**HyNECC: Hypersonic NonEquilibrium Comparison Cases**

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**1. Objective**

With the recent availability of QCT-based state-specific rates and the many proposed relaxation and reaction models, and the presentation of new experimental data on non-equilibrium high temperature flows, it will be advisable for the *nonequilibrium CFD community* to adopt a common set of benchmark cases. Ideally, these cases would elucidate both the validity of various approaches and the underlying reasons for differences in results.

While the ultimate goal of the study is to include CFD/NS nonequilibrium solvers, we recognize that the initial formulation of test cases reflects a DSMC-oriented approach. It is hoped that initial discussions will generate the necessary interest and feedback to modify and add to the test cases and make them sufficiently general and robust to allow for the wider CFD community.

The goals of this study are

(1) Comparison of rates produced by different models and implementations at

(a) equilibrium

(b) two- or three-temperature regimes

(c) quasi-steady state (QSS)

(2) Projecting the differences and similarities in models and rates onto realistic nonequilibrium hypersonic flow conditions

(3) Comparison with available experimental data in order to understand how well or poorly state-of-the-art solvers predict different flows

(4) Find properties and conditions most indicative and most sensitive to models, parameters, and implementations

(5) Provide specific feedback to the experimental community on conditions, properties, and flows of interest.

(6) Establish clear, straightforward set of benchmarks for future code and model development

To achieve the goals, we propose to evaluate numerical accuracy and uncertainty of physical models and numerical approaches for modeling real gas effects in high temperature hypersonic flows through code-to-code and code-to-measurement comparison of four main benchmarks: relaxation rates, flow properties, surface parameters, and radiation signatures. The cases are assumed to be run by code experts, in “production mode”, so only the basic parameters of the problem are defined here. Solver-related parameters such as collision models and grid refinements are left to the discretion of the experts and/or the capability of the solver involved. Sensitivity studies of the impact of these parameters on results are of interest, but are not otherwise addressed at this stage.

**2. Overview of Test Cases**

The proposed test cases include three modeling configurations of increasing complexity: (i) 0D spatially homogeneous high-temperature heat bath, (ii) 1D normal shock wave, (iii) axially symmetric hypersonic, high enthalpy flow. The configuration (i) provides the opportunity to directly compare equilibrium and non-equilibrium rates of vibrational excitation and chemical reactions under conditions that emulate those behind strong shock waves. The configurations (ii) and (iii) are based on recent measurements where the spatial distribution of flow properties, in one case, and surface parameters, in the other case, have been obtained using modern experimental facilities and techniques. In both cases, the experimental conditions are characterized by strong thermal and chemical non-equilibrium in the flow. The first set of test cases uses the conditions and data from the shock tube measurements of Ibraguimova et al. [1-3] which provide vibrational temperatures of O2 in a shock under strongly non-equilibrium conditions. These temperatures, evaluated from the absorption data on the Schumann-Runge UV band of O2, are based on contributions from vibrational levels through at least *v*=10 and are not potentially-distorted ones based on only the *v1*/*v0* ratio. The second set of test cases is not finalized at this time yet, and two possibilities are currently discussed. The first possibility is to use the measurements [4-6] of pressure and heat flux distributions over a double cone configuration in LENS XX expansion tunnel, where dry air was taken as a test gas at total enthalpies from 5 MJ/kg to 22 MJ/kg (free stream velocities from 3.2 to 6.5 km/s, respectively). The second possibility is to use the measurements of surface properties over a cylinder, presented in Ref. [13], with some additional detail given in Ref. [14], where the test gas was also air, and free velocities ranged from 4.8 to 6 km/s.

**3. TC1: Spatially Homogeneous Heat Bath**

*3.1. Flow Conditions*

3.1.1. A fixed-temperature bath is proposed for the evaluation of chemical reaction rates, in which separate mode temperatures (translational, rotational, and vibrational) are set, with Maxwell-Boltzmann state distributions enforced at the prescribed temperatures.

(a) In the DSMC method, a fixed-temperature bath can be modeled as a spatially uniform box with specular walls where the gas translational, rotational, and vibrational temperatures are all kept at their prescribed values. The chemical reaction rates should be calculated even though no internal energy transfer or chemical reactions should be allowed (i.e. the reaction events are counted but not modeled).

(b) For continuum CFD, such a bath reduces to the calculation of chemical reaction rates determined as functions of total or translation-rotational and vibrational temperatures.

(c) In the QCT framework, the methodology described in Ref. [10] may be used to evaluate the reaction rates. In that work, a large number of representative collisions between given species in an ensemble of particles characterized by one or more temperatures is used to calculate the rate.

