DEVELOPMENT OF A SUB-GRID MODEL OF A DIESEL PARTICULATE FILTER

George Muntean, David Rector, Delbert L. Lessor, Darrell R. Herling, and Mohammad A. Khaleel
Pacific Northwest National Laboratory

The U.S. Environmental Protection Agency's (EPA) 2007 heavy- duty diesel engine exhaust emissions standards mandate a 90-percent reduction in particulate matter over current levels. The majority opinion in the diesel industry is that these standards are, by implication, mandating exhaust particulate filtration for diesel engines. Currently there is no commercially viable filtration technology that can be universally applied to all on-highway heavy-duty diesel engines. Several key technical hurdles that must be overcome in order for diesel particulate filters to become practical include: filter plugging, thermal failures, size, cost, filtration performance, and durability.

The resolution of these issues requires a detailed systems-level understanding. This includes the diesel engine's characteristics and the application duty cycle in order to understand the temperature of exhaust gas and its constituents. It also includes a characterization of installation requirements and the individual aftertreatment-device performance to understand filtration effectiveness, durability, and fuel-economy impacts.

In order for the diesel industry to meet the quickly approaching EPA regulations, the industry requires modeling capabilities. These models can be used to optimize the engine-control strategies in order to help determine the physical dimensions of the catalyst system and to simulate numerous real-world applications, which are prohibitively expensive to test in the field. Regardless of the specific question being answered, a critical key component of these models is the representation of the soot oxidation rate. This term directly influences most of the macroscopic phenomena of interest, including filtration efficiency, heat transfer, back pressure, and substrate geometries.

One key technical challenge relates to the fact that particulate filter soot regeneration remains a poorly understood and inadequately characterized phenomenon. Current sub-grid models use gross simplifications to represent the carbonaceous soot oxidation rates. All phenomena that occur on the finest length scales (approximately less than 100 microns) are typically lumped together into a single Arhenius-type equation with curve-fitted, pre-exponential and activation energy terms. Furthermore, intrinsic soot cake properties, such as packing density, permeability, and heat transfer coefficients, are poorly understood. Improvements in these sub-grid model formulations will improve the ability of engineers to model the filter on a device scale and lead to better systems optimization capabilities and improved design tools.

This paper will report on improved sub-grid representations of the local oxidation reactions by employing detailed sub-grid modeling techniques. These techniques involve the use of a lattice Boltzman modeling approach coupled with validation via both

in-situ and ex-situ experiments. This approach resolves length scales, which are orders of magnitude below those typical of a standard computational fluid dynamics (CFD) representation of an aftertreatment device. This improved resolution allows for the characterization of functionality not previously employed in the CFD analysis. Sub-grid modeling results will be presented describing the interactions of the soot-cake layer evolution with the substrate structure and catalyst materials.