# DIAGNOSTICS AND MODELING

# Chemical Kinetic Modeling

## OVERVIEW

The mechanical engineering profession has the momentous challenge to provide transportation and energy without significantly degrading the environment. To meet this challenge the combustion community needs advanced engineering resources that can facilitate the economical research an development of low emission combustor designs. Understanding the underlying chemistry behind combustion is critical in combustor design. Chemical kinetic that occur in the reaction involve hundreds species and thousands of elementary reactions. Despite these challenges, modern computer software is available that can calculate these reaction rates for given condition in order to quantify the combustion environment. Two commercially available software programs are CHEMKIN and DARS. Cantera is another program that is freely available. These programs can calculate Figure 1 shows an example of the concentration of species across a thin laminar flame front calculated in CHEMKIN. In this example propane is burn to completion, and near the flame the concentration of carbon monoxide momentary peaks before it is oxidized itself into water and carbon dioxide.

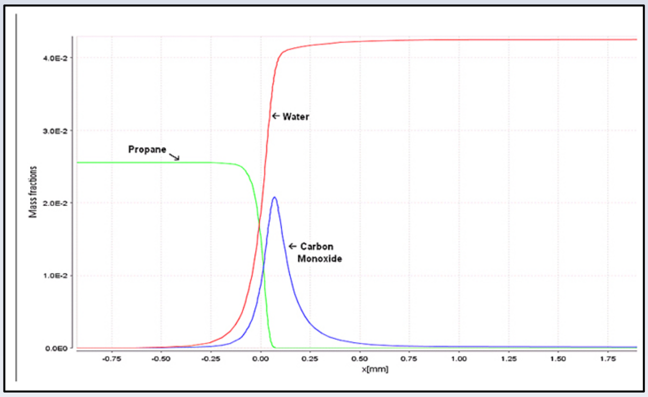


**Figure 1 : Species concentration across a flame front for a laminar propane flame**

The programs have several modules for setting up simulations. These include reactors such as perfectly or well stirred reactors, plug flow reactors, turbulent flamelet simulators, diesel or SI or HCCI engine simulators. Additional analysis tools in the programs allow for a sensitivity analsys of the most dominant reactions along with reaction pathways so one can visualize the process of oxidation of the fuel into its intermediate species and final products. Figure 2 shows the reaction pathway of ethane as it oxidizes.

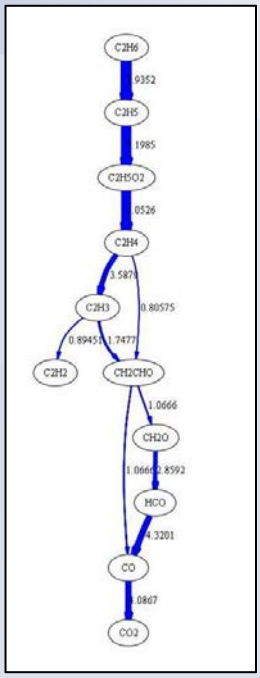


**Figure 2: Oxidation pathway of ethane**

Many of these reactions are both temperature and pressure dependent, therefore the reactions dominant at high pressures in gas turbines many not necessarily be the same as those dominant in atmospheric experiments. Therefore any new chemical mechanisms currently available need to be tested and validated at these extreme conditions before they can be considered reliable. Figure 3 shows comparison of several chemical kinetic models used in CHEMKIN to calculate the ignition delay time of the alkane fuels, methane, ethane and propane. The results are compared to experimental data obtained at this laboratory. The comparison found that one of the models compared favorably, while the other did not. There is a great deal of effort to optimize these models to the combustion conditions found in gas turbines today.

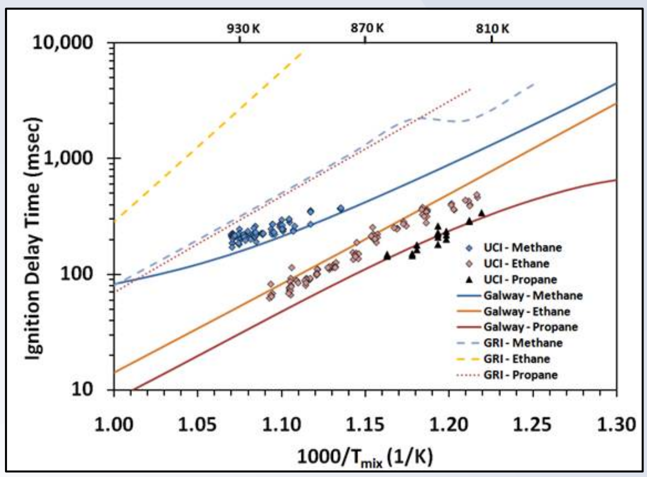


**Figure 3: Comparison of chemical mechanisms to experimental ignition delay results**

## RECENT PUBLICATIONS/PAPERS


**AUTOIGNITION OF METHANE, ETHANE AND PROPANE IN TURBULENT HIGH PRESSURE AND INTERMEDIATE TEMPERATURE FLOWS (2009).** Presented at the 6th US National Meeting of the Combustion Institute, Paper 22C1, May (D.J. Beerer, V.G. McDonell, and G.S. Samuelsen, L. Angello)

**INTERPRETATION OF FLOW REACTOR BASED IGNITION DELAY MEASUREMENTS (2009).** Presented at the ASME Gas Turbo Expo, Paper GT2009-60269, June (D.J. Beerer, V.G. McDonell, and G.S. Samuelsen, L. Angello)

**AUTOIGNITION OF HYDROGEN AND AIR INSIDE A CONTINUOUS FLOW REACTOR WITH APPLICATION TO LEAN PREMIXED COMBUSTION (2008).** Journal of Engineering for Gas Turbines and Power, Vol. 130 051507-1 to 8. September Issue (D.J. Beerer, V.G. McDonell)

**AUTOIGNITION CORRELATIONS FOR PIPELINE NATURAL GAS AT LOW AND INTERMEDIATE TEMPERATURES (2007).** AIAA J. Prop. and Power, Vol 23, No. 3, pp. 585-592. (J.H. Chen, V.G. McDonell, and G.S. Samuelsen)

**EXPERIMENTAL STUDY OF IGNITION DELAY FOR APPLICATION TO HYDROGEN AND SYNGAS FIRED LEAN PREMIXED GAS TURBINE ENGINES (2007).** Presented at the 5th US National Meeting of the Combustion Institute, Paper E01, March (D.J. Beerer, V.G. McDonell)


## PERSONNEL


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