Reverse Flow Catalytic

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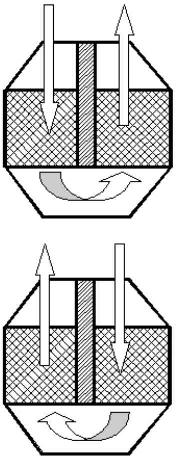
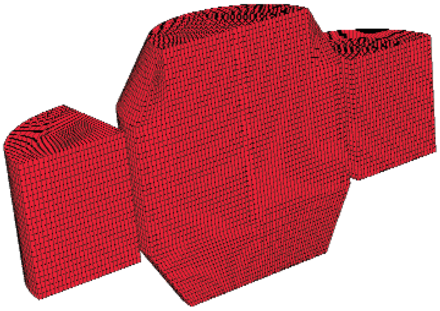


The compact reverse flow catalytic converter used for automotive applications; a rotating valve at the top is used to change flow direction



The surface mesh used; the second computation zone for the solid temperature is shown outside the actual catalytic converter in the middle

THERE IS INCREASING INTEREST in the use of natural gas to fuel automobiles. New fuels, however, may require redesign of the catalytic converters used to reduce emissions of carbon monoxide, hydrocarbons and nitrogen oxides. The natural gas engine poses a challenge for emissions control because, under some operating conditions, the exhaust temperature is too low to achieve reaction in the converter. Under these conditions, the catalytic flow reversal reactor (CFRR) offers potential. In the CFRR, the feed is periodically switched between the two ends of the reactor. Switching the feed allows energy to accumulate in the reactor, resulting in high temperatures that can sustain a reaction. Although CFRRs have been used in industrial applications, their use in automobiles presents difficulties. The large gas velocity requires a switching time of about 5 to 15 seconds. One recent design uses a single cylindrical monolith core, separated into two halves by a flow divider. A rotating valve on the top directs the flow into one side or the other. At the University of Alberta, 3D simulations of this system have been performed using FLUENT to help optimize the system design. The model has been validated with experimental results using the exhaust from a natural gas engine.

The 3D model of the full catalytic reactor contains porous catalytic sections consisting of a monolith support coated with a catalytic washcoat, and open sections. The catalytic sections are modeled using the porous media option, and the permeability is adjusted to account for the channels. In the flow direction, the permeability is based on experimental pressure drop measurements. To discourage flow in the transverse directions, it is set one to two orders of magnitude higher. The flow through the catalyst section is laminar, and in the open sections, the standard k-ε turbulence model is used.

Two approaches have been used to model the reactor. In the homogeneous model (the single zone model, or SZM), the solid and fluid phase properties are not differentiated, whereas in the heterogeneous model (the dual zone model, or DZM) separate equations are used for the fluid and solid phases. In the SZM, the catalyst sections are modeled as a porous medium, with the bulk thermal properties being used along with an apparent thermal conductivity. The DZM uses two computational zones. The first zone covers the entire reactor geometry, including the monolith and empty sections, the wall, the insulation, and the fluid phase. The fluid phase is treated the same as in the SZM; that is, the monolith sections are modeled using the porous media option with laminar flow. The second computational zone accounts for the solid temperature. This zone is built by duplicating the meshed domain of the porous sections into a new domain, which is identified as a solid in FLUENT. The density and thermal conductivity for this solid are effective properties. The bulk density and an anisotropic effective thermal conductivity are used to account for the porosity. A mesh of 64,500 cells is used for the SZM, and one of 90,710 cells is used for the DZM.

The conservation equations are solved in each computational cell, and the two zones are coupled by source terms. A matching process is done by a user-defined function (UDF) before starting the flow solution. The link between each pair of fluid and solid cells is established. During the solution, relevant information is abstracted from each fluid cell and its corresponding solid cell. Exchange terms are computed and used as source terms during the next iteration. The source terms include heat and mass transfer terms, reaction rates, and thermal energy generation terms, which are calculated using UDFs.

The boundary conditions imposed are mass flowrate and temperature at the inlet, and heat loss from the reactor by convection to the surrounding air. The interface between the catalytic monoliths and the inside reactor wall is treated differently for the two approaches. In the case of an SZM, there is one continuous phase throughout the domain, and thus no need to impose a thermal boundary condition between the monolith surface and the wall. For the DZM, continuity of flux at the wall is achieved

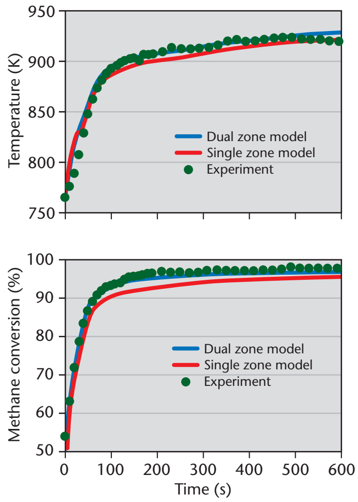
Converter Heats Up

through the fluid phase, and thus an adiabatic boundary condition is imposed at the surface of the catalyst sections.

