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Re-evaluation of the Nusselt number for determining the interfacial heat and mass transfer coefficients in a flow-through monolithic catalytic converter

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ABSTRACT

The two-equation porous medium model has been widely employed for modeling the flow-through monolithic catalytic converter. In this model, the interfacial heat and mass transfer coefficients have been usually obtained using the asymptotic Nusselt and Sherwood numbers with some suitable assumptions. However, previously it seemed that there existed some misunderstanding in adopting these Nusselt and Sherwood numbers. Up to now, the Nusselt number based on the fluid bulk mean temperature has been used for determining the interfacial heat and mass transfer coefficients. However, the mass and energy balance formulations in the two-equation model indicate that the Nusselt number should be evaluated based on the fluid mean temperature instead of the fluid bulk mean temperature. Therefore, in this study, to correctly model the heat and mass transfer coefficients, the Nusselt number based on the fluid mean temperature was newly obtained for the square and circular cross-sections under two different thermal boundary conditions (i.e., constant heat flux and constant temperature at the wall). In order to do that, the present study employed the numerical as well as analytical method.

1. Introduction

As a part of efforts to reduce exhaust emissions from vehicles, the use of flow-through type monolithic catalytic converters has been substantially increased during the past several decades. As worldwide automobile emission legislations become tighter, its technology is also developing so fast. In order to reduce developing cost in experiments, the numerical modeling is in high demand for the analysis and design.

In modeling the catalytic converter, the porous medium approach has been widely adopted while considering the trade-offs between cost and accuracy. Most of previous works have employed the two-equation model, in which gas phase (i.e., exhaust flow) and solid phase (i.e., catalyst/washcoat and substrate) are, respectively, viewed as individually continuous medium. Thereby, the phase-averaged solution is obtained for each phase (Kaviany, 1995; Quintard and Whitaker, 2000).

In the two-equation porous medium model, interfacial heat and mass transfer coefficients are crucial factors which describe linkages between gas and solid phases. These coefficients have been mostly obtained using asymptotic Nusselt and Sherwood numbers with some proper assumptions. Several Nusselt numbers employed in the literatures are summarized in Table 1. Note that it is enough to utilize only the Nusselt number for obtaining both transfer coefficients because Sherwood number is assumed to be the same as Nusselt number from the heat and mass transfer analogy, which implies that if the bulk flow configuration is the same in both problems and if the wall boundary condition is the same, the mass transfer result can be obtained directly from the heat transfer result (Bejan, 1995).

The values listed in Table 1 were originated from the following earlier works. For a square channel, Clark and Kays (1953) presented fully developed Nusselt numbers for different boundary conditions using the finite difference method. The reported value is 3.63 under the axially constant heat transfer rate per unit length with constant peripheral wall temperature (**H1** boundary condition), while 2.89 under the uniform wall temperature peripherally as well as axially (**T** boundary condition). More refined finite difference solutions are given in Shah and London (1978) such that 3.60795 for **H1** and 2.976 for **T**. For a round channel, there exists an analytic solution of 48/11 for **H1** (Incropera and DeWitt, 2002; Shah and London, 1978), while an infinite series solution of 3.6567935 is reported for **T** (Shah and London, 1978).

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Table 1
Asymptotic Nusselt and Sherwood numbers generally employed in the literatures to determine the interfacial heat and mass transfer coefficients

References	Asymptotic Nusselt and Sherwood number
Siemund et al. (1996), Jeong and Kim (2000)	2.89
Chen and Cole (1989)	2.982
Taylor (1999)	2.97
Keren and Sheintuch (2000)	3.66

However, it seemed that there were previously some mistakes in applying the Nusselt numbers to obtain interfacial heat and mass transfer coefficients. Until now, all the asymptotic Nusselt numbers adopted in the earlier works have been based on the fluid bulk mean temperature. However, according to the two-equation model formulation in those works, the Nusselt numbers should be based on the fluid mean temperature, not on the fluid bulk mean temperature. In order to correct this error, the current study first provides some discussions on the formulation of the two-equation model together with appropriate Nusselt numbers, and then newly derives the Nusselt numbers based on the fluid mean temperature using the numerical as well as the analytical method for circular and square cross-sections under **H1** and **T** boundary conditions. Particularly regarding the solution method, the present work employs the non-dimensional technique as in Clark and Kays (1953).

