Uncertainty Quantification of Expanding High-Enthalpy Air Flows

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Abstract. In the present work, we study the sensitivity of expanding hypersonic air flows in the HEG facility with respect to the thermochemical relaxation rates and reservoir conditions, along with the impact of uncertainties in the rates and reservoir conditions on uncertainties of the free-stream parameters. A simplified 1-D formulation of the flow equations is utilized to allow for simultaneous variation of a large number (10) of uncertain parameters. The simulation results show large uncertainties in the vibrational temperature of oxygen and molar fractions of oxygen-containing species, mainly due to uncertainties in the reservoir parameters and data on thermochemical relaxation rates of molecular oxygen.

Keywords: shock tunnel, thermochemical relaxation, numerical simulation, uncertainty quantification, hypersonic flow

1 Introduction

Hypersonic ground test facilities use flow expansion to achieve conditions similar to those of high-velocity hypersonic re-entry in order to provide experimental data for spacecraft design. The simulation of the operation of such facilities is needed for estimation of the free-stream conditions, interpretation of experimental data, as well as verification of computational models. In shock tunnel facilities, such as the High Enthalpy Shock Tunnel Göttingen (HEG) [7], the flow is stagnated in order to achieve the required enthalpies; as it then expands through a nozzle section, thermochemical relaxation and subsequent freezing of the flow takes place, potentially leading to a chemically and vibrationally non-equilibrium flow at the nozzle exit [2]. The modeling of hypersonic flows is complicated by significant uncertainties in the data on the thermochemical relaxation rates, as well as the often significant impact on the choice of models to describe the relaxation processes [10, 18, 5, 6].

In recent years, more attention and effort has been devoted to consistent analysis of the impact of the uncertainties in the thermochemical relaxation rates on various quantities of interest (such as surface heat fluxes) in high-enthalpy flows; however most of the effort has been focused on flows behind strong shock waves [21, 22, 1]. Expanding flows have received less attention, even though their analysis is required for accurate estimation of free-stream uncertainties that

are in turn used in the aforementioned post-shock simulations of shock tunnel experiments; and the computed free-stream conditions may be quite sensitive to the choice of thermochemical relaxation rates [8]. Several recent studies have focused on improvements of modeling expanding flows in experimental facilities: in Gimelshein & Wysong [4], the impact of chemical reaction rates on nitric oxide production was studied, along with the role of variations in the reservoir density and temperature. It was shown that vibration-dissociation coupling has a large effect on O_2 and NO concentrations for a high-enthalpy HEG condition. In Gu et al. [6], the applicability of two-temperature models (as compared to higher-fidelity state-specific models) to simulations of nozzle flows was investigated, along with the possibility of simplification of vibrational relaxation modeling. It was shown that the presence of non-Boltzmann vibrational energy distributions at the nozzle exit has little impact on the flow further downstream behind a shock around the test body; as such, simplified models that assume a Boltzmann vibrational distribution may be sufficient for the computation of free-stream conditions in shock tunnels. In [15], we performed a sensitivity analysis and uncertainty quantification study of expanding binary flows of N_2/N and O_2/O, with the aim of verifying the developed framework and providing preliminary results to reduce the parameter space in uncertainty quantification/sensitivity analysis studies of air flows.

The objective of the present work is to expand our uncertainty quantification and sensitivity analysis framework to air flows, and assess the role that the uncertainties in reservoir conditions and thermochemical relaxation rates play in high-enthalpy air flows characteristic of HEG conditions.

2   Governing Equations

In the present work, we assume that the nozzle flow is steady, inviscid, and quasi-one-dimensional. This allows to use a simplified system of equations, and greatly reduces the required computational time. As numerous simulations with varying parameters are required for the uncertainty quantification and sensitivity analysis studies, the ability to rapidly perform multiple simulations is crucial.

