Wall effects characterization for thermal dispersion in porous media: importance of a parsimonious parameterization.

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Abstract. Thermal dispersion in a granular medium results from the combined effects of heat diffusion in both the fluid and solid phases and of thermal conduction in the fluid. These phenomena require some kind of averaging in order to be modelled at the mesoscopic scale. A model using a local mean ‘enthalpic’ temperature and a filtration velocity has been developed previously. A different model that takes into account wall effects is derived here. A sensitivity analysis of the local temperature output shows that some parameters are correlated, and cannot be estimated. So a reduced model with less many parameters is derived and a least square parameter estimation technique based on a Bayesian approach with external a priori information is designed. Experimental results for the estimation of the resulting reduced set of parameters are presented.

1. Introduction
This study concerns heat transfer inside a fixed-bed chemical reactor. In order to maintain an operating process under control, a reliable model is needed. A fixed bed reactor is composed of a granular medium through which a fluid flows: heat transfer is governed by thermal dispersion phenomena (conduction and convection). In practice, the conservation equations of momentum and of thermal energy cannot be solved because the local structure of the material is not precisely known. So modelling is commonly made at the mesoscopic scale. In order to derive a reduced model for heat transfer, techniques such as volume averaging of the local equations can be implemented. This paper briefly presents some of the models resulting from these techniques in the core of the bed and near its wall where local change of porosity modifies the flow as well as
heat transfer [1] [2]. Starting from a first reference homogeneous model, we set up a more pertinent non-homogeneous analytical model to describe the temperature field in the bed and close to its walls. The number of parameters in this model can be controlled by a sensitivity analysis. So this model is finally reduced by replacing the near-wall layer by a specific boundary condition. A second sensitivity analysis allows to distinguish three kinds of parameters in this last model: those that are fixed, those that are freely estimated (initialized to nominal or measured values in a non linear estimation algorithm), and the remaining parameters that are constrained through a Bayesian approach. This method of parsimonious parameterization allows the estimation of the parameters that are looked for.

2. The reference models H1
We consider a one-temperature model [3] : The temperature field in the bed corresponds to an enthalpic averaged temperature $T_H$, defined locally at point P (center of a sphere of diameter D and volume V) :

$$T_H(P, t) = \frac{1}{(\rho Cp)_l V(P, D)} \int_{V(P, D)} (\rho Cp)(P') T(P') dV(P') \quad (1)$$

with $(\rho Cp)_l = \epsilon (\rho Cp)_f + (1-\epsilon) (\rho Cp)_s$.

$\epsilon$ is the average porosity in our granular medium, $(\rho Cp)_f$ and $(\rho Cp)_s$ are respectively the volumetric heat capacities of the fluid and solid phases. This $T_H$ temperature corresponds to a spatial filtering of the local temperature field using volumetric heat capacities as weights. The 2D heat equation can be written as follows for a uniform Darcy velocity $u$ in the $x$ direction in the porous medium :

$$(\rho Cp)_t \frac{\partial T}{\partial t} = \lambda_x \frac{\partial^2 T}{\partial x^2} + \lambda_y \frac{\partial^2 T}{\partial y^2} - (\rho Cp)_f u \frac{\partial T}{\partial x} + s \quad (2)$$

with $T = T_H$ (we drop the subscript now), $s$ a volumetric heat source and $\lambda_x$ and $\lambda_y$ constant dispersion coefficients. If we now consider that the porous bed is limited by an infinite length plane solid wall located at $y=0$ and heated from $x=0$ to $x=l$ with a uniform and constant (in time) surface power $W$ starting at $t=0$, the heat source $s$ can be reported into the boundary and initial conditions that become :

$$-\lambda_y \frac{\partial T}{\partial y} = W(H(x) - H(x-l))H(t) = \varphi_{exc}(x, t) \quad \text{for } y = 0$$

$$T \to 0 \text{ for } x = \pm \infty \quad T \to 0 \text{ for } y = + \infty \quad T = 0 \text{ at } t = 0$$

