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Numerical Study on Forced Regeneration of Wall-Flow Diesel Particulate Filters

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ABSTRACT

A computational model which describes the combustion and heat transfer that takes place during forced regeneration of honeycomb structured wall flow type diesel particulate filter was developed. In this model, heat released by the soot- oxygen reaction, convection heat transfer in the gas phase, conductive heat transfer in solid walls, and heat transfer between the gas and wall of each honeycomb cell at various radial positions in a filter are calculated. Each honeycomb cell was modeled as one solid phase and two gas phases and these three phases were divided in the axial direction into small elements. Conductive heat transfer between the small solid elements and convection heat transfer between the small gas elements were calculated for each small time increment. Conductive radial heat transfer between honeycomb cells was also calculated. By comparison between calculated results with this model and experimental results under available limited conditions, the accuracy of the calculation model was verified. Filter temperature distributions were calculated for a wide range of material thermal properties, various cell structures and various filter shapes. Using the calculated temperature distributions, thermal stress analyses were performed for various filter designs and materials to discuss the relative merits of materials and structures. As conclusions, effects of material properties and structural design on filter durability in respect to thermal stress during forced regeneration are presented and favorable material selection and an example of stress relief design are proposed.

INTRODUCTION

While the diesel engine is more favorable for the purpose of environmental protection than a spark-ignition engine in terms of its higher thermal efficiency and reduced volume of CO_2 emissions, it has the disadvantage of emitting particulates, and the reduction of this emission is strongly desired. As information on the influences that this substance exerts on human health has been reported, the societal demands to promote a reduction of particulate emissions are thought to further strengthen the regulations in this area.

The most effective method for responding to these demands is to install a filter in the exhaust system, and the type of filter that currently excels in collecting diesel particulates is the wall-flow type made of a ceramic material. Currently, there are several issues that the diesel particulate filter (DPF) confronts. The most important issue among them is the prevention of the breakage of the filter due to the thermal load that is applied to it during regeneration. Breakage occurs primarily in two forms. One is damage through melting, as the material is exposed to high temperatures that exceed its thermal resistance threshold. The other are the cracks created through thermal stress. Therefore, it is desirable for the material to have a higher thermal resistance and a characteristic that resists the creation of thermal stress. Meanwhile, it is also necessary to devise a system that will not apply a high thermal load to the DPF, with one of the solutions being the continuous regeneration system. However, it is difficult to effect continuous generation with all operating conditions. Soot loads the DPF during low exhaust temperature operating conditions, during which regeneration is impossible. Thus, the removal of soot through some form of forced combustion is considered impossible except on certain heavy-duty vehicles (HDVs) that operate constantly with high-load conditions.

The purpose of our reserach is to analyze, through numerical calculation, the characteristics that are needed in the material used for the wall-flow type DPF, with the premise of forced regeneration. Numerous studies have already been reported concerning the simulation calculation of the combustion and regeneration of soot

transfer coefficient at the peripheral surface of the DPF and activation energy of the soot oxidation reaction were tuned through comparison with the actual test results. In the reference papers[1-2], a quasi one-dimensional model and the reaction equation are reported. Basically the quasi one-dimensional model and Arrhenius reaction parameters in these references were used. Another paper [10] presented a 2-D thermal conduction model in which quasi one-dimensional models are connected axisymmetrically with the thermal conductance between them. This method is thought to be useful for estimating the temperature distribution and thermal stress of DPFs . More detailed 2-D models for one set of an inlet cell and an outlet cell of a DPF are presented in other papers [8,9]. These models can predict the flow and the reaction more precisely than the quasi one-dimensional model, however, it takes more computational time to estimate the whole DPF temperature distribution. Then, in the research here, the quasi one- dimensional model was selected for the description of one set of an inlet cell and an outlet cell. These quasi one-dimensional models are put side by side with the thermal conductance between them. Through this model, the temperature distribution was estimated by varying the materials, cell structures, and DPF sizes. We used this temperature distribution to carry out stress analyses in order to research the material characteristics and structure that are needed.

