**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) two-dimensional or/and 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 configuration (ii) is 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. The configuration (iii), as discussed below, is still not finalized, and *is currently deferred* until all possible options are carefully reviewed and analyzed. The 1D 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 2D set of test cases, not finalized at this time yet, includes two possibilities currently being discussed, but is not limited by them. 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.

**3.1.3. *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.

*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. Adiabatic bath

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

For all baths: 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.

The run matrix for an adiabatic bath is given in Table 3.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Test Case | Bath | Collision Type | Tt =Tr | Tv |
| TC1.1 | Fixed Tt, Tr, Tv | N2-N2 | 4,000 K, 6,000 K, 8,000 K,  10,000 K,  15,000 K | 4,000 K, 6,000 K, 8,000 K, 10,000 K,  15,000K  Tv≤Tt |
| TC1.2 | Fixed Tt, Tr, Tv | N2-N | 4,000 K, 6,000 K, 8,000 K,  10,000 K,  15,000 K | 4,000 K, 6,000 K, 8,000 K, 10,000 K,  15,000K  Tv≤Tt |
| TC1.3 | Fixed Tt, Tr, Tv | O2-O2 | 4,000 K, 6,000 K, 8,000 K,  10,000 K,  15,000 K | 4,000 K, 6,000 K, 8,000 K, 10,000 K,  15,000K  Tv≤Tt |
| TC1.4 | Fixed Tt, Tr, Tv | O2-O | 4,000 K, 6,000 K, 8,000 K,  10,000 K,  15,000 K | 4,000 K, 6,000 K, 8,000 K, 10,000 K,  15,000K  Tv≤Tt |

*Table 1. Initial number density = 1025 1/m3*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 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. Initial number density = 1025 1/m3*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 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 |
| TC1A.3 | Adiabatic | Air: 79% N2, 21% O2 | 15,000 K | 300 K |

*Table 3. Initial number density = 1025 1/m3*

**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**

The 2D set of test cases is being deferred until the optimum configuration and conditions are finalized.

At this time, 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]

Although two options are considered, 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. Suggestions and ideas related to TC3 conditions selection are most welcome.

*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.

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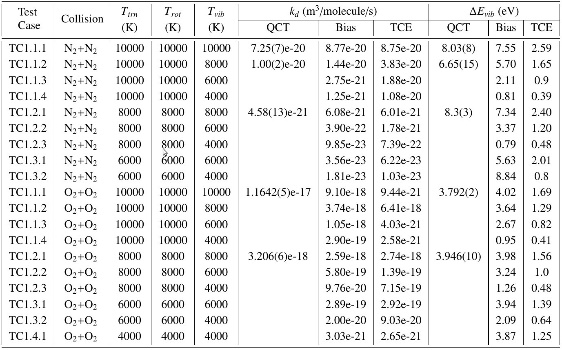
**APPENDIX. Initial results.**

The summary of initial results is shown below for TC1 and TC2.

***TC1: with contribution from R. Chaudhry and M. Grover***

The dissociation reaction rates *kd* obtained by two different approaches for fixed-temperature nitrogen and oxygen baths are shown in Table 7. The first approach is QCT, which uses potential energy surfaces of Ref. [15] for nitrogen and [16, 17] for oxygen. The second approach is DSMC, for which two dissociation models are used, the total collision energy (TCE) [18] and the extended Bias [19, 20] models. The parameters of the Bias model were chosen in Ref. [21] to reasonably reproduce several experimental and theoretical results, while the parameters of the TCE model used here provide the best fit to the Bias model reaction rates at equilibrium. As expected, the equilibrium reaction rates for the TCE and the Bias models are close. Comparing the corresponding equilibrium and non-equilibrium cases, lines 1 and 2, one can see that decreasing vibrational temperature from 10,000 K to 8,000 K results in approximately a factor of 7 decrease in rate for QCT and the Bias model, and a less than a factor of three decrease for TCE.

