Int. J. Heat Mass Transfer. Vol. 26, No. 1, pp. 49-54, 1983
Printed in Great Britain

0017-9310/83/010049-06 $03.00/0

TRANSIENT ANALYSIS OF PACKED-BED THERMAL STORAGE SYSTEMS

A. E. SAEZ and B. J. MCCOY
Department of Chemical Engineering, University of California, Davis, CA 95616, U.S.A.

(*Received* 8 *October* 1981 *and in final form* 24 *May* 1982)

Abstract — A model, including longitudinal thermal dispersion and intraparticle conduction, is developed to describe the transient response of a packed column with a time-varying inlet temperature. The model can be applied to a diabatic column with uniform and constant ambient temperature, or to a perfectly insulated system. The expression for the temperature response within the column as a function of time and axial position is obtained by expanding the solution to an impulse of heat at the inlet in terms of either Hermite or Laguerre polynomials. The response to an arbitrary inlet temperature transient, found via a convolution integral, is expressed as a single quadrature. The response to a step input is an algebraic expression.

NOMENCLATURE

- a_c, external area per unit volume of the column;
- a_s, surface area of spheres per unit column volume;
- c_p, specific heat capacity of the fluid;
- c_{ps}, specific heat capacity of the solid spheres;
- d_c, column diameter;
- h_c, overall heat transfer coefficient for heat losses from the column to the environment;
- h_s, fluid-to-particle heat transfer coefficient;
- k_s, thermal conductivity coefficient of solid particles;
- k_{zz}, effective axial thermal conductivity coefficient;
- m_n, nth temporal moment;
- r, radial coordinate in spherical particles;
- R, radius of spherical solid particles;
- t, time;
- T, fluid temperature;
- T_s, solid particle temperature;
- T_0, fluid temperature at column entrance;
- T_e, temperature of environment;
- v_0, superficial velocity, εv;
- z, column length.

Greek symbols

- ε, interparticle void fraction;
- ρ, fluid density;
- ρ_s, solid particle density;
- θ_0, strength of input impulse;
- μ_n, normalized nth temporal moment;
- Δ_3, contribution of third-order term in expansions (39) and (43).

INTRODUCTION

PACKED beds are commonly used as energy storage systems or heat regenerators, for example, in solar and geothermal applications. The objective of this paper is to develop a mathematical model for the simulation of such systems, which will aid in their design, operation and control. Emphasis is placed on understanding the limitations of the assumptions of the model. We present an analytical solution for the model, avoiding numerical solution techniques for partial differential equations.

The model gives the fluid and average particle temperatures as functions of time and axial distance in a packed bed subjected to an arbitrary temperature input. The model applies to a diabatic column, but can be reduced to the adiabatic (perfectly-insulated) column if the wall heat transfer coefficient is negligible. The key to the method presented here is the representation of the response to an impulse of heat at the column entrance as an expansion in the temporal moments of the response. As is well known, such moments can be calculated from the Laplace transform of the temperature. Using the convolution theorem we show that the transient behavior of the bed can be presented as a simple quadrature, for any varying input temperature. The step-function input has a response represented by a simple algebraic equation. This technique has been demonstrated as effective in describing breakthrough curves for various mass transfer and chemical reaction phenomena in packed beds [1, 2].

Because of inaccuracies in the determination of the effective axial thermal conductivity coefficient, k_{zz}, and especially the fluid/particle heat transfer coefficient, h_s, it may be difficult to distinguish between results of the several models under certain ranges of operating conditions. However, in general, before such parameters can be readily estimated from experimental data, an accurate model whose limitations are understood in detail is needed.

Dixon and Cresswell [3] present a model for packed-bed heat transfer that smooths the intraparticle temperature, but allows for radial and axial solid temperature gradients in the column. This two-phase model is proposed mainly for catalytic reactors, where wall heat transfer is significant.

Wakao *et al.* [4] classify the models of heat transfer in packed beds, and argue why the "dispersion concentric" model, identical to the model of the present paper without heat losses, is preferable. They provide correlations for axial thermal dispersion coefficients as well as particle-to-fluid heat transfer coefficients. Shen *et al.* [5] provide a Fourier series solution for this model.

Sagara *et al.* [6] used the same model to interpret pulse response data for water flowing through a column packed with porous spheres. They considered gas as well as liquid systems and pointed out that radiation effects are unimportant in packed beds at gas temperatures below 400°C, and that particle-to-particle conduction is significant only for small particle sizes.

