



# DEPARTMENT OF MECHANICAL ENGINEERING Purdue School of Engineering and Technology

## SUMMER 2004 SEMINAR SERIES

---

Date: **Thursday, July 22, 2004**

Time: **1:30 pm – 2:30 pm**

Room: **SL 165**

**Everyone is invited**

---

### **The Development of a CFD Chemistry ODE Solver for Ethylene Fuel**

(Thesis Defense)

**Keith Bandi**

*Graduate Student in Mechanical Engineering, IUPUI.*

**Abstract.** The combustion process occurring within a combustor is characterized by chemical reactions and mixing. Fuel and air are mixed, ignited, and burned. This process allows for the heat release needed to drive many propulsion systems. This project revolves around the development of a chemistry solver for the combustion of Ethylene (C<sub>2</sub>H<sub>4</sub>) and oxygen, and its implementation into a computational fluid dynamics (CFD) solver. A reduced kinetic model for the combustion of Ethylene was selected. This model contains three reactions and six species. Each reaction has a different set of forward and reverse reactions rates. Here, reverse reactions are modeled using the NASA GRC chemical database and the forward reaction rates were obtained from literature. The goal for this chemistry solver is to determine the concentration of each species involved in the reaction at a given temperature. The law of mass action represents the net production of each species mathematically. The six species in the model lead to a system of six nonlinear equations with six unknowns. The desire to solve for the concentration of species at different times requires transient conditions to be considered rather than equilibrium conditions. A system of six nonlinear equations requires a numerical method to solve. When solving the chemistry model as a stand alone program, a Runge-Kutta fourth order accurate explicit method is used to allow the concentration of each species to converge at a given temperature and at a given time. With verification that the model is accurate, it has been implemented into a CFD Navier-Stokes solver for high Mach number flows and combustion.

A smaller aspect of this work concerns the development of supersonic expansion nozzle design program. The principles behind this program are considerably different than the ones for the chemistry solver and the programs appear to be unrelated. Each program however was written for the same overall project. In this presentation of research, both programs will be discussed with emphasis placed on the chemistry solver and its inclusion into the CFD solver.

**About the Speaker.** Keith Bandi obtained his B.S. in Mechanical engineering from IUPUI in 2002. He is the recipient of the Melba Schumacher Engineering and Technology Endowment Scholarship, and the NASA Indiana Space Grant consortium scholarship. He is currently a research assistant in the Department of Mechanical Engineering, IUPUI, working in the areas of Computational Fluid Dynamics and Chemical Kinetics. His thesis advisors are Dr. Andrew Hsu (major advisor), Dr. Razi Nalim, and Dr. Sivakumar S. Krishnan.