Multiphase Reacting Flow Modeling of Singlet Oxygen Generators for Chemical Oxygen Iodine Lasers

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Singlet oxygen generators are multiphase flow chemical reactors used to generate energetic oxygen to be used as a fuel for chemical oxygen iodine lasers. In this paper, a theoretical model of the generator is presented along with its solutions over ranges of parameter space and oxygen maximizing optimizations.

The singlet oxygen generator (SOG) is a low-pressure, multiphase flow chemical reactor that is used to produce molecular oxygen in an electronically excited state, i.e. singlet delta oxygen. The primary product of the reactor, the energetic oxygen, is used in a stage immediately succeeding the SOG to dissociate and energize iodine. The gas mixture including the iodine is accelerated to a supersonic speed and lased. Thus the SOG is the fuel generator for the chemical oxygen iodine laser (COIL). The COIL has important application for both military purposes — it was developed by the US Air Force in the 1970s — and, as the infrared beam is readily absorbed by metals, industrial cutting and drilling.

The SOG appears in various configurations, but the one in focus here is a crossflow droplet generator SOG. A gas consisting of molecular chlorine and a diluent, usually helium, is pumped through a roughly rectangular channel. An aqueous solution of hydrogen peroxide and potassium hydroxide is pumped through small holes into the channel and perpendicular to the direction of the gas flow. So doing causes the solution to become aerosolized. Dissociation of the potassium hydroxide draws a proton from the hydrogen peroxide generating an HO_2 radical in the liquid. Chlorine diffuses into the liquid and reacts with the HO_2 ion producing the singlet delta oxygen; some of the oxygen diffuses back into the gas phase.

The focus of this work is to generate a predictive multiphase flow model of the SOG in order to optimize its design. The equations solved are the so-called Eulerian-Eulerian form of the multiphase flow Navier-Stokes equations wherein one set of the equations represents the gas phase and another equation set of size m represents the liquid phase. In this case, m is representative of the division of the liquid phase into distinct representations of the various droplet sizes distributed in the reactor. A stabilized Galerkin formulation is used to solve the equation set on a computer. The set of equations is large. There are five equations representing the gas phase: continuity, vector momentum, heat. There are 5m representing the liquid phase: number density, vector momentum, heat. Four mass transfer equations represent the gas phase constituents and there are m advection diffusion equations representing the HO_2 ion concentration in the liquid phase. Thus we are taking advantage of and developing algorithms to harness the power of large parallel computing architectures to solve the steady-state form of these equations numerous times so as to explore the large parameter space of the equations via continuation methods and to maximize the generation of singlet delta oxygen via optimization methods.

Presented here will be the set of equations that are solved and the methods we are using to solve them. Solutions of the equations will be presented along with solution paths representing varying aerosol loading—the ratio of liquid to gas mass flow rates—and simple optimizations centered around maximizing the oxygen production and minimizing the amount of entrained liquid in the gas exit stream. Gas-entrained liquid is important to minimize as it can destroy the lenses and mirrors present in the lasing cavity.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

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