Developing a Consistent Chemical Kinetic Model for Electron Beam Irradiation of Humid Air

THEODORE DIBBLE, KAREN SCHMITT, DAVID-ANTHONY MURRAY, SUNY-Environmental Science and Forestry — A chemical kinetic model has been assembled to assist in better understanding the mechanisms underlying hydroxyl radical production via electron beam irradiation of humid air. Thermodynamic determination of the feasibility of particular product sets was used to eliminate certain reactions proposed previously, dynamical models were used to guide the choice of product sets, and updated rate constants were obtained from the current literature. Tracers were also used to determine the major reactions producing and destroying hydroxyl radical, because of its role in removing pollutants from irradiated air. Modeling results for selected species have been presented for 1 atmosphere of air at 298.15 K and 50% relative humidity, at doses of 1, 5, 10, 25, and 50 kGy delivered over 0.8 seconds to a static sample. The concentrations of the most abundant ions, radicals, and stable reaction products are reported, and the major reactions producing and destroying hydroxyl radical are quantified.

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