ON THE OBSERVABILITY OF HEAT DISPERSION PARAMETERS OF THE PSEUDOHOMOGENEOUS MODEL OF HEAT TRANSFER IN PACKED BEDS

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Solution has been obtained of the pseudohomogeneous model of heat dispersion in a packed bed under simultaneous radial and axial dispersion of heat using Danckwerts' boundary condition. The obtained solution has been used to evaluate parameters of the model from experimental data based on the least sum of square deviations of the temperature profiles. Maps have been constructed of the joint confidence regions in the parameter domain. The results have shown the method to be suitable for the determination of radial thermal dispersion while suppressing the effects of structural disturbances of the bed near the containing walls.

Systems with solid particles passed by one or more fluid phases exist in a variety of technological operations, which utilize its large available interfacial surface and low degree of mixing of fluid phases. The first of these features is important for high intensity of the process, while the low degree of the so called axial mixing is advantageous, for instance, for the continuous mode of operation of chemical reactors as it preserves selectivity achieved in the batch operation. The low degree of radial mixing is, as a rule, not favoured particularly in the processes requiring removal or supply of heat. Efficient use of packed bed systems for processes involving heat transfer is thus vitaly dependent on the knowledge of the dispersion of heat in these systems.

Net heat transfer in beds passed by gas is compounded of mutual interactions of the three basic transport mechanism: conduction, convection and radiation in both the gas and the solid phase. Beveridge and Haughey[1] list 10 mechanisms for the generalcase of heat transfer. Individual mechanisms depend in a different way on the hydrodynamics of the flow and are mutually coupled. This considerably complicates the scale-up and modelling of the system without detailed quantitative understanding of their physical nature[2]. Due to the different character of the interactions the ability of the bed to disperse heat is anisotropic and the effective thermal conductivity depends on the direction. The introduced notions of the radial and axial thermal dispersion are not in fact very appropriate for the anisotropy of heat dispersion actually relates to the gas velocity vector rather than the frame of coordinates. Ideally, as axial should be termed that component of the effective conduction heat flux vector parallel to the gas velocity vector, while as radial should we regard the component of the heat flux perpendicular to the velocity vector.

Various mathematical models have been used in practice to describe the heat transfer in a packed bed. Two-phase models solve separately the energy balances of both phases which exchange heat. Their parameters are coefficients of thermal diffusivity and the fluid-to-particle and bed-to-wall heat transfer coefficients. The single-phase models view the bed, including the flowing fluid, as a pseudohomogeneous medium and express the overall energy balance by a single equation. Parameters of these models are the effective thermal conductivities of the bed and the bed-to-wall heat transfer coefficient. Vortmeyer and Schaefer[3] proved equivalence of both types of models by deriving corresponding single-phase model from the two-phase one under the sufficient condition of equality of the second derivatives of temperature of the solids and the gas with respect to the axial coordinate.

More recently however, Dixon and Cresswell[13] derived, on the basis of an approximate collocation method solution, relations between parameters of the pseudohomogeneous and the two-phase model, leading to identical temperature profiles. The applied two-phase model admits existence of axial dispersion of heat in both phases and the relations of equivalence do not require the assumption of equality of temperatures of phases or their second derivatives.

Existing experimental methods are essentially of two kinds. Dynamic measurements examine the development of the inlet temperature signal[4–7] after passing through the system and the results are processed usually by the two-phase models.

With static methods of measurements the most frequent arrangement is that of a cylindrical bed heated across the wall. Wakao[8] have shown that if there are no heat sources or sinks within the bed, the temperature of the solids and the fluid phase are nearly identical, which makes the two-phase models essentially inapplicable. The static measurements are thus processed mostly by the single-phase, pseudohomogeneous models. A two-dimensional form of such model has been derived by Froment[9] and further modified by Gunn and Khalid[10] who incorporated axial thermal dispersion.

Recent literature is rich on experimental data and correlations, *e.g.*[11–14]. The results of individual authors, however, differ often significantly. Wakao and coworkers[11] put forth as a cause of these differences the choice of the mathematical model and reevaluated available experimental data with the aid of the modified „dispersion concentric" model. Gunn and Khalid[10] explain the differences by the neglect of the axial dispersion term and thus, in principle, also by the choice of the model.

