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Bayesian estimation of heat transport parameters in fixed beds

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Abstract—An approach based upon Bayes Theorem has been developed to resolve two major difficulties encountered in earlier experimental investigations concerned with the estimation of parameters for heat transfer in fixed beds. The first difficulty is in obtaining estimates of the Nusselt and Peclet groups with appropriate confidence intervals, and the second is the considerable variation found in the Peclet and Nusselt groups in the range of intermediate Reynolds number. In a new experimental investigation it has been found that estimates of the Peclet and Nusselt groups could be changed in a correlated way without changing the variance of experimental error about the theoretical values, an interaction that precluded the accurate estimation of either parameter. The Bayesian approach identified a confidence region linking the Nusselt and Peclet groups from earlier work, and a confidence region for the two parameters obtained in the new investigation; the best estimates were obtained where the two confidence regions overlapped. In the final presentation the parameter values and independent estimates of parameter accuracy were found to be consistent with correlations established on the basis of earlier work, but with greatly improved confidence regions for the Nusselt and Peclet groups expressed as functions of Reynolds number.

INTRODUCTION

THE PREDICTION of heat transfer in packed beds of gas–solid systems is a topic of continuing interest to chemical engineers, as it is an important factor for the modelling and operation of fixed bed processes. Many experiments have been carried out for the purpose of estimating the parameters in a model of known mathematical form (Littman *et al.* [1], Littman and Sliva [2], Gunn and de Souza [3], Gunn [4] and Dixon and Cresswell [5]). Several models have been proposed for the description of the phenomena of heat transfer in packed beds under steady and unsteady state conditions. They may be categorised as single and two phase models. It is important to select the appropriate model to ensure the reliability of the heat transfer parameters obtained and to carry out statistical tests on the model to test for its validity. According to Gunn [6] there are three principal criteria that should be met in a satisfactory model; they are as follows:

1. The first is that the form of the experimental response should be satisfactorily represented by the theoretical response according to statistical tests designed to examine the validity of models such as the variance ratio test (i.e. F test) and the Chi^2 test.

2. The second criterion is that the parameters of the model found from a set of different experiments should be physically consistent from one experiment to another.

3. The third criterion is that the parameters of the model should depend upon the physical properties of the fluid and solid in a manner that is consistent with the established laws of fluid mechanics and heat transfer.

A major criticism of much of the experimental work on heat transfer is that only rarely have statistical techniques of model validation been employed (Narayanan [7] and Sabri [8]). There are a small number of experimental reports on heat transfer and of this small number most authors have reported transport parameters for a preferred model without subjecting their experiments to error analysis to examine the distribution of residual errors.

In one-phase models the bed is approximated by a homogeneous medium (Damkohler [9], Yagi *et al.* [10], and Vortmeyer and Schaefer [11]). In two-phase models both phases exchange heat and interphase transport processes are accounted for separately (Schumann [12], Littman *et al.* [1], Littman and Sliva [2], and Gunn and de Souza [3]).

Although single phase models are relatively simple in form they cannot include heat transfer between particle and fluid (Yagi *et al.* [10]). The solid and the fluid temperatures are assumed to be the same even though there are differences between the temperatures when a reaction of significant thermicity takes place in the porous interior or at the surface of the particles. Although homogeneous models reduce the complexity of the computations, the transport and reaction parameters within the models effectively lump contributions from intraparticle and fluid particle processes into the parameter values. Thus, in effect, transport and kinetic coefficients in single-phase models are empirical, and can only be related to more fundamental properties by reference to other more realistic models.

Two-phase models are thus more realistic and more satisfactory in representing two-phase behaviour. Three basic types may be defined according to whether

NOMENCLATURE

c	specific heat of fluid [J kg^{-1} K^{-1}]
C_p	specific heat of solid [J kg^{-1} K^{-1}]
d	diameter of particle [m]
D_L	axial thermal dispersion [W m^{-1} K^{-1}]
e	porosity
h	heat transfer coefficient [W m^{-2} K^{-1}]
K_f	heat capacity of fluid [J m^{-3} K^{-1}]
K_s	heat capacity of solid [J m^{-3} K^{-1}]
q_c	rate of heat transfer/unit volume of solid [W m^{-3}]
r	particle radial coordinate [m]
R	radius of particle [m]
T	temperature of fluid [K]
T_p	temperature of particle [K]
t	time [s]
V	superficial velocity [m s^{-1}]
Z	bed axial coordinate [m].

Greek symbols

λ	thermal conductivity of fluid [W m^{-1} K^{-1}]
μ	viscosity of fluid [kg m^{-1} s^{-1}]
ρ	density of fluid [kg m^{-3}].

Dimensionless groups

N	Nusselt group, hd/λ
Pe	Peclet group, $VK_f d/D_L$
Pe_f	defined following equation (11)
Pr	Prandtl group, $K_f\mu/(\lambda p)$
Re	Reynolds group, $dV\rho/\mu$.

axial dispersion is related to temperature gradients in the solid phase, fluid phase or both phases. Littman *et al.* [1] included dispersion terms in both the solid and the fluid-phase equations. There is a problem in separating the two dispersion terms as they are interconnected. In this model known as the continuous-solid phase model (Wakao and Kaguei [13]) the particle phase is regarded as continuous. However, this model may not depict satisfactorily the phenomena of heat transfer in packed beds because intraparticle temperature and concentration distributions have not been included. The model is not suitable for beds with particles of significant size if intraparticle concentration or temperature gradients are significant although it can be useful if intraparticle gradients are not important (Vortmeyer and Berninger [14]). Littman and Sliva [2] proposed a two-phase model which only included dispersion in the solid phase and is thus suitable for low flow rates where intraparticle effects are not significant.

The fluid-phase dispersion model has been widely used for the analysis of unsteady state heat transfer in packed beds (Gunn and de Souza [3]). In this model, the total dispersion is attributed to the fluid-phase and the temperature distribution within the solid phase is considered. This model provides a satisfactory description of the heat transfer process in packed beds that contain particles of considerable size that cannot be considered isothermal. Intraparticle effects have not been accounted for in two-phase models except the fluid-phase dispersion model. Gunn [6] has also shown that the fluid-phase dispersion model satisfies the three principal criteria for a satisfactory model.

Several workers have employed dynamic analysis for parameter estimation (Littman *et al.* [1], Goss and Turner [15], Turner and Otten [16], Gunn and de Souza [3] and Narayanan [7]). Of the usual techniques for dynamic response, analysis of a step change, of a pulse change, and of a periodic change are experimentally convenient, and of these, pulse response analysis, although not as sensitive as frequency response is convenient and accurate when analysed by sensitive and responsive instrumentation.

Most of the experimental investigations into dynamic response have been carried out on packed beds of spheres with estimation procedures concerned with final point estimates of the heat transfer parameters. The parameter estimation procedures which have been followed for functions which are linear in the parameters, were usually aimed at achieving a point estimate by applying a least squares optimisation method. Sensitivity analyses were then carried out at the optimum to calculate the variance–covariance matrix, from which the accuracy of the estimate can be evaluated (Davies and Goldsmith [17]). This procedure is strictly justified only when the model equations are linear in the parameters. For non-linear systems Draper and Smith [18] pointed out the importance of good starting values to enable an iterative technique to converge to the optimal condition. Thus, if there are several local minima besides the global minimum, poor starting values may result in convergence to a point possessing a high variance. They pointed out that available knowledge should be utilised in order to achieve good starting values and suggested carrying out a grid search in order to select starting points which would allow the solution to converge.