The system of equations describing a chemically reacting vibrationally non-equilibrium flow takes on the following form [13]:

$$\frac{d\left(\rho_c v S\right)}{dx} = S R_c^{chem}, \ c = 1, \ldots, N_s, \tag{1}$$

$$\rho v \frac{dv}{dx} = -\frac{dp}{dx}, \tag{2}$$

$$\frac{dh}{dx} + v \frac{dv}{dx} = 0, \tag{3}$$

$$\frac{d\left(\rho_c S v E_v^c\right)}{dx} = S R_c^{vibr}, \ c = 1, \ldots, N_m. \tag{4}$$

Here x is the coordinate along the nozzle axis, $S = S(x)$ is the cross-sectional area of the nozzle, ρ_c is the density of species c, v is the flow velocity, R_c^{chem} is the

chemical relaxation term, ρ is the flow density, p is the pressure, h is the enthalpy, E_v^c is the vibrational energy (per unit mass) of molecular species c, R_c^{vibr} is the vibrational relaxation term, N_s is the number of chemical species in the flow, N_m is the number of molecular species in the flow. Despite the inability of the utilized approach to model the viscous boundary layer, a corresponding correction can be incorporated by performing a viscous 2-D axisymmetric simulation, extracting the boundary layer thickness and using an effective nozzle profile $\hat{S}(x)$ [17].

In the present work, we consider a five-component air flow: $N_2/O_2/NO/N/O$. Vibrational relaxation due to VT exchanges was computed using the Landau–Teller formula with the Millikan–White expression for VT relaxation times [12]. For VV exchanges of vibrational energy between O_2 and N_2, the empirical correlation proposed by Klomfass was used [9]:

$$\tau_{cd}^{VV} = \frac{1}{nk_{cd}^{VV}}, \quad k_{cd}^{VV} = \hat{K}_{cd}^{VV}\sqrt{k_{cc}^{VT}k_{dd}^{VT}\exp\left(\left(\theta_c - \theta_d\right)/T\right)}. \tag{5}$$

Here τ_{cd}^{VV} is the VV relaxation times for molecules of species c colliding with molecules of species d; k_{cd}^{VV} is the corresponding VV rate coefficient, k_{cc}^{VT} is the VT rate coefficient, θ_c is the characteristic vibrational temperature of molecular species c, and $\hat{K}_{cd}^{VV}$ is a constant factor.

The exchange reactions were computed assuming no influence of the reactant and product vibrational temperatures. For dissociation reactions, the Treanor–Marrone model [11] was used to account for the preferential dissociation from higher-lying vibrational levels and compute the vibrational energy loss/gain due to dissociation and recombination reactions.

3   Uncertainty Quantification

3.1   Generalized Polynomial Chaos

In order to compute the impact of the uncertainties in the reservoir parameters and thermochemical relaxation rates on the flow, we utilise the generalized Polynomial Chaos (gPC) [19] approach. Compared to traditional Monte–Carlo methods, for moderate parameter space dimensions, far fewer model evaluations are needed. In the present work, we use the non-intrusive approach, which allows us to treat the solver of the system of governing equations Eqn. (1)–(4) as a "black box" and thus does not require solving additional equations.

Denoting the vector of uncertain model parameters as $\mathbf{w}$, and assuming that all these uncertain parameters are independent random variables, a quantity of interest Y (such as pressure, temperature, etc.) can be represented in the following form:

$$Y(x,\mathbf{w}) \approx \sum_{i=0}^{N} c_i(x)P_i(\mathbf{w}). \tag{6}$$

Here $c_i(x)$ are the unknown expansion coefficients (which are dependent on the spatial location x), and P_i are the expansion polynomials (of order i up to N),

which are chosen to be orthogonal with respect to the parameter distributions and are known beforehand. Due to the orthogonality of the polynomials, the coefficients of the expansion are given through the following expression:

$$c_i = \frac{\langle Y, P_i \rangle}{\langle P_i, P_i \rangle}, \quad \langle a, b \rangle = \int ab d\mathbf{w}. \tag{7}$$