THEORY

We consider a column of length L packed with spheres of diameter $2R$, such that $L \gg 2R$. We assume that fluid flow in the column is incompressible, viscous heating is negligible, the physical properties of the fluid are constant, the temperature on the surface of a particle is uniform, heat conduction directly from particle to particle is negligible, temperature and velocity profiles across the column are uniform, and radiant heat transfer between particles is negligible. In addition, if the column is surrounded by an environment of uniform and constant temperature, T_e, the equation for the interparticle fluid temperature, $T(t, z)$, as a function of time and axial position is

$$\varepsilon \rho c_p \left(\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial z}\right) = k_{zz}\frac{\partial^2 T}{\partial z^2} - a_s h(T - T_s) - a_c h_c (T - T_e). \quad (1)$$

Here ε is the interparticle void fraction, ρ and c_p are the density and heat capacity of the fluid, $v_0 = \varepsilon v$ is the fluid volumetric flow rate per unit column cross-section area, i.e. the superficial velocity, $a_s = 3(1 - \varepsilon)/R$ is the area of spheres per unit column volume, h_s is the fluid-to-particle heat transfer coefficient, a_c is the external area per unit volume of the column, and h_c is the overall heat transfer coefficient for heat losses from the column to the environment. The effective axial thermal conductivity coefficient, k_{zz}, accounts for conduction as well as hydrodynamic dispersion of heat longitudinally in the column. Channeling near the wall can be a problem unless the particle diameter is much less than the column diameter.

An order of magnitude analysis shows that radial temperature gradients across the column are negligible if

$$h_c d_c / 2k_{rr} \ll 1$$

where $d_c/2$ is the column radius, and k_{rr} is the radial thermal dispersion coefficient. The constraint is satisfied if the column is well-insulated (h_c is small), when the column diameter is small, or when heat transfer radially is large.

We have ignored the effect of the wall heat capacity, an approximation that is valid when the thermal diffusivity of the wall times the wall thickness squared is much smaller than the transient time.

The equation for the temperature of the spheres as a function of time and radial position inside the sphere, $T_s(t, r)$ is

$$\rho_s c_{ps}\frac{\partial T_s}{\partial t} = k_s \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_s}{\partial r}\right) \quad (2)$$

where ρ_s and c_{ps} are the mass density and specific heat capacity of the solid, and k_s is the thermal conductivity coefficient of the solid. Note that T_s also varies with z, as indicated by the coupling boundary condition. When heat losses are negligible, equations (1) and (2) reduce to the model for heat transfer in packed beds proposed previously [4–7].

Equations (1) and (2) may be solved for appropriate initial and boundary conditions. At the surface of the particles we require the heat flux to be continuous,

$$h_s (T - T_s)_{r=R} = -k_s \frac{\partial T_s}{\partial r}\bigg|_{r=R} \quad (3)$$

which serves to couple equations (1) and (2). At the column inlet we have the arbitrary input temperature $T_0(t)$ i.e.

$$T(t, 0) = T_0(t). \quad (4)$$

For a column very long compared to sphere diameter,

$$T(t, \infty) = \text{finite}. \quad (5)$$

Boundary conditions for T_s are equation (3) and

$$T(t, 0) = \text{finite}. \quad (6)$$

We assume that the bed is initially at the environment temperature, T_e,

$$T(0, z) = T_e, \quad (7)$$

$$T_s(0, r) = T_e. \quad (8)$$

The case when $T_s(t = 0)$ is not uniform over the column can in principle be solved with the present method. However, if the initial condition is not a simple function, the algebraic complexities may be problematic.

MOMENTS

The moment technique, widely applied in modeling chromatographic columns [1] and sometimes in the analysis of heat transfer in packed beds, [6], will be used to represent the average temperature of air and particles in the packed bed as functions of time and axial distance. The moments are integrals of a distribution function, $\psi(t)$,

$$m_n = \int_0^\infty t^n \psi(t)\,\mathrm{d}t, \qquad n = 0, 1, 2, \ldots \quad (9)$$

The normalized nth moment is defined by

$$\mu'_n = m_n/m_0, \qquad n = 0, 1, 2, \ldots \tag{10}$$

and the central moments are

$$\mu_n = \frac{1}{m_0}\int_0^\infty (t - \mu'_1)^n \psi(t)\,dt, \qquad n = 2, 3, \ldots \tag{11}$$

The Laplace transform of $\psi(t)$ is a generating function for the moments

$$m_n = (-1)^n \frac{d^n \bar{\psi}}{ds^n}\bigg|_{s=0} \tag{12}$$

Letting

$$\psi = T - T_e \tag{13}$$

and

$$\psi_s = T_s - T_e \tag{14}$$

and applying Laplace transformation to equations (1)–(6), allow us to calculate the moments for the air temperature relative to the environmental temperature

$$m_0(z) = m_0(0)\exp(\lambda z), \tag{15}$$

$$\mu'_1(z) = \mu'_1(0) + \delta_3 z, \tag{16}$$

$$\mu_2(z) = \mu_2(0) + \delta_4 z \tag{17}$$

where

$$\lambda = \frac{1}{2}[\alpha - (\alpha^2 + u)^{1/2}] \tag{18}$$

$$\alpha = \varepsilon\rho\, c_p v_0/k_{zz}, \tag{19}$$

$$u = 4 h_c a_c/k_{zz}, \tag{20}$$

$$\delta_3 = \{\varepsilon\rho c_p/[k_{zz}(\alpha^2 + u)]\} \times \{1 + [(1-\varepsilon)\rho_s c_{ps}]/\varepsilon\rho c_p\} \tag{21}$$

and

$$\delta_4 = [2/(\alpha^2 + u)^{3/2}](\varepsilon^2\rho^2 c_p^2/k_{zz}^2)(1+\delta_0)^2 + [2/(\alpha^2+u)^{1/2}][\rho_s^2 c_{ps}^2 R^2(1-\alpha)/3k_{zz}]\left(\frac{1}{Rh_s} + \frac{1}{5k_s}\right). \tag{22}$$

with

$$\delta_0 = \frac{1-\varepsilon}{\varepsilon}\frac{\rho_s c_{ps}}{\rho c_p}. \tag{23}$$

