



FORTH/ICE-HT

SEMINAR SEMINAR

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THEME: Detailed modelling of reactive processes

PLACE: FORTH/ICE-HT auditorium

DATE: Wednesday, 13th of June, 2007

TIME: 17:00

ABSTRACT: The work in my research group is focused primarily on sophisticated modelling of reactive processes. A detailed understanding of reactions, and how they affect various industrially important phenomena, is a critical need today. The emphasis is on a handful of systems of particular relevance – pollution mitigation in automobiles; gasification of coal; combustion in engines, and so on.

Nitrogen oxides coming out of automotive exhaust continue to pose severe health risks. Future emission standards are expected to be extremely stringent. At the same time, new generations of automobiles are expected to utilize fuel in a better way as well. The popularly used catalytic converter has a severe limitation at conditions where excess of oxygen is present. In lean-burn petrol, CNG, and diesel engines, therefore, the ability of the catalytic converter to reduce nitrogen oxide emissions is poor. Selective catalytic reduction, where an additional 'reductant' species is introduced in order to assist in NO reduction, is proposed as a solution in these cases. In our studies, we have explored, through the development and validation of detailed catalytic reaction mechanisms, the ability of various metal catalysts to reduce NO at a variety of conditions. A combination of mathematical modelling and experimental studies have yielded fundamental knowledge about this important reaction system.

In India, more than 30% of the available coal deposits are at large depths underground, wherein conventional mining is not feasible. These deposits are currently not utilised. The Underground Coal Gasification (UCG) technique, which involves the in-situ reaction of coal in order to generate useful product gas, provides great potential for utilisation of these coals. The UCG process is a complex one, involving multiple gaseous and gas-solid reactions, evolution of solid structures, mass and heat transfer, among other things. Successful implementation of UCG technology requires detailed analysis of the 'UCG reactor' (the cavity in the underground coal seam); evaluation of geomechanical aspects such as subsidence, and environmental aspects including impacts on surrounding aquifers. In our work, we are systematically developing tools for comprehension of UCG. Some aspects dealt with are: Experimental determination of kinetic constants for the pyrolysis, combustion and gasification of various Indian coals, Reactor modeling to evaluate effect of inlet and other parameters on product gas quality, Computational Fluid Dynamic and other modelling for study of the coal/char cavity growth, and so on.

In this talk, I will introduce our work on NO reduction, discuss a study on feasibility of UCG for Indian coals, and present results from a Packed Bed Reactor model for UCG that we have developed recently.