Once the set of uncertain model parameters $\mathbf{w}$ and their distributions have been chosen, along with the desired order of the polynomial expansion N the quadrature appearing in Eqn. (7) can be evaluated numerically. For a chosen quadrature rule, a set of sample points of $\mathbf{w}$ is generated, along with the associated weights, the model is evaluated using the sampled values of the uncertain parameters, and the quadrature is calculated in order to obtain the coefficients c_i. Smolyak sparse grids [3] are used for evaluation of the quadrature in order to reduce the number of model evaluations required. In the present work, 2nd order polynomial expansions are used, as in our previous work [15], they were found to provide sufficient convergence of the statistical properties being investigated (mean, standard deviation, sensitivity indices). Once the expansion coefficients c_i have been computed, relevant statistics can be calculated, such as the mean and standard deviation of the flow quantities of interest (for example, temperature at the nozzle exit), as well as the sensitivity of these flow quantities with respect to the uncertain model parameters (via Sobol sensitivity indices). The total Sobol sensitivity index of quantity of interest Y with respect to uncertain model variable w_i is defined as

$$S_{tot,i} = 1 - \frac{\mathrm{Var}_{\mathbf{w}_{\sim \mathbf{i}}}\left(E_{w_i}\left(Y|\mathbf{w}_{\sim \mathbf{i}}\right),\right)}{\mathrm{Var}(Y)} \tag{8}$$

where Var is the variance, E is the expectation, and $\mathbf{w}_{\sim \mathbf{i}}$ is the vector of all uncertain model variable except variable w_i. The values of the Sobol indices are proportional to the influence the corresponding parameter has on the flow uncertainty: values close to 1 mean a strong influence of the parameter, and small values mean a weak influence.

3.2   Parametrization of Uncertainty Sources

In order to perform the uncertainty quantification and sensitivity analysis study, we need to choose the uncertain model parameters w which we want to incorporate into our analysis. Unlike our previous studies in binary N_2/N and O_2/O mixtures, the much larger number of relaxation pathways in air prohibits the simultaneous consideration of all possible chemical and vibrational relaxation rates. Thus, additional reduction of the possible parameter space is required. The uncertainties in the reservoir pressure p_r and temperature T_r where taken to be $\pm 5\%$ of the reference values p_r^0, T_r^0 for the conditions considered, as given in [7].

In the present work, we assume the nitric oxide in the flow to be in vibrational equilibrium, due to its very short vibrational relaxation times [14]. Our previous

study found that the role of the high-temperature Park correction [16] to VT relaxation times was found to be small due to the rapid freezing of the flow [15]. Thus the value of it was kept fixed in the present work.

In the current analysis, we consider uncertainties in the following VT relaxation times: N_2 in collisions with N, and O_2 in collisions with O atoms. This is motivated by several factors. First of all, available experimental and quasi-classical trajectory computational data on these times exhibit the largest degree of discrepancy. Secondly, these VT relaxation times are much shorter than relaxation times of molecule-molecule collisions. Due to the presence of oxygen (which has a low dissociation energy), a significant fraction of oxygen atoms are present in the flow; at the high enthalpy condition considered in the present work, nitrogen also experiences a noticeable degree of dissociation in the critical cross-section. Thus, a sufficient fraction of atoms is present in the flow to have a noticeable impact on the vibrational relaxation.

We took the VT relaxation times τ_{cd}^{VT} for collisions of molecules of species c with particles of species d to be given by the Millikan–White [12] expression $\tau_{cd,MW}^{VT}$ and the Park high-temperature correction $\tau_{cd,P}^{VT}$:

$$\tau_{cd}^{VT} = \tau_{cd,MW}^{VT} + \tau_{cd,P}^{VT}. \tag{9}$$

The Millikan–White formula gives the pressure-corrected VT relaxation times in the following form:

$$p\tau_{cd}^{VT,MW} = \exp\left(A_{cd}\left(T^{-1/3} - B_{cd}\right) - 18.42\right). \tag{10}$$

While the A_{cd}, B_{cd} coefficients can be varied independently to introduce uncertainty in the vibrational relaxation data, doing so may lead to uncharacteristically low or high values of the VT relaxation times. Thus, we took these coefficients to be linearly dependent on a single model parameter α_{cd}^{VT}. The single uncertain parameter $\alpha_{VT,cd}$ is taken to be uniformly distributed between 0 and 1, and the coefficients of the linear dependence were chosen based on analysis of existing experimental and QCT data for VT relaxation times. The use of a single parameter (instead of two) also allows to reduce the dimension of the space of uncertain parameters, lowering the number of model evaluations required.

