunity to verify and validate both our solvers, FV and RD, with the basic non reactive Navier-Stokes model, before coping with the more challenging cases (run 40 and 42) in thermo-chemical nonequilibrium.
\[
\begin{array}{|c|c|c|c|c|}
\hline
M_\infty & \rho_\infty [kg/m^3] & U_\infty [m/s] & T_\infty [K] & T_w [K] \\
\hline
11.5 & 0.0005515 & 2713 & 138.9 & 296.1 \\
\hline
\end{array}
\]

Table 6.1: Free stream and wall conditions for double cone (run 35).

The computations have been run on a relatively coarse structured mesh with 256x128 cells kindly provided by Dr. Nomelis. Detailed views of the mesh around the two most critical points, namely the leading edge and the junction between the two cones are shown in Fig. 6.3a and 6.3b.

![Zoom around the leading edge.](image1.png)

![Zoom on the junction between the two cones.](image2.png)

Figure 6.3: Detailed views of the coarse structured mesh (256x128 cells) for the double cone.

The numerical solutions are compared among each other and against experiments in Figs. 6.4 and 6.5 in terms of surface pressure and heat flux. In particular, we show results with

- AUSM+up (Sec. 5.2.1.5), weighted MUSCL reconstruction (Sec. 5.2.2.1) and Van Leer limiter (Sec. 5.2.3.2);
- AUSM+, least square reconstruction (Sec. 5.2.2.2) and Venkatakrishnan limiter (Sec. 5.2.3.1);
- Roe (Sec. 5.2.1.1), MUSCL extrapolation and Van Leer limiter;
- modified Steger Warming (Sec. 5.2.1.4), least square reconstruction and Venkatakrishnan limiter.
Figure 6.4: Surface pressure with FV schemes for double cone (run 35).

Figure 6.5: Surface heat flux with FV schemes for double cone (run 35).
In all the four schemes, the high order reconstruction has been performed in update variables \( \mathbf{P} = [p, \mathbf{u}, T] \). In the case of both surface quantities, AUSM+ and modified Steger Warming in combination with Venkatakrishnan limiter seem to give the results more in agreement with the experimental measurements. The merit for this can probably be attributed to the multidimensional character of the least square reconstruction and the Venkatakrishnan limiter compared to the more uni-directional MUSCL approach. The results obtained by us agree qualitatively and quantitatively well with those shown in [42], where several schemes have been tested, but with a more accurate MUSCL formulation, involving 5 points in the face-based stencil.

The same simulation has been performed with the second order accurate Bx RD scheme (see Sec. 5.3.2.3). Since our RD Navier-Stokes solver works only on grids composed of triangles, the original structured mesh used for the previous computations has been split into triangles, while keeping approximately the same number of degrees of freedom. In fact, RD is a vertex centered method and the number of vertices is equal to the number of cell centers, except for boundary effects.

The temperature field corresponding to the RD solution is shown in Fig. 6.6, where a zoomed view with some overposed streamlines near the junction between the first and second cone is also presented, in order to better visualize the flow behaviour in the separation bubble. The convergence history in Fig. 6.7 corresponds to the first order RD computation (N scheme) starting from an initial uniform flowfield: it shows an example of almost quadratic convergence achieved by the implicit Newton method in such a complex testcase. The second order simulation with Bx was restarted from the fully converged first order solution, leading to a less optimal convergence history, with a maximum CFL equal to 25.

The surface pressure and heat flux calculated by the Bx scheme are shown in Figs. 6.8 and 6.9 and compared with the modified Steger Warming solution (i.e. the best result in Figs. 6.4 and 6.5) and the available experimental data. The superior shock capturing of the RD approach yields an impressive improvement in the numerical solution if compared to the standard FV method, in particular on the heat flux distribution on the first cone and on the detection of the bubble size, which almost perfectly match the experiments on this rather coarse mesh. This result alone indicates RD as a strong candidate for enhancing the accuracy of double cone flow simulations on unstructured grids.
Figure 6.6: Temperature field given by Bx scheme in run 35 with a zoom on the separation region.

Figure 6.7: Convergence history in terms of pressure residual for run 35 with N scheme and user-defined CFL law.
**Figure 6.8:** Surface pressure with Bx and modified Steger Warming for run 35.

