Materials & Coatings

A Model of Reduced Kinetics for Alkane Oxidation Using Constituents and Species for N-Heptane

When certain variables are judiciously combined, a self-similarity appears, allowing for a compact chemistry reduction mechanism that predicts ignition time.

NASA's Jet Propulsion Laboratory, Pasadena, California

The reduction of elementary or skeletal oxidation kinetics to a subgroup of tractable reactions for inclusion in turbulent combustion codes has been the subject of numerous studies. The skeletal mechanism is obtained from the elementary mechanism by removing from it reactions that are considered negligible for the intent of the specific study considered. As of now, there are many chemical reduction methodologies.

A methodology for deriving a reduced kinetic mechanism for alkane oxidation is described and applied to n-heptane. The model is based on partitioning the species of the skeletal kinetic mechanism into lights, defined as those having a carbon number smaller than 3, and heavies, which are the complement of the species ensemble. For modeling purposes, the heavy species are mathematically decomposed into constituents, which are similar but not identical to groups in the group additivity theory.

From analysis of the LLNL (Lawrence Livermore National Laboratory) skeletal mechanism in conjunction with CHEMKIN II, it is shown that a similarity variable can be formed such that the appropriately non-dimensionalized

global constituent molar density exhibits a self-similar behavior over a very wide range of equivalence ratios, initial pressures and initial temperatures that is of interest for predicting n-heptane oxidation. Furthermore, the oxygen and water molar densities are shown to display a quasi-linear behavior with respect to the similarity variable. The light species ensemble is partitioned into quasi-steady and unsteady species. The reduced model is based on concepts consistent with those of Large Eddy Simulation (LES) in which functional forms are used to replace the small scales eliminated through filtering of the governing equations; in LES, these small scales are unimportant as far as the overwhelming part of dynamic energy is concerned.

Here, the scales thought unimportant for recovering the thermodynamic energy are removed. The concept is tested by using tabular information from the LLNL skeletal mechanism in conjunction with CHEMKIN II utilized as surrogate ideal functions replacing the necessary functional forms. The test reveals that the similarity concept is indeed justified and that the combustion tempera-

ture is well predicted, but that the ignition time is over-predicted, a fact traced to neglecting a detailed description of the processes leading to the heavies chemical decomposition. To palliate this deficiency, functional modeling is incorporated into this conceptual reduction in addition to the modeling the evolution of the global constituent molar density, the enthalpy evolution of the heavies, the contribution to the reaction rate of the unsteady lights from other light species and from the heavies, the molar density evolution of oxygen and water, and the mole fractions of the quasi-steady light species.

The model is compact in that there are only nine species-related progress variables. Results are presented showing the performance of the model for predicting the temperature and species evolution. The model reproduces the ignition time over a wide range of equivalence ratios, initial pressure, and initial temperature.

Thermally Conductive Tape Based on Carbon Nanotube Arrays

This material can be used for thermal management of microelectronic packages and electronic systems.

Goddard Space Flight Center, Greenbelt, Maryland

To increase contact conductance between two mating surfaces, a conductive "tape" has been developed by growing dense arrays of carbon nanotubes (CNTs, graphite layers folded into cylinders) on both sides of a thermally conductive metallic foil. When the two mating surfaces are brought into contact with the conductive tape in between, the CNT arrays will adhere to the mating surface.

The van der Waals force between the contacting tubes and the mating surface provides adhesion between the two mating surfaces. Even though the thermal contact conductance of a single tube-to-tube contact is small, the tremendous amount of CNTs on the surface leads to a very large overall contact conductance.

Interface contact thermal resistance rises from the microroughness and the macro-

scopic non-planar quality of mating surfaces. When two surfaces come into contact with each other, the actual contact area may be much less than the total area of the surfaces. The real area of contact depends on the load, the surface roughness, and the elastic and inelastic properties of the surface. This issue is even more important at cryogenic temperatures, where materials become hard and brittle and vacuum is