TRANSIENT RADIATIVE HEAT TRANSFER IN CHEMICAL REACTIVE SYSTEMS

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The analysis of radiation heat transfer within a chemically reactive system, in which the chemical species, their phases, and their properties vary with time as the reaction progresses, is a complex transient problem found in such areas as combustion, atmospheric sciences, and high-temperature material processing. Part of the complexity derives from the fact that the variation of the radiative properties of the reacting system depends on the chemical reaction rate, which in turn is a function of temperature and radiation absorption. Another important field of application is solar thermochemistry. Solar thermochemical reactors make use of concentrated solar radiation as the source of high-temperature process heat. Examples of solar thermochemical processes include the thermal decomposition of limestone, the thermal reduction of metal oxides, and the thermal gasification of coal. The direct irradiation of the chemical reactants provides efficient energy transfer to the reaction site, bypassing the limitations imposed by indirect heat transfer through the reactor walls. Modeling such directly-irradiated solar chemical reactors is crucial for anticipating the consequences of a given design decision on the reactor's performance.

A transient model coupling radiative transfer to chemical kinetics is examined for a suspension of chemical reacting particles that are exposed to an external source of concentrated thermal radiation. The endothermic decomposition of $CaCO_3(s)$ into CaO(s) and $CO_2(g)$ is selected as the model heterogeneous reaction. The particle suspension is modeled as a non-isothermal, non-gray, absorbing, emitting, and Miescattering media. The Monte Carlo and finite volume methods are applied for solving the mass and energy conservation equations. MPI parallelization is applied to minimize computational time. Two cases are considered: non-shrinking and shrinking particles. In the former case, radiation absorption is superior, resulting in a faster reaction rate. In the latter case, the radiative properties vary strongly with time as the reaction progresses because of the decreasing size parameter. Both cases are compared in terms of their temperature profiles and reaction extents.