**Figure 6.9:** Surface heat flux with Bx and modified Steger Warming for run 35.
The overestimation of the heat flux on the first cone can be furtherly reduced, and get closer to the experiments, by including a frozen vibrational energy content in the free stream conditions and considering the effect of vibrational relaxation as demonstrated in [108] on the same specific testcase.

### 6.1.1.2 Double cone: run 40

The nominal conditions for this low enthalpy (5.38 MJ/kg) configuration are given in Table 6.2.

<table>
<thead>
<tr>
<th>$M_{\infty}$</th>
<th>$\rho_{\infty} ,[kg/m^3]$</th>
<th>$U_{\infty} ,[m/s]$</th>
<th>$T_{\infty} ,[K]$</th>
<th>$T_{w} ,[K]$</th>
<th>$y_N$</th>
<th>$y_{N_2}$</th>
<th>$T_w ,[K]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.6</td>
<td>0.00253</td>
<td>3104</td>
<td>172</td>
<td>2617</td>
<td>0</td>
<td>1</td>
<td>294</td>
</tr>
</tbody>
</table>

**Table 6.2:** Free stream conditions for double cone (run 40).

This testcase has a truly unsteady nature, at least numerically, and it doesn’t reach steady state convergence. The solution which is presented hereafter depicts the situation on a certain moment during the computation when numerical results and experiments were in a reasonably good agreement. Our simulation has been performed with the AUSM+ scheme in combination with least square reconstruction and Venkatakrishnan’s limiter on the 512x1024 quadrilateral cells mesh provided by Dr. Nompelis and used in [42, 105]. The flow is modeled as a neutral nitrogen mixture ($N_2$-$N$) in thermo-chemical nonequilibrium with a 2 temperature model. The corresponding reaction rate coefficients are given in [105]. Mach number and roto-translational temperature contours and isolines are presented in Figs. 6.10 and 6.11. In this case, no chemical reactions occur and molecular nitrogen remains the only component present in the whole flow field. Figs. 6.12 and 6.13 show a good agreement between experimental and computed surface pressure and heat flux up to the corresponding peaks, but both physical quantities are overpredicted on the second cone past the impingement point. This effect is probably due to the least square reconstruction algorithm applied to the supersonic outlet boundary condition that, at the time in which the simulation was performed, was not preserving a zero gradient for the extrapolated variables, leading to some inconsistency in the flowfield upstream.
Figure 6.10: Mach number field for run 40 (FV AUSM+).

Figure 6.11: Roto-translational temperature for run 40 (FV AUSM+).
Figure 6.12: Surface pressure vs. experiments for run 40 (FV AUSM+).

Figure 6.13: Surface heat transfer vs. experiments for run 40 (FV AUSM+).
6.1.1.3 Double cone: run 42

The nominal conditions for this high enthalpy (9.17 MJ/kg) configuration are listed in Table 6.3.

<table>
<thead>
<tr>
<th>$M_\infty$</th>
<th>$\rho_\infty [kg/m^3]$</th>
<th>$U_\infty [m/s]$</th>
<th>$T_\infty [K]$</th>
<th>$T_\infty^v [K]$</th>
<th>$y_N$</th>
<th>$y_{N_2}$</th>
<th>$T_w [K]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.5</td>
<td>0.001468</td>
<td>3849.3</td>
<td>268.7</td>
<td>3160</td>
<td>0</td>
<td>1</td>
<td>294.7</td>
</tr>
</tbody>
</table>

Table 6.3: Free stream conditions for double cone (run 42).

The results here shown for this testcase have been run with the CRD solver for the 2-temperature model and nitrogen mixture as described in run 40. In particular, the second order accurate blended Bxc scheme has been employed. Since this novel method works, for the moment, only on simplex cells (triangles in 2D and tetrahedra in 3D), Nompelis’s intermediate mesh (256x512 in this case) has been split into triangles, as in run 35.

From the Mach number and roto-translational temperature contours/isolines presented in Figs. 6.14 and 6.15 we can see the excellent shock capturing properties of the CRD method. The vibrational temperature of molecular nitrogen is shown in Fig. 6.16, clearly indicating a non negligible presence of thermal nonequilibrium in the flow, particularly in the boundary layer and downstream of the bow shock, where the roto-translational temperature is higher. Unlike the previous case, i.e. run 40, a moderate dissociation of molecular nitrogen into atoms occurs, as highlighted from the contours/isolines of atomic nitrogen mass fractions in Fig. 6.17. Because of the effect of the chemistry-vibration-chemistry coupling, the region affected by chemical dissociation has also the highest vibrational temperature.