The question of determining a confidence interval for the final estimate is important. The suitability of the experiments for optimising the parameters has sometimes not been taken into consideration. It should be emphasised that unless point estimates are accompanied by an estimate of their accuracy they are of little use. Sabri [8] applied the linearisation procedure to a steady state heat transfer model in estimating the axial and radial dispersion coefficients and wall heat transfer coefficient. The principal elements of the variance–covariance matrix gave the standard errors for the parameters, and a wide variation in standard errors for the same parameters was found in different experiments.

From previous work which was carried out we may conclude that:

1. It is important to select the appropriate model to ensure the reliability of the heat transfer parameters obtained and to carry out statistical tests on the model to test for its validity.
2. Intraparticle effects should be included as they can play an important role in the heat transfer process.
3. Estimation procedures of earlier workers have been mainly concerned with obtaining final point estimates of the heat transfer parameters. None of the work related the final estimates to prior information as suggested by Bayes' Theorem, a possible way of providing more comprehensive parameter estimates by using other information.

There are two difficulties which are encountered in parameter estimation problems. The first is the sensitivity of the experiment to the parameters. Gunn *et al.* [19] measured radial temperature distributions when air passed through a fixed bed heated at the wall. The inclusion of the axial dispersion coefficient in the model provided good agreement between the theoretical and experimental temperature profiles when radial transport parameters were obtained, even though tests showed that the sensitivity of the model to the axial dispersion term was low. Transient experiments without radial gradients gave a much better estimate of the axial dispersion term (Gunn and de Souza [3] and Dhingra *et al.* [20]).

The second difficulty is interaction between parameters. In dynamic response experiments axial dispersion of heat dominates at low Reynolds numbers (Gunn and de Souza [3], and Narayanan [7]) and thus the experiment is insensitive to the particle fluid heat transfer coefficient. As the Reynolds number increases both axial dispersion and particle fluid transfer affect the heat transfer processes. The interaction between these two parameters appeared in the form of a scatter when the values of the estimated Peclet and Nusselt groups were plotted against Reynolds number in the range from 1.0 to 300.0 (Gunn and de Souza [3], and Narayanan [7]).

A Bayesian analysis of the dynamic response of a fixed bed of particles to a pulse of heat has been attempted in the estimation of particle thermal conductivity and heat capacity (Gunn and Misbah [21]). Figure 1 shows the dependence of the sum of squares of the experimental temperature deviations from the actual values upon Nusselt and Peclet groups based upon values of the particle thermal capacity and conductivity estimated from the Bayesian Analysis. The banana-shaped contours show cusps and sharp complexities. The function possesses a complex rough surface topology with multiple local minima. The dependence of the sum of squares upon the parameter values shown in Fig. 1 may be described as a fairly shallow region in which several minima lie, surrounded by regions in which the sum of squares increases sharply. Model validation tests such as the F ratio test indicate that if the model is valid at the minimum then the entire shallow region is a region of model validity in that the test gives a high probability that the model is valid without significant variation in the entire region. A variation of the order of 10% in the sum of squares does not affect the validity of the model, and we refer to this region as the 'indifference region'.

Therefore in view of the complexity of the topology of the surface a parameter estimation procedure that terminates in the indifference region is satisfactory. There is no significant statistical basis for dis-

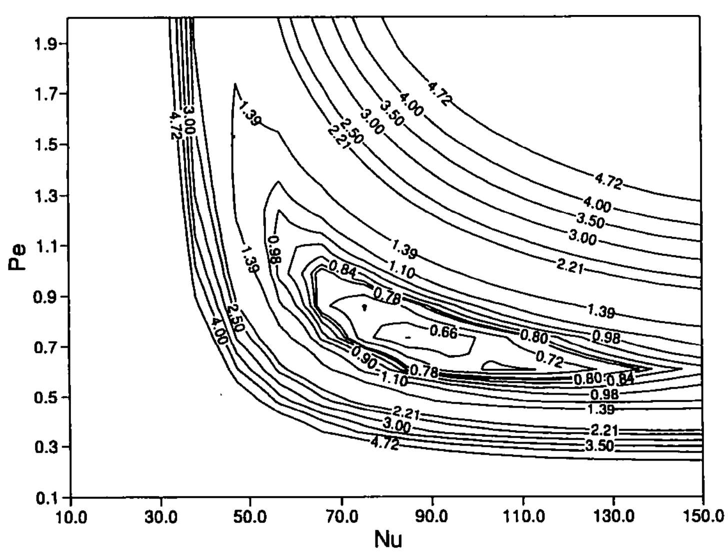

FIG. 1. Contours of the S.S. × 10^{-7} for glass spheres at $Re = 263$.

criminating amongst the different minima in this region.

The purpose of this paper is to extend the Bayesian method to provide estimates of parameter accuracy for the Nusselt and Peclet groups characterising fixed bed transport processes, and in particular to resolve a major and difficult interaction between these two parameters. The resolution of this interaction is found to comprise transport relationships established previously, as well as the present experiments, and to explain the wide variation of these two parameters in the range of intermediate Reynolds numbers found in earlier work.

DESCRIPTION OF EXPERIMENTAL EQUIPMENT

Dynamic methods have been frequently used in experimental investigations into heat transfer characteristics of packed beds mainly because a wider range of transport modes are stimulated in an experiment, and response to a wide range of impressed functions can be measured. Of the usual techniques for dynamic response, analysis to a step change, a pulse change and a periodic change are often used.

In this study a series of experiments into the dynamics of pulse response of beds of spherical particles was examined. A flow diagram for the experimental equipment is shown on Fig. 2. The experimental set-up consisted of the flow control systems, the tracer input system and the tracer detection system. The flow system comprised the air supply, the experimental column and inlet section, and the packing materials which were glass ballotini spheres. Two sizes of spheres were examined in the experiments: 0.5 and 6.0 mm in diameter. The tracer input system comprised the pulse generator and a grid heater, while the tracer detection system consisted of the temperature sensors, the resistance bridges and a recorder. Air flowing through the packed bed was metered by one of the rotameters which had a total capacity in the range 1–370 l min^{-1}. The air from the flow meters was first passed through an inlet section, which housed three inlet sensors to be described later. The inlet section was made of tufnol and was packed with 2 mm glass spheres to act as a distributor. Experimental columns were made of perspex of internal diameter 89 mm and lengths of 50 and 80 mm. The columns were held between tufnol flanges by means of tie rods. The pulse heat input was generated by a thyristor circuit and a grid heater. The grid heater consisted of 200 strands of 0.025 mm diameter tungsten wire, each 5 cm long, attached to two conducting supports, one of which was connected to a taut spring to allow for expansion of wires on heating. The voltage supplied to the heater was constant and was controlled by a timing circuit.

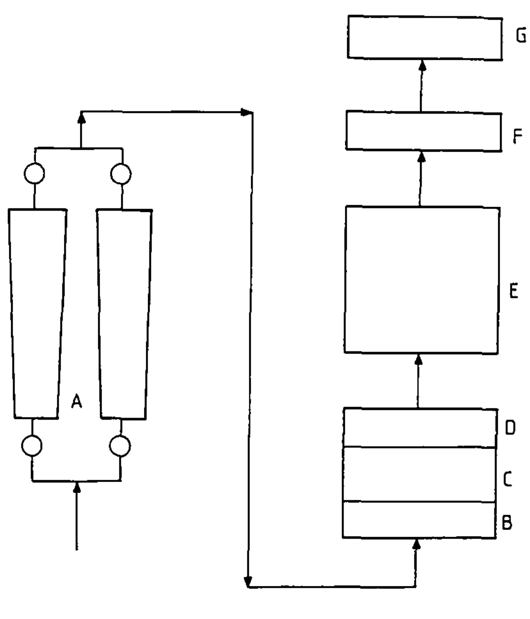

FIG. 2. Block diagram of experimental set-up.

