An Advanced 1D 2-Layer Catalyzed Diesel Particulate Filter Model to Simulate: Filtration by the Wall and Particulate Cake, Oxidation in the Wall and Particulate Cake by NO2 and O2, and Regeneration by Heat Addition

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Abstract:
A numerical model to simulate the filtration and regeneration performance of catalyzed diesel particulate filters (CPFs) was developed at Michigan Technological University (MTU). The mathematical formulation of the model and some results are described. The model is a single-channel (inlet and outlet) representation of the flow while the thermal and catalytic regeneration framework is based on a 2-layer approach. The 2-layer model can simulate particulate matter (PM) oxidation by thermal and "catalytic" means of oxidation with O\textsubscript{2}.

Several improvements were made to this basic model and are described in this paper. A model to simulate PM oxidation by NO\textsubscript{2}/Temperature entering the particulate filter and oxidizing the PM in the two layers of the PM cake was developed. This model can be used to simulate the performance of filters with catalyst washcoats and uncatalyzed filters placed downstream of diesel oxidation catalysts (DOCs), as in the continuously regenerating traps, CRT's. A sub-model that simulates the production of NO to NO\textsubscript{2} in the washcoat of the CPF, and integrates with the NO\textsubscript{2}-PM oxidation model to simulate the higher oxidation rates (due to greater availability of NO\textsubscript{2}) in catalyzed continuously regenerating traps, CCRT's, was developed. An oxidation model to simulate PM oxidation by O\textsubscript{2} and NO\textsubscript{2} in the pores of the filter wall, which can cause the pressure drop of the filter to rapidly decrease with time, is described. The wall oxidation model was able to explain the disproportionate decreases in CPF pressure drop with respect to PM mass in the filter, which was seen at MTU. To ensure proper integration of the wall oxidation model with the overall filtration/oxidation model, a parametric model to simulate the particle filtration by the PM cake layer was developed. The wall and PM cake layer filtration and oxidation models were able to simulate sudden and rapidly decreasing pressure drops...
drops with time, with high oxidation rates in and on the filter wall while still predicting high particle filtration efficiencies. The CPF model was also modified to include a heat addition source term in the energy balance of the filter wall. This model can simulate the effect of heat generation inside a filter due to heat addition by external means. Some results from the use of this model are also presented.

A 1-D DOC model previously developed at MTU was coupled to the CPF model using Fortran Mex-Files and Matlab S-functions in Simulink to simulate DOC-CPF system performance. This integrated model can be used to simulate the filtration and oxidation performance of CRT\textsuperscript{sR} and CCRT\textsuperscript{sR} technologies or other DOC and CPF designs.