Reply to Comments by Vortmeyer and Berninger on the Paper "Theoretical Prediction of Effective Heat Transfer Parameters in Packed Beds (*AIChE J.*, 25, 663, 1979)"

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The authors are grateful for this opportunity of clearing up the disagreements which appear to exist between their work and the results of Vortmeyer and Berninger. In fact, there are no discrepancies. The case considered by the authors was that of *steady state* heat transfer in a packed tubular bed with heat exchange at the wall, the motivation ultimately being that of designing a non-isothermal non-adiabatic catalytic reactor employing an effective continuum model.

On the other hand, Vortmeyer and Berninger address themselves to quite a different problem. They deal with the problem of predicting the *dynamic state* of an adiabatic packed bed, the so-called thermal regenerator problem.

The optimal relations between effective heat transfer parameters and those of the two-phase model are *quite* different in the two cases, as we demonstrate in the simplified example given below. This should not be surprising, since it has already been pointed out by Jackson (1977) in a related problem of determining the effective diffusivity of a porous medium that different estimates of this parameter can accrue between steady state and transient analyses. Indeed, Jackson showed further that different estimates are to be expected between different transient techniques. Despite these rather serious limitations of effective continuum models they continue to enjoy widespread use and it is important, therefore, to establish the correct correlations of the parameters to be employed in particular modelling and design problems.

As a vehicle for illustrating our ideas we consider a case similar to that given by Vortmeyer and Berninger but generalized to consider heat exchange between the fluid phase and the surroundings at temperature T_c, the heat exchange being regarded as a lumped process with overall heat transfer coefficient U. This model permits a non-uniform steady state temperature profile to be established through the bed. To simplify the model further, we neglect axial conduction in the solid phase relative to that in the fluid, although it should be noted that inclusion of this mechanism presents no special mathematical problems. The transient two-phase energy equations are written as:

Fluid:

$$\epsilon \cdot \rho_f \cdot c_f \cdot \frac{\partial T}{\partial t} = -\dot{m}_f c_f \frac{\partial T}{\partial x} + k_f \frac{\partial^2 T}{\partial x^2} + ah(\theta - T) + \frac{4U}{D_t}(T_c - T) \quad (1)$$

Solid:

$$(1-\epsilon)\rho_s c_s \frac{\partial \theta}{\partial t} = ah(T - \theta) \quad (2)$$

The simplifying boundary conditions are employed:

$$t < 0 \quad 0 \le x \le \infty \quad T = \theta = T_c \quad (3)$$

$$t \ge 0 \quad x = 0 \quad T = T_{\text{in}} \quad (4)$$

$$x \to \infty \quad T \to T_c \quad (5)$$

Equations 1–5 can be solved to give the following result, expressed in terms of the Laplace transform $\hat{T}^*(\eta)$ of the dimensionless fluid temperature $T^* = (T - T_c)/(T_{\text{in}} - T_c)$:

$$\hat{T}^*(\eta) = \frac{G_1(s)}{s} \quad (6)$$

where

$$G_1(s) = \exp\left\{(1-\beta)\frac{\text{Pe}_f}{2}\eta\right\} \quad (7)$$

and

$$\beta = \left(1 + \frac{4\gamma}{\text{Pe}_f}\right)^{1/2} \quad \gamma = sH + M + \frac{sN}{s+N}, \quad \eta = \frac{x}{D_p}$$

with

$$H = \frac{\epsilon\rho_f c_f}{(1-\epsilon)\rho_s c_s}, \quad M = \frac{4U}{\dot{m}_f c_f}\left(\frac{D_p}{D_t}\right) \quad N = \frac{ahD_p}{\dot{m}_f c_f}, \quad \text{Pe}_f = \frac{\dot{m}_f c_f D_p}{k_f}$$

The corresponding solution of the one-phase continuum model can be written as

$$\hat{v}^*(\eta) = \frac{G_2(s)}{s} \quad (8)$$

where

$$G_2(s) = \exp\left\{(1-\beta')\frac{\text{Pe}_{\text{eff}}}{2}\eta\right\} \quad (9)$$

and

$$\beta' = \left[1 + \frac{4}{\text{Pe}_{\text{eff}}}\left\{M_{\text{eff}} + (1+H)s\right\}\right]^{1/2}$$

with

$$M_{\text{eff}} = \frac{4U^{\text{eff}}}{\dot{m}_f c_f}\left(\frac{D_p}{D_t}\right), \quad \text{Pe}_{\text{eff}} = \frac{m_f c_f D_p}{k_{ax}^{\text{eff}}}$$