The tracer detection system consisted of four temperature sensing elements, two resistance bridge networks and a recorder. Three of the sensors were placed in the inlet section so that the entire exit gas flow from the rotameters passed over them. The inlet sensors were mounted on rectangular tufnol frames and housed in the inlet section. Two of the inlet sensors were placed in a resistive bridge which was connected to a recorder and gave an output indication of the integrity of the instrument system. The third input sensor, carefully balanced with the outlet sensor was placed in a second bridge. The signal from the second bridge, due to the out of balance voltage generated by changes in gas temperature, was passed into an inbuilt amplifier in the two channel recorder (Tekman model 800). All sensors were made of tungsten wire 0.025 mm diameter and wound over rectangular tufnol frames 30 mm × 10 mm. The four sensors were wound to resistances of 36.8, 36.7, 37.6 and 37.4 Ω and placed in the resistance bridges that were balanced by highly stable standard resistances of 50 Ω (3 ppm $°\text{C}^{-1}$) when no heat was applied to the grid heater.

The experimental scheme was set to obtain two sets of responses for beds 50 mm and 80 mm in length. To determine an accurate temperature distribution from the experiment it was necessary to correct for the end effects of the bed, effects due to the inlet section and output detection. The correction was incorporated in the experimental results by using two lengths of bed, each chosen to give a response that could be measured accurately for different particle sizes and flow rates. When a steady base line was attained, a temperature pulse was imposed upon a steady gas flow metered to the experimental bed by passing a current through the

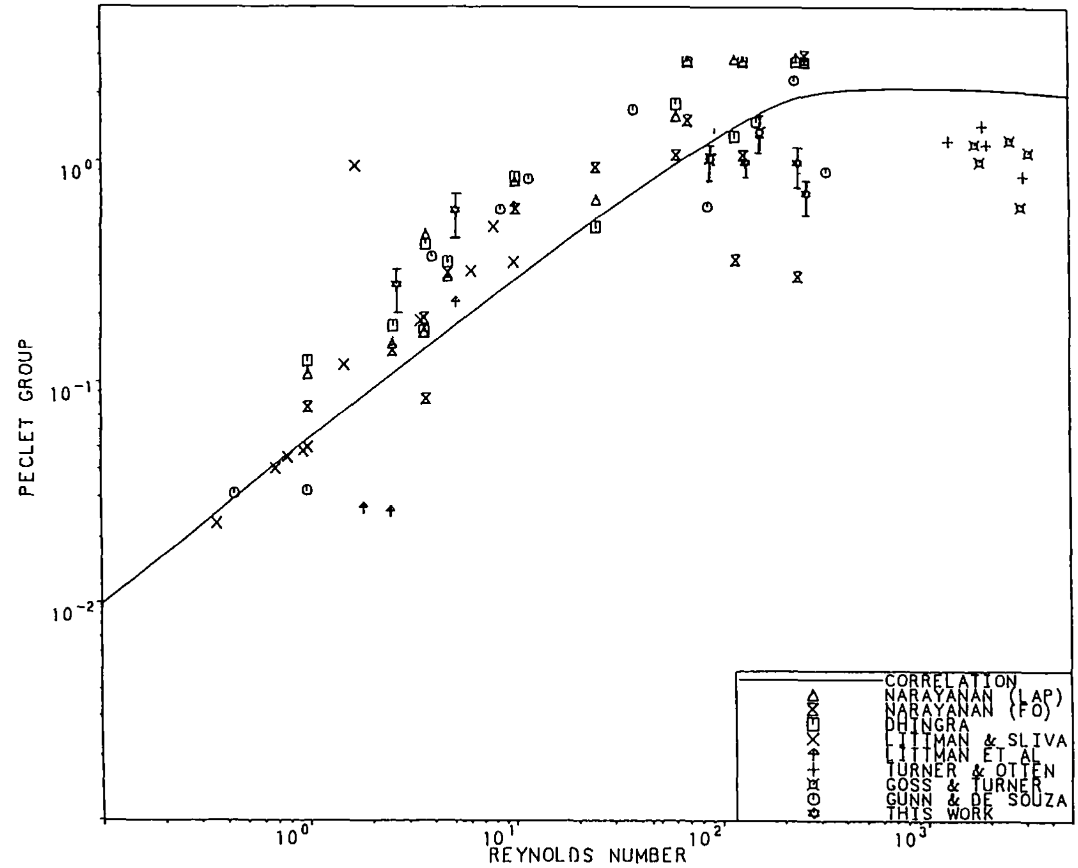

FIG. 3. Peclet groups reported in various studies.

grid heater for a measured period of 30 s. The out of balance voltage generated by the increase in gas temperature was fed to a two channel recorder of 100 μV full scale maximum sensitivity.

The response measured for the 50 mm bed, represented the input pulse, and the response measured for the 80 mm bed represented the output pulse for a bed of length equal to the difference, i.e. 30 mm in length.

THEORY

The fluid-phase dispersion model

The fluid-phase dispersion model has been widely used for the analysis of unsteady state heat transfer in packed beds, Gunn and de Souza [3] and Dhingra *et al.* [20]. In this model, the total dispersive flow assumed proportional to the fluid-phase temperature gradient and the temperature distribution within the solid particle is considered. The partial differential equations describing this model are as follows:

For the fluid phase

$$D_L \frac{\partial^2 T}{\partial Z^2} - K_f V \frac{\partial T}{\partial Z} - K_f \frac{\partial T}{\partial t} - q_c \frac{(1-e)}{e} = 0 \quad (1)$$

subject to the boundary conditions

$$VT_o = VT - \frac{D_L}{K_f} \frac{\partial T}{\partial Z} \quad \text{at } Z = 0 \quad (2)$$

and

$$\frac{\partial T}{\partial Z} = 0 \quad \text{at } Z = l. \quad (3)$$

For the solid phase,

$$\frac{\partial T_p}{\partial t} = \frac{\lambda}{K_s} \left[\frac{\partial^2 T_p}{\partial r} + \frac{2}{r} \frac{\partial T_p}{\partial r} \right]. \quad (4)$$

The fixed bed equation is linked to the particle equation by the boundary condition

$$\lambda \left(\frac{\partial T}{\partial n} \right) = h(T - T_p) \quad \text{at the surface of heat transfer} \quad (5)$$

where n is the inward directed normal at the particle surface.

The form of the differential equation allows any convenient temperature datum to be chosen.