Figs. 6.18a and 6.19a show the comparison between experimental and computed heat flux and surface pressure. The CRD solver yields a resolution competitive with the one given by Nompelis’s finite volume solver, but requiring only one quarter of the degrees of freedom. This emerges clearly from comparing Figs. 6.18a and 6.18b for the pressure surface, Figs. 6.19a and 6.19b for the heat flux, where the reference results are taken from [105] and they were computed on a finer 512x1024 cells mesh.
**Figure 6.14:** Mach number field for run 42 (CRD Bxc).

**Figure 6.15:** Roto-translational temperature for run 42 (CRD Bxc).
Figure 6.16: Vibrational temperature $T_{N_2}^v$ for run 42 (CRD Bxc).

Figure 6.17: Atomic $N$ mass fraction for run 42 (CRD Bxc).
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6.1.2 Cylinder 3D (DLR)

This experiment was performed in HEG wind tunnel at DLR (Germany). The configuration is a circular cylinder with diameter 90 mm and a length (including shaped holder) of 380 mm, placed with its axis transverse to the...
flow. The measurements on the cylinder have been carried out at two different total enthalpies (HEG conditions 1 and 2, 22.4 MJ/kg and 13.5 MJ/kg, respectively) and with air as a test gas. At those experimental conditions, the flow in the shock layer is subject to nonequilibrium chemical relaxation phenomena, leading to a modification of the gas properties (temperature, density, \ldots), which in turn causes changes in shock properties, such as shape and stand-off distance. A preliminary study on a similar configuration but with different free-stream flow conditions is reported in [106].

A blind numerical study on the two selected configurations have been conducted within the RTO contest, so that experimental measurements have been made available to participants only after the delivery of the computational results. The partially unstructured mesh for this case has been generated with ANSYS Gambit with the precious help of Janos Molnar. It is composed by 3426300 hexaedral cells: a global view of the surface mesh (except for the inlet boundary that has been blanked for visualization purposes) and a zoom near the tip of the cylinder can be seen in Figs. 6.20 and 6.21a. In particular, the sharp corner of the cylinder has been rounded up in order to avoid singularities in the solution, as shown in Fig. 6.21b, while the shaped holder has not been included in the model.

The implicit cell centered finite volume solver with AUSM+ flux, weighted least square reconstruction and Venkatakrishnan limiter has been used for computing both the flow conditions. A 3-temperature model (including roto-translational $T$, $T_{N_2}^v$, $T_{O_2}^v$) for thermo-chemical nonequilibrium has been applied to this case. The flow is modeled as a 5-species air mixture with reaction rate coefficients given by [120].

### 6.1.2.1 Cylinder HEG: condition 1

The HEG reservoir and free stream data for the measurements are listed in Table 6.4. The free stream Mach number, which is not specified in the table, is $M_\infty = 8.8$. Furthermore, the free stream vibrational temperatures $T_{N_2}^v$ and $T_{O_2}^v$ have been assumed in equilibrium with the roto-translational temperature, while $T_w = 300 \, K$ is imposed as wall temperature.

<table>
<thead>
<tr>
<th>$\rho_\infty [kg/m^3]$</th>
<th>$U_\infty [m/s]$</th>
<th>$T_\infty [K]$</th>
<th>$y_N$</th>
<th>$y_O$</th>
<th>$y_{N_2}$</th>
<th>$y_{NO}$</th>
<th>$y_{O_2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001547</td>
<td>5956</td>
<td>901</td>
<td>0.65e-6</td>
<td>0.2283</td>
<td>0.7543</td>
<td>0.01026</td>
<td>0.00713</td>
</tr>
</tbody>
</table>

**Table 6.4:** Free stream conditions for HEG cylinder (condition 1).

Figures 6.22a and 6.22b show respectively the isolines and contours of Mach
number and roto-translational temperature. In the latter case, a maximum temperature of 17000 K is reached.

The contours and isolines of the mass fractions of atomic species, oxygen and nitrogen, are shown in 6.23a and 6.23b, while the mass fractions of the corresponding molecules are presented in 6.24a and 6.24b: it can be easily seen that the overall composition of the mixture remains frozen to the free stream values, except for some unperceivable variations clearly due to some small numerical inaccuracy. The latter is especially located near the corner between the far field and symmetry plane, where the shock hits the side boundary: a slightly bigger domain or just a finer mesh in the region past the cylinder would probably have avoided this trouble.