3.1.2. A fixed translational temperature Tt bath is suggested for the evaluation of rotational and vibrational relaxation times r and v and quasi-steady state (QSS) reaction rates.

(a) For DSMC, the Tt isothermal bath may be modeled as a spatially uniform box with specular walls where the gas translational temperature is kept constant at a given value. This can be done either by not changing molecular velocities after collisions, or re-sampling the particle velocities from the corresponding Maxwellian distribution every time step.

(b) For continuum CFD, the internal energy relaxation times and QSS rates are evaluated in a spatially homogeneous gas cell where the translational temperature is kept constant during the simulation, while the rotational and vibrational temperatures and species concentrations are allowed to change with time.

(c) QCT approach is not easily amenable to the calculation of vibrational and/or rotational relaxation rates. One of the possible ways to obtain and verify such rates is to use state-specific transition rates obtained by QCT in a solution of master equations (see, for example, [11]). One can also use the direct molecular simulation (DMS) method [12], which embeds trajectory calculations within a standard DSMC simulation, and thus allows one to directly evaluate vibrational and rotational relaxation rates.

For r and v evaluation, no chemical reactions are allowed, only energy exchange between vibrational, rotational, and translational modes. The relaxation proceeds from the initial state specified in Table 1, and the r and v values are obtained using the e-folding approach [7,8]: the rotational and vibrational relaxation times are the times at which the vibrational and rotational energies *Er* and *Ev* rise from their initial values *Er,i* and *Ev,i* to

where *Er,f* and *Ev,f* are the rotational and vibrational temperatures at the translational (i.e. their final) temperature Tt.

The vibrational rate constant for the 10 transition is also of interest here, and is sought for TC1.5 and TC1.6.

For the QSS dissociation rate evaluation in TC1.7 and TC1.8, both chemical reactions and internal energy transfer are allowed.

*3.2. Desired Output*

3.2.1. Fixed-temperature bath (TC1.1 through TC1.4)

The following relaxation property:

* dissociation reaction rate kd (m3/(molecule s))
* average vibrational energy of dissociating molecules
* average difference between the vibrational energy of reactants and reaction products

3.2.2. Tt isothermal bath (TC1.5 through TC1.8)

The following gas properties as a function of time:

* rotational temperature (TC1.5 through TC1.8)
* vibrational temperature (TC1.5 through TC1.8)
* atomic nitrogen (TC1.7) and atomic oxygen (TC1.8) mole fractions

The following relaxation properties:

* rotational relaxation time r (s) for TC1.5 and TC1.6
* vibrational relaxation time v (s) for TC1.5 and TC1.6
* vibrational rate constant k10 (molecule/s) for TC1.5 and TC1.6
* QSS dissociation reaction rate kd at the end of the simulation (m3/(molecule s)) for TC1.7 and TC1.8

3.2.3. A summary of the models used. The approach used to split the internal energies into vibrational and rotational parts, if applicable.

*3.3 Run Matrix*

The run matrix for a fixed-temperature bath is given in Table 1. Here, Tt, Tr, Tv are translational, rotational, and vibrational temperatures, respectively.

The run matrix for the Tt isothermal bath is shown in Fig. 2. Here, only the translational temperature does not change during the simulation, while the rotational and vibrational temperatures do, and the values given in the right column are their initial values. Initial gas composition is either pure nitrogen or pure oxygen. For TC.5 and TC.6, chemical reactions should be turned off, and only internal energies (temperatures) change with time. Cases TC1.7 and TC1.8 include both internal energy relaxation and dissociation reactions. For TC1.7, the initial number density and total simulation time are 1025 molecule/m3 and 50 s, respectively. For TC1.12, the initial number density and total simulation time are 1025 molecule/m3 and 0.2 s, respectively. For models that do not rely on the multi-temperature approach (e.g, grouping method or DMS method), the rotational or vibrational temperatures can be computed a posteriori even though they are not used explicitly in the calculations.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Test Case | Bath | Collision Type | Tt =Tr | Tv |
| TC1.1 | Fixed Tt, Tr, Tv | N2-N2, N2-N  O2-O2, O2-O | 10,000 K | 4,000 K, 6,000 K, 8,000 K, 10,000 K |
| TC1.2 | Fixed Tt, Tr, Tv | N2-N2, N2-N  O2-O2, O2-O | 8,000 K | 4,000 K, 6,000 K, 8,000 K |
| TC1.3 | Fixed Tt, Tr, Tv | N2-N2, N2-N  O2-O2, O2-O | 6,000 K | 4,000 K, 6,000 K |
| TC1.4 | Fixed Tt, Tr, Tv | N2-N2, N2-N  O2-O2, O2-O | 4,000 K | 4,000 K |