The partial differential equations were solved by applying a finite difference method, the Alternating Phase Implicit Method which was developed by Dhingra *et al.* [20]. These workers employed the basic idea of the ADI method (Peaceman and Rachford [22])

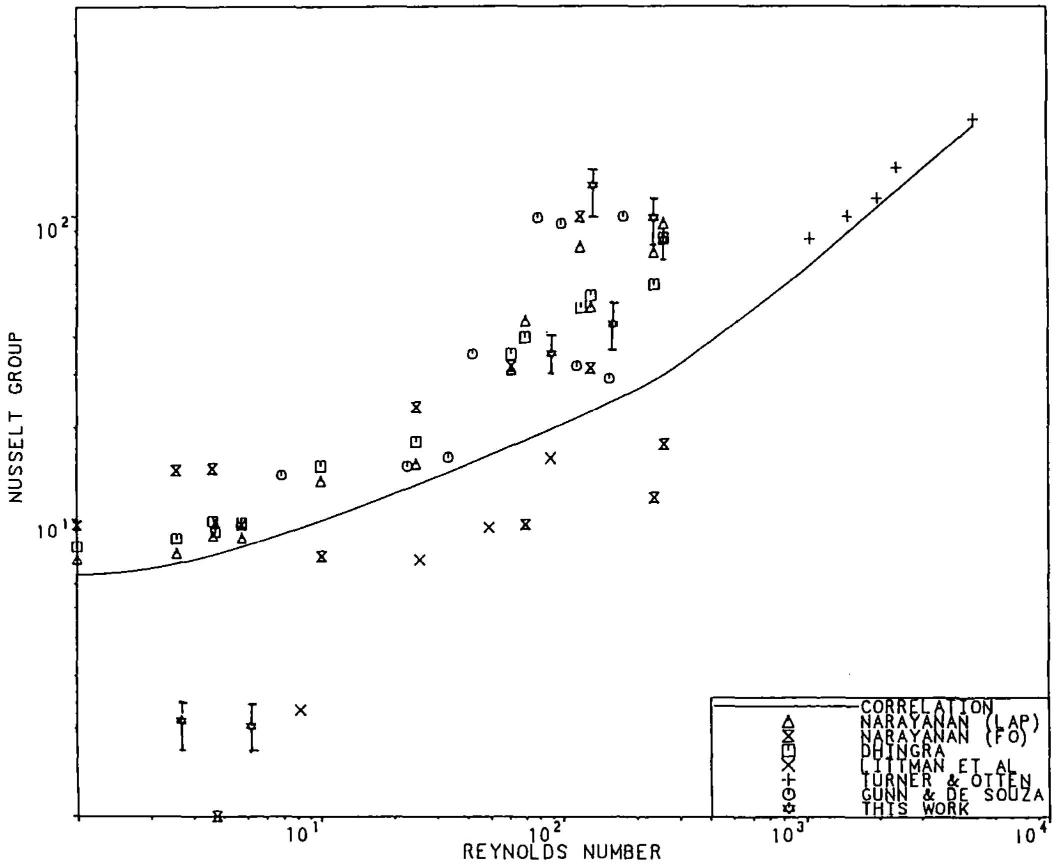

FIG. 4. Nusselt groups reported in various studies.

for solving two equations, bed and particle in the fluid phase dispersion model. They developed a scheme to alternate an implicit–explicit formulation between two phases. For a fixed bed packed with spherical particles the alternation was between axial coordinates for the bed, and the coordinate of radial symmetry for the spherical particles. This discretization technique is stable for all Δt but requires merely the solution of several tridiagonal equation sets for each time step movement. The method consists of representing one of the second order space derivatives fully implicitly and others explicitly then solving to the new time level (t_{j+1}). When the set of tridiagonal equations has been solved, the t_j level is deleted and then the t_{j+2} time level is calculated from the t_{j+1} values. The implicit–explicit representation is then reversed for the following new time step (t_{j+3}). The algorithm developed was as follows:

1. Explicit bed equation
2. Implicit particle equation
3. Explicit particle equation
4. Implicit bed equation.

The alternation in coordinates to represent derivatives explicitly or implicitly is necessary in order to ensure stability of the computations. Central differences were used to expand the space derivatives and a forward difference representation was used for the time derivatives. In the tridiagonal equation set, each equation has exactly three unknowns in a particular order except for the first and last equations which have exactly two unknowns. A direct elimination method that utilises the banded nature of the matrix is applied to obtain the solution.

Bayes Theorem and its application

In Bayes Theorem (Bard [23]), the posterior probability density of a parameter θ, $P^*(\theta)$ is related to the prior probability density $P_o(\theta)$ by the likelihood function L

$$P^*(\theta) \propto L(\theta)P_o(\theta). \tag{6}$$

The likelihood is a function of θ and ψ is the true parameter value. It may be described as follows:

$$Y = F(X, \theta) + \varepsilon \tag{7}$$

where Y is the vector of dependent variables, θ are the parameters and X is the vector of independent variables.

$$\varepsilon(\theta) = Y - F(X, \theta) \tag{8}$$

where $\varepsilon(\theta)$ is the difference between the observed and

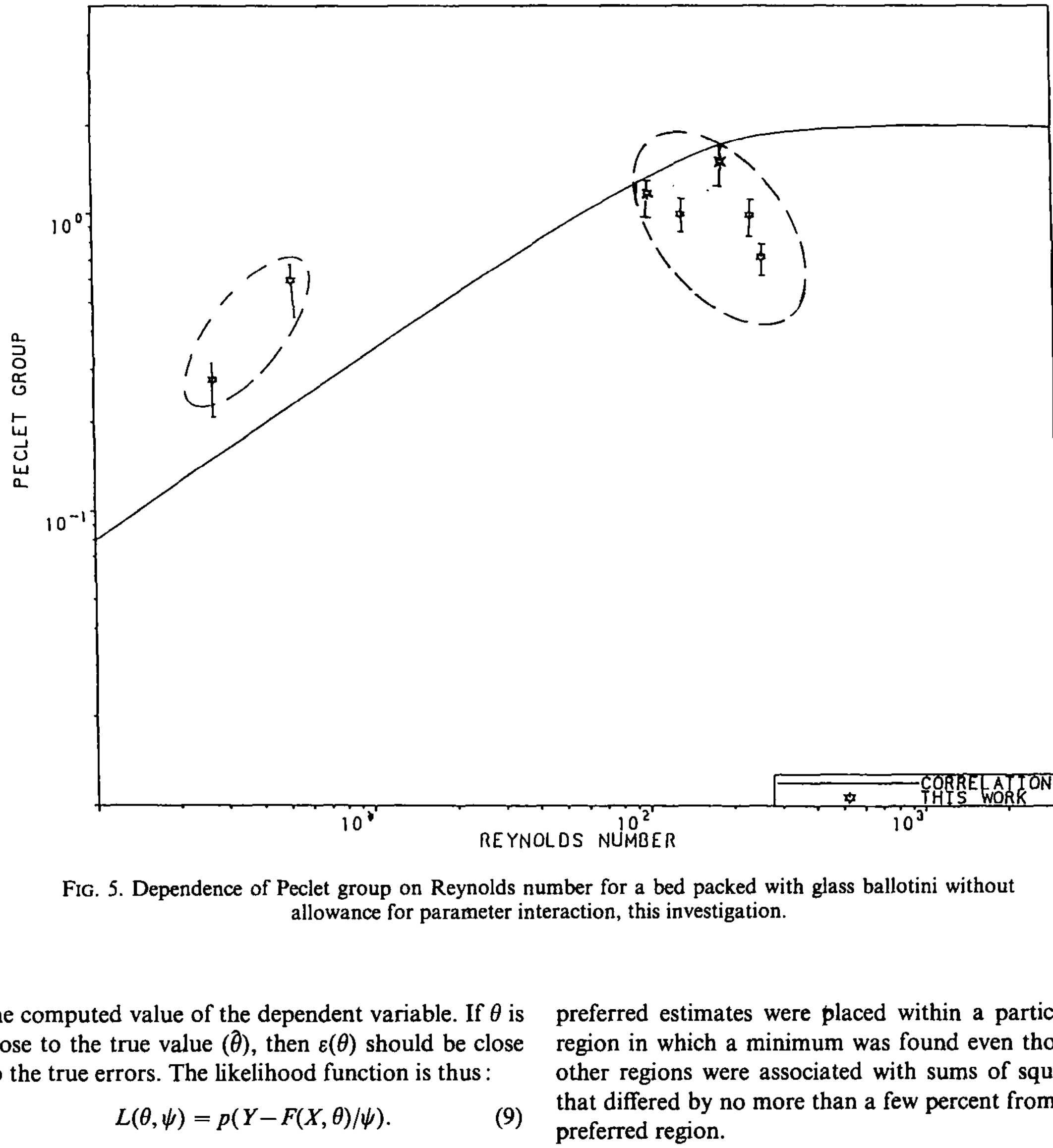

FIG. 5. Dependence of Peclet group on Reynolds number for a bed packed with glass ballotini without allowance for parameter interaction, this investigation.

the computed value of the dependent variable. If θ is close to the true value ($\hat{\theta}$), then $\varepsilon(\theta)$ should be close to the true errors. The likelihood function is thus:

$$L(\theta, \psi) = p(Y - F(X, \theta)/\psi). \tag{9}$$

We simply seek to identify properties of the optimisation search that will allow equation (6) to be realised with $L(\theta)$ as the maximum likelihood estimator for $P(\theta)$.