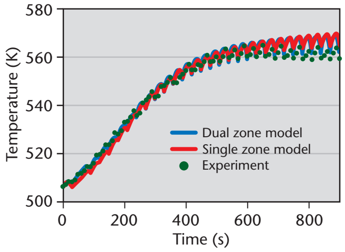
The only curve-fit parameters in the model are the kinetic rate constants, which were obtained from ten steady-state uni-directional flow experiments conducted in the University of Alberta's engine lab. The model was then tested against transient uni-directional flow experiments, also performed in the lab. In the latter experiments, the engine operating conditions were gradually changed, producing a transient response. The outlet temperatures and methane conversion predicted by the two models were found to be in good agreement with measurements, even though the DZM temperature and conversion were both predicted to be higher than the SZM values. Furthermore, the outlet temperature was found to be higher than in the experiment, while the methane conversion at the outlet was found to be slightly lower. This result indicates a discrepancy between the model and experiments in the calculation of heat loss. The numerical results for the uni-directional flow also show that there is not a large difference in the predictions of the SZM and the DZM. Considering the experimental error, the observed difference is insignificant. Computationally, the DZM uses more CPU time for a given simulation. The number of computational nodes in the DZM is higher, and because the fluid and solid calculations are coupled, a smaller time step is needed to provide an equivalent solution.

For low temperature feeds, reverse flow is required to heat the reactor adequately so that conversion can occur. In a second set of experiments, the reactor started at steady-state in uni-directional flow, and then the reverse flow mode was activated. While in reverse flow mode, the average reactor temperature was found to increase, as expected. The numerical results show how the reversing flow keeps a hot spot in the central portion of the reactor, so that methane conversion is possible.

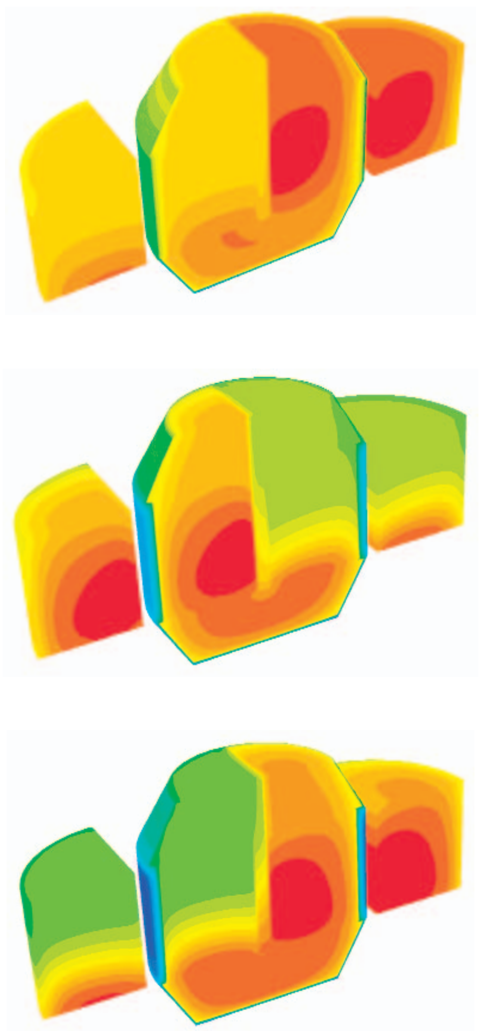
Overall, the reverse flow catalytic converter offers a practical method for achieving methane conversion in the emissions from a natural gas engine. The DZM offers superior model prediction when there are large differences in solid and fluid temperatures resulting from sharp changes in the inlet conditions. It is required for reverse flow in most conditions, and perhaps for uni-directional flow with sudden large changes in exhaust gas temperature. ■



Comparison of the reactor outlet temperature (top) and methane conversion at the outlet (bottom) for the experiments and the two models for the transient uni-directional flow case



Average reactor temperature during the reverse flow process; the temperature rise reflects the accumulation of thermal energy in the reactor



Temperature fluctuations in the catalytic converter fluid (middle) and solid (outer) zones for the DZM as the exhaust flow enters from alternating sides at the top