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TABLE 1. FIRST THREE MOMENTS OF THE ONE AND TWO-PHASE MODELS

Moment	One-Phase Model	Two-Phase Model (Fluid Phase)
m_0	$\exp\left\{(1-\beta_0')\frac{\mathrm{Pe}_{\mathrm{eff}}\eta}{2}\right\}$	$\exp\left\{1-\beta_0)\frac{\mathrm{Pe}_f\eta}{2}\right\}$
m_1	$\frac{\eta(1+H)}{\beta_0'}$	$\frac{\eta(1+H)}{\beta_0}$
μ_2	$\frac{2\eta(1+H)^2}{\beta_0'^3\,\mathrm{Pe}_{\mathrm{eff}}}$	$\frac{2\eta}{\beta_0}\left\{\frac{1}{N}+\frac{(1+H)^2}{\mathrm{Pe}_f\beta_0^2}\right\}$
	$\beta_0'=\left(1+\frac{4M_{\mathrm{eff}}}{\mathrm{Pe}_{\mathrm{eff}}}\right)^{1/2}$	$\beta_0'=\left(1+\frac{4M}{\mathrm{Pe}_f}\right)^{1/2}$

It is pertinent to compare statistical moments of the two transfer functions $G_1(s)$ and $G_2(s)$ as a basis for matching the two models. The zero moment (m_0), first moment (m_1) and second central moment (μ_2) are defined by

$$m_0 = G(s)|_{s\to 0} \quad m_1 = \frac{-(dG/ds)_{s\to 0}}{m_0}, \quad \mu_2 = \frac{(d^2G/ds^2)_{s\to 0}}{m_0} - m_1^2 \tag{10}$$

The first three moments are shown in Table 1.

Case 1—Zero Moment Matching

If one were concerned primarily with matching *steady state* profiles of the two models to provide effective transport parameters for subsequent *steady state* reactor modelling, then matching of the zero moments is optimal. This case is shown schematically in Figure 1(a). Note that the dynamic responses are relatively poorly matched. In this case,

$$M_{\mathrm{eff}} = M, \quad P_{\mathrm{eff}} = \mathrm{Pe}_f, \tag{11}$$

as could be deduced from considering the steady state equations alone. This was the case considered previously by the authors.

Case 2—First and Second Moment Matching

On the other hand, if interest centres on matching the shapes of the transient temperature profiles it is expedient to match first and second moments. This case is shown schematically in Figure 1(b).

Note here that in the non-adiabatic case the final steady states are relatively poorly matched. Now,

$$\frac{1}{\mathrm{Pe}_{\mathrm{eff}}} = \frac{1}{\mathrm{Pe}_{\mathrm{f}}}\left\{1+\frac{4M}{(1+H)^2}\right\} + \frac{1}{N(1+H)^2} \tag{12}$$

and

$$M_{\mathrm{eff}} = \frac{M}{\left\{1+\frac{(4M+\mathrm{Pe}_f)}{N(1+H)^2}\right\}} \tag{13}$$

It is interesting here to compare Eq. 12 with Eq. 7 in Vortmeyer and Berninger's paper. For $k_s = 0$ (the case considered here) their Eq. 7 becomes

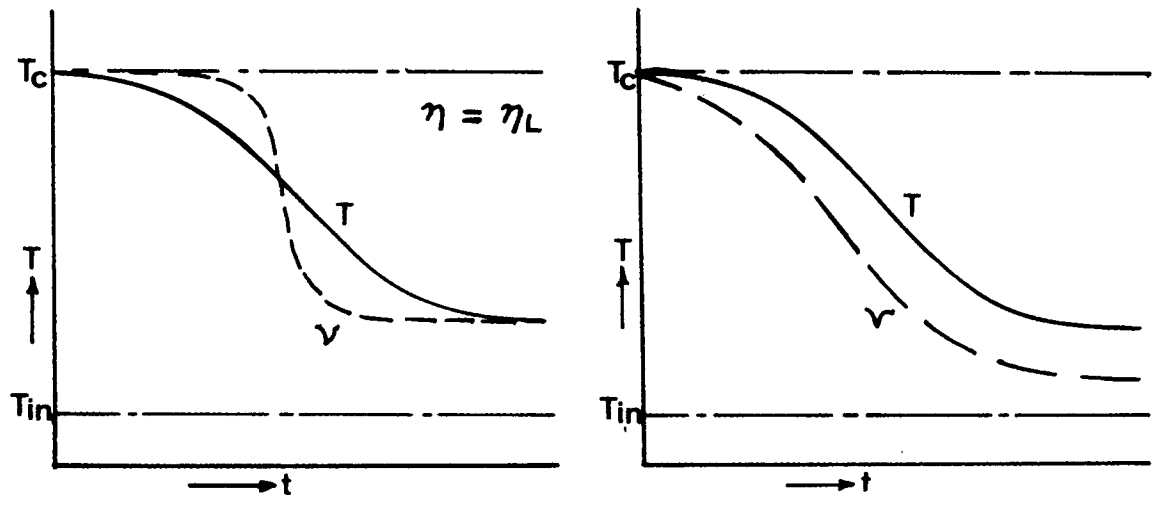
$$\frac{1}{\mathrm{Pe}_{\mathrm{eff}}} = \frac{1}{\mathrm{Pe}_f} + \frac{1}{N} \tag{14}$$

Equation 14 and the more general relation 12 become identical *only* if $M = 0$ and $H = 0$—i.e., the case of an adiabatic bed and a gaseous fluid. For a liquid mobile phase $H \sim 0(1)$, Eq. 14 is completely inappropriate.