Computed and measured surface pressure and heat flux versus angle ($0^\circ$ corresponds to the stagnation point) are shown in Figs. 6.25a and 6.25b in three different sections in the spanwise direction ($z/L = 0$, $z/L = 0.5$, $z/L = 0.95$, the latter being close to the tip of the cylinder). On the one hand, the agreement with the experiments is remarkably good for the pres-

Figure 6.20: Global view of the unstructured surface mesh.
Figure 6.21: Detailed views on the cylinder surface mesh.

Figure 6.22: Contours/isolines of Mach number and roto-translational temperature for the HEG cylinder (condition 1) with FV AUSM+.

sure, whose peak reaches about 50 kPa. On the other hand, the peak heat flux on the symmetry plane, 7 MW/m², is underestimated by roughly 12% which is considered acceptable also in view of the experimental uncertainties.

The matching with the experiments could be probably improved by assum-
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Figure 6.23: Contours/isolines of atomic $O$ and $N$ mass fractions for the HEG cylinder (condition 1) with FV AUSM+, showing the chemically frozen flowfield.

(a) Mass fractions of atomic oxygen  (b) Mass fractions of atomic nitrogen

Figure 6.24: Contours and isolines of $O_2$ and $N_2$ mass fractions for the HEG cylinder (condition 1) with FV AUSM+, showing the chemically frozen flowfield.

(a) Mass fractions of molecular oxygen  (b) Mass fractions of molecular nitrogen

ing some catalytic activity at the wall, as shown in [93] for a number of 2D cases in similar conditions.
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6.1.2.2 Cylinder HEG : condition 2

The free stream conditions are presented in Table 6.5. The free stream mach number is \( M_\infty = 8.7 \), while, also in this case, the free stream vibrational temperatures \( T_{N_2}^v \) and \( T_{O_2}^v \) have been considered in equilibrium with the roto-translational temperature. The wall temperature is again \( T_w = 300 \) K as in the previous case.

<table>
<thead>
<tr>
<th>( \rho_\infty [kg/m^3] )</th>
<th>( U_\infty [m/s] )</th>
<th>( T_\infty [K] )</th>
<th>( y_N )</th>
<th>( y_O )</th>
<th>( y_{N_2} )</th>
<th>( y_{NO} )</th>
<th>( y_{O_2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00326</td>
<td>4776</td>
<td>694</td>
<td>0</td>
<td>0.07955</td>
<td>0.7356</td>
<td>0.0509</td>
<td>0.1340</td>
</tr>
</tbody>
</table>

Table 6.5: Free stream conditions for the HEG cylinder (condition 2).

Figs. 6.26a and 6.26b show respectively the isolines and contours of Mach number and roto-translational temperature. In the latter case, a maximum temperature of 11500 K is reached.
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Figure 6.26: Contours/isolines of Mach number and roto-translational temperature for the HEG cylinder (condition 2) with FV AUSM+.

Figure 6.27: Contours and isolines of mass fractions of atomic O and N for the HEG cylinder (condition 2) with FV AUSM+, showing a perfectly chemically frozen flowfield.

The contours and isolines of the mass fractions of atomic species, oxygen and nitrogen, are shown in 6.27a and 6.27b, while the mass fractions of the corresponding molecules are presented in 6.28a and 6.28b. Also in this case,
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Figure 6.28: Contours and isolines of mass fractions of $O_2$ and $N_2$ for the HEG cylinder (condition 2) with FV AUSM+, showing a perfectly chemically frozen flowfield.

Figure 6.29: Computed surface pressure and heat flux vs. experimental measurements for the HEG cylinder (condition 2) with FV AUSM+.

The overall composition of the mixture remains frozen to the free stream values. In particular, the mass fraction of atomic nitrogen remains identically zero. The solution is smooth even near the corner between the far field and
symmetry plane, which was causing some small trouble in Condition 1. Computed and measured surface pressure and heat flux versus angle are shown in Figs. 6.29a and 6.29b in the same three sections in the spanwise direction as for the previous condition. The maximum pressure is about 64 kPa, while the peak heat flux reaches 5.0 MW/m² on the symmetry plane and 6.4 MW/m² near the tip. The agreement with experiments is remarkably good for both the surface quantities.