This equation can be solved through the thermal quadrupoles method. This method uses a Laplace transformation in time and a Fourier transformation for the $x$ coordinate and allows a solution for the two layer models presented in section 3. It can be shown that if $2N$ harmonics are considered in the Fourier transformation, the direct-inverse Fourier transform pair for the temperature is :

$$\tilde{T}_n(y, t) = \int_{-L}^{L} e^{-i\alpha_n x} T(x, y, t) dx \text{ and } T(x, y, t) = \frac{1}{2L} \sum_{N=1}^{N} \tilde{T}_n(y, t) e^{i\alpha_n x} \quad (3)$$
In this expression, $a_n$ is equal to $n^2/2$, with $n$ a natural integer, and $L >> l$ is a large enough characteristic length in the $x$ dimension. Finally the expression for harmonic $\tilde{T}_n(y,t)$ is:

$$
\tilde{T}_n(y,t) = \frac{W}{i\alpha_n \pi \lambda_y(\rho C_p) t} \left( 1 - e^{-i\alpha_n} \right) \int_0^t e^{-(\rho C_p) t^2} e^{-\left( \frac{\lambda_x}{(\rho C_p) t} \right)^2} e^{-\left( \frac{\lambda_y}{(\rho C_p) t} \right)^2} e^{-\left( \frac{\lambda_z}{(\rho C_p) t} \right)^2} t \, dt
$$

Testu [4] set up the following two correlations for the two dispersion coefficients:

$$
\frac{\lambda_x}{\lambda_f} = \frac{\lambda_x}{\lambda_f} + 0.126 Re^{1.45} = \frac{\lambda_x}{\lambda_f} + 0.211 Pe^{1.45} \quad \text{for} \ 12 < Re < 130
$$

$$
\frac{\lambda_y}{\lambda_f} = 6.4 + 0.079 Re = 6.4 + 0.11 Pe \quad \text{for} \ 16 < Re < 130
$$

These correlations have been derived for an air flow of Darcy velocity through a bed of monodisperse spherical beads. Averaging this function over the thickness $\delta$ of the near wall region (with $\delta = d/2$ for example) yields a near wall porosity value $\epsilon'$ as well as a core region value $\epsilon$. Application of Ergun’s equation for pressure drop in these two regions (averaged filtration velocities $u'$ and $u$) allowed Martin to derive a correlation of the form $u'/u = f(Re, \epsilon, \epsilon'/\epsilon)$. It is thus possible to write the heat dispersion equation (2) in the two regions with different sets of total volumetric heat capacities (1) and dispersion coefficients given by Testu’s correlations (4):

| Core region | Near-wall region |
|-------------|------------------|
| $(\rho C_p) \frac{\partial T}{\partial t} = \lambda_x \frac{\partial^2 T}{\partial x^2} + \lambda_y \frac{\partial^2 T}{\partial y^2} - (\rho C_p) f u' \frac{\partial T}{\partial x}$ | $(\rho C_p) \frac{\partial T}{\partial t} = \lambda_x' \frac{\partial^2 T}{\partial x^2} + \lambda_y' \frac{\partial^2 T}{\partial y^2} - (\rho C_p) f u' \frac{\partial T}{\partial x}$ with $-\lambda_y' \frac{\partial T}{\partial y} = \varphi_{exc}(x,t)$ for $y = 0$ |

We have $T \to 0$ for $x = \pm \infty$ and $T = 0$ for $t = 0$

The interface condition is:

$$T(x, \delta^+, t) = T(x, \delta^-, t) \quad \text{and} \quad -\lambda_y' \frac{\partial T}{\partial y}(x, \delta^+, t) = -\lambda_y' \frac{\partial T}{\partial y}(x, \delta^-, t)$$

These two problems can be solved by the quadrupoles method:

$$T(x, y, t) = \frac{1}{2L} \sum_{-N+1}^N \tilde{T}_n(y, t) e^{i\alpha_n x} \quad \text{with} \quad \alpha_n = \frac{n \pi}{L}$$
where $\tilde{T}_n(y,t)$ is the inverse Laplace transform of the $\tilde{T}_n(y,p)$ harmonic:

$$
\tilde{T}_n(y,p) = \frac{1}{\lambda_y k_n} \frac{\lambda'_y k'_n \cosh(k'_n(y-\delta)) - \lambda_y k_n \sinh(k_n(y-\delta))}{\lambda'_y k'_n \cosh(k'_n(\delta)) + \lambda_y k_n \sinh(k_n(\delta))} \frac{W}{\nu \alpha_n} (1 - e^{-i\alpha_n}) \quad \text{for } y \leq \delta
$$