De Wasch and Froment[15], as well as other authors, pointed at the length dependence of the parameters of heat transfer in packed beds. From the standpoint of this length dependence Li and Finlayson[12] classified various experimental and data processing methods. These authors showed that some methods provide effective means of the parameters for the given depth of the packed section and reevaluated available experimental data to obtain asymptotic values free of the length effect.

The length dependence of the parameters is a serious shortcoming for scale-up and data transfer and clearly the principal source of discrepancy of results of various authors. Although positively detected[15] for all parameters of pseudohomogeneous single-phase and two-phase models, this fact is forseen by neither of the existing models. Nor is there an unambiguous explanation for the length dependence.

Botterill and Denloye[16] presumed different thermal dispersions and gas velocities in the bulk of the bed, exhibiting constant porosity and in the region adherring to the wall. These authors derived a theoretical, pseudohomogeneous model which treats both regions separately and hence respects the inherent inhomogeneity of the bed and its consequences for heat transfer.

This paper presents solution of the pseudohomogeneous model with axial dispersion of heat for the case of radially distributed temperature profile in the inlet gas. This method is in principle analogous to the method of heating the bed through the jacket, but the heat is not supplied across the geometrically least representative part of the bed. The effect of bed irregularities, increased porosity and increased gas velocity in the wall region may thus, to a large extent, be eliminated. The aim of this work has been to test the possibility of evaluating the radial and axial thermal diffusivities from such experiments.

THEORETICAL

Steady state heat transfer in a cylindrical bed is described by the following partial differential equation in the dimensionless form as

$$\frac{1}{Pe_L}\frac{\partial^2 T}{\partial z^2} + \frac{1}{r\,Pe_R}\frac{\partial T}{\partial r} + \frac{1}{Pe_R}\frac{\partial^2 T}{\partial r^2} - \frac{R}{d_p}\frac{\partial T}{\partial z} = 0\,, \tag{1}$$

where

$$T = (T' - T'_E)/(T'_1 - T'_E) \tag{2}$$

$$r = r'/R \tag{3}$$

$$z = x/R \tag{4}$$

and appropriate boundary conditions.

Thermal losses through an insulated wall into the surroundings of constant temperature and infinite thermal capacity are expressed by the boundary conditions

$$-\partial T/\partial r = HT \quad \text{for} \quad r = 1\,, \tag{5}$$

where

$$H = hR/k_R\,. \tag{6}$$

Radially distributed, axially symmetric inlet temperature profile it given by the initial condition in the following form

$$\begin{aligned} T = T_1 = 1 \quad &\text{for} \quad 0 \leqq r \leqq r_1\,; \quad z = 0 \\ T = T_2 \quad &\text{for} \quad r_1 < r \leqq 1\,; \quad z = 0\,. \end{aligned} \tag{7}$$

For a bed of finite length Z one has to specify one more condition. For no heat dispersion across the outlet cross-section we can write

$$\partial T/\partial z = 0 \quad \text{for} \quad z = Z\,. \tag{8}$$

Solution of the above stated model has been described in detail in the previous work[17]. Solution was obtained with the above conditions for a semi-infinite bed and a bed of a finite length, Z. For brevity let us put

$$A = Gc_{PF}R/k_L = R\,Pe_L/d_p \tag{9}$$

$$B = Gc_{PF}R/k_R = R\,Pe_R/d_p\,. \tag{10}$$

For the purpose of processing the experimental temperature profiles measured at the bed exit we are concerned with the theoretical temperature profile for $z = Z$:

$$T = \sum_{n=1}^{\infty} \frac{2\alpha_n[(T_1 - T_2)\,r_1\,J_1(\alpha_n r_1) + T_2\,J_1(\alpha_n)]\,J_0(\alpha_n r)}{(\alpha_n^2 + H^2)\,J_0^2(\alpha_n)} \,. \cdot \frac{2Y\exp\left[AZ(\frac{1}{2} - Y)\right]}{\frac{1}{2} + Y - (\frac{1}{2} - Y)\exp(-2AZY)}\,. \tag{11}$$

where

$$Y = \sqrt{[\tfrac{1}{4} + (\alpha_n^2/AB)]}\,.$$

Eq. (7), specifying the inlet temperature conditions, does not meet the balance of thermal fluxes across the inlet surface. As shown by Danckwerts[18] a more rigorous formulation is following

