An axi-symmetric shock-tube model has been developed to simulate shock propagation and reflection in both non-reactive and reactive flows. Simulations were performed for the full shock-tube geometry of the high-pressure shock tube facility at Texas A&M University.

The numerical method was first applied to the problem of axi-symmetric inviscid flow then viscous effects were incorporated which allowed for the modeling of the non-idealities in the shock tube; notably the non-ideal transient behavior in the shock-tube nozzle section, heat transfer effects from the hot gas to the shock tube side walls, the reflected shock/boundary layer interactions known as bifurcation, and the contact surface/bifurcation interaction resulting into driver gas contamination.

Both the inviscid and the viscous non-reactive models provided a baseline for the combustion model which involved elementary chemical reactions and required the coupling of the chemistry with the flow fields thereby requiring tremendous computational resources. Combustion modeling focused on the ignition process behind the reflected shock wave in a Hydrogen test gas mixture at practical power generation conditions. The numerical study revealed that the test conditions in the shock-tube endwall behind the reflected shock wave are highly non-uniform for test gas mixtures involving diatomic and polyatomic gases. The sudden interaction of the incident shock wave with the endwall and the initiation of bifurcation result into the formation of localized hot spots in the shock tube endwall corners, thereby promoting premature autoignition. Consequently, the assumption of ideal flow properties before ignition takes place does not hold valid.

The multi-dimensional, time-dependent numerical simulations resolved all of the relevant scales, ranging from the size of the system to the reaction zone scale. The robustness of the numerical model and the accuracy of the simulations were assessed through validation with the analytical ideal shock tube theory and experimental data.

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Approved for distribution by Dr. Alain Kassab, Committee Chair, on February 18, 2010.

The public is welcome to attend.