$$
\tilde{T}_n(y,p) = \frac{e^{-k_n(y-\delta)}}{\lambda_y k_n \sinh(k_n(\delta)) + \lambda'_y k'_n \cosh(k'_n(\delta))} \frac{W}{\nu \alpha_n} (1 - e^{-i\alpha_n}) \quad \text{for } y \geq \delta
$$

with $k^2_n = \frac{(\rho C_p)_{\nu}}{\lambda_y} + \frac{\lambda'_y}{\lambda_y} + \frac{i \alpha_n (\rho C_p)_{fu}}{\lambda_y}$ and $k'^2_n = \frac{(\rho C_p)'_{\nu}}{\lambda'_y} + \frac{\lambda'_y}{\lambda'_y} + \frac{i \alpha_n (\rho C_p)'_{nu'}}{\lambda'_y}$.

A simple verification was made for this model, by replacing all the parameters of the near-wall region by the parameters of the core region: this "homogeneous" simulation is then compared to the first model H1: the two models agree perfectly.

Model H2 can be used with a set of parameters derived from the literature.

The difference between the two models (contrast curves) is shown in Figure 1. The heat distribution is slightly different depending on whether the near-wall layer is taken into account or not. But this simulation was made with parameters from the literature: precise parameters values still need to be estimated in order to get a more predictive model.

**Figure 1:** Thermal contrast $T_{H2} - T_{H1}$ between the H1 and H2 models for $\delta = d/2$ ($W = 1000 W.m^{-2}$, $u = 0.325 m.s^{-1}$, $d = 2 mm$)

**Figure 2:** Experimental thermocouples position

Sensitivity analyses implemented for this model show that its parameters are correlated. So a correct estimation of the too-many parameters is not possible, and this model has to be reduced in order to estimate pertinent parameters. This corresponds to an underparametrization. The reduced model is derived from a thickness averaging of the original version of the H2 heat equation over the thickness $\delta$ of the near wall region:

$$
(\rho C_p)'_{\nu} \frac{\partial T^m}{\partial t} = \lambda'_x \delta \frac{\partial^2 T^m}{\partial x^2} + \varphi_{exc} - \varphi_{int} - (\rho C_p)'_{fu} \delta \frac{\partial T^m}{\partial x}
$$
with:
\[ T^m = 0 \text{ for } t = 0 \]
\[ \varphi_{int}(x, t) = -\lambda_0 \frac{\partial T}{\partial y}(x, \delta^+, t) \]
\[ T^m \to 0 \text{ for } x = \pm\infty \]

In order to close the problem we need a relation between \( T^m \) and the interface flux \( \varphi_{int} \). Transverse dispersion coefficient \( \lambda'_y \) cannot be used anymore. So a kind of constant heat transfer coefficient \( h \) must be used. In the Laplace-Fourier domain, this relation can be written:

\[ \tilde{\varphi}_{int,n}(\delta, p) = h(\tilde{T}_{m,n}(p) - \tilde{T}_n(\delta, p)) \]

Finally, the temperature harmonics in the Laplace Fourier domain are:

\[
\begin{align*}
\tilde{T}_{m,n}(p) &= \frac{W(1-e^{-il\alpha n})}{ip\alpha_n} \frac{1+h/\lambda y_kn}{h+k_y(1+h/\lambda y_kn)} \\
\tilde{T}_n(y, p) &= \frac{W(1-e^{-il\alpha n})}{ip\alpha_n} \frac{h(e^{-h_k(y-\delta)})}{h\lambda y_kn+k_y(\lambda y_kn+h)} \text{ for } y > \delta
\end{align*}
\]

The use of (3) with a numerical Laplace inversion allows the calculation of \( T(x, y > \delta, t) \) and \( T^m(x, t) \)

4. Experimental device

The objective of this part is to present our experimental device for estimating the parameters of the HR model by inverting thermocouples output. The fixed bed is composed of a central plate heated on both of its faces by two foil electrical resistances and filled with spherical glass beads with uniform air flow parallel to it. Thermocouples have been embedded in the bed at known (nominal) positions, see figure 2. Step heating has been applied and the corresponding temperatures have been recorded. Assuming
that the thermocouple positions are known, and that the Darcy velocity of the fluid is
deducted from the output of a hot wire sensor in the downstream duct, linking bed and
fan, the recorded thermograms which are obtained can be used to estimate the model
parameters. A sensitivity study (see Figure 3) shows that the parameters of model HR
are correlated. So external information is needed for their estimation.

