

High Temperature Flow Simulations: Reduced Models and Data Validation

E. Kustova^{a)}, O. Kunova, D. Kravchenko, M. Melnik

Saint Petersburg State University, 7/9 Universitetskaya nab., St. Petersburg, 199034, Russia

^{a)} Corresponding author: e.kustova@spbu.ru

Modern aerospace applications require modeling nonequilibrium high-temperature and high-enthalpy flows. Accuracy of flow simulations depends on many factors: the level of detail in the flow description, fidelity of available data on the reaction and relaxation rates, numerical precision. Computational cost is also crucial for the choice of an appropriate model; depending on the required accuracy, kinetic or continuum flow descriptions can be implemented. Among continuum approaches, the state-to-state (STS) flow description is the most detailed and accurate; its implementation, however, requires data on all kinds of vibrational energy transitions and state-specific reaction rate coefficients. Moreover, for gas mixtures involving polyatomic species with multiple vibrational modes, STS simulations become prohibitively expensive since one has to solve several thousands of master equations for the vibrational state populations.

In this talk, we first discuss the possibility of reducing the STS models to multi-temperature ones without considerable loss of accuracy. For CO₂ mixtures, we show that multi-temperature simulations using direct averaging of the state-specific reaction and transition rates provide fairly good agreement with full STS simulations [1, 2]. The advantages of such a hybrid approach are: 1) the set of several thousand master equations is reduced to a few relaxation equations; 2) vibrational-chemical coupling is modeled naturally, without need for some phenomenological models; 3) the approach does not use the Landau-Teller relaxation equations having many limitations under strongly nonequilibrium conditions [3]. On the other hand, the proposed approach still requires the full set of rate coefficients for state-specific chemical reactions and vibrational energy transitions; this data remains the main source of uncertainty. In the second part of the talk, we discuss validation of the state-specific reaction rate coefficients for oxygen and air on the basis of shock tube experiments [4-6]. Several models of different fidelity are assessed: SSH [7], FHO [8], Marrone-Treanor dissociation model with various parameters [9-12]. In particular, we show an important role of partial vibrational relaxation between incident and reflected shocks for correct reproducing the reflected shock experiments.

ACKNOWLEDGEMENTS

This study is supported by the Saint Petersburg State University, Project No. 93022273.

REFERENCES

- [1] A. Kosareva, O. Kunova, E. Kustova, and E. Nagnibeda, *Phys. Fluids*, **33**, 016103 (2021).
- [2] A. Kosareva, O. Kunova, E. Kustova, and E. Nagnibeda, *Phys. Fluids*, **34**, 026105 (2022).
- [3] E. Kustova, G. Oblapenko, *Phys. Fluids*, **27**, 016102 (2015).
- [4] L.B. Ibraguimova, A.L. Sergievskaya, V.Y. Levashov, O.P. Shatalov, Y.V. Tunik, I.E. Zabelinskii, *J. Chem. Phys.*, **139**, 034317 (2013).
- [5] V. Gorelov, M. Gladyshev, A. Kireev, I. Yegorov, Y. Plastinin, G. Karabadzhak, *J. Thermophys. Heat Tran.*, **12**, pp. 172–179 (1998).
- [6] J. W. Streicher, A. Krish, R.K. Hanson, *Phys. Fluids*, **33**, 056107 (2021).
- [7] R. Schwartz, Z. Slawsky, K. Herzfeld, *J. Chem. Phys.*, **20**, pp. 1591–1599 (1952).
- [8] I. Adamovich, S. Macheret, J. Rich, C. Treanor, *J. Thermophys. Heat Tran.*, **12**, pp. 57–65 (1998).
- [9] P. Marrone, C. Treanor, *Phys. Fluids*, **6**, pp. 1215–1221 (1963).
- [10] O. Kunova, E. Kustova, A. Savelev, *Chem. Phys. Lett.*, **659**, pp. 80–87 (2016).
- [11] L. Campoli, O. Kunova, E. Kustova, M. Melnik, *Acta Astronautica*, **175**, pp. 493–509 (2020).
- [12] M. Pogosbekyan, A. Sergievskaya, *Russ. J. Phys. Chem. B*, **12**, pp. 208–218 (2018).