ANALYSIS MODEL

MODEL - Fig. 1-a and Fig. 1-b show type specimen diagrams of the model. The quasi one-dimensional model shown in Fig. 1-a has been placed in the radial direction as shown in Fig. 1-b to create a two-dimensional thermal conduction model in which the flow of heat in the radial direction through solid wall is taken into account. As shown in Fig. 1-a, the basic one-dimensional model consists of the gas in the inlet cell, filter solid wall, and the gas in the outlet cell. The single solid wall that separates the inlet and outlet cells and 1/4 of the gas in the cells that sandwiches the wall have been rendered into a model. Independent quasi one-dimensional models for the gas flows were created, and, in terms of their combination in the radial direction, only the thermal conductance through the solid wall was taken into account. The volume of soot and its heat capacity were ignored, and it is assumed that the combustion heat is created in the solid wall. Furthermore, it is assumed that the gas that flows into the wall attains the same temperature as the solid wall. Because the surface area in the porous wall material is adequately large, the gas and the solid material have an extremely efficient heat transfer, and this assumption is considered to be justifiable. Based on the results of the observation of the experiments, it is assumed that soot evenly loads on one side of the filter wall.

EQUATIONS - The general equations for the gas and the solid wall are described below. In the research presented in this paper, equations for momentum conservation are not solved. Instead of that, assuming the constant gas density, mass flow rates at each position are calculated as mentioned later. A calculation of pressure is not performed .

Continuity

$$\partial\rho/\partial t + \partial(\rho_g u)/\partial x + \partial(\rho_g v)/\partial \xi = 0$$

Momentum Conservation

$$\partial(\rho_g u)/\partial t + \partial(\rho_g uu)/\partial x + \partial(\rho_g uv)/\partial \xi$$

$$= \partial p/\partial x + \mu\partial^2 u/\partial x^2$$

$$\partial(\rho_g v)/\partial t + \partial(\rho_g uv)/\partial x + \partial(\rho_g vv)/\partial \xi$$

$$= - \partial p/\partial \xi + \mu\partial^2 v/\partial \xi^2 - \mu v/k_{eq}$$

Energy Balance

(Gas)

$$\partial(\rho_g C_p T)/\partial t + \partial(\rho_g u C_p T)/\partial x + \partial(\rho_g v C_p T)/\partial \xi$$

$$= hS(T_s - T)$$

(Solid Wall)

$$\partial(\rho_s C_s T_s)/\partial t - \partial^2(\lambda_s T_s)/\partial x^2 - \partial^2(\lambda_s T_s)/\partial y^2$$

$$= hS(T - T_s) + q_r - \partial(\rho_g v C_p T)/\partial \xi$$

The last term in the equation for solid wall corresponds to the enthalpy transfer by the wall-flow gas. h is the heat transfer coefficient between the gas and wall. S is wall surface area per unit volume of the gas. q_r is the heat release rate from soot oxidation reaction.

$$q_r = H_L \, d[m_p]/dt$$

Here, $[m_p]$ is the soot mass in a unit volume. H_L is calorific value of soot combustion. The value of H_L =33000 kJ/kg was used. The formula below has been applied to calculate the oxidation reaction rate of the soot[1,2,3].

$$dm_p/dt = a \, m_p[O_2]\exp(-E_a/RT)$$

The values of the frequency factor a=300000m^3/kgs, and the activation energy E_a = 105000kJ/kmol were used.

As an experimental result, pressure drop through the wall with a uniformly distributed soot layer had been expressed by following equation:

$$[\Delta p_f]_{\text{uniform soot}} = C_1(C_2 + t_p)\,\mu v \qquad [Pa]$$

t_p: apparent soot layer thickness [m]

μ: viscosity of gas [Pa s]

C_2: constant = 0.7×10^{-5} [m]

This means the flow resistance through the wall with a soot layer is a linear function of the soot layer thickness. This relationship has been used to calculate the flow rates at each position of the DPF during regeneration where the soot distribution is uneven.