Analysis of the VV relaxation times computed using the empirical expression of Klomfass (5) showed excellent agreement with recent experimental data on O_2-N_2 VV relaxation times [20] if the factor $\hat{K}_{cd}^{VV}$ was taken to be equal to 4 (in the original work of Klomfass it is equal to 1). Thus, in the present study, $\hat{K}_{cd}^{VV}$ was assumed to be uniformly distributed between 3 and 5, which corresponds to a 25% uncertainty in the VV relaxation times, this is comparable to the 30%-40% experimental uncertainty reported by Streicher et al. [20].

In the present case of the five-component air flow, 17 chemical reactions are included in the simulation: 15 dissociation reactions (3 molecular species, each with 5 possible collision partner species) and 2 exchange reactions. Of course, considering the impact of uncertainties in all the associated reaction rates

simultaneously would require an exorbitant amount of computations, therefore, some simplification have been made. We use a single parameter to vary the dissociation rates of a specific molecule, and thus we have to consider only 5 uncertainties in the reaction rates: 3 dissociation rates (of N_2, O_2, and NO), and the two Zeldovich exchange reactions $N_2+O \rightarrow NO+N$ and $NO+O \rightarrow O_2+N$. As in our previous work [15], we parametrize the dissociation rate coefficients in the following fashion:

$$k_{cd}^{diss}(T) = (a_{cd}^{diss} + b_{cd}^{diss}T)k_{cd,Park}^{diss}(T), \tag{11}$$

where $k_{cd,Park}^{diss}$ are the values computed using the Arrhenius expression and data from Park [16], and a_{cd}^{diss}, b_{cd}^{diss} are linear functions of a parameter α_c^{diss}. The coefficients for the linear dependence were chosen so that a wide rang of possible values is covered, based on existing experimental and QCT data. As already mentioned, a single α_c^{diss} parameter governs all the uncertainties in the dissociation of a molecule of species c simultaneously. Whilst a simplification, such a parametrization still allows us to determine uncertainty in which dissociation/recombination rate data of which particular species has the most significant impact on the flow, and in future studies, a detailed investigation of the sensitivity to the partner-specific dissociation rates is planned. The 2 Zeldovich exchange reactions were parametrized in the same fashion as the dissociation reactions. Our previous studies in binary flows of N_2/N and O_2/O showed the relatively small impact of uncertainties in the vibration-dissociation coupling parameters (the U_{TM} parameter in case of the Treanor–Marrone model) due to recombination playing a larger role in expanding flows. Thus, the high-temperature Park correction as kept fixed, along with the U_{TM} parameter, which was taken to be equal to $3T$.

Thus, to summarize, we consider in total 10 uncertain parameters and their associated distributions: 2 reservoir parameters, 2 parameters governing VT relaxation, 1 parameter governing VV exchanges, 3 parameters governing dissociation rates, and 2 parameters governing exchange reaction rates. All the distributions were taken to be uniform.

4   Results

We consider an air flow characteristic of condition H22R0.20 [7] in the HEG shock tunnel. The condition has a reservoir pressure p_r of 35 MPa, reservoir temperature T_r of 9100 K, and total enthalpy of 22 MJ/kg. The contoured Mach 10 Nozzle V profile was used.