*Table 1*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Test Case | Bath | Gas | Tt | Tr,initial=Tv,initial |
| TC1.5 | Tt fixed, Tr and Tv vary | N2 | 4000 K, 6,000 K, 8,000 K, 10,000 K, 15,000 K | 300 K |
| TC1.6 | Tt fixed, Tr and Tv vary | O2 | 4000 K, 6,000 K, 8,000 K, 10,000 K, 15,000 K | 300 K |
| TC1.7 | Tt fixed, Tr and Tv vary | N2 | 10,000 K | 300 K |
| TC1.8 | Tt fixed, Tr and Tv vary | O2 | 8,000 K | 300 K |

*Table 2*

**4. TC2: Normal Shock Wave in Dissociating O2**

*4.1. Geometry*

While it is possible to model the normal shock wave in one-dimensional configuration, it is recommended for the sake of consistency to model it in 2D. For CFD, that allows one to avoid the calculation of Rankine-Hugoniot conditions at the downstream boundary. For DSMC, in addition to the above, there will be no shock front movement in the upstream or downstream direction due to boundary condition fluctuations or incomplete thermal or chemical relaxation resulting in gas properties near the downstream boundary being slightly different from those dictated by the Rankine-Hugoniot conditions. In the 2D setup, it is important that the geometry is large enough so that the solution along the stagnation line matches that in a one-dimensional shock. It is suggested to compute a flow over a 30 cm plate of an arbitrary thickness, placed perpendicular to the free stream. Fully specular in DSMC, and adiabatic in CFD, reflection should be set at the plate surface. The solution for a normal shock wave for the 2D case should then be extracted along the symmetry axis (stagnation streamline) of the flow.

*4.2. Desired Output*

4.2.1. The following gas properties along the stagnation line

* total number density (molecule/m3)
* O mole fraction
* overall translational temperature (K)
* rotational temperature of O2 (K)
* vibrational temperature of O2 (K)
* vibrational level populations at the point where the vibrational temperature is maximum

4.2.2. A summary of the problem setup and solution procedure. Basic assumptions and models used, such as thermodynamic and transport data, collision models (elastic, inelastic, and reacting collisions), boundary condition description, grid sizes, as well as convergence criteria. An expert opinion as to the validity of the results, or any indicators that suggest the code or its algorithms or models may not be applicable to the problem.

4.2.3. An estimate of computational resources required (platform, memory, number of processors and CPU-time), and of the problem setup and postprocessing time (man-hours).

*4.3. Run Matrix*

The run matrix is given in Table 3. Symbol ∞ denotes here the equilibrium upstream condition.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Test Case | Free Stream Gas | p∞, Torr | U∞, m/s | T∞, K |
| TC2.1 | 100% O2 | 2 | 3,070 | 300 |
| TC2.2 | 100% O2 | 0.8 | 4,440 | 300 |

*Table 3.*

**5. TC3: Two-Dimensional Hypersonic Flow**

We are currently considering two options:

**Option 1**: flow over a double cone, with flow conditions of Refs. [4-6]

**Option 2**: flow over a cylinder, with flow conditions of Refs. [13-14]

Two options are considered since none of them is ideal. The double-cone experiments have been shown to be difficult to match numerically, with at least some of the difference attributed to uncertainties in the free stream conditions. The cylinder experiments are 3D, and even though the spanwise distance is four times larger than the diameter, some 3D effects may still be present. Also, the cylinder surface was proven to be catalytic, and thus surface reactions need to be accounted for in numerical simulations in order to reproduce the data.

*5.1. Geometry*

***Option 1***

The flow is axially symmetric, and the geometry is a 25°/55° double cone. The base diameter of the front and back cones is 3.381 in and 10.309 in, respectively. There is also a 1.574 in thick cylinder attached at the aft end of the back cone. For a coordinate system with origin at the leading edge of the front cone, and the flow direction from left to right, the describing vertices are given in Table 4.

|  |  |  |
| --- | --- | --- |
| Point | x, mm | y, mm |
| leading edge | 0 | 0 |
| aft end of the front cone | 92.085 | 42.94 |
| aft end of the back cone | 153.69 | 130.925 |
| aft end of the cylinder | 170.9 | 130.925 |
| center of cylinder base | 170.9 | 0 |

*Table 4*

The cone boundary condition is isothermal with full accommodation at 300 K.

