η = dimensionless concentration defined by Eq. 24 or 29
ν_{ij} = stoichiometric coefficient
τ = relaxation time for dissolution or precipitation

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R & D NOTES

Comments on the Paper, Theoretical Prediction of Effective Heat Transfer Parameters in Packed Beds by Anthony Dixon and D. L. Cresswell [*AIChE J.*, 25, 663 (1979)]

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One of the paper's main topics is the discussion on the equivalence between two phase and pseudohomogeneous mathematical models for packed bed analysis. Our previous work (Vortmeyer and Schaefer, 1974) which was related to the same problem is shortly discussed and criticized as being severely restricted by our assumptions. This criticism implies that obviously Dixon and Cresswell have found a more general method in order to connect both types of models. However a closer inspection of their work reveals that the obtained results are incorrect. For the sake of clearness we consider the adiabatic packed bed with a large ratio d_t/d_p. The transient, two-phase energy equations are written as:

fluid:

$$\epsilon \cdot \varphi_f \cdot c_f \cdot \frac{\partial T}{\partial t} = -\dot{m}_f c_f \frac{\partial T}{\partial x} + k_f \frac{\partial^2 T}{\partial x^2} + ah(\Theta - T) \quad (1)$$

solid:

$$(1-\epsilon)\varphi_s c_s \frac{\partial \Theta}{\partial t} = k_s \frac{\partial^2 \Theta}{\partial x^2} + ah(T - \Theta) \quad (2)$$

The right hand sides of both Eqs. 1 and 2 correspond to Eqs. 1 and 2 in the paper of Dixon and Cresswell (1979). The radial terms are neglected because they are unimportant for that what we want to demonstrate. Furthermore, by including transient terms in our Eqs. 1 and 2, we have generalized the equations of the paper of Dixon and Cresswell (1979). Equation 3 represents the energy equation of the pseudohomogeneous model:

$$[\epsilon \rho_f c_f + (1-\epsilon)\rho_s c_s] \frac{\partial \theta}{\partial t} = k_{ax}^{\text{eff}} \frac{\partial^2 \theta}{\partial x^2} - \dot{m}_f c_f \frac{\partial \theta}{\partial x} \quad (3)$$

The problem is how both types of models are interrelated concerning temperatures and axial dispersion coefficients. From the physical point of view certainly the two phase model is more realistic since it describes the heat transfer process between fluid and solid if, e.g., a packed bed is heated by a hot gas stream or if in a packed bed chemical reactor the heat of reaction is transferred from the catalyst surface to the fluid. The problem of equivalence is solved if it is known: i) how T and Θ of the two phase model are related to θ of the one phase model; and ii) how the axial dispersion coefficients of both models are interconnected.

Vortmeyer and Schaefer (1974) provided an answer by assuming the second derivatives of fluid and solid temperature profiles to be approximately the same

$$\frac{\partial^2 T}{\partial x^2} \cong \frac{\partial^2 \Theta}{\partial x^2} \quad (4)$$

Applying this condition to Eqs. 1 and 2 of the two phase model

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Vortmeyer and Schaefer (1974) obtained the following one phase model equation

$$(1-\epsilon)\rho_s c_s \frac{\partial \Theta}{\partial t} = \left(k_s + k_f + \frac{\dot{m}_f^2 c_f^2}{ha}\right) \times \frac{\partial^2 \Theta}{\partial x^2} - \dot{m}_f c_f \frac{\partial \Theta}{\partial x} \quad (5)$$

A comparison with Eq. 3 reveals that

$$\theta = \Theta \quad (6)$$

and

$$k_{ax}^{\text{eff}} = k_s + k_f + \frac{\dot{m}_f^2 c_f^2}{ha} \quad (7)$$

The one phase model of Dixon and Cresswell (1979) is obtained by the assumption that the fluid phase temperature profile of the two phase model is identical with the temperature profile of the pseudohomogeneous model.

By a comparison of both profiles Dixon and Cresswell (1979) obtained the relations

$$k_{ax}^{\text{eff}} = k_s + k_f \quad (8)$$

$$\theta = T \text{ by assumption} \quad (9)$$

The following pseudohomogeneous model equation is recommended.

$$(1-\epsilon)\rho_s c_s \frac{\partial T}{\partial t} = (k_s + k_f) \frac{\partial^2 T}{\partial x^2} - \dot{m}_f c_f \frac{\partial T}{\partial x} \quad (10)$$

Since both methods leading to pseudohomogeneous models are not exact, we feel that the quality of the approximations can only be evaluated if the solutions of Eqs. 1 and 2 are compared with the solutions of the homogeneous models (Eqs. 5 and 10). Differences in the solutions of the pseudohomogeneous models are expected since they differ in their axial effective conductivities k_{ax}^{eff} by the term $\dot{m}_f^2 c_f^2/ha$ which was derived by Vortmeyer and Schaefer (1974). This term takes account of the dispersion effect caused by the heat transfer process in the two phase model. Dixon and Cresswell (1979) have not obtained an analogeous term. We therefore can predict that the temperature profiles calculated from model (Eq. 10) will exhibit increasing deviations from the two phase model solutions if the Reynolds number is raised. The equations were solved subject to the following boundary conditions (somewhat simplified at the inlet).