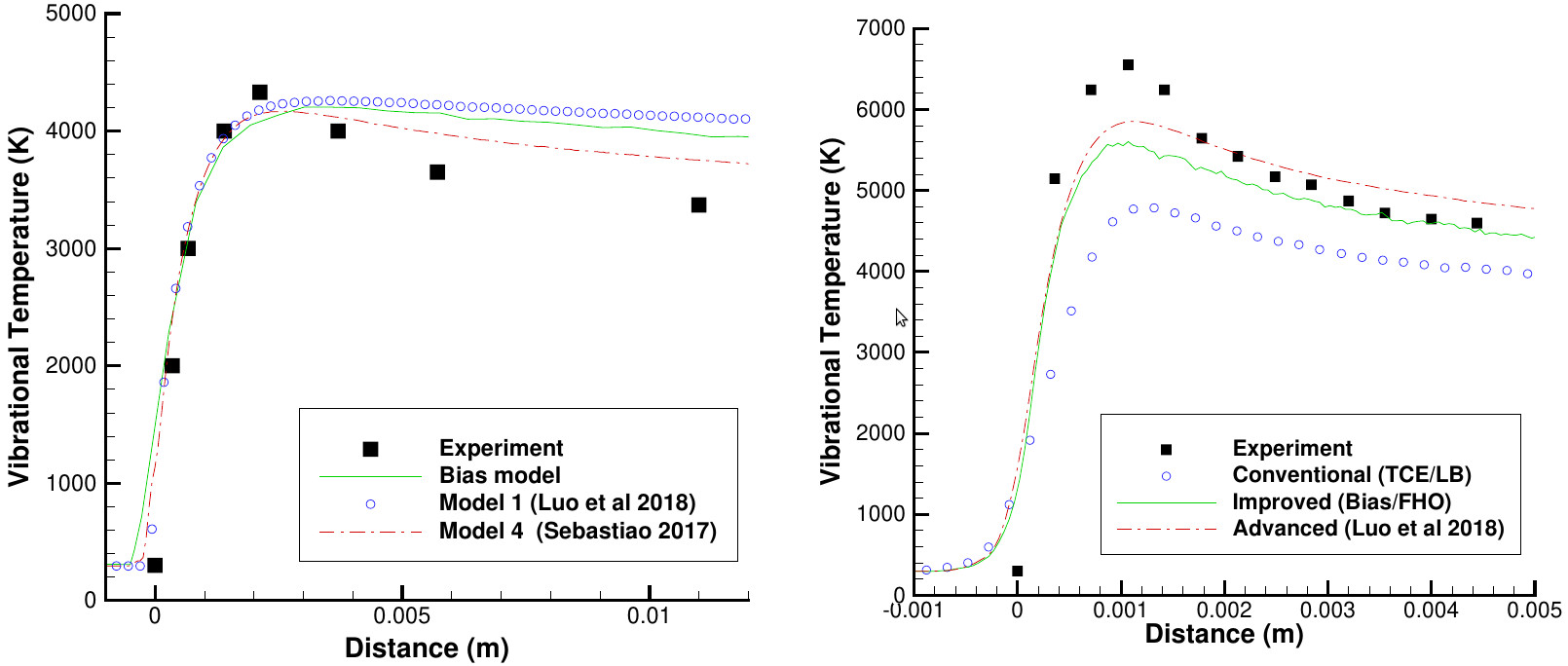
In addition to the dissociation rates, the average vibrational energy removed per dissociation ∆*Evib* is also shown in Table 7, and that is where the most significant differences are observed. According to QCT, as the vibrational temperature decreases from 10,000 K to 8,000 K, ∆*Evib* decreases by about 20% for nitrogen, and increases 4% for oxygen. For the Bias model, it decreases for both gases - about 32% for N2 and 10% for O2. Even though there is some difference between QCT and the Bias model, their ∆*Evib* values are still reasonably close. The energy change for the TCE model, however, is quite different. For both gases considered here, it is much lower than in QCT - about 3 times for both N2 and O2. Much higher removal of vibrational energy due to dissociation in QCT and the Bias model than in the TCE model may have significant implications in non-equilibrium flows, especially those where the vibrational bias of the dissociation reactions is important.

Table 7. *Comparison of different models in N2 and O2 homogeneous heat baths.*

***TC2: with contribution from A. Alexeenko and I. Sebastião***

All gas macroparameters are of interest in HyNECC, including translational and internal temperatures, species mole fractions, and bulk velocity, as well as the molecular velocity and internal energy distribution functions. The most important of those is the vibrational temperature profile, as it provides an opportunity to compare to the experimental results of Ref. [2]. The result of such a comparison for a shock velocity of 3.07 km/s is illustrated in Fig. 1 (left) where the vibrational temperatures obtained by different models of the DSMC method are shown. Here, Bias model denotes the Bias model for dissociation and recombination and the FHO-FR [22] model for the vibration-translation energy transfer. Model 4 of Ref. [23] uses a maximum-entropy and an ab-initio based models for the VT transfer and dissociation in atom-molecule collisions, and the Larsen-Borgnakke and Macheret-Friedman models for the VT transfer and dissociation in molecule-molecule collisions, respectively. Model 1 is the most advanced model shown here as it provides an improvement in the implementation of the Macheret-Friedman model [24] for dissociation as compared to Model 4. It can be seen that there is very good agreement between the Bias model and Model 1, whereas Model 4 predicts a somewhat lower vibrational temperature, especially downstream from the peak. All three models differ from the measurements of Ref. [2], which manifests significantly faster after-peak relaxation. Some caution needs to be exercised when comparing to the experimental data, since the error bar associated with the determination of absorption cross sections and their processing and conversion to vibrational temperature is up to 20%.

The Bias model and Model 1 of Ref. [24] are shown in Fig. 1 (right) for a shock velocity of 4.44 km/s. Similar to the previous case, the vibrational temperatures obtained by Model 1 and the Bias model are relatively close, with the former approximately 250 K higher. While the peak vibrational temperature for the advanced Model 1 is somewhat closer to that obtained experimentally than the Bias model, it is still almost 1,000 K lower. Moreover, after-peak relaxation is slower in both Model 1 and the Bias model than in the experiment. Note that the difference between the Bias model and Model 1 is much smaller than the experimental error bar of 10-20%. The conventional model is also shown here, based on the TCE and LB models. For that model, the maximum vibrational temperature is even lower than in the more advanced models, while the slope after the peak is similar. The higher maximum in Model 1 and the Bias model than in the conventional model is due to lower dissociation rate before and near the peak as a result of the vibration-dissociation coupling. While the vibrational temperatures for the Bias model and Model 1 are relatively close, the vibrational distribution functions were found to differ. The distributions functions obtained by these two models are given in Fig. 2 for a shock velocity of 3.07 km/s at the location of maximum vibrational temperature. There is little difference in populations of lower levels, but for levels above 25, the difference approaches an order of magnitude. It is attributed partially to the vibration-dissociation coupling approach, but mostly to the vibration-vibration energy transfer which was taken into consideration in the Bias model.

Fig. 1 *Vibrational temperature profiles in a 1D oxygen shock wave with a free stream velocity of 3.07 km/s (left) and 4.44 km/s (right).*