The experimental bed was recently disassembled, and the exact position of the
thermocouples were measured once again : they were slightly different from their original
positions. The reason for this deviation is that the glass beads slightly moved the
thermocouples when the bed was constructed. So their exact positions always need
to be estimated. The same conclusion is valid for the Darcy velocity, because of the
inaccuracy of the measuring instrument.

5. Parameters estimation and first experimental results

Model HR involves 3 kinds of parameters in our estimation strategy:

- arbitrary and insensitive parameters : \( \delta \) is arbitrary fixed to the half of a bead
diameter, and \( h \) and \( \lambda_x \) that are quasi-insensitive in the model (see figure 3) : they
can be fixed in agreement with literature. These two kinds of parameters are called
"given parameters" and noted \( \beta_g \) here;

- unknown parameters : \( u' \) is completely unknown (no prior information) and is freely
estimated ; So we set \( \beta_{fe} = u' \);

- parameters that are sensitive, but correlated with the \( \beta_{fe} \) parameters. A prior
information of the level of their value is available (measurement, correlation or
nominal value). Parameters \( x_i, y_i, (\rho C_p)'_t \) and \( u \) are supposed to be known. They
can be estimated with constraints, and are noted \( \beta_{sk} \) here.

So the parameter vector which must be estimated is only \( \beta = (u', u, (\rho C_p)'_t, x, y) = 
(\beta_{fe}, \beta_{sk}) \). Estimation of the model parameters is implemented through a minimization
of a modified least square sum :

\[
S(\beta) = \frac{1}{\sigma_T^2} \sum_{j=1}^{m} \sum_{i=1}^{n} (T_{exp}(t_j, x_i) - T_{mod}(t_j, \beta_g, \beta))^2 + \frac{1}{\sigma_x^2} \sum_{i=1}^{n} (x_{i}^{nom} - x_i)^2 \\
+ \frac{1}{\sigma_y^2} \sum_{i=1}^{n} (y_{i}^{nom} - y_i)^2 + \frac{1}{\sigma_{(\rho C_p)'_t}^2} ((\rho C_p)'_t^{nom} - (\rho C_p)'_t)^2 + \frac{1}{\sigma_u^2} (u^{nom} - u)^2
\]

The first term of this sum is the least square classical term. The other terms
 correspond to a Bayesian approach for any parameter for which no precise information
is available (parameters "supposed to be known" \( \beta_{sk} \)). All the parameters and the
measurements are assumed to be independent Gaussian random variables, with known
means and covariance matrices. Their a priori variance \( \sigma_j^2 \) are chosen as follows : \( \sigma_x^2 \)
and \( \sigma_y^2 \) can be chosen from the order of magnitude of the possible thermocouple junction
displacement. \( \sigma_u^2 \) can be fixed thanks to the knowledge of the accuracy of the hot wire
velocity sensor. \( \sigma_{(\rho C_p)'_t}^2 \) is deducted from a 10% uncertainty on \( \epsilon' \). All these constants
quantify the defiance we have in the corresponding prior information. Moreover the measurement errors are assumed to be uncorrelated and additive.

A simple Gauss-Newton minimization algorithm is used. Around the minimum \( \hat{\beta} = (\hat{u}, \hat{\rho C P})_t, \hat{x}, \hat{y} \) of sum \( S \), one can write (for \( n=1 \) thermocouple):

\[
T(\hat{\beta}) \approx T(\beta) + X(\beta)(\hat{\beta} - \beta) \quad \text{and} \quad \beta_{sk} = (\beta_{sk} - \beta) + (\hat{\beta}_{sk} - \hat{\beta})
\]

with \( \hat{\beta} \) solution of:

\[
\nabla_{\beta} S(\hat{\beta}) = -\frac{2}{\sigma_T^2} X^t(\hat{\beta}) (T_{exp} - T(\hat{\beta})) - 2 \left[ \begin{array}{ccc} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{array} \right] \left( \begin{array}{c} \sigma_T^2 \\ \rho C P \\ \frac{1}{2} \end{array} \right) \left( \begin{array}{c} \hat{u} \\ \hat{x} \epsilon \\ \hat{y} \epsilon \end{array} \right) = 0
\]