$$T_{z=0_-} = T_{z=0_+} - (1/A)\,(\partial T/\partial z)_{z=0_+}\,. \tag{12}$$

The model was further solved with Danckwerts' condition, Eq. (*12*), again for a semi-infinite bed as well as the bed of finite length, Z. The temperature profile at the bed exit ($z = Z$) is given by

$$T = \sum_{n=1}^{\infty} \frac{2\alpha_n[(T_1 - T_2)\,r_1\,J_1(\alpha_n r_1) + T_2\,J_1(\alpha_n)]\,J_0(\alpha_n r)}{(\alpha_n^2 + H^2)\,J_0^2(\alpha_n)} \,. \cdot \frac{2Y\exp\left[AZ(\frac{1}{2} - Y)\right]}{(\frac{1}{2} + Y)^2 - (\frac{1}{2} - Y)^2\exp(-2AZY)}\,. \tag{13}$$

For same inlet conditions we obtained also solution for the case of negligible axial dispersion. This involved solution of Eq. (*1*) in the absence of the first term on the left hand side. The theoretical outlet temperature profile then reads

$$T = \sum_{n=1}^{\infty} \frac{2\alpha_n[(T_1 - T_2)\,r_1\,J_1(\alpha_n r_1) + T_2\,J_1(\alpha_n)]\,J_0(\alpha_n r)}{(\alpha_n^2 + H^2)\,J_0^2(\alpha_n)} \exp\left(-\frac{\alpha_n^2}{B}Z\right). \tag{14}$$

The quantity α_n in Eqs (*11*), (*13*) and (*14*) is the n-th root of the characteristic equation

$$\alpha_n J_1(\alpha_n) - H J_0(\alpha_n) = 0 . \qquad (15)$$

For a perfectly adiabatic arrangement of the experiment, *i.e.* for $H = 0$, all above solutions must be supplemented by the zero-th term of the infinite series in the form

$$T_1 r_1^2 + T_2(1 - r_1^2) . \qquad (16)$$

EXPERIMENTAL

Apparatus

The measurements were carried out in column 50 mm in diameter with the packed bed height between 40 and 112 mm. The packing was steel and lead balls between 1 and 3 mm in diameter. The flowing gas was in all cases air whose flow rate was metered by a bank of rotameters. After metering the air was lead into the heater creating an axially symmetric inlet temperature profile (see Eq. (*7*) for $T_1 > T_2$) by heating 20% of the air stream. Both the heated and the cold part of the air stream were separated mutually by a teflon ring and directed into the space above bed. Their temperature was gauged by a set of eight thermocouples. The temperature profile in the outlet air was measured by a set of 20 thermistors, asymmetrically distributed over the outlet column cross-action.

Data Processing

The set of data from each experiment consisted of temperatures T_1, T_2, determining the inlet temperature profile, twenty temperatures T_n, measured at the outlet in radial positions r_n, and the superficial mass velocity of air, G. All temperatures were referred to the temperature of the surroundings, according to Eq. (*2*).

The theoretical temperatures at the bed outlet were expressed from Eqs (*11*), (*13*) and (*14*). Optimization of parameters of these models was carried out as a nonlinear regression[19] using the BSOLVE algorithm[20]. The calculations were carried out on an EC 1033 computer in double precision arithmetic. The objective function was the residual sum of square deviations, RSQ:

$$RSQ = \sum_{n=1}^{20} [T_{exp}(r_n, Z) - T_{calc}(r_n, Z)]^2 . \qquad (17)$$

Optimized values of model parameters were initially the dimensionless quantities A, B, H, defined by Eqs (*9*), (*10*) and (*6*). The third parameter, equivalent to the Biot number, was later replaced by the dimensionless parameter C, defined as follows:

$$C = H/B = h/Gc_{PF} . \qquad (18)$$

This was done in accord with the results of Lerou and Froment[21] who found that the optimization proceeds more rapidly with the parameter C, which is independent of the radial thermal diffusivity.

The first estimate of the parameter A was taken so as to make $Pe_L = 2$. The first estimate of the parameter B was taken from the results of Gunn and Khalid[10]. In view of the thermal insulation of the wall and expected small thermal losses, the initial estimate of the parameter C was taken low, namely $C = 1 \times 10^{-3}$.

For all experiments the optimization was performed with at least two sets of initial estimates in order to approach the optimum from different directions. Typical comparison of the measured and theoretical temperature profiles is shown in Fig. 1.

