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COMPUTATION OF HYPERSONIC FLOW USING HIGH FIDELITY AEROTHERMOCHEMISTRY

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Hypersonic vehicles fly faster than Mach 5 (about 3,000 mph) and may re-enter from space or cruise through the atmosphere at high altitude. The strong shock wave formed around the vehicle creates very high temperatures that lead to excitation of the internal energy modes of the air and eventually to chemical reactions. The state of the art for modeling this aerothermochemistry consists of a phenomenological two-temperature (2T) approach in which the translational and rotational energy modes are assumed to be in equilibrium and the vibrational mode is modeled using a separate energy equation with a characteristic relaxation time. Coupling between the translational and vibrational modes for dissociation chemistry is accounted for using the geometric mean of the two temperatures in Arrhenius rate coefficients. Evaluation of the 2T model using experimental data acquired in shock tubes and shock tunnels reveals that it is often not accurate in modeling aerothermochemistry and critical vehicle surface properties such as pressure and heat transfer.

As an alternative to the 2T model, we are pursuing a high fidelity, multi-step approach in which molecular dynamics is employed with an ab initio potential energy surface to calculate cross sections of transitions between individual quantized energy states of oxygen molecules. The cross sections are subsequently integrated to yield temperature dependent rates of state-to-state (STS) transitions. The temperature-dependent rates can be employed in Master Equation analyses of heat baths, and in flow simulations of shock tubes and shock tunnels. In this presentation, results are presented from all stages of the multi-step approach, and assessment provided of the information and solutions generated through direct comparisons with experimental measurements.

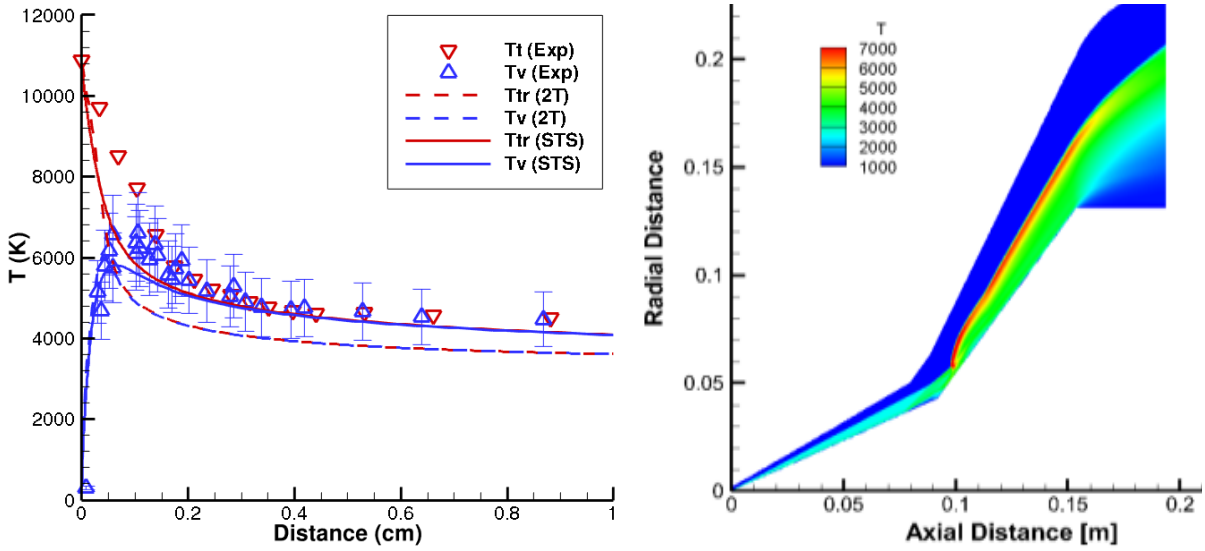

Figure 1: Assessment of high fidelity computation of: (a) Mach 12 shock wave; (b) Mach 12 flow over a double cone.