Figure 1 shows the computed flow properties along the nozzle axis, with a range of one standard deviation around the mean value shown by the shaded region. The annotated text gives the values at the nozzle exit and the associated relative uncertainty in percent. We observe a strong influence of the considered model uncertainties on the vibrational relaxation of O_2 and the molar fraction of oxygen-containing species ($O/O_2/NO$). A significant relative uncertainty of
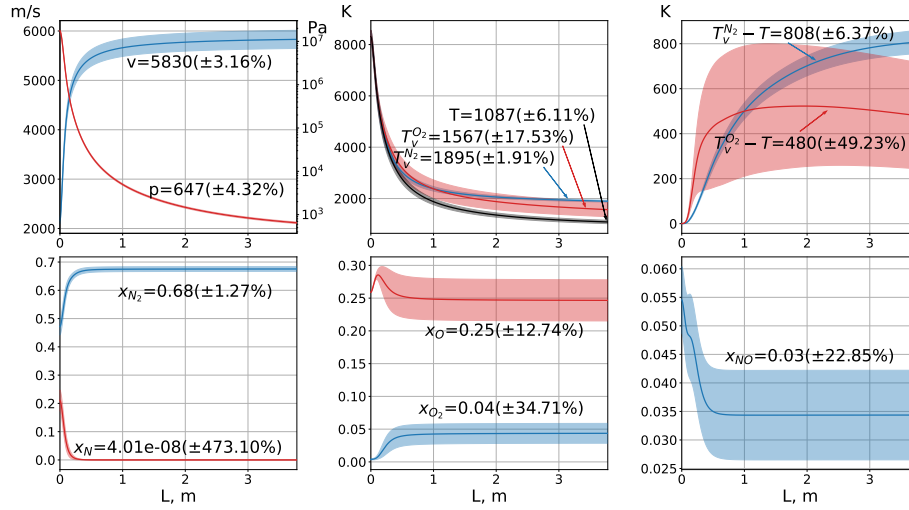
Fig. 1. Flow properties computed along the nozzle axis; shaded regions denote a range of one standard deviation, solid lines show the mean values.
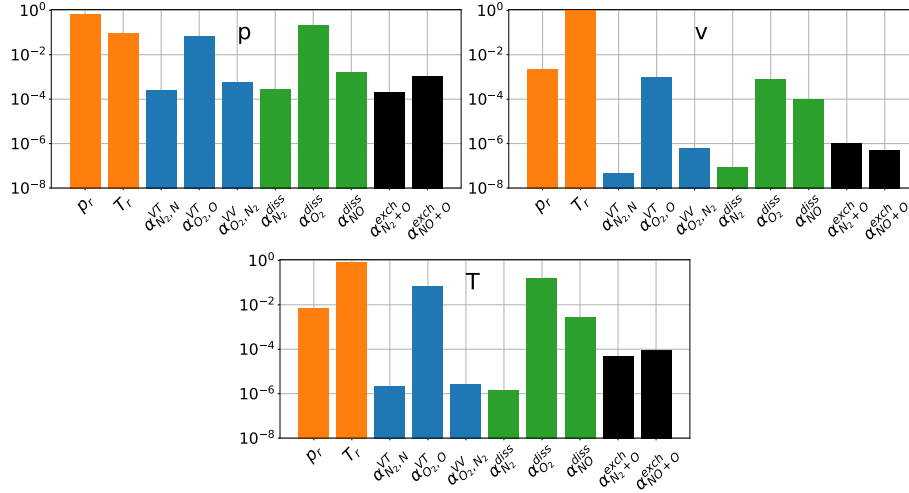

Fig. 2. Total Sobol sensitivity indices of pressure, velocity, and temperature at the nozzle exit with respect to the uncertain model parameters.

the molar fraction of atomic nitrogen at the nozzle exit is also present, however, the absolute values of the atomic nitrogen concentration are extremely low, and as such, we do not investigate this quantity further.