Maximum likelihood is attained by achieving a minimum least squares estimate, under conditions that may reasonably be expected to apply (Bard [23]).

The procedure used for the estimation of parameters was to define the sum of the squares of deviations between experimental and theoretical temperatures, and to use an optimisation routine to minimise the sums of squares by changing the parameter values. Because of the form of the objective function illustrated in Fig. 1, it was found that when the optimisation routine due to Rosenbrock [24] was used when seeking four or more parameters, the final estimates were placed within 'the indifference region' for a range of initial values taken from an estimated prior distribution. When three or less parameters were sought it was found that the procedure was more sensitive to the minima illustrated in Fig. 1, and the preferred estimates were placed within a particular region in which a minimum was found even though other regions were associated with sums of squares that differed by no more than a few percent from the preferred region.

If the initial estimates were taken from a range of values that corresponded to a fairly wide initial choice, the final estimates when four or more parameters were varied possessed the salient properties of Bayesian posterior densities (Gunn and Misbah [21]). This method was extended here to provide estimates for all four parameters, while including a resolution of a particularly difficult parameter interaction.

EXPERIMENTAL RESULTS

The experimental results in the form of the time variation of temperatures from beds of different lengths were fed as input data to a computer program which was developed to estimate the heat transfer parameters. Parameter estimates were obtained by calculating a variance of experimental measurements about predicted values for parameters by applying the criterion of least squares. The values of the axial dispersion coefficient, heat transfer coefficient, thermal conductivity and heat capacity of solid associated

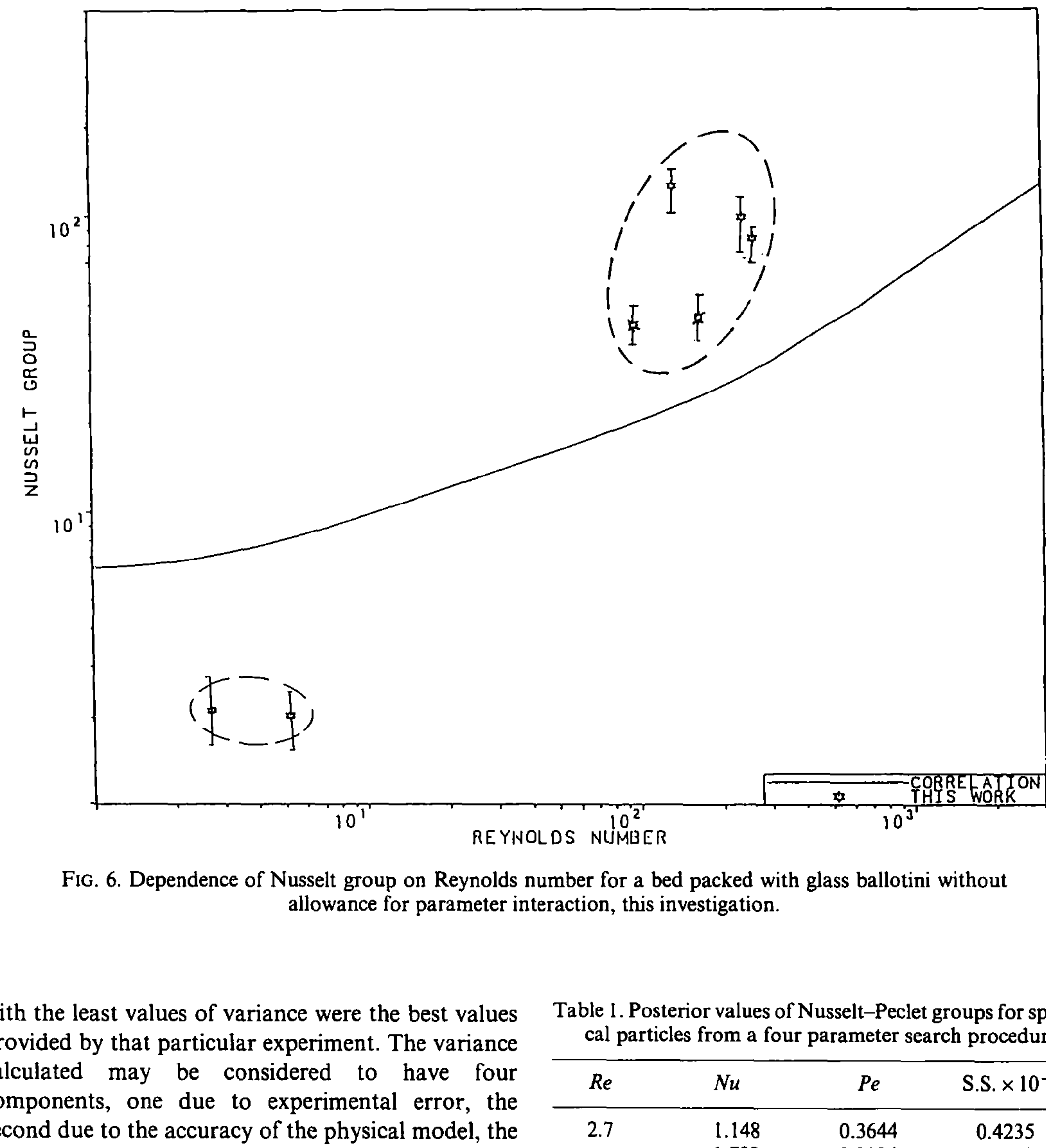

FIG. 6. Dependence of Nusselt group on Reynolds number for a bed packed with glass ballotini without allowance for parameter interaction, this investigation.

with the least values of variance were the best values provided by that particular experiment. The variance calculated may be considered to have four components, one due to experimental error, the second due to the accuracy of the physical model, the third due to the minimisation routine applied, and the fourth due to the numerical error. It was shown that the variance could be mostly described by the experimental error, that the contribution of the minimisation routine and numerical error could be neglected, and that the model gave a good description of the experimental results (Misbah [25]).

When the optimisation procedure was carried out over the range of the prior density it became apparent that the posterior densities so obtained gave realistic estimates of the accuracy of the parameter estimates and the ratio of the standard deviation of the posterior to prior densities reflected the accuracy of that experiment for that parameter.