6.2 Stardust Sample Return Capsule

The Stardust Sample Return Capsule (SRC) was launched in February 1999 with the aim of retrieving samples of interstellar dust from the tail of the WILD-2 comet. The capsule reentered Earth atmosphere in January 2006 at a speed of 12.6 km/s, which corresponds to the fastest and most energetic reentry of any artificial vehicle to date. The Stardust observation data recorded by several optical instruments aboard the NASA DC-8 Airborne observatory offers a precious opportunity to compare simulation to flight data at hypervelocity [25, 92, 153]. Figure 6.30a shows the Stardust capsule as seen from NASA’s DC-8 Airborne Laboratory aiming at exploring the conditions during reentry from the light emitted by the fireball caused when the capsule streaked through the sky. The aircraft was located near the end of the trajectory. The participating researchers were from NASA Ames, the SETI Institute, the University of Alaska, Utah State University, Lockheed Martin, U.S. Air Force Academy, the University of Kobe (Japan) and Stuttgart University. A closer look at the capsule after its landing is given in Fig. 6.30b.

In this section we present the results of the simulation of a few points points belonging to the flight trajectory of Stardust, corresponding to 34s, 51s and 66s after the reentry in Earth atmosphere. Since the entry of the capsule was nearly ballistic [153], an axisymmetric simulation offers a quite good approximation of the reality and has allowed us to save a lot of computational cost compared to a fully 3D configuration. All our computations have been performed with the AUSM+ scheme, which is exceptionally robust and deliver carbuncle free solutions even at these very high velocities (> 12 km/s at 34s), at least on meshes with cells sufficiently stretched in the direction tangential to the shock. Second order accuracy has been achieved by means of the least square reconstruction in combination with the Venkatakrishnan limiter. An example of mesh used for our calculations and a zoomed view around the capsule can be found respectively in Figs. 6.31 and 6.31b.
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Figure 6.30: Views of the Stardust capsule during the reentry phase and after landing.

(a) Stardust capsule streaking through the sky as seen from NASA’s DC-8 Airborne Laboratory on January 15th, 2006
(b) Stardust capsule after the landing

As far as the physical model is concerned, the 2-temperature Park model for ionized mixtures has been adopted, together with the reaction rates for the chemical nonequilibrium given by [120] and a radiative and local thermo-chemical equilibrium condition have been imposed at the wall. The numerical results given by our baseline solver (without any specific adjustment of chemical rates or thermodynamic properties) will be compared with those obtained with the NASA DPLR code in [25, 92, 153]. The differences be-
between DPLR and our aerothermodynamic solver are considerable from both the numerical and physical modelling point of view. In particular, DPLR uses a modified Steger-Warming scheme similar to the one presented in Sec. 5.2.1.4, a third order accurate MUSCL reconstruction, a 3-temperature model where the rotational temperature is separated from the translational one, transport properties based on mixing rules and different chemical reaction rates. Moreover, while we assume LTE at the wall, DPLR simulations have been run with full catalicity only for ions.

### 6.2.1 81.02 Km, t=34 s, Max entry speed, $M_\infty = 41.9$

At this point of the reentry trajectory the capsule reached its maximum speed, which also corresponds to the maximum velocity ever experienced by an artificial object flying within Earth atmosphere. The corresponding flow conditions are given in Table 6.6. It is estimated that at this point the transition between continuum and non-continuum regimes occurs, with $Kn \approx 0.005$ based on the diameter of the capsule.

<table>
<thead>
<tr>
<th>$M_\infty$</th>
<th>$\rho_\infty \text{[kg/m}^3\text{]}$</th>
<th>$U_\infty \text{[m/s]}$</th>
<th>$T_\infty \text{[K]}$</th>
<th>$p_\infty \text{[Pa]}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>41.9</td>
<td>0.00001269</td>
<td>12385.12016</td>
<td>217.63406</td>
<td>0.79216</td>
</tr>
</tbody>
</table>

**Table 6.6:** Free stream conditions for Stardust at $t = 34$s.

![Mach number and streamlines around the capsule at t=34s with FV AUSM+](image-url)
Figure 6.33: Roto-translational and vibrational temperatures at t=34s with FV AUSM+.

