Multiscale Modeling/Simulation for Gas-Phase Chemistry and Materials Design: Computational Tools and Applications

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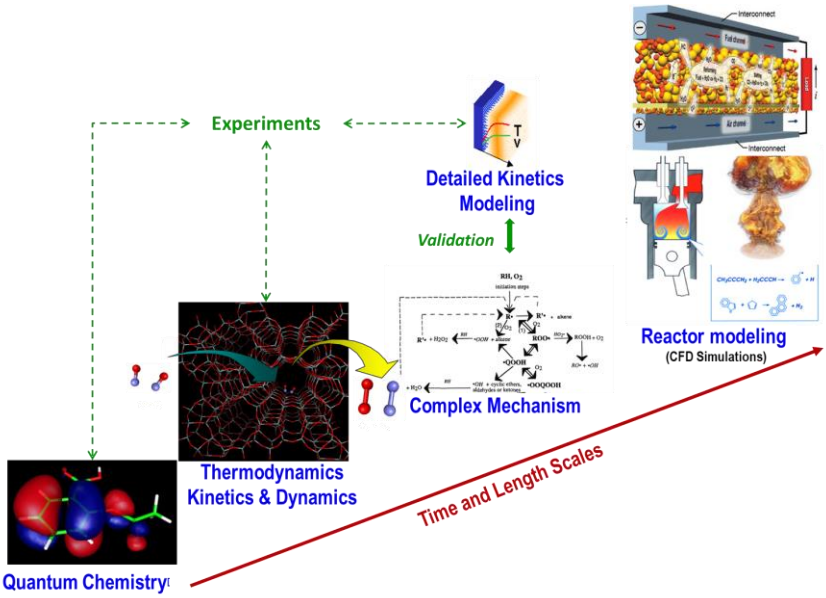
Computational modeling and simulation have served not only as a powerful post-facto tool for validating existing principles and knowledge but also as a strong predictive tool in the discovery of new knowledge in science and engineering. Recent advances in information technology, algorithm, and scientific methods, which allow faster and more accurate calculations for more realistic systems, have laid a solid foundation for bridging the time and length scale from fundamental science to real engineering challenges. In this talk, a demonstration of how to bridge fundamental chemistry/physics and reaction engineering modeling/simulation will be presented in two domains: *(1) gas-phase chemistry* and *(2) catalysts/materials design (complex chemical processes on surfaces).* In gas-phase chemistry, examples for understanding and modeling atmospheric chemistry and low-temperature combustion of hydrocarbon/alternative fuels will be discussed in detail. Then, the demonstration of how to design better catalysts for complex chemical systems will be presented. To facilitate the multiscale applications, main features of our in-house computational tools, namely, *MultiSpecies-MultiChannel (MSMC)*[1] for complex gas-phase systems and *Surfkin*[2] for gas-surface reactions, will be introduced. New methodologies and approaches (e.g., machine learning) for such interests will also be discussed.



Multiscale approach from fundamental chemistry and physics to reactor modeling and simulation.

Keywords: Multiscale, Modeling, Simulation, Gas-phase Chemistry, Materials Design, Thermodynamics, and Kinetics.

References:

1. Duong, M. V.; Nguyen, H. T.; Truong, N.; Le, T. N. M.; Huynh, L. K. *International Journal of Chemical Kinetics* 2015, **47** (9), 564-575 (website: https://sites.google.com/site/msmccode/).
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