Molecular simulation and computational techniques for the multiscale simulation of acccidental fires

박명남, 신동일*
명지대학교 화학공학과
(dongil@mju.ac.kr*)

The application of quantum mechanics and molecular simulation methods can yield new insights into the thermal reactivity of large molecules and nanoscale structures. In this research, we are interested in using molecular simulation and other computational techniques to gain theoretical insights into accidental fires in chemical and energy industries, at the molecular level. Time-accurate, full physics simulations of accidental fires require consideration of fundamental gas and condensed phase chemistry, structural mechanics, turbulent reacting flows, convective and radiative heat transfer, and mass transfer. The objective is to provide a system comprising a problem-solving environment in which fundamental chemistry and engineering physics are fully coupled with nonlinear solvers, computational steering, visualization and experimental data verification. We are also investigating the coupling of the micro-scale and meso-scale contributions to the macroscopic application in order to provide full-physics accuracy and the effective utilization of the Grid computing environment and consisting supercomputers.