Figure 6.34: Temperatures profiles on the stagnation line at t=34s computed with COOLFluiD and the solvers in [25].
The Mach number field around the capsule is shown in Fig. 6.32, where the superposed streamlines indicate the location of the recirculation bubble. The roto-translational and vibrational temperature contours corresponding to this trajectory point are presented in Fig. 6.33. In particular, the peak post-shock roto-translation temperature reaches 53000 K, while the maximum vibrational temperature is 13400 K. The temperature profiles on the stagnation line are shown in Fig. 6.34 together with the solutions computed in [25] with the Direct Simulation Monte Carlo (DSMC) method and the DPLR code. For the latter case, two solutions with different physico-chemical models, i.e. baseline (b) and modified (m), are given. Our solution is close to the (m) case in terms of roto-translational temperature and it predicts a vibro-electronic temperature that falls right in between the DSMC results for the electronic and vibrational temperature. The stagnation line profiles for the neutral species number densities in the air mixture are plotted in Fig. 6.35 (COOLFluiD) and 6.36 ([25]). Similarly, the number densities of all ionic components and electrons obtained with COOLFluiD are shown in Fig. 6.37, while only the number densities of \(N^+\) and \(N_2^+\) are shown in 6.38, because other data were not available in [25] for comparison. If we compare the behaviour of the ionic and electron species close to the wall (a logarithmic scale has been adopted to simplify this analysis), our results differ considerably with those of [25]. This is partially justified by the fact that we apply a LTE model at the wall, while [25] imposes full catalycity to ions (that recombine into their neutral atoms and molecules) and atoms (that recombine into molecules).

Generally speaking, the many differences in the thermo-chemical modeling, in the numerical scheme and in the mesh resolution between the DPLR simulations and ours can reasonably justify the partial disagreement between the two solutions.

### 6.2.2 61.76 Km, t=51 s, Peak heating point, \(M_\infty = 35.3\)

This trajectory point corresponds to the maximum thermal load, achieved at \(M_\infty = 35\). The flow free stream conditions are listed in Table 6.7.

<table>
<thead>
<tr>
<th>(M_\infty)</th>
<th>(\rho_\infty[kg/m^3])</th>
<th>(U_\infty[m/s])</th>
<th>(T_\infty[K])</th>
<th>(p_\infty[Pa])</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.3</td>
<td>0.00021100</td>
<td>10871.38098</td>
<td>234.95243</td>
<td>14.21781</td>
</tr>
</tbody>
</table>

**Table 6.7:** Free stream conditions for Stardust at t = 51s.

The flowfield around the capsule is shown in Fig. 6.39a in terms of Mach number contours and velocity streamlines. COOLFluiD’s solution is in per-
Figure 6.35: Stagnation line profiles for the number densities of the neutral species at t=34s with COOLFluiD (FV AUSM+).

Figure 6.36: Stagnation line profiles for the number densities of the neutral species at t=34s in [25].
Figure 6.37: Stagnation line profiles for all number densities of the ionic and electron species at $t=34s$ with COOLFluiD (FV AUSM+).

Figure 6.38: Stagnation line profiles for the number densities of $N^+$ and $N_2^+$ and electrons at $t=34s$ in [25].
fect agreement with the one in Fig. 6.39b, yielded by the DPLR code. Herein, the length of the capsule for our simulation have been taken from [25] (0.5 m) and is slightly different from the size adopted in [153] (0.56 m), but this have no relevant effect in our code to code comparison. In particular, the three recirculation bubbles that can be identified in the after-body are located in the same positions (relatively to the capsule) and have very similar sizes.

Fig. 6.40 shows the surface heat fluxes calculated by the two solvers and the agreement between the two solutions is again pretty impressive, especially on the predicted peak value. The only remarkable difference consists in a little overshoot due to thickening of the boundary layer on the shoulder which is not properly resolved by COOLFluiD, probably because the mesh was not sufficiently fine in that region.

![Mach number and velocity streamlines at t=51s.](image)

(a) COOLFluiD solution (FV AUSM+)  (b) Solution given by NASA DPLR in [153]

**Figure 6.39:** Mach number and velocity streamlines at t=51s.

6.2.3 50.98 Km, t=66 s, \(M_\infty = 20.3\)

The conditions for this trajectory point are shown in Table 6.8.

<table>
<thead>
<tr>
<th>(M_\infty)</th>
<th>(p_\infty[kg/m^3])</th>
<th>(U_\infty[m/s])</th>
<th>(T_\infty[K])</th>
<th>(p_\infty[Pa])</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.3</td>
<td>0.00085435</td>
<td>6504.45316</td>
<td>255.83878</td>
<td>62.78974</td>
</tr>
</tbody>
</table>

**Table 6.8:** Free stream conditions for Stardust at \(t = 66s\).

The surface heat fluxes computed with COOLFluiD and with DPLR in [153] are presented in Figs. 6.41a and 6.41b (dashed line), showing a good agreement. In the latter picture, an additional curve corresponding to the heat
Figure 6.40: Surface heat flux profile for the Stardust capsule at t=51s.

