



## Wolfson Department of Chemical Engineering Special Seminar

Lecture Hall 6, Wolfson Department of Chemical Engineering,

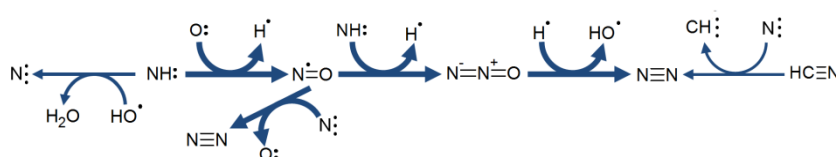
Wednesday, December 7, 2016 at 13:30

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## Automated Reaction Mechanism Generation

The ultimate goal of chemical kinetic modeling is to make predictions: given our current understanding of chemistry, what do we expect to happen in a particular reacting mixture under certain specified reaction conditions? Specifically, detailed kinetic models are necessary for simulating today's complex processes, especially as increasing environmental regulations require the identification of trace products. Detailed combustion models become very tedious to construct manually (and are error-prone) as the number of reactions and intermediate species increase, making computer-generated models favorable for this task. The open-source Reaction Mechanism Generator software (RMG, *see* [rmg.mit.edu](http://rmg.mit.edu)), developed at the Green Group at MIT, is designed to automatically constructs kinetic models composed of elementary chemical reaction steps and answer such questions. This software generates efficient kinetic models tailored for the specific fluid composition and condition. The rate-based algorithm reduces a very large chemical mechanism (about hundreds of thousands of elementary reactions) into an efficient model which consists of the most significant reactions (hundreds to a few thousands). Even more importantly, the algorithm automatically predicts missing data, since many kinetic and thermodynamic parameters are not available from ab initio quantum calculations or experimental measurement. Recently, RMG was enhanced with nitrogen chemistry in addition to C\H\O; hhis new capability incorporated is expected to prove very helpful as the community moves to incorporate nitrogen chemistry in kinetic models.



Refreshments will be served at 13:15