Improving Gas Reactor Design With Complex Non-Standard Reaction Mechanisms in a Reactive Flow Model

Marc Day, Lawrence Berkeley National Laboratory
John Sullivan, ALZETA Corporation

Need
Fluorinated gases are critical to many high-tech industries (e.g. manufacturing of semiconductors, flat panel displays, LEDs, photovoltaic cells, etc.). Fluorinated gases have very high global warming potentials (GWPs), and the most stable have atmospheric lifetimes of thousands of years. For environmental reasons, release of these gases must be minimized. They can be destroyed chemically, but some, such as perfluorocarbons (PFCs) contain extremely strong C-F bonds that require a significant amount of thermal energy to break. In this project, we seek to dramatically improve the energy-efficiency of this process.

Approach
A “burn-wet” exhaust gas abatement device uses combustion energy (typically from natural gas or propane) to break C-F bonds, provide a reactive environment for formation of HF, and then capture and neutralize HF in a wet scrubber downstream of the thermal reactor. Care must be taken to avoid conditions favoring the formation of CF₄ from fluorine or fluoride-containing byproducts entering the reaction chamber.

Optimizing the process
- Chemical reactions for PFCs are very sensitive to the thermal and chemical environment. Successful devices have multiple injection points for fuel, air, etc. It is difficult to determine/ optimize system dynamics experimentally.
- Simulation of these systems can be extremely expensive (large, complex reaction networks, disparate temporal and spatial scales).
- Traditional CFD inefficient for low Mach number systems (time-stepping governed by unimportant transport of acoustics).
- Leads to large number of cells, small time step, and thus massive computing resources!

Approach – cont’d
LBNL’s reacting flow code, LMC¹
- “Low Mach number” solver, removes acoustics (and the need to evolve them!) from the numerics
- Dynamic, solution-adaptive mesh refinement (AMR) localizes fine mesh around regions of interest
- Modern numerical methods for robust, efficient simulation of stiff nonlinear coupled dynamics
- Developed for massively parallel HPC platforms

Expected Results
Using LMC with HPC resources, we will map out device performance vs hardware design and process flow controls.

We expect substantial iterative refinement of the process (between levels of details of the simulation necessary to capture key experimental profiles).

Will require the design of an efficient sampling of multidimensional space involving the key process parameters

Benefits
Target industries (semiconductor, flat-panel display, LED and photovoltaic) are very important economically to the US. In 2014 the US EPA put in place the “Greenhouse Gas Reporting Rule,” requiring manufacturers to monitor and report greenhouse gas (GHG) emissions. This rule has created a better understanding of pollutant emissions and energy usage related to the control of fluorinated gas emissions. This project addresses the energy and environmental issues related to perfluorocarbon use.

Device & Model
The PFC chemical reaction model is based on previous work²
- Accurately simulates 1- and 2- carbon fluorinated compound decomposition.
- Hydrocarbon kinetics will be modeled using one of several CH₄ combustion models

Begin with simple cylindrical setup, and add more accurate inlet geometries as needed

References