Figure 6.41: Surface heat flux profile for the Stardust capsule at t=66s.

A full and a zoomed view of the flowfield surrounding the capsule in terms of roto-translational and vibro-electronic temperature is shown in 6.42. In
this case, in the post-shock region on the stagnation line the peak roto-translational and vibro-electronic temperatures reach 14150 K and 9200 K respectively.

![Contour and isolines of roto-translational and vibrational temperatures for the Stardust capsule at t=66s.](image)

**Figure 6.42:** Contour and isolines of roto-translational and vibrational temperatures for the Stardust capsule at t=66s.

### 6.3 EXPERT Vehicle

The European re-entry vehicle EXPERT (EXPERimental Re-entry Test-bed) [103] is part of the ESA aerothermodynamic research program aiming to design a low cost hypersonic flight vehicle for measurement of aerothermodynamic phenomena and thus also validating the numerical codes. The goal of EXPERT is to achieve low cost re-entry experiments focused on flying "problems for design"; that is, complex fluid dynamic phenomena such as boundary layer/ shear layer transition, viscous interactions, flow separation and re-attachment, shock-boundary layer interactions, surface catalysis, blackout and plume-flowfield interactions.

The results to be presented shortly concern the investigation of two points on the trajectory followed by the EXPERT vehicle during the reentry phase. The first one is the point of maximum convective heating (Condition 1),
whereas the second trajectory point has been chosen in order to investigate flow conditions characterized by a stronger thermal and chemical nonequilibrium (Condition 2).

As we shall see in the following, the condition of maximum heating is characterized by relatively low speed and high pressure, reducing in this way the extent of thermal and chemical nonequilibrium. The location of the two points within the reentry trajectory (as foreseen till June 2007) are highlighted in Fig. 6.43, while the corresponding flow conditions are shown in Table 6.9.

<table>
<thead>
<tr>
<th></th>
<th>$M_\infty$</th>
<th>$p_\infty [Pa]$</th>
<th>$U_\infty [m/s]$</th>
<th>$T_\infty [K]$</th>
<th>$T_w [K]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>condition 1</td>
<td>14</td>
<td>668.1</td>
<td>4286.5</td>
<td>233.61</td>
<td>1000</td>
</tr>
<tr>
<td>condition 2</td>
<td>18.4</td>
<td>2</td>
<td>5040</td>
<td>186.4</td>
<td>1650</td>
</tr>
</tbody>
</table>

**Table 6.9**: Free stream conditions for the EXPERT simulations.

### 6.3.1 Condition 1, $M_\infty = 14$

This condition, corresponding to a low altitude trajectory point characterized by relatively high free stream pressure and temperature, has been selected in order to test different physical models presented in Chapter 4. In particular, the results given by the two LTE models with fixed (LTE-
FEF) and variable elemental fractions (LTE-VEF) are compared against each other and against the solution obtained in Chemical Nonequilibrium (CNEQ) and TCNEQ simulations. Hereby, LTE and CNEQ simulations have been run with the AUSM+ scheme, while the Roe scheme described in Sec.5.2.1.1 has been used for TCNEQ, in combination with the carbuncle fix in [144]. All computations have been performed on a 2D axisymmetric structured mesh with 12600 cells, which is shown in Fig. 6.44a and Fig. 6.44b. The temperature flowfields yielded by the four different models are shown in Fig. 6.45a for the chemical equilibrium case (LTE-FEF and LTE-VEF) and in Fig. 6.45b for the nonequilibrium cases (CNEQ and TCNEQ). More detailed views of the flowfield around the vehicle nose are presented in Figs. 6.46a and 6.46b. While the two LTE models give no visible difference on the temperature, the overall flowfield appears a bit different in the two nonequilibrium cases.

![Computational mesh](image)

(a) Global view.  
(b) Zoom around the vehicle.