Wall flow resistance $R_f(i, j)$ at each position is:

$$R_f(i,j) = t_{eq}(i,j) / k_{eq}(i,j)$$

$$= 1.06 \times 10^9 (0.7 \times 10^{-5} + t_p(i,j)) \quad [1/m]$$

$k_{eq}(i,j)$: apparent permeability of wall with soot [m^2]
$t_{eq}(i,j)$: thickness of wall with soot [m]

For the purpose of simplifying the calculation, it is assumed that the density of the gas is not affected by the temperature in calculating the inner axial gas flow speed in the inlet cell at each position in the DPF, the wall flow speed, and the inner axial gas flow speed in the outlet cell. Furthermore, it is assumed that the flow direction of the wall gas flow to be perpendicular to the wall.

Furthermore, because the pressure loss in the flow path direction in the cell is very small as compared with the wall flow pressure loss when soot has been loaded, this can be ignored in determining the flow rate of each area through the distribution of the wall flow resistance. Rendering the total flow rate of the two-dimensional thermal conduction model to be Q'_m, the wall flow rate at the position (i,j) is:

$$q_m(i,j) = Q'_m / R(i,j) / (\Sigma(1/R(i,j)))$$

The apparent wall flow speed v (i, j) is:

$$v(i,j) = q_m(i,j) / (s \rho_g \Delta x)$$

The inner axial flow speed at each position in inlet cells and outlet cells, respectively, are as follows:

Inlet cell

$$u_{in}(i,j) = [\sum_{k=i+1}^{k=n} q_m(k,j)] / (\rho_g s^2/4)$$

Outlet cell

$$u_{out}(i,j) = [\sum_{k=1}^{k=i} q_m(k,j)] / (\rho_g s^2/4)$$

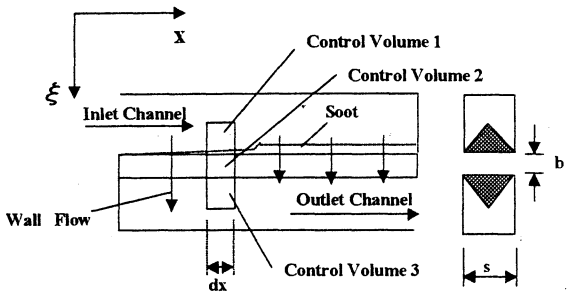

Fig.1 –a Quasi one-dimensional model

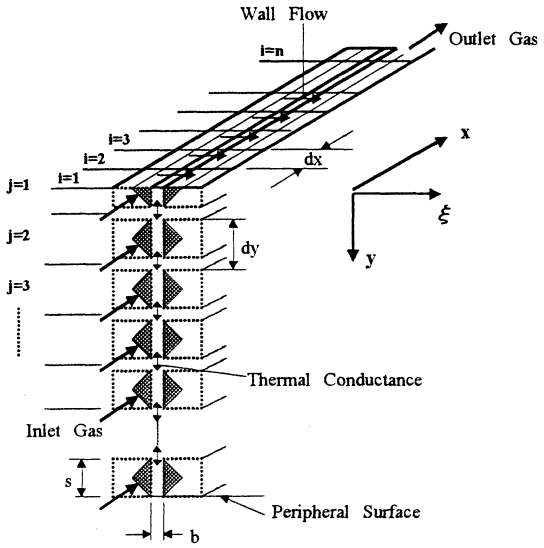

Fig.1-b 2-D thermal conduction model

Based on the aforementioned assumptions, solving the momentum equations is not necessary and the energy balance is simplified to the equations given below.

The up wind difference of first order precision is used to discretize the space–differencial terms for convection in the x direction, and a central difference of first order precision is used to discretize the space-differencial terms for thermal conduction in the solid wall. Each term on the right side of the equations for gas correspond to the enthalpy that flows into a control volume, the enthalpy that flows out from a control volume and the heat transfer between the gas and wall during the time increment dt.

In the equation for the solid wall, the first term on the right side corresponds to the enthalpy that flows into the wall with the gas that flows through the wall. The second term and the third term are the heat transfer between the gas and the wall. The forth term corresponds to the enthalpy that flows out from the wall with the gas that flows through the wall. The temperature of the gas that flows out from the wall is assumed to be the same as the wall temperature. The fifth and the sixth

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