SAND2007-3909P

A Simulation and Design Capability for Singlet-Oxygen Generators for Chemical Oxygen Iodine Lasers

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 SOG is the initial stage in the chemical oxygen iodine laser (COIL), which has important application for both military purposes—it was initially developed by the US Air Force in the 1970s—and, as the infrared beam is readily absorbed by metals, for industrial cutting and drilling.

The SOG is a complex multiphase reacting-flow system, with a gas mixture of chlorine and helium reacting with dispersed droplets of an aqueous solution of hydrogen peroxide and potassium hydroxide (Figure 1). The primary product of the reactor, the energetic oxygen, is subsequently used in the COIL to dissociate and energize iodine, which in turn is accelerated to a supersonic speed and lased. Researchers at the Air Force Research Laboratory approached Sandia researchers to develop a computational simulation and design capability for the SOG based on our expertise in developing advanced algorithms for reacting flow simulation on HPC platforms.

A multidisciplinary team of Sandians from organizations 1437, 1416, 1411 and 1514 are working under a WFO-MIPR contract with the AFRL to create a multiphase reacting flow model within the PDE-solution research tool Charon to predict flow and conversion and attending efficiencies, utilizations and yields in various configurations of the SOG reactor. The multiphase model that was chosen is the so-called Eulerian-Eulerian form of the Navier-Stokes equations wherein one set of the equations represents the gas phase and another equation “m” sets of equations represents the liquid phase, for “m” representative droplet sizes. This formulation can lead to over 50 coupled PDEs solved over complex geometries, and thus we are developing algorithms to harness the power of large parallel computing architectures to solve the steady-state and transient forms of these equations.

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.

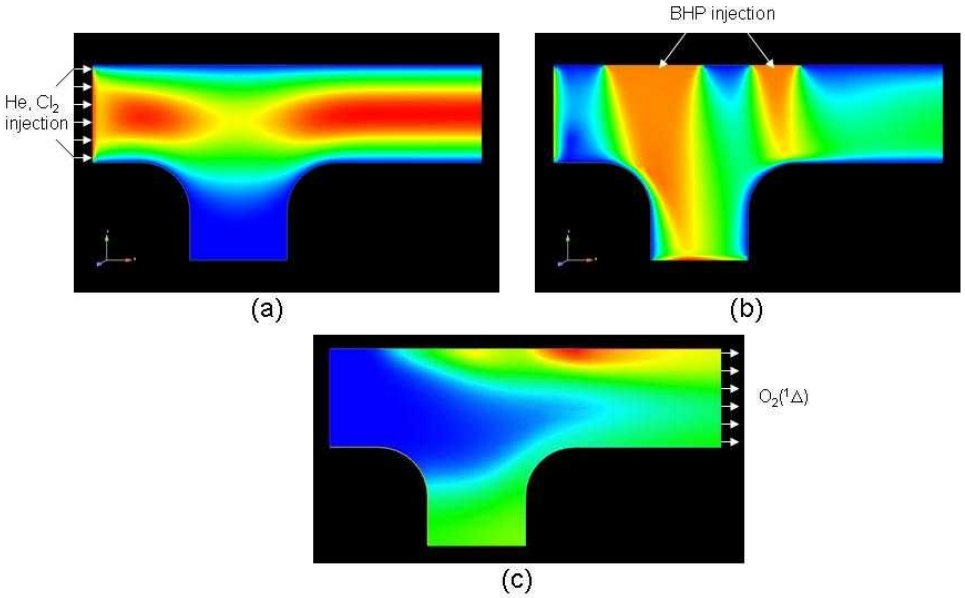

Figure 1: Various quantities in the multiphase reacting flow SOG reactor. (a) is contours of gas (He & Cl_2) velocity magnitude. (b) is contours of the velocity magnitude of aqueous BHP. (c) is contours of the target product singlet delta oxygen.