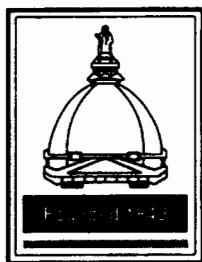


# AEROSPACE & MECHANICAL ENGINEERING



**2004 COLLOQUIUM 2005  
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**INFORMAL COFFEE PERIOD BEFORE THE SEMINAR IN ROOM 365, ENGR. BLDG.  
UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA 46556**

**SPEAKER:** **Ms. Xiaolin Zheng**  
Department of Mechanical and Aerospace Engineering  
Princeton University  
Princeton, New Jersey

**TOPIC:** **IGNITION OF HYDROGEN  
AND HYDROCARBONS  
IN CONVECTIVE-DIFFUSIVE SYSTEMS**

**DATE:** Tuesday, April 19, 2005

**TIME:** 3:30 p.m.

**PLACE:** 138 DeBartolo Hall

## **Abstract**

Control of ignition is crucial for the satisfactory performance of combustors and for the prevention of fires and explosions. Compared to the high-temperature chemistry governing steady burning and extinction, the low- to intermediate-temperature chemistry relevant for ignition is more complex. The level of complexity is further elevated when ignition takes place in a non-uniform medium and as such is also affected by convective-diffusive transport. Such intricacies will be illustrated by first considering the ignition of a lean premixed hydrogen/air mixture by a counterflowing heated nitrogen stream. Experimental results backed by computational simulation show that, compared to the three explosion limits for homogeneous mixtures, ignition now takes place at higher temperatures and exhibits five limits over the pressure range investigated, and that such a behavior can be largely explained by the reduced residence time and the self enrichment of the original fuel-lean mixture through the preferential diffusion of the highly mobile hydrogen. We then examine the nonpremixed ignition of a nitrogen-diluted dimethyl ether (DME) stream by a counterflowing heated air stream, again experimentally and computationally, and demonstrate the importance of accurate description of the low-temperature chemistry by comparing the performance of two existing mechanisms. The third component of the seminar is a study on the thermochemistry, chemical reaction pathways and reaction kinetics of the isobutenyl radical oxidation through *ab initio* calculations. The potential energy diagrams for the first and second O<sub>2</sub> addition were constructed, and the high-pressure limit rate constants for each reaction channel were determined as functions of temperature for further kinetic model development.