THE AXIAL DISPERSION COEFFICIENT AND HEAT TRANSFER COEFFICIENT AND THE RESOLUTION OF THE PARAMETER INTERACTION

The axial dispersion coefficients and heat transfer coefficients for the spherical particles were expressed

Table 1. Posterior values of Nusselt–Peclet groups for spherical particles from a four parameter search procedure

Re	*Nu*	*Pe*	S.S. $\times 10^{-7}$
2.7	1.148	0.3644	0.4235
	1.739	0.3134	0.4252
	2.289	0.2621	0.4416
	2.295	0.256	0.4482
	1.452	0.3332	0.4242
	2.355	0.2349	0.4556
	3.393	0.1968	0.494
	2.343	0.26	0.4925
91	25.19	2.301	0.6754
	34.48	1.457	0.67476
	38.5	1.369	0.67592
	44.19	1.217	0.67926
	31.61	1.667	0.67376
	39.17	1.328	0.67659
	37.06	1.387	0.67559
	37.42	1.368	0.67584
	29.88	1.802	0.67378
240	74.81	1.221	0.9261
	93.89	0.9605	0.9023
	114.9	0.8804	0.8969
	129.7	0.8662	0.8937
	110.5	0.9134	0.8979
	102.3	0.9341	0.8995
	94.68	0.9593	0.9018
	75.62	1.218	0.9243

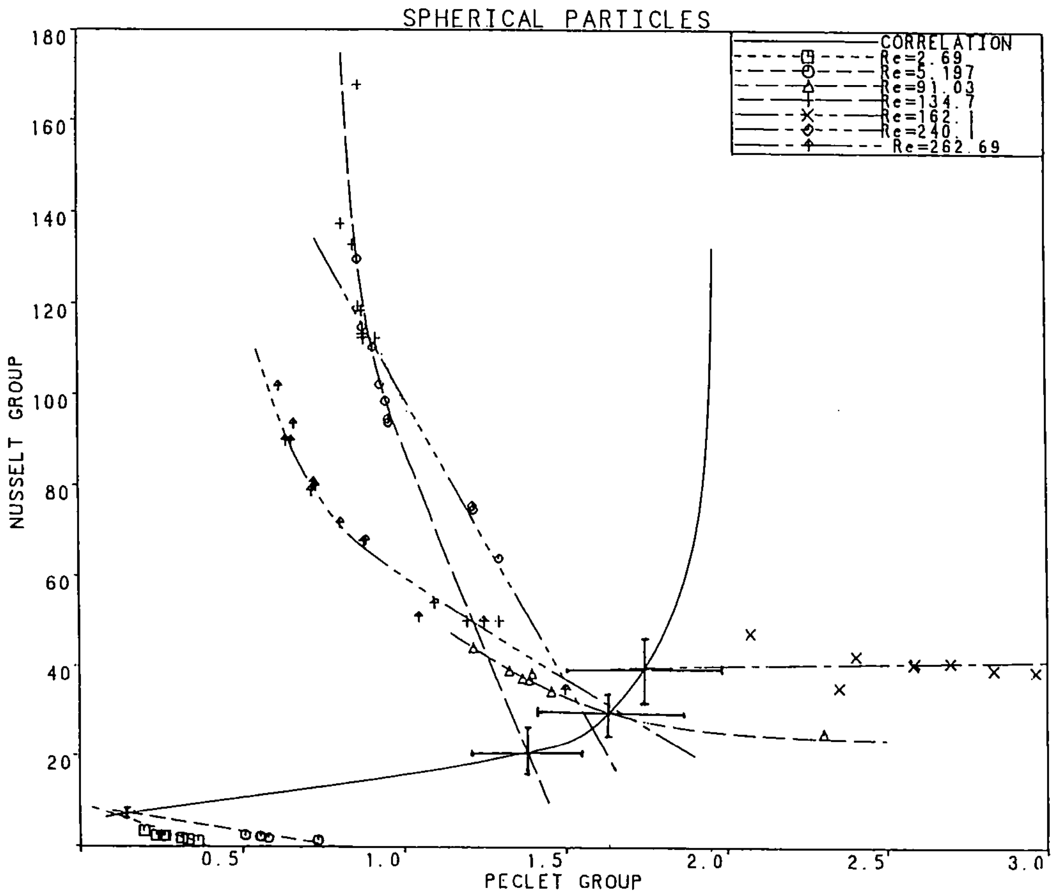

FIG. 7. Peclet–Nusselt groups for packed bed of glass ballotini showing trajectories.

in terms of the dimensionless groups Peclet and Nusselt. On completing the parameter search on the heat capacity and the thermal conductivity for spherical particles, their mean values were calculated from the Bayesian procedure (Gunn and Misbah [21]) and the parameter optimisation procedure was carried out for estimating Nusselt and Peclet groups.

The experimental work on the glass spheres covered a range of Reynolds number from 2.7 to 263. Consistent results were obtained by following the Bayesian approach in the parameter estimation procedures as only estimates which were located in the indifference region were considered. Thus both the Peclet and Nusselt groups and their corresponding standard deviations were quantified.

The calculated values of the Peclet and Nusselt groups were plotted against Reynolds number in Figs. (3) and (4) where they are compared with estimates from other work, Littman *et al.* [1], Littman and Sliva [2], Goss and Turner [15], Turner and Otten [16], Gunn and de Souza [3], Gunn *et al.* [26] and Vortmeyer and Adam [27]. The solid curves plotted in these figures are the representation of the equations proposed by Gunn and Vortmeyer [28] and Gunn [4] for the calculation of Peclet and Nusselt groups.

Gunn and Vortmeyer combined the effect of both conduction and convection in the calculation of the dispersion coefficient

$$\frac{1}{Pe} = \frac{1}{Pe_f} + \frac{\lambda_o}{\lambda \, Re \, Pr}. \tag{10}$$

Equation (10) represents the summation of a low Reynolds Number asymptote, $\lambda_o/(\lambda \, Re \, Pr)$ and a high Reynolds Number asymptote $1/Pe_f$. The value of λ_o/λ depends upon the fluid and particle thermal conductivities only and values are given by Gunn and Vortmeyer. The group Pe_f depends only upon particle Reynolds number for a given bed. For beds of spheres Pe_f may be expressed (Gunn [6]),

$$Pe_f = \frac{2p}{1-p}, \quad \text{with } p = 0.17 + 0.33\exp(-24/Re).$$

The low Reynolds number asymptote is based upon steady state measurements such as those of Vortmeyer and Adam [27] and earlier workers, and upon dynamic experiments at very low Reynolds number such as those of Gunn and de Souza [3]. The particle fluid heat transfer coefficient in the fluid-phase dispersion model is not stimulated at steady state, while at low Reynolds number the transfer of heat from particle to fluid in dynamic response is so slow that

