Hybrid reduced order model for N_2-N_2 interactions for application to dissociation and energy transfer processes

Oral Presentation

Robyn L. Macdonald[†], Richard L. Jaffe[‡], Marco Panesi[†]

[†]*University of Illinois at Urbana Champaign, 104 S Wright Street, 302 Talbot Lab, Urbana, IL 61801*
[‡]*NASA Ames Research Center, Moffett Blvd, Mountain View, CA 94035*

Recent work in the aerothermodynamics community has focused on the development of reduced-order models for thermo-chemical non-equilibrium which avoid the restrictive assumptions of multi-temperature models and the prohibitive cost associated with State-to-State (StS) models. In the present work, this is accomplished by lumping energy states together and assuming groups of states are roughly in equilibrium. As a result, the non-equilibrium behavior of a gas can be captured at a reduced computational cost from a full StS simulation.

In this work, we present a hybrid grouping model for studying energy transfer and dissociation in a mixture of nitrogen molecules due to N_2-N_2 reactions. This is accomplished by making use of a grouping strategy informed by data from the N_2-N StS kinetic data.[1] However, due to the massive computational cost associated with constructing StS data for the N_2-N_2 system, the kinetic data for the hybrid grouping model are calculated using the quasi-classical trajectory (QCT) method by sampling states for trajectory within the groups.[2,3] This general framework is called the Maximum-Entropy Quasi-Classical Trajectory (ME-QCT) method. The primary challenge associated with this method is that rates for reverse grouped reactions cannot be obtained through detailed balance at a group level, due to the variation of group internal temperatures. To construct the full model for N_2-N_2 grouped kinetics using the ME-QCT method, detailed balance is invoked at the microscopic level, allowing for the calculation of the full kinetic data from QCT.

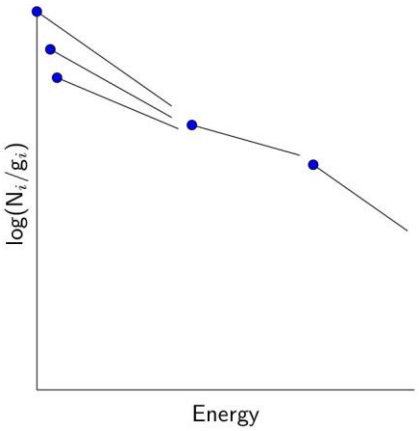

Fig.1: Schematic of hybrid grouping strategy where low lying energy states are grouped according to vibrational quantum number and high lying energy states are grouped according to energy.

Results will be presented using the full ME-QCT model for the N_2-N_2 system in an isothermal and isochoric reactor simulation. In addition, simple CFD test cases for a one-dimensional standing shock and for a quasi-one-dimensional nozzle will be used for demonstration of the ME-QCT method. This method allows for the calculation of non-equilibrium behavior for the N_2-N_2 system without the prohibitive cost of a full StS simulation. Moreover, it enables the construction of a unified model for the dissociating and recombining non-equilibrium flows.

ACKNOWLEDGEMENTS

Ms. R. Macdonald was supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program. Dr. M. Panesi was supported by the Air Force Office of Scientific Research Young Investigators Program FA9550-15-1-0132 with Program Officer Dr. Ivett Leyva. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the AFOSR or the US government.

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