The apparently arbitrary approximation $\partial^2 T/\partial x^2 \simeq \partial^2\theta/\partial x^2$ employed by Vortmeyer and Schaefer (1974) can now be given a sounder basis, since it turns out to be equivalent to matching 2nd moments of the temperature response curves.

Finally, it is important to assess the differences between the parameter correlations obtained from steady state and transient state model matching within the context of available experimental data. In Figure 2 we present data obtained from *steady state* heat transfer measurements. These data cover both the adiabatic and non-adiabatic cases, as well as extending over wide ranges of particle thermal conductivity, particle size and tube diameter.

It is hardly surprising, therefore, that the data show considerable scatter, making quantitative comparisons of different correlations rather meaningless. Nevertheless, some conclusions can be drawn as regards the qualitative trends in the data. The correlation for k_{ax}^{eff} suggested by Vortmeyer and Berninger (their Eqn 7) is shown as the dotted curve, whereas the relation $k_{ax}^{\mathrm{eff}} = k_s + k_f$ is given by the solid curve. The dotted curve was constructed using the data in Table 1 of Vortmeyer and Berninger's paper, except that a ratio of $k_s/k_g = 18$, rather than 6 was employed. The former figure is the more appropriate for metallic packings, whereas the latter is more suitable for glass and ceramic packings. It is important to note that Vortmeyer and Berninger's correlation possesses a *maximum*, occurring at a modest value of the Reynolds number, well within the range of Reynolds numbers covered experimentally. Now, despite the scatter of the data, one *cannot* detect a maximum in *any* of the individual $\mathrm{Pe}_{\mathrm{eff}}$ vs. Re data sets. The overriding trend



(a) Zero Moment Matching (b) 2nd Moment Matching

Figure 1. Relating one-phase and two-phase models by matching of moments.

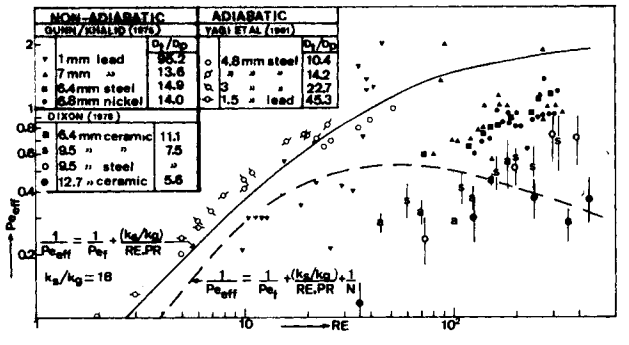


Figure 2. Comparison of parameter relations with "steady state" experimental data.

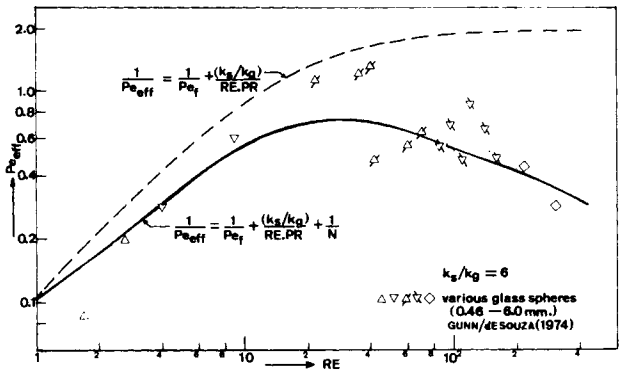


Figure 3. Comparison of parameter relations with "dynamic state" experimental data.

is for Pe_{eff} to increase monotonically with Re, in line with the correlation $k_{ax}^{eff} = k_s + k_f$, obtained from steady state model matching.

On the other hand, according to our argument, *dynamic* heat transfer measurements should show up the virtue of Vortmeyer and Berninger's correlation while revealing also the paucity of the "steady state" correlation for k_{ax}^{eff}. This is indeed confirmed in Figure 3 for data on glass spheres of various sizes.

Since our original paper, one of the authors (Dixon, 1980) has provided a numerical comparison of the one-phase and two-phase models and presented experimental data tending to confirm the validity of the parameter relations.

NOTATION

All heat transfer parameters defined in terms of total area (void + non-void) normal to the direction of heat transfer.

a = specific interfacial surface area
c_f = fluid specific heat
c_s = solid specific heat
D_p = particle diameter
D_t = tube diameter
h = apparent fluid/solid heat transfer coefficient
k_{ax}^{eff} = axial effective conductivity (one-phase model)
k_f = axial conductivity of the fluid
k_s = axial conductivity of the solid
$\dot{m}_f$ = superficial fluid mass velocity
T = fluid temperature
T_c = coolant temperature
T_{in} = fluid temperature at inlet
t = time
U = apparent fluid/coolant heat transfer coefficient
U_{eff} = effective overall heat transfer coefficient (one-phase model)
x = axial co-ordinate

Greek Letters

ϵ = bed porosity
θ = solid temperature
ρ_f = fluid density
ρ_s = solid density

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