2. General formulations on the catalytic converter

According to the literatures employing the two-equation porous medium approach to model the cylindrical automobile catalytic converters such as Chen et al. (1988), Guojiang and Song (2005), Keren and Sheintuch (2000), Koltsakis and Stamatelos (1997), Oh and Cavendish (1982), and Zygourakis (1989), typical differential equations describing the mass and energy transport between two phases can be expressed in two-dimensional axisymmetric domain as follows:

Gas phase mass balance equation for species i:

$$\varepsilon\frac{\partial C_{g,i}}{\partial t} = -\varepsilon u_g \frac{\partial C_{g,i}}{\partial x} - k_{m,i}a_{sf}(C_{g,i} - C_{s,i}). \tag{1}$$

Solid phase mass balance equation for species i:

$$(1-\varepsilon)\frac{\partial C_{s,i}}{\partial t} = k_{m,i}a_{sf}(C_{g,i} - C_{s,i}) - a_c \sum R_i. \tag{2}$$

Gas phase energy balance equation:

$$\varepsilon\rho_g c_{p,g}\frac{\partial T_g}{\partial t} = -\varepsilon\rho_g c_{p,g} u_g \frac{\partial T_g}{\partial x} + h_{sf}a_{sf}(T_s - T_g). \tag{3}$$

Solid phase energy balance equation:

$$(1-\varepsilon)\rho_s c_{p,s}\frac{\partial T_s}{\partial t} = (1-\varepsilon)k_{s,x}\frac{\partial^2 T_s}{\partial x^2} + (1-\varepsilon)k_{s,r}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T_s}{\partial r}\right) - h_{sf}a_{sf}(T_s - T_g) + a_c\sum(-\Delta H_i)R_i. \tag{4}$$

The above formulation set of Eqs. (1)–(4) resulted from the intrinsic phase-averaging for the general form of conservation equations. Each primitive variable (i.e., C_g, C_s, T_g, and T_s) and u_g represent the intrinsic phase-averaged quantities defined as (Nield and Bejan, 1992; Quintard and Whitaker, 2000)

$$\phi_\alpha \equiv \frac{1}{V_\alpha}\int_{V_\alpha}\phi\,\mathrm{d}V, \tag{5}$$

where α means the phase (i.e., gas or solid).

In order to describe the channel flow configuration, the Darcy flow model or the fully developed laminar flow model has been usually employed. The Darcy flow model (Bejan, 1995; Kaviany, 1995; Nield and Bejan, 1992) assumes that the flow has a uniform velocity profile over the channel cross-section so that no slip condition does not hold at the wall. Here, since the axial velocity can be easily obtained from the Darcy law; $u_D = K/\mu(-\mathrm{d}P/\mathrm{d}x)$, the momentum equation is not required to be solved. Note in this model that the Nusselt numbers presented in Table 1 cannot be used because they are obtained under the fully developed laminar flow assumption. Actually, the Nusselt numbers for the Darcy flow are larger than those for the fully developed laminar flow. Refer to the values produced by Asako et al. (1988) for the slug flow (i.e., longitudinally uniform over the cross-section) in several cross-sections. For a physical viewpoint, the fully developed laminar flow model is more realistic one. In this model, local velocities are known for several simple cross-section geometries so that the phase-averaged velocity present in Eqs. (1) and (3) can be obtained from their integration. In actual problems, it is easily estimated using the simple relation, $u_g = Q/A_p$ with the known intake volumetric flow rate. Therefore, as for the Darcy flow model, it is not necessary to solve the momentum equation here. Note that, although Eqs. (1) and (3) are expressed as an one-dimensional form, they are not physically one-dimensional.

There are possibly two options depending on the region of the intrinsic phase-averaging. First, the averaging is carried out over the entire monolith cross-section, which yields one-dimensional velocity and concentrations all over the monolith. Second, the averaging is performed for each channel and then Eqs. (1)–(3) are solved line by line along radial direction. This gives multi-dimensional velocity and concentrations over the monolith. Note that, for both cases, the solid temperature can be obtained multi-dimensionally.

3. Proposing new Nusselt number

In the formulation set from Eqs. (1) to (4), one of the most important tasks is how to obtain the interfacial transfer coefficients for heat, h_{sf} and mass of ith species, $k_{m,i}$. Meanwhile, these two coefficients have been usually determined through the following way.

First, h_{sf} is calculated from the definition of Nusselt number as

$$Nu \equiv \frac{h_{sf}d_h}{k_g}, \tag{6}$$

where the Nusselt number is usually assumed to be a constant. Its theoretical background is that, for a circular or square channel whose cross-section shape does not change axially, the Nusselt number approaches an asymptotic value as the flow becomes thermally fully developed under **H1** or **T** boundary condition. Here, the flow is assumed to be already hydrodynamically fully developed, which is reasonable because the Prandtl number of exhaust gases from vehicles has a near unity and thereby the hydrodynamic and thermal entrance lengths are in the same order of magnitude. In addition, for real-world vehicle operating conditions, the hydrodynamic entrance length is very short. For example, if an air at 600 K passes through a monolith of 400/6.5 (cell density [cells/in^2]/wall thickness [m in]) configuration with 0.11 m outer-diameter at 20 l/s volumetric flow rate, the single channel Reynolds number based on the fluid mean velocity becomes approximately 43.9. Referring to Wiginton and Dalton (1970) in which the dimensionless length defined by $L_{hy}/(d_h Re)$ is reported to 0.09, the hydrodynamic entrance length is calculated to about 4.3 mm.

Second, $k_{m,i}$ is obtained from the definition of Sherwood number as

$$Sh \equiv \frac{k_{m,i}d_h}{D_i}, \tag{7}$$