Two phase model:

$$\begin{array}{llll} t < 0 & 0 \le x \le x_L & T = T_0 & \\ & & \Theta = T_0 & \\ t \geq 0 & x = 0 & T = \Theta = T_{\text{in}} & (11) \\ & x = x_L & \dfrac{\partial T}{\partial x} = \dfrac{\partial \Theta}{\partial x} = 0 & \end{array}$$

Pseudohomogeneous models: for Eq. 5 for Eq. 10

$$\begin{array}{lllll} t < 0 & 0 \le x \le x_L & \Theta = T_0; & T = T_0 & \\ t \geq 0 & x = 0 & \Theta = T_{\text{in}}; & T = T_{\text{in}} & (12) \\ & X = x_L & \dfrac{d\Theta}{dx} = 0; & \dfrac{dT}{dx} = 0 & \end{array}$$

The fluid phase dispersion coefficient k_f was evaluated from the data of Edwards and Richardson (1968) which are correlated as

$$\frac{1}{Pe_f} = \frac{0.73\,\epsilon}{\text{RePr}} + \frac{0.5}{1 + \dfrac{9.7\,\epsilon}{\text{RePr}}} \quad (13)$$

The effective conductivity k_s which is assumed to be the conductivity of a fixed bed without flow was evaluated from the relation of Krupiczka (1967). The heat transfer numbers h were calculated from the following correlations:

$1 < \text{Re} < 13$ $\quad \text{Nu} = 0.89\,\text{Re}^{0.41}$ (Littman and Sliva 1970) (14)

$$\left.\begin{array}{ll} 13 < \text{Re} < 180 & \text{Nu} = 1.75\,\text{Re}^{0.49}\,\text{Pr}^{1/3} \\ 180 < \text{Re} & \text{Nu} = 1.03\,\text{Re}^{0.95}\,\text{Pr}^{1/3} \end{array}\right\} \text{(Bird, Steward and Lightfoot 1960)} \quad (15)$$

Other data are listed in Table 1. Temperature profiles were calculated for four different Reynolds numbers Re = 5, 15, 100 and 1000, they are plotted in dimensionless coordinates, Figures 1a, b, c, d:

$$\left[\Theta^* = \frac{\Theta - T_0}{T_{\text{in}} - T_0},\ T^* = \frac{T - T_0}{T_{\text{in}} - T_0},\ \eta = x/x_L\right]$$

From the graphical representations, it is seen clearly that the temperature profiles predicted by the pseudohomogeneous model of Vortmeyer and Schaefer (1974) agree much better with the solutions of the two phase model than the profiles which are obtained from the model of Dixon and Cresswell (1979). This defect had to be expected because the latter authors do neglect the dispersion effect by heat transfer in their pseudohomogeneous model.

Furthermore, it may be noted that in a number of previous papers Vortmeyer and coworkers have made extensive use of the equivalent one phase model (Eq. 5) in order to predict fixed bed chemical reactor behavior (1974, 1975, 1978) and cyclic operation of heat regenerators (1976, 1978).

NOTATION

a	= specific interfacial surface area
c_f	= fluid specific heat
c_s	= solid specific heat
dp	= pellet diameter
d_t	= tube diameter
h	= fluid/solid heat transfer coefficient calculated by Eqs. 14 to 15
k_f	= dispersion of the fluid from Eq. 13
$k_s = k_0^{eff}$	= conductivity of the fixed bed without flow
$k_{f\ \text{molecular}}$	= molecular conductivity of the fluid
$\dot{m}_f$	= mass flow rate per unit cross section
T	= temperature of the fluid phase
x_L	= length of the reactor

Dimensionless Parameters

Nu	= Nusselt number $h \cdot dp/k_{f\ \text{molecular}}$
Pe_f	= Peclet number $\dot{m}_f \cdot c_f \cdot dp/k_f$
Pr	= Prandtl number
Re	= Reynolds number $\dot{m}_f \cdot dp/\eta$

Greek Letters

ϵ	= mean bed voidage
η	= fluid viscosity
Θ	= temperature of the solid phase
ρ_f	= fluid density
ρ_s	= solid density

TABLE 1. DATA FOR HEAT TRANSFER CALCULATION

a	$= 6(1-\epsilon)/d_p$	m^{-1}
c_f	= 1013	$J\,kg^{-1}\,K^{-1}$
c_s	= 837.4	$J\,kg^{-1}\,K^{-1}$
d_p	$= 3\ 10^{-3}$	m
h	calculated from Eqs. 14 to 15	$W\,m^{-2}\,K^{-1}$
k_f	calculated from Eq. 13	$W\,m^{-1}\,K^{-1}$
$k_s = k_0^{eff}$	= 0.1826	$W\,m^{-1}\,K^{-1}$
k_f molecular	= 0.0307	$W\,m^{-1}\,K^{-1}$
T_0	= 293	K
T_{in}	= 433	K
ϵ	= 0.4	—
η	$= 21.3889\ 10^{-6}$	$kg\,m^{-1}\,s^{-1}$
ρ_f	= 0.994	$kg\,m^{-3}$
ρ_s	= 2480	$kg\,m^{-3}$
Pr	= 0.706	—

