

CHEMICAL AND BIOLOGICAL ENGINEERING DEPARTMENT SEMINAR SERIES

***Catalytic Fuel Reforming: A mechanistic understanding***

Presented by: Marco J. Castaldi, Assistant Professor, Columbia University

Time: Wednesday, April 15; 3:15 – 4:30 pm

Location: Perlstein Hall Auditorium

**Abstract**

There has been a large effort to produce hydrogen from various hydrocarbon sources. For example, reforming of liquid logistic fuel has become important for a variety of applications such as remote power production via PEMFC and SOFC as well as ICE combustion enhancement with synthesis gas. In landfill gas to energy projects (LFGTE), reforming a portion of the LFG to produce syngas that can be mixed with the remaining un-processed LFG to yield a more reactive mixture to enhance the combustion performance is being done. In addition, conversion of LFG to syngas for feedstock to a Fischer Tropsch process to yield liquid fuels are being developed. To understand the reactions governing these processes, we have done reactor testing coupled to mechanistic model development.

The performance issues associated with logistic fuel reforming were investigated in a series of experiments, for steam to carbon (S/C) ratios between 1.6 and 2.2 and oxygen to carbon (O/C) ratios between 0.8 and 1.1. A reaction mechanism was developed using tetradecane as a surrogate to capture the major reactions, which was then validated using experimental data. The significance of each major reaction class as the reaction proceeds through the reactor was considered and integrated into an existing C7 mechanism.

To investigate the viability of reforming LFG, auto-thermal reforming (ATR) was employed as a way to reduce carbon formation potential and eliminate the need for external heat requirements. Experiments were performed with 1:1 and 1.4:1.0 CH<sub>4</sub>:CO<sub>2</sub> ratios at 5,000-8,000 hr<sup>-1</sup> space velocities from 20°C to 800°C at 1 atm total pressure. Oxygen was introduced at a 0.46:1.0 O<sub>2</sub>:CH<sub>4</sub> ratio at temperatures ranging from 250°C to 550°C. It has been found that during ATR operation, in addition to methane combustion and dry reforming, partial oxidation, steam reforming and water-gas shift reactions are dominant. The methane combustion and partial oxidation provide the required heat and reactive chemical species that lead to greater conversion of CH<sub>4</sub> to H<sub>2</sub> and CO, and higher H<sub>2</sub>:CO ratios compared to CH<sub>4</sub>/CO<sub>2</sub> reforming alone. Furthermore, ATR produces an H<sub>2</sub>:CO ratio that varies from approximately 1.0 to 2.0 as a function of the reactor temperature. This allows for the tuning of H<sub>2</sub>:CO, depending on the application.

This presentation will discuss the experimental findings and the insights developed from the modeling efforts.

**Biography**

Marco Castaldi was born in New York City and received his B.S. ChE (Magna cum Laude) from

Manhattan College. His Ph.D. is in Chemical Engineering from UCLA and he has minors in Advanced Theoretical Physics and Astrophysics. Marco has a number of inventions as a result of his research, supported by 6 issued and 2 pending US patents. One innovation makes catalytically assisted combustion in gas turbines practically feasible. This research has been published in a refereed publication resulting in the "Best Applications Paper" Award by the Gas Turbine Institute of ASME International. He was recently awarded The Gas Turbine Award for his contributions in 2005. The other inventions relate to the development of Water Gas Shift and Preferential CO oxidation reactors for fuel processing applications related to fuel cell engines. Marco J. Castaldi is an Assistant Professor in the Earth & Environmental Engineering Department (Henry Krumb School of Mines), Columbia University where he has been since 2004. He teaches in the area of combustion chemistry and processes. He is currently involved in research in the area of environmentally benign energy technologies some of which are being patented by Columbia. This includes waste to energy, greenhouse gas reforming, methane production from methane hydrates and hydrogen production from coal.

Prof. Castaldi is very active in the American Society of Engineering Education. He also participates in the Summer Research Program for Science Teachers and "Shadow Day" where students of Puerto Rican decent who are the first in their families to go to college participate in graduate student research. Prof. Castaldi was awarded by the School of Engineering and Applied Science of Columbia University, the distinguished 2006 Distinguished Faculty Teaching Award.