Substituting (5) into this expression and setting \( \beta^{(k)} = \hat{\beta}, \beta^{(k-1)} = \beta, \beta_{sk}^{(k)} = \hat{\beta}_{sk} \) and \( \beta_{sk}^{(k-1)} = \beta_{sk} \) yields, after linearization, the following iterative algorithm:

\[
\beta^{(k)} = \beta^{(k-1)} + \left[ X^t(\beta^{(k-1)}) X(\beta^{(k-1)}) + \sigma_T^2 R \right]^{-1} \left( X^t(\beta^{(k-1)}) (T_{exp} - T(\beta^{(k-1)})) + \sigma_T^2 R (\beta_{sk}^{(k-1)} - \beta_{sk}^{(k-1)}) \right)
\]

In these equations, \( \beta \) is the parameter vector, \( X \) is the sensitivity matrix and \( R \) is some kind of regulation matrix. In this example, only one thermocouple is used, but the same algorithm can be applied to several thermocouples. \( T_{exp} \) is then a sequence of the corresponding experimental temperature vectors (one vector per thermocouple).

The convergence criteria is triple: the algorithm stops if the parameter vector \( \beta \) does not vary more than one percent per iteration, if a critical number of iterations have been reached (this number was fixed to 30 here), or if the temperature residuals are lower than the experimental signal noise. In this case, the model cannot be closer to the experimental signal than the noise level.

So this iterative algorithm must be correctly initialized, otherwise the convergence criteria will not be met. Positions \( x \) and \( y \) are initialized at the nominal measured position for the thermocouple. These nominal values are the values designed during the construction of the fixed-bed. The Darcy velocity in the core region \( u \) is initialized through the velocity measurement in the duct (hot wire sensor). And finally the Martin correlation allows to initialize both porosity \( \epsilon \) and Darcy velocity \( u' \) in the near wall region. This porosity is then used to initialize the heat capacity in this region \( (\rho C P)_t \). The dispersion coefficient \( \lambda_x, \lambda_y \) and \( \lambda_x' \) are initialized from the Testu correlation, using the initialized velocities \( u \) and \( u' \).

Table 1 sums up the first results which were obtained for an experimental inversion of a thermocouple output (with \( \sigma_T = 0.02C; W = 100W; d = 2mm; \epsilon = 0.365; \epsilon_{nom} = 0.487 \)). The corresponding residuals (not shown here) are not correlated and of the same level as the measurement noise \( \sigma_T \).
Table 1: An example of an single thermocouple inversion (SI units)

| \(\beta_j\) | \(\beta^{\text{nom}}_j\) | \(\sigma^{\text{nom}}_j\) | \(\beta^{(0)}\) | \(\hat{\beta}\) |
|--------------|-----------------|-----------------|----------------|----------|
| \(u\)        | 0.290           | 0.1012          | 0.290          | 0.248    |
| \((\rho C_p)\)' | 1.0676.10^6    | 10^5            | 1.0676.10^6    | 9.96.10^5|
| \(u'\)       | -               | \(\infty\)     | 0.550          | 0.526    |
| \(x\)        | 0.120           | 0.001           | 0.120          | 0.1154   |
| \(y\)        | 0.005           | 0.001           | 0.005          | 0.0055   |

6. Conclusion

The main objective of this paper was to present a pertinent model for wall effects in dispersion of heat by a fluid flowing through a packed bed with the most parcimonious parametrization. This model has to be constructed with the parallel design of an efficient inversion technique allowing estimation of the most sensitive parameters. A reference heat transfer model for the homogeneous core region of the bed was first constructed. A more refined model that takes into account the wall effects was derived then. This model was too largely parameterized for a correct parameter estimation. So the last step was to reduce this model to be able to determine all the active parameters. A specific estimation technique has to be designed. A sensitivity analysis allowed to sort the parameters of the model into three class: (i) arbitrary or insensitive parameters, that is parameters whose effects on the model response are weak and whose estimation is not necessary (and not possible); (ii) parameters that are sensitive and that can be either freely estimated (without prior information or constraint) or (iii) estimated with prior information (nominal or literature values or correlations or external measured values) in order to decorrelate them in the signal. This last class concerns the supposedly known parameters. A corresponding Bayesian estimation technique was designed and applied to a single thermocouple experimental signal with success. Future work will be devoted to inverting several thermocouples signals in order to validate and improve the characterization of this thermal wall effect.

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