For optimum values of the parameters $b(m)$ ($b(m)$ being identical with either A, B or C) the covariance matrix, **V**, was evaluated under the assumption of the normal distribution of errors of the experimental data and parameters.

$$\mathbf{V} = [(1/\sigma^2)\mathbf{J}.\mathbf{J}^T]^{-1} \qquad (19)$$

J in this equation is the Jacobi matrix of derivatives of the model function with respect to parameters and $\mathbf{J}^T$ is the corresponding transpose matrix. Inversion of the matrix on the right hand side of Eq. (19) was accomplished by Gauss elimination. The variance σ^2 was approximated by the relation

$$\sigma^2 = RSQ_{min}/(n - m), \qquad (20)$$

where n is the number of experimental data and m is the number of parameters.

The covariance matrix served to obtain standard deviations, $\sigma(m)$, the cross correlation coefficients, $\varrho(m_1, m_2)$ and the variational coefficients, $v(m)$

$$v(m) = 100\sigma(m)/b(m) \quad [\%] \qquad (21)$$

for individual parameters.

Strictly speaking, the above considerations apply to problems linear with respect to parameters. This assumption in our case is not fulfilled even approximately. The following conclusions are thus valid with sufficient accuracy only in the close neighbourhood of the optimum. In the reamining part of the parameter domain the conclusions may be regarded only as qualitative.

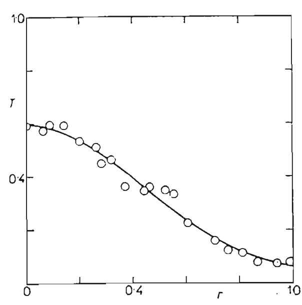

FIG. 1

Typical computed and experimental radial temperature profiles in outlet gas (3 mm steel balls, 60 mm bed depth)

In order to better illustrate the observability of individual parameters and their cross correlations, maps of joint confidence regions were constructed for several experiments. This consisted of calculating the residual sum of square deviations in individual points of the parameter domain, corresponding to the $(1 - \alpha)$ level of the F distribution for $(n - m)$ degrees of freedom.

RESULTS

Axial Dispersion

Solution of the above mathematical model for the given experimental conditions did not yield values of the coefficient of axial thermal dispersion. In a wide range of values the residual sum of square deviations was insensitive to the parameter A. Fig. 2 shows typical pattern of the confidence regions in the Pe_L–Pe_R space. For the majority of experiments the parameter A converged to the high values $(k_L \to 0)$ and the obtained results were identical with the model neglecting axial dispersion, Eq. (*14*). The parameters A and B were found mutually uncorrelated $\varrho(AB) < 0{\cdot}1$.

In only isolated cases (high air flow rates) did the routine converge to low values of the parameter A, but their standard deviations were larger than the value of the parameter proper. In these cases, in addition, a strong cross correlation was detected of the parameters A and B $(\varrho(AB) > 0{\cdot}8)$, which adversely affected optimizations of the parameter B. Owing to the overall loss of sensitivity, decreased also the parameter B with decreasing A while the corresponding change of the residual sum of square deviations was small. As a consequence, the accuracy of determination of the parameter B was impaired and its variational coefficient increased to about 20%. For these experiments the data were reevaluated using the model with neglected axial dispersion.

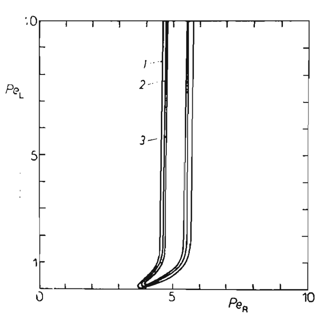

FIG. 2

Map of joint confidence regions in the radial Peclet number *versus* axial Peclet number domain (constructed from data from experiment shown in Fig. 1). *1* $\alpha = 0{\cdot}01$, *2* $\alpha = 0{\cdot}05$, *3* $\alpha = 0{\cdot}1$

Radial Dispersion

The change of the parameter B, incorporating the effect of the radial thermal dispersion, affected the residual sum of square deviations most markedly. The variational coefficient ranged between 2 and 6%. Higher than these $v(B)$ values displayed experiments at high air rates and on shallow beds, when the inlet temperature profile was little deformed, and, on the contrary, for very low air rates, when the putlet profile was already too flat.

Fig. 3 shows the map of the confidence regions for the parameters Pe_R and C.