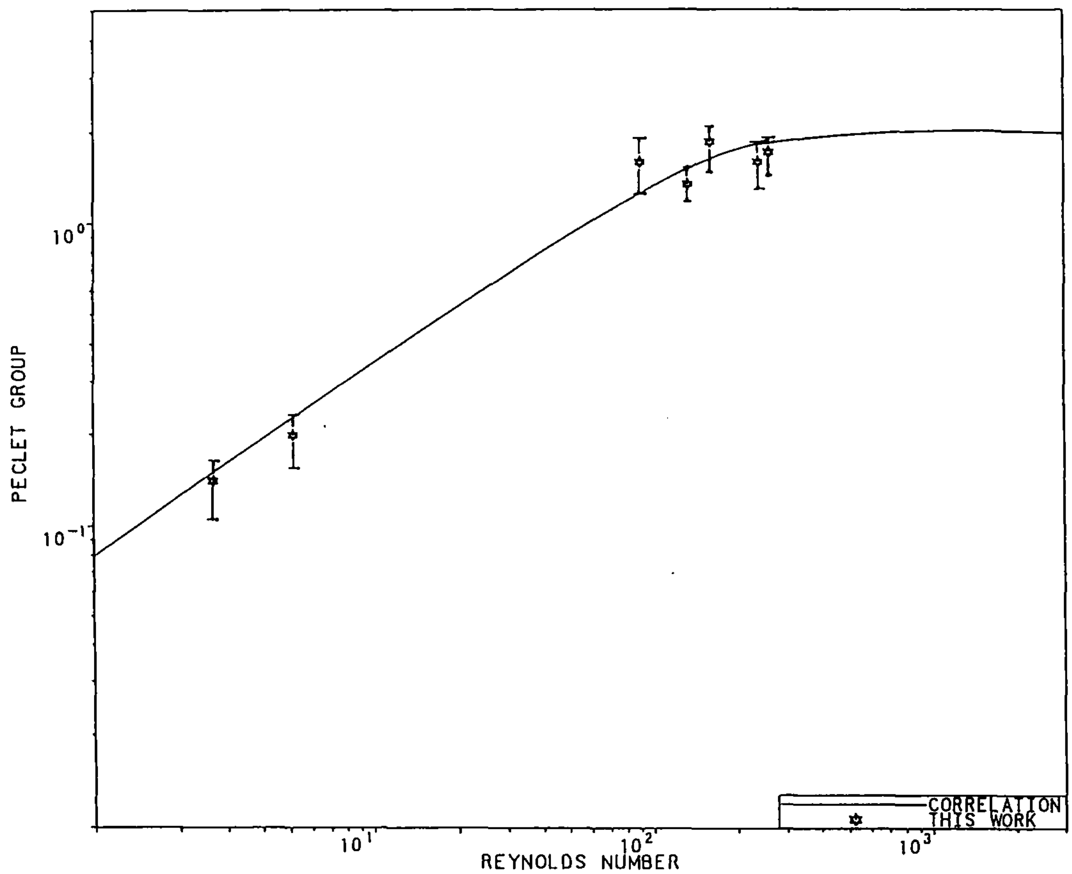

FIG. 8. Dependence of Peclet group on Reynolds number when parameter interaction has been accounted for.

the response is affected only by the coefficient of axial dispersion.

The high Reynolds number asymptote $1/Pe_r$ is mainly determined by measurements of *mass* dispersion in beds of impermeable particles.

Thus, although equation (10) has been used to describe experimental results from experiments similar to those described in this paper, the substantial basis of equation (10) is founded upon different types of experiment.

The equation presented by Gunn [4] for the prediction of the dependence of Nusselt group upon Reynolds number is

$$Nu = (7-10e+5e^2)(1+0.7\,Re^{0.2}Pr^{1/3}) + (1.33-2.4e+1.2e^2)Re^{0.7}Pr^{1/3}. \quad (11)$$

Equation (11) is based upon a low Reynolds Number asymptote of 4.0 found by analysis of two-dimensional heat transfer between fluid and enveloping surfaces and a large Reynolds number asymptote that represents steady state measurements of heat transfer such as those of Denton [29] and many others. The models of this period did not include axial dispersion but since the effect of axial dispersion at high Reynolds number is small (Gunn and de Souza [3]) the calculations of heat transfer coefficient were not affected. Equation (11) also describes the experimental values of mass transfer coefficient by means of the analogy between heat and mass transfer. Equation (11) is therefore founded on experiments and theory that differ from experiments of the type described in this study.

Figure 3 shows the dependence of the experimental Peclet groups reported by several workers upon the Reynolds groups; it covers a range of Reynolds numbers from 0.06 to 4600. The scatter in the Peclet group is clear for Reynolds numbers between 1.0 and 300. Although experiments at low Reynolds number are difficult because of the increased environmental variability, the effect of the heat transfer becomes negligible at Reynolds number less than 1.0. At low Reynolds number (Gunn and de Souza [3]) thermal dispersion dominates and the effect of the fluid particle heat transfer may be neglected. Thus the scatter of the Peclet group at low Reynolds number is reduced.

In the intermediate range of Reynolds number the scatter of the Nusselt and Peclet groups is significant. This scatter could be attributed to the type of dynamic

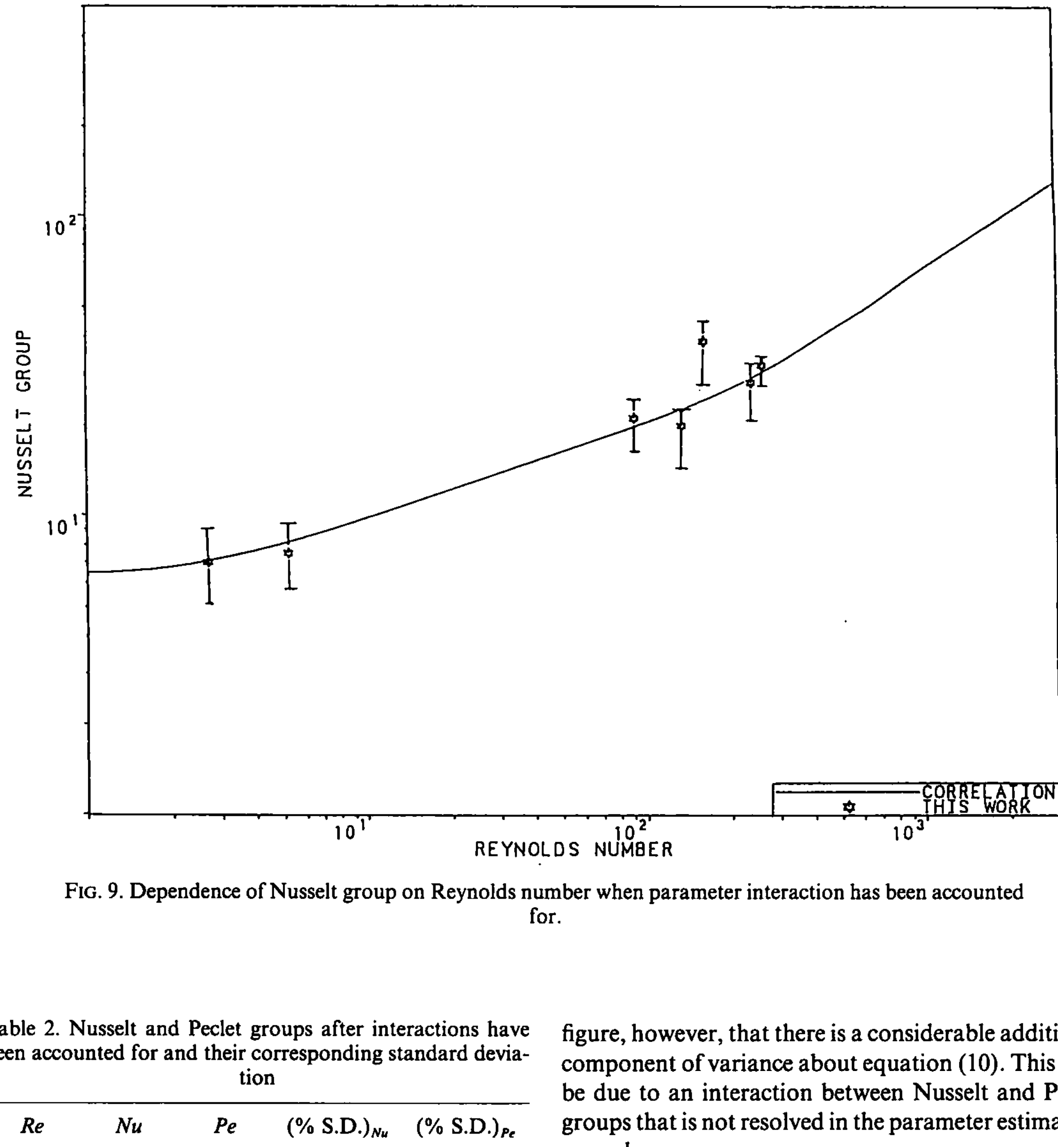

FIG. 9. Dependence of Nusselt group on Reynolds number when parameter interaction has been accounted for.