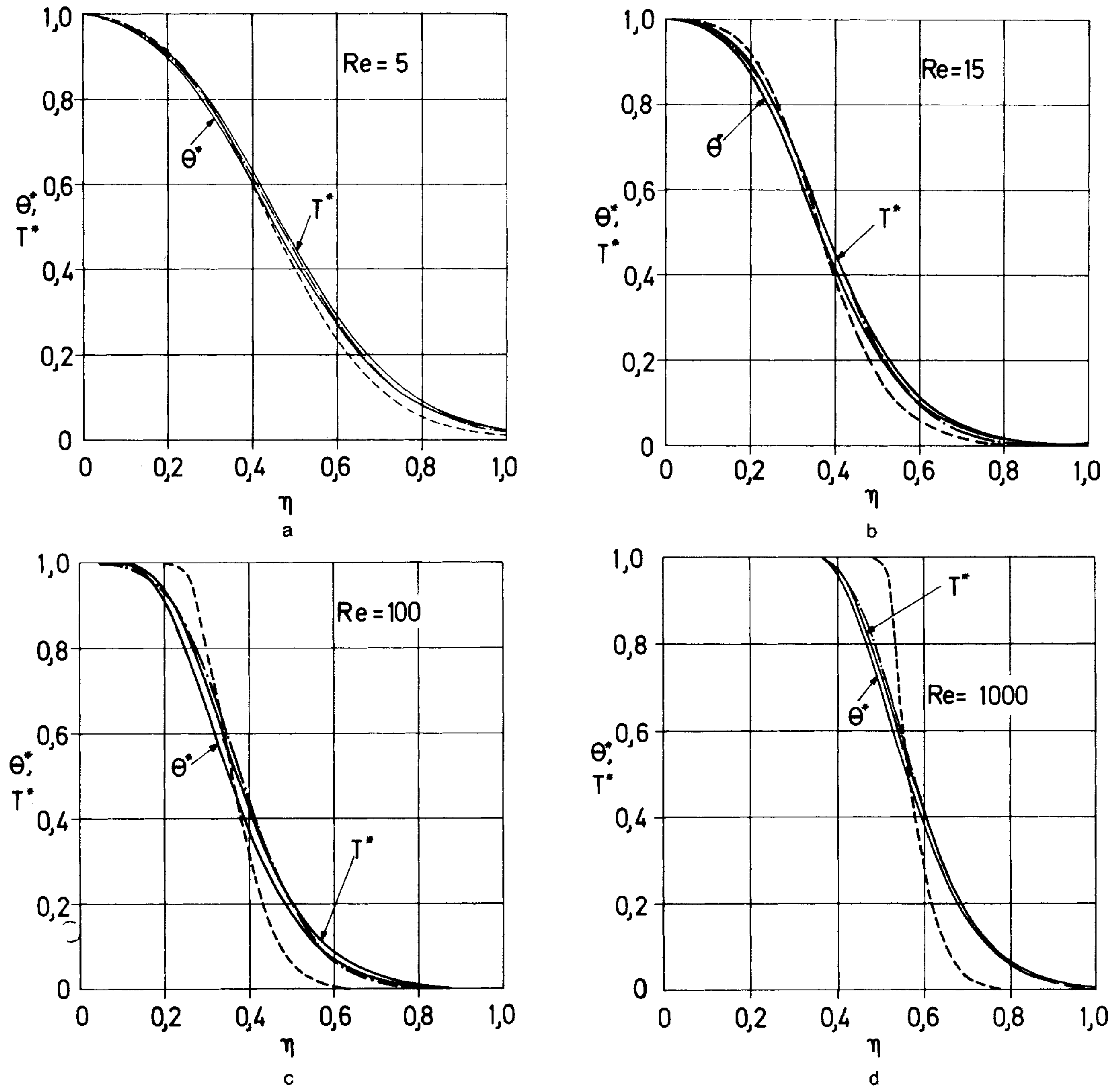

Figure 1. Comparison of temperature profiles ——— two phase model -------- pseudohomogeneous model of Dixon/Cresswell — • — • — pseudohomogeneous model of Vortmeyer/Schaefer. a) Re = 5; x_L = 0.1 m; t = 1400 s, b) Re = 15; x_L = 0.1 m; t = 400 s, c) Re = 100; x_L = 0.2 m; t = 125 s, d) Re = 1000; x_L = 1.0 m; t = 100 s

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See letter to the editor on page 526 of this issue.

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