The Wall Heat Transfer Coefficient

As expected, the accuracy of determination of the parameter C was not high due to the thermal insulation of the wall and due to the fact that the temperature in the wall region was close to the temperature of the surroundings. The net heat flux across the wall was minimal, particularly at high air rates.

The cross correlation of the parameter B and C showed only for low air velocities, while in other cases was insignificant $\varrho(BC) < 0{\cdot}2$.

CONCLUSIONS

The pseudohomogeneous model of Gunn and Khalid[10] was solved for Danckwert's boundary condition and the axially symmetric, radially distributed temperature profile in the inlet gas. The obtained solution was used to process experimental data. Optimum values of the model parameters were obtained by minimizing the residual sum of square deviations. Statistical analysis of the experimental data con-

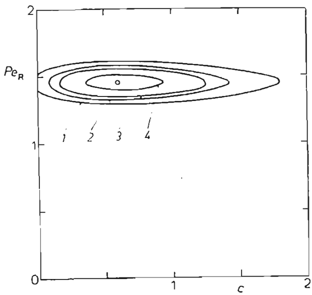

FIG. 3

Map of joint confidence regions in the radial Peclet number *versus* Biot over radial Peclet number domain (constructed from data for 1 mm steel balls, and 83 mm bed depth. *1* $\alpha = 0{\cdot}01$, *2* $\alpha = 0{\cdot}05$, *3* $\alpha = 0{\cdot}1$, *4* $\alpha = 0{\cdot}5$

sisted of calculating the covariance matrix, standard deviations of parameters and their cross correlations.

The obtained results indicate that the described method of measurement and data processing yields values of Pe_R with a high precision. Pe_L is not observable; the results mostly converge to high values and the standard deviations of the parameter are comparable with the value of the parameter or even higher. The results of Pe_R are little sensitive to the value of Pe_L, which enables utilization of the simpler model with neglected axial dispersion. For this reason it is impossible to assess the significance of the solution with Danckwerts' boundary condition, which, of course, from the standpoint of the thermal balance is more rigorous.

The wall heat transfer coefficient was not observable for already the experimental conditions (insulation, the form of the inlet temperature profile) were purposly adjusted as to make it insignificant. The results of Pe_R at low values of the heat transfer coefficient are little sensitive to heat transfer across the wall. This further offers the possibility of simplifying the model to the adiabatic case.

From these conclusions there follows the applicability of our experimental techniques for measurement of the radial thermal dispersion in packed beds. The found low sensitivity to the phenomenon of axial dispersion thus inherently suppresses the so called end effects. In addition, the nearly adiabatic course of the experiment suppresses the influence of the inhomogeneous regions of the bed where the particles contact the wall. The obtained radial dispersions thus approach the results for the radially unconfined bed. This fact may be significant for a succesfuly scale-up to larger systems.

LIST OF SYMBOLS

A, B, C	defined by Eqs (*9*), (*10*), (*18*) (−)
b(m)	general parameter of the model
c_{PF}	specific heat of fluid [J/kg K]
d_p	particle diameter [m]
G	superficial mass velocity [kg/m^2 s]
h	wall heat transfer coefficient [W/m^2 K]
H	defined by Eq. (*6*) [−]
J_0, J_1	Bessel functions
k_L, k_R	axial and radial effective thermal conductivity [W/m K]
m	number of parameters of the model [−]
n	number of experimental points, summation index [−]
$Pe_L = Gc_{PF}d_p/k_L$	axial Peclet number [−]
$Pe_R = Gc_{PF}d_p\mathrm{L}k_R$	radial Peclet number [−]
$r = r'/R$	dimensionless radial coordinate [−]
r'	radial coordinate [m]
R	column radius [m]
T	dimensionless temperature defined by Eq. (*2*) [−]

T_1, T_2	dimensionless inlet temperatures [—]
T', T'_E	temperature and temperature of the surroundings [K]
$v(m)$	variational coefficient defined by Eq. (*21*)
$\mathbf{V}$	covariance matrix
x	axial coordinate [—]
$z = x/R$	dimensionless axial coordinate [—]
Z	dimensionless bed depth [—]
α	significance level [—]
α_n	roots of Eq. (*15*) [—]
$\varrho(m_1, m_2)$	cross correlation coefficient of parameters m_1, m_2
$\sigma(m)$	standard deviation of parameter $b(m)$ [—]

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