Table 2. Nusselt and Peclet groups after interactions have been accounted for and their corresponding standard deviation

Re	*Nu*	*Pe*	(% S.D.)$_{Nu}$	(% S.D.)$_{Pe}$
2.7	6.8	0.14	29.2	22.4
5.2	7.3	0.15	24.8	16.2
91.0	29.0	1.7	22.4	14.0
134.7	20.0	1.40	17.19	4.8
162.0	39.0	1.75	24.3	11.5
240.0	22.0	1.65	23.3	13.3
262.7	31.5	1.82	12.0	13.9

experiments carried out, the method of parameter estimation (whether accurate estimates were obtained or not), the deviation which is inherent in each experiment (for example, the repacking of particles in the bed is accompanied by a standard deviation ± 10–15%, Gunn and Pryce [30]) and finally parameter interaction.

The standard errors of the Peclet group estimated from the posterior distribution are shown as vertical lines for the results of this investigation; the standard errors were found to be almost completely due to the experiments since errors from the numerical analysis were found to be negligible. It is obvious from this figure, however, that there is a considerable additional component of variance about equation (10). This may be due to an interaction between Nusselt and Peclet groups that is not resolved in the parameter estimation procedure.

The corresponding experimental results for the dependence of the Nusselt upon the Reynolds group are shown in Fig. 4. At low Reynolds number only those experimental results taken from analyses that have included the effect of axial dispersion have been considered. The scatter of the Nusselt group at low Reynolds number is expected since axial dispersion dominates. Estimates of parameter error are again included in vertical lines, and as for Fig. 4, there appears to be a considerable additional component of scatter about equation (11). The pattern of interaction between the two groups may be identified by plotting the experimental results of this investigation alone.

Figure 5 shows the experimental estimates of the Peclet group, and Fig. 6 shows the estimates of the Nusselt group.

For Reynolds numbers 2.7 and 5.2 the estimates of the Peclet group are significantly above equation (10), but the corresponding estimates of the Nusselt groups lie significantly below equation (10), while at Reynolds number of 91, 135, 162, 240 and 263, Peclet groups significantly below equation (10) corresponded to Nusselt numbers significantly above equation (11). These regions are identified as ellipses in Figs. 5 and 6. Indeed it appears that the Nusselt and Peclet groups are highly correlated.

In the parameter estimation procedure different initial values of the Nusselt and Peclet groups were selected and subsequently different pairs of Nusselt and Peclet groups resulted. Table 1 lists the values of the Nusselt and Peclet groups obtained in the search procedure.

It is clear that these different pairs possess variances that do not differ significantly; the maximum variation is of the order to 10%. The F ratio test showed that a difference of this magnitude is statistically not significant.

Thus unique pairs of Peclet and Nusselt groups cannot be found because of parameter interaction. When a high Nusselt group is estimated a corresponding low value of Peclet group would be obtained and if a low Nusselt group is estimated a high Peclet group is obtained. This adds a difficulty as single values cannot be selected. Therefore unique *Nu–Pe* pairs are not obtained even though the pairs of values at each flow rate are all associated with similar values of variances.

To resolve this interaction a Bayesian approach was adopted. This was done by combining the parameter values obtained from the experiments with the previous values reported in the literature to achieve a *Nu–Pe* pair which satisfied all the information present and accounted for the interaction. The different sets of the Nusselt and Peclet pairs obtained from the parameter search were plotted in Fig. 7, where it may be seen that pairs of the two groups lie on individual trajectories for each experiment; and that the experimental variance on the trajectories is approximately constant. It has been established on the basis of a great many investigations of different types, that the dependence of Peclet and Nusselt groups upon Reynolds number may be reasonably predicted by equations (10) and (11).

In the Bayesian interpretation equations (10) and (11) represent prior information.

Both the experimental estimates and the prior information are illustrated in Fig. 7. If the trajectory of the Nusselt and Peclet groups obtained from the experiments is to be compatible with previous investigations both curves should intersect. The intersection is the point at which both the experimental analysis and prior information obtained from other investigations are satisfied—a Bayesian approach.

The same behaviour was found for all flow rates examined in this series of experiments. The *Nu–Pe* trajectory for the seven flow rates examined are shown in Fig. 7, together with the confidence region obtained from the intersection of the trajectories. The full line on this figure corresponds to equations (10) and (11) and the confidence region for four flow rates has been indicated by the confidence limits for each parameter. The points which were obtained from the intersection of the *Nu–Pe* trajectories with the derived relationships are plotted against Reynolds numbers in Figs. 8 and 9; for each point the standard error estimated for the posterior probability density is shown. From these figures it is clear that the *Nu–Pe* groups which were obtained from the joint confidence region are close to the values calculated from equations (10) and (11), both based upon the results of several other investigations.

The individual estimates of the parameter values and their standard errors are shown in Fig. 8 for the Peclet group and in Fig. 9 for the Nusselt group as functions of Reynolds number. It may be observed that the greater proportions of points in each figure lie within a standard deviation of the respective correlating relationships, equations (10) and (11). It should be emphasised that although the correlations have been used to resolve the parameter interaction, the method adopted to resolve the interaction does not consider the experimental points to lie on the previously established correlations since the Reynolds group, the correlating parameter, is not directly expressed in the resolution illustrated in Fig. 7. If the correlations are to describe the results of this investigation it would be expected that some two thirds of the experimental points would lie within a standard deviation of the correlations. This is clearly so in both Figs. 8 and 9, and therefore the experimental estimates of Peclet and Nusselt groups both support, and are supported by, the respective correlations, equations (10) and (11).

Therefore from Figs. 8 and 9, it is clear that the Bayesian approach adopted for the resolution of the interaction problem was successful in providing parameter values, all of which were compatible with the previously derived correlations.

Table 2 lists the values of the Nusselt and Peclet groups which lie in the joint confidence region with their standard deviations calculated from the four parameter optimisation search.

The standard deviations shown agree with the qualitative conclusions from other work and support the Bayesian nature of the search procedure when the number of parameters was four or more.

The effectiveness of the Bayesian method described here may be gauged from a comparison of Fig. 3, a general collection of the results of this investigation without allowance for parameter interaction and of the experimental results of earlier investigations for the Peclet group, with Fig. 8. The departure of the experimental results of this investigation from the correlation of equation (10) has been greatly reduced. Since dynamic experiments of the type described here have been used by earlier workers such as Gunn and Narayanan [31], Littman and Sliva [2] and Turner and Otten [16], it would be expected that the difficulty of parameter interaction between the Nusselt and Peclet groups would also contribute to a scattering of results.

A comparison of the corresponding Figs. 4 and 9 for the dependence of Nusselt number upon Reynolds group gives exactly the same conclusions for the Nusselt group and the correlating equation (11).

The analysis suggests that the scatter in the experimental results of earlier workers is mainly due to parameter interaction between the Nusselt and Peclet groups in the analysis of dynamic, and perhaps sometimes, steady state response. Thus, unless allowance is made for the interaction by a method such as described in this paper, the experimental results will exhibit a scatter that does not reflect the quality of the experiment, just the interaction.

The second benefit of the Bayesian analysis is the estimate of the parameter error for both the Nusselt and Peclet groups found by this calculation of a posterior probability density for the parameter from a prior probability density. In contrast to the linearised variance–covariance analysis the parameter accuracies estimated in this way agree well with experimental and other evidence for the accuracy of these two parameters. As the parameter error can be obtained by a well-defined procedure found to be reliable in this paper, it is possible that the method may be extended to the analysis of other situations in heat and mass transfer.

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