***Option 2***

The flow is two-dimensional, and the geometry is a 9 cm diameter circle that represents a cross section of a 9 cm diameter, 38 cm spanwise cylinder used in the experiment [13].

*5.2. Desired Output*

5.2.1. Overall surface properties (properties of the gas at the surface) along the double-cone surface as a function of X coordinate (to make them compatible with published measured results), in spreadsheet form and SI units. The surface properties of interest are

* pressure (N/m2)
* skin friction (N/m2)
* heat flux (W/m2)

5.2.2. Gas properties

**Option 1**

The following gas properties along the line Y=100 mm in spreadsheet form and SI units:

* overall translational temperature (K)
* overall number density (molecule/m3)
* species mole fractions
* species rotational temperature (K)
* species vibrational temperature (K)
* local Reynolds number based on the reference length of 131 mm

**Option 2**

The following gas properties along the stagnation stream in spreadsheet form and SI units:

* overall translational temperature (K)
* overall number density (molecule/m3)
* species mole fractions
* species rotational temperature (K)
* species vibrational temperature (K)
* local Reynolds number based on the reference length of 90 mm

5.2.3. **Option 1** only: the temporal change in

* the number density a spatial point (X,Y)=(92mm,46mm)
* heat flux along the surface

5.2.4. Flowfield data files suitable for 2D contour plotting with Tecplot. Variables of interest are similar to those given in 5.2.2.

5.2.5. A summary of the problem setup and solution procedure. Basic assumptions and models used, such as thermodynamic and transport data, collision models (elastic, inelastic, and reacting collisions), boundary condition description, grid sizes, as well as convergence criteria. An expert opinion as to the validity of the results, or any indicators that suggest the code or its algorithms or models may not be applicable to the problem.

5.2.6. An estimate of computational resources required (platform, memory, number of processors and CPU-time), and of the problem setup and postprocessing time (man-hours).

*5.3. Run Matrix*

The run matrix is given in Table 5 for **Option 1** and Table 6 for **Option 2**. Symbol ∞ denotes here the equilibrium free stream condition.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Test Case | Free Stream Gas | ∞, kg/m3 | U∞, m/s | T∞, K | Kn |
| TC3.1 | 76.5% N2 & 23.5% O2 | 4.99∙10-4 | 3,246 | 175 | 7.7e-4 |
| TC3.2 | 76.5% N2 & 23.5% O2 | 9.64∙10-4 | 6,497 | 652 | 2.5e-4 |
| TC3.3 | All free stream conditions of TC3.2; Chemical reactions turned off | | | | |
| TC3.4 | All free stream conditions of TC3.2; Perfect gas\* with specific heat ratio of 1.4 | | | | |

*Table 5. Cases TC3.1 and TC3.2 correspond to experimental cases Run 1 and Run 4 of*

*Ref. [6], respectively. Knudsen numbers are based on the double cone radius of 131 mm.*

\* In DSMC, perfect gas should be modeled as gas mixture with only translational and rotational modes active

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Test Case | Free Stream Gas | p, Pa | U∞, m/s | T∞, K | Kn |
| TC3.1 | 73.6% N2, 13.4% O2, 5.1% NO, 7.9% | 687 | 4,776 | 694 | 2.5e-4 |
| TC3.2 | O75.4% N2, 0.7% O2, 1% NO, 22.9% O | 476 | 5,956 | 901 | 5.8e-4 |
| TC3.3 | All conditions of TC3.1, plus catalytic recombination at the surface | | | | |
| TC3.4 | All conditions of TC3.2, plus catalytic recombination at the surface | | | | |

Table 6. *Cases TC3.1 and TC3.2 correspond to experimental cases HEG III and HEG I of*

*Ref. [13], respectively. Knudsen numbers are based on the cylinder diameter of 90 mm.*

*5.4. IR Signature Calculation*

The macroparameters along the Y=100mm line will be used to compute IR emission from the fundamental transition of NO in the 4.9-5.6m range. The objective is to examine the impact of numerical uncertainties and models on the IR emission. Specair software [8] will be used in IR emission calculations.

Note that all signature calculations may only be considered preliminary; they can’t substitute for a full collisional-radiative model. Moreover, significant difference in radiances may indicate the need for the development of such models.

**6. Tentative Timeline**

* January 2019, discussion of next steps aimed at finalizing test conditions for TC1 and TC3
* Summer 2019, presentation of comparative results and possible next steps (AIAA Thermophysics Conference, DSMC 2019 Workshop).

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