**HyNECC: Hypersonic NonEquilibrium Comparison Cases**

*S. Gimelshein and I. Wysong*

with contributions of A. Alexeenko, D. Andrienko, E. Josyula, D. Levin, and M. Panesi

and numerical results from A. Borner, O. Tumuklu & D.Levin, and R. Chaudhry

**Phase 1: 5-species air in 0D adiabatic bath and**

**a 2D 6km/s flow over a cylinder**

**1. Objective**

With the recent availability of QCT-based state-specific rates and the many proposed relaxation and reaction models, and the prospects 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.

This document describes a Phase I proposal to be completed in 2020 focusing on just two initial cases. Contributions for the Phase I cases are sought before 30 Sept 2020 in order for analysis to be performed and a publication documenting the results to be written and submitted by 31 Dec 2020.

The goal of this study is the evaluation of the impact of the numerical method, models, rates, and implementations, on

1. gas properties in a 0D adiabatic bath under conditions reproducing those behind strong shock waves, and
2. gas and surface properties for air flow over a cylinder at a flow velocity of 6km/s and a Knudsen number of 6e-4 (HEG-I flow conditions).

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. TC1: Spatially Homogeneous Heat Bath**

*2.1. Flow Conditions*

**2.1.3. *An adiabatic 0D bath*** that conserves energy is proposed as a highly-simplified approximation to a post-shock case for comparison of models. The initial condition will have number density of the initial species (either pure N2, pure O2, or N2/O2 air-like mixture) of 1e25m3/s and separate mode temperatures (translational, rotational, and vibrational), with Maxwell-Boltzmann state distributions enforced at the prescribed temperatures. Relaxation and chemical reactions will take place in accordance with the given models used. Bath results should be reported for a period of 400 ns if possible.

*2.2. Desired Output*

2.2.3. Adiabatic bath

Contributed results should provide the following gas properties as a function of time:

* vibrational temperature for each species and for the overall gas as function of time
* translation and rotation temperature for the gas as function of time
* mole fractions for each species as function of time

Contributed results should provide adequate references to define the assumptions, equations and models used and a complete listing of input parameters used including:

* transport properties
* any input parameters used for the internal energy transfer models
* input parameters for equilibrium, multi-temperature, and/or state-to-state specified reaction rates
* parameters used for mode energy removed or added per reaction and/or post-reaction energy distribution method
* method, equations, and parameters used for reverse reactions and Keq(T)

The run matrix for an adiabatic bath is given in Table 1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Test Case | Bath | Collision Type | Tt =Tr | Tv |
| TC1A.1 | Adiabatic | N2-N2, N2-N  Initial gas: pure N2 | 20,000 K | 300 K |
| TC1A.2 | Adiabatic | O2-O2, O2-O  Initial gas: pure O2 | 10,000 K | 300 K |
| TCA.3 | Adiabatic | Air: 79% N2, 21% O2 | 15,000 K | 300 K |

*Table 1. Initial number density = 1e25 m3/s*

**3. TC2: Two-Dimensional or Three-Dimensional Hypersonic Flow**

The Phase I 2D/3D case is flow over a cylinder measured in the HEG tunnel, with flow conditions of Refs. [1-2] 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. However, as noted in Ref. [1], where both 2D and 3D computations were presented, the 3D effect on surface properties near the centerline is negligible. Thus, a 2D setting may be used for comparison with the data, and is proposed in this TC. Note also that the cylinder surface in the experiment was proven to be catalytic, and thus surface reactions need to be accounted for in numerical simulations to reproduce the data.

*3.1. Geometry*

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 [1].

*3.2. Desired Output*

3.2.1. 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)

3.2.2. Gas properties

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

3.2.4. Flowfield data files suitable for 2D contour plotting with Tecplot. Variables of interest are similar to those given in 3.2.2.

3.2.5. 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.

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

*3.3. Run Matrix*

The run matrix is given in Table 2. Symbol ∞ denotes here the equilibrium free stream condition. The baseline case TC2.1 should include dissociation and exchange reactions only (no recombination).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Test Case | Free Stream Species Mass Fractions | p, Pa | U∞, m/s | T∞, K | Kn |
| TC2.1 | O75.4% N2, 0.7% O2, 1% NO, 22.9% O | 476 | 5,956 | 901 | 5.8e-4 |
| TC2.2 | All conditions of TC2.1, plus gas-phase recombination | | | | |
| TC2.3 | All conditions of TC2.2, plus fully catalytic recombination at the surface | | | | |

Table 2. The test case *corresponds to experimental case HEG I of*

*Ref. [1]. Knudsen number is based on the cylinder diameter of 90 mm.*

**6. References**

[1] S. Karl, J. Martinez-Schramm, and K. Hannemann, “High enthalpy cylinder flow in HEG: a basis for CFD validation,” AIAA Paper 2003-4252 (2003).

[2] D. Knight, J. Longo, D. Drikakis, D. Gaitonde, A. Lani, I. Nompelis, B. Reinmann, L. Walpot, “Assessment of CFD capability for prediction of hypersonic shock interactions,” Progr. Aerospace Sciences 48-49, 8-26 (2012).