

^(®) Hard-X-Ray/Soft-γ-Ray Imaging Sensor Assembly for Astronomy A pixilated scintillator is coupled with an array of avalanche photodiodes.

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An improved sensor assembly has been developed for astronomical imaging at photon energies ranging from 1 to 100 keV. The assembly includes a thallium-doped cesium iodide scintillator divided into pixels and coupled to an array of high-gain avalanche photodiodes (APDs). Optionally, the array of APDs can be operated without the scintillator to detect photons at energies below 15 keV. The array of APDs is connected to compact electronic readout circuitry that includes, among other things, 64 independent channels for detection of photons in various energy ranges, up to a maximum energy of 100 keV, at a count rate up to 3 kHz. The readout signals are digitized and processed by imaging software that performs "on-the-fly" analysis.

The sensor assembly has been integrated into an imaging spectrometer, along with a pair of coded apertures (Fresnel zone plates) that are used in conjunction with the pixel layout to implement a shadow-masking technique to obtain relatively high spatial resolution without having to use extremely small pixels. Angular resolutions of about 20 arc-seconds have been measured. Thus, for example, the imaging spectrometer can be used to (1) determine both the energy spectrum of a distant x-ray source and the angular deviation of the source from the nominal line of sight of an x-ray telescope in which the spectrometer is mounted or (2) study the spatial and temporal development of solar flares, repeating γ ray bursters, and other phenomena that emit transient radiation in the hard-x-ray/soft- γ -ray region of the electromagnetic spectrum.

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Implified Modeling of Oxidation of Hydrocarbons

Only a few dozen molecular and radical species are included in calculations.

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A method of simplified computational modeling of oxidation of hydrocarbons is undergoing development. This is one of several developments needed to enable accurate computational simulation of turbulent, chemically reacting flows. At present, accurate computational simulation of such flows is difficult or impossible in most cases because (1) the numbers of grid points needed for adequate spatial resolution of turbulent flows in realistically complex geometries are beyond the capabilities of typical supercomputers now in use and (2) the combustion of typical hydrocarbons proceeds through decomposition into hundreds of molecular species interacting through thousands of reactions. Hence, the combination of detailed reaction-rate models with the fundamental flow equations yields flow models that are computationally prohibitive. Hence, further, a reduction of at least an order of magnitude in the dimension of reaction kinetics is one of the prerequisites for feasibility of computational simulation of turbulent, chemically reacting flows.

In the present method of simplified modeling, all molecular species involved

in the oxidation of hydrocarbons are classified as either light or heavy; heavy molecules are those having 3 or more carbon atoms. The light molecules are not subject to meaningful decomposition, and the heavy molecules are considered to decompose into only 13 specified constituent radicals, a few of which are listed in the table. One constructs a reduced-order model, suitable for use in estimating the release of heat and the evolution of temperature in combustion, from a base comprising the 13 constituent radicals plus a total of 26 other species that include the light molecules and related light free radicals. Then rather than following all possible species through their reaction coordinates, one follows only the reduced set of reaction coordinates of the base.

The behavior of the base was examined in test computational simulations of the combustion of heptane in a stirred reactor at various initial pressures ranging from 0.1 to 6 MPa. Most of the simulations were performed for stoichiometric mixtures; some were performed for fuel/oxygen mole ratios of 1/2 and 2. The following are among the conclusions drawn from the results of these simulations:

Constituent Radical	δh^0	δh^c	δh^f
$ m CH_3$ (methyl)	-42.0	714	188
$ m CH_2$ (methylene)	-20.8	614.3	411
m CH (methylidyne)	≈ -7	≈ 507	≈ 603
$ m C_2H_3$ (vinyl)	62.5	1,212	237

Some of the Constituent Radicals included in the simplified model are listed with some of their pertinent thermodynamic properties. The listed properties, all in units of kilojoules per mole, are the heat of formation (δh^0) , the heat of combustion (δh^0) , and the heat of component-to-free transition (δh^0) . Other pertinent properties, omitted for the sake of simplicity, are coefficients in an equation for partial molar heat capacity as a function of temperature.