**Figure 6.44:** Computational mesh (12600 cells) for the EXPERT vehicle.

In Fig. 6.47 we compare the temperature profiles on the stagnation lines for the four models. The shock stand-off distance is slightly bigger in the TCNEQ case, but this is expected, because of the slightly higher post-shock temperature. As far as the LTE models are concerned, they yield different results inside the boundary layer, because of the demixing phenomenon. To better understand the latter, Fig. 6.48 shows temperature and species mass fractions profiles on the stagnation line only for LTE-FEF and LTE-VEF. A logarithmic scale is used on the $x$ axis, in order to better visualize the
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(a) LTE-FEF (top) vs. LTE-VEF (bottom)  
(b) CNEQ (top) vs. TCNEQ (bottom)

**Figure 6.45:** Contour/isolines of temperature for the EXPERT vehicle in condition 1 \( (M_\infty = 14) \) with different models.

(a) LTE-FEF (top) vs. LTE-VEF (bottom)  
(b) CNEQ (top) vs. TCNEQ (bottom)

**Figure 6.46:** Temperature field around the nose of the EXPERT vehicle in condition 1 \( (M_\infty = 14) \) with different models.
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Figure 6.47: Comparison of the stagnation line profiles of temperature for LTE-FEF, LTE-VEF, CNEQ and TCNEQ in condition 1 ($M_\infty = 14$).

Figure 6.48: Stagnation line profiles of temperature and species mass fractions for LTE-FEF and LTE-VEF in condition 1 ($M_\infty = 14$).
behaviour inside the boundary layer, where the demixing effect causes an increase of the oxygen element (and corresponding atomic) concentration, and a decrease of nitrogen element (and corresponding atomic) concentration with respect to the case with constant elemental fractions. As underlined in [141], the presence of oxygen tends to increase in the direction opposite to the temperature gradient at relatively low temperatures (below a certain threshold which varies with pressure), while the inverse situation occurs at higher temperatures. This trend, which is mainly due to the non-monototic behaviour with respect to temperature of the elemental thermal demixing coefficient $D^T_O$ in Eq. 4.18 [79, 141], is clearly identifiable in Fig. 6.49, where the gradient of elemental fraction of oxygen presents a sign change from negative to positive: after the gradient inversion, the elemental fraction of oxygen increases with the decrease of temperature while approaching the wall.

The temperatures (roto-translational and vibrational for TCNEQ, the only temperature for CNEQ) and composition on the stagnation line with nonequilibrium conditions are presented in Fig. 6.50.
Figure 6.50: Comparison of the stagnation line profiles of temperature and species mass fractions for TCNEQ and CNEQ in condition 1.

6.3.2 Condition 2, \( M_\infty = 18.4 \)

This 3D computation has been run in parallel on a 3.3 million hexaedra mesh (generated by Fabio Pinna), on up to 316 AMD64 processors on KU Leuven cluster. The geometry includes 4 open flaps (with the same angle), which anyway don’t affect significantly the flowfield, since the secondary shocks generated in front of them don’t interact with the bow shock. A global view of the surface mesh is presented in Fig. 6.51 while zoomed views near the nose and flap regions, including the surface mesh on the symmetry boundary, are shown in Figs. 6.52a and 6.52b.

The Liou Steffen AUSM scheme has been used for this computation. In this case, we have restricted ourselves to the multi-temperature model described in Sec. 4.3.3 and 5-species air mixture with reaction rate coefficients given by [120]. The full three dimensional flowfield can be viewed in Figs. 6.54 and 6.55 in terms of Mach number and roto-translational temperature respectively.
Figure 6.51: Global view of the wall surface mesh for the EXPERT vehicle.

(a) Zoom on the wall and mirror mesh surfaces near the nose
(b) Zoom on the wall and mirror mesh surfaces near one flap

Figure 6.52: Detailed views on the surface mesh for the EXPERT vehicle.
Figure 6.53: Partitioned surface mesh for the EXPERT vehicle.

The contours and isolines of vibrational temperatures of $N_2$ and $O_2$ are presented in Figs. 6.56 and 6.57, showing a considerable degree of thermal nonequilibrium, since the fields of both temperatures are very far from the one in Fig. 6.55. In particular, while the peak roto-translational temperature is higher than 12100 K, the post-shock vibrational temperatures are about 6300 K for $T_{N_2}^v$ and 5100 K for $T_{O_2}^v$.

In this simulation, however, the boundary layer is very likely not to be accurately resolved in 3D, due to the relative coarseness of the grid near the body (the first cell size is about 1 mm) and therefore the heat flux is not shown here. Further investigation on finer meshes and validation against results obtained by other codes would therefore be needed.