Next we consider the sensitivity of the different flow parameters at the nozzle exit to uncertainties in the reservoir parameters and thermochemical relaxation
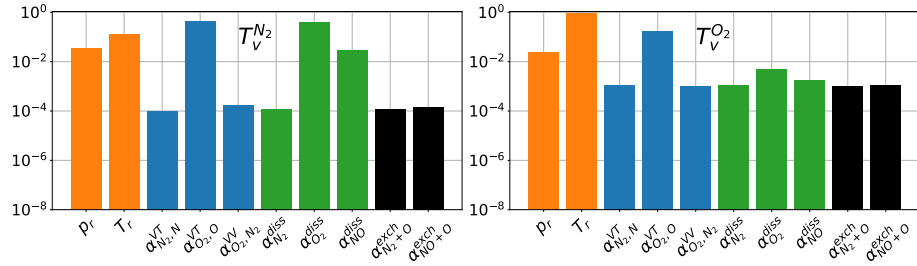
Fig. 3. Total Sobol sensitivity indices of vibrational temperatures at the nozzle exit with respect to the uncertain model parameters.
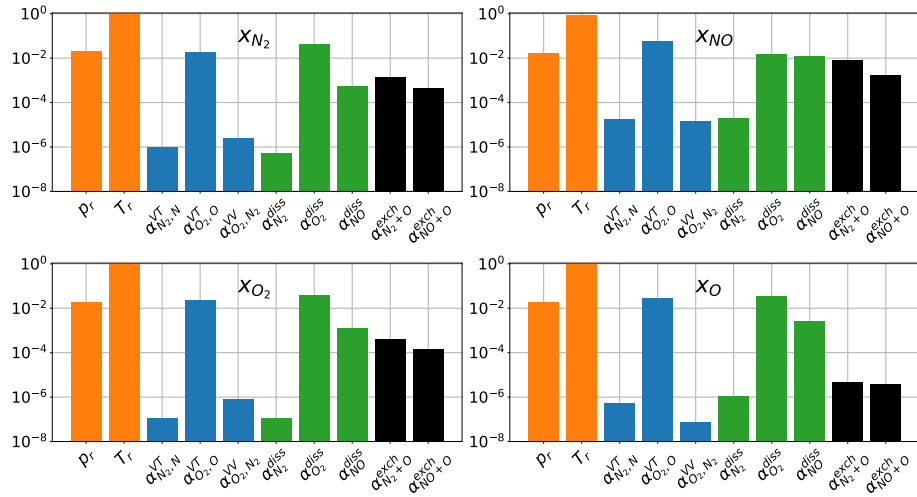

Fig. 4. Total Sobol sensitivity indices of species' molar fractions at the nozzle exit with respect to the uncertain model parameters.

rates. Figures 2–4 show the total Sobol sensitivity indices S_{tot} with respect to uncertainties in the reservoir parameters (shown by orange bars), parameters governing VT and VV relaxation (blue bars), parameters governing dissociation reaction rates (green bars), and parameters governing exchange reaction rates (black bars). As expected, and seen on Fig. 2, only the reservoir temperature has any noticeable impact on the flow velocity. The flow temperature is strongly influenced not only by the reservoir temperature, but also by the VT relaxation of oxygen (due to both the large uncertainties in the O_2-O VT relaxation times and their low values) and the dissociation–recombination of O_2. As such, uncertainties in these quantities, along with uncertainty in the reservoir pressure, have the strongest effect on the uncertainty in the pressure at the nozzle exit.

For the vibrational temperatures at the nozzle exit, the VV relaxation time uncertainty has little impact on the flow, as seen on Fig. 3. This is due to the

VV relaxation times being significantly larger than VT relaxation times, coupled with the rapid freezing of the flow. From Fig. 3 we also see a surprisingly large influence of the uncertainty in the VT relaxation rate and the dissociation rate of oxygen on the vibrational temperature of N_2. Analyzing the sensitivities of the molar fractions presented on Fig. 4, we see a significant sensitivity of all of the constituent species' molar fractions to the uncertainties in the VT relaxation of O_2 and dissociation–recombination of O_2. This suggests the following explanation for the strong sensitivity of $T_v^{N_2}$ to uncertainties in thermochemical relaxation rates of O_2: due to the preferential dissociation model of Treanor–Marrone, the vibrational relaxation of O_2 has a strong impact on its dissociation, which in turn affects the fraction of atomic oxygen available for the $N_2+O \rightarrow NO+N$ Zeldovich reaction. This reaction leads to a change in the vibrational temperature of N_2; thus, it is through this three-step process that the VT relaxation of O_2 affects vibrational relaxation of N_2.

5   Conclusions

We performed an uncertainty quantification and sensitivity analysis study of an expanding hypersonic air flow in the HEG nozzle. For the condition considered, apart from uncertainties in the reservoir conditions, the most significant source of uncertainty in the flow parameters at the nozzle exit were uncertainties in the data on O_2-O VT relaxation rate and uncertainties in the data on dissociation rate coefficients of O_2 and NO. The vibrational temperature of O_2, and molar fraction of O_2, O, and NO all exhibited significant (at least 10%) uncertainties at the nozzle exit. Further planned extensions to the present work include accounting for vibrational non-equilibrium of NO, incorporation of vibration-chemical coupling into the exchange reaction modeling, and a more detailed analysis of uncertainties in specific dissociation–recombination pathways on the flow.

6   Acknowledgments

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