It can be shown that the moments for the diabatic case reduce to the following moments for the adiabatic case [6] when the column heat transfer coefficient vanishes

$$m_0(z) = m_0(0), \tag{24}$$

$$\mu'_1(z) = \mu'_1(0) + (z/v)(1+\delta_0), \tag{25}$$

$$\mu_2(z) = \mu_2(0) + (2z/v)\left[\delta_1 + \frac{k_{zz}}{\varepsilon\rho c_p v^2}(1+\delta_0)^2\right]. \tag{26}$$

In addition, the third central moment for the adiabatic column is

$$\mu_3(z) = \mu_3(0) + (3z/v)\left[\delta_2 + \frac{4k_{zz}}{\varepsilon\rho c_p v^2}\delta_1(1+\delta_0) + \frac{4k_{zz}^2}{\varepsilon^2\rho^2 c_p^2 v^4}(1+\delta_0)^3\right] \tag{27}$$

where

$$\delta_1 = \frac{1-\varepsilon}{\varepsilon}\frac{\rho_s^2 c_{ps}^2}{\rho c_p}\frac{R^2}{15}\left(\frac{1}{k_s} + \frac{5}{h_s R}\right), \tag{28}$$

$$\delta_2 = \frac{1-\varepsilon}{\varepsilon}\frac{\rho_s^3 c_{ps}^3 R^4}{\rho c_p}\left(\frac{12}{945 k_s^2} + \frac{4}{45 h_s R k_s} + \frac{1}{27 h_s^2 R^2}\right) \tag{29}$$

The zeroth moment, m_0, is constant with z when heat losses are negligible.

To model the dynamics of the heat storage in the packed bed, we need the single-particle average temperature, defined as

$$\langle T_s \rangle = \frac{3}{R^3}\int_0^R T_s r^2\,dr. \tag{30}$$

Taking the volume average of equation (2) over one particle, and using boundary conditions (3) and (6) gives

$$\rho_s c_{ps}\frac{\partial\langle\psi_s\rangle}{\partial t} = \frac{-3h_s}{R}[\psi_s(R) - \psi]. \tag{31}$$

Equation (31) may be Laplace-transformed and the moments found with equation (12)

$$m_{0s} = m_0, \tag{32}$$

$$\mu'_{1s} = \mu'_1 + \frac{\rho_s c_{ps} R^2}{3}\left(\frac{1}{5k_s} + \frac{1}{h_s R}\right), \tag{33}$$

$$\mu_{2s} = \mu_2 + \frac{\rho_s^2 c_{ps}^2 R^4}{9}\left(\frac{13}{175 k_s^2} + \frac{2}{5k_s h_s R} + \frac{1}{h_s^2 R^2}\right). \tag{34}$$

The results show as expected that the zeroth moments for the particle and fluid temperature are identical. The first and second particle moments show delays with respect to the fluid moments, and reduce to fluid moments for very large values of k_s and h_s.

TEMPERATURE PROFILE

The temperature response for a delta function (impulse) input can be expressed as a series expansion in orthogonal polynomials [1, 2]. Both Hermite and Laguerre polynomials have been used for this purpose [7]. The Hermite polynomials have a weighting function $\exp(-x^2)$, so that the first term in the series represents a Gaussian distribution, and higher order terms account for deviations to the Gaussian shape. The Laguerre polynomials have a Poisson distribution as a weighting function, providing an advantage over Hermite polynomials since the expansion is zero for $t \leq 0$.

For the delta function input, i.e.

$$T(z=0,t) - T_e = \theta_0 \delta(t) \quad (35)$$

we have

$$m_0(0) = \theta_0,\ \mu'_1(0) = 0,\ \mu_2(0) = 0,\ \mu_3(0) = 0, \ldots$$

Expressing the response to the delta function in terms of Hermite polynomials gives

$$T - T_e = m_0 \exp(-x^2) \sum_{n=0}^{\infty} a_n(z) H_n(x) \quad (36)$$

where

$$x = (t - \mu'_1)/(2\mu_2)^{1/2}. \quad (37)$$

The first term of the expansion corresponds to a Gaussian distribution centered at μ'_1 with standard deviation $\mu_2^{1/2}$. The coefficient of the expansion can be found from the orthogonality relation for Hermite polynomials to be

$$a_0(z) = 1/(2\pi\mu_2)^{1/2}, \quad (38)$$
$$a_1(z) = 0,$$
$$a_2(z) = 0,$$
$$a_3(z) = \mu_3/24(\pi\mu_2^3)^{1/2}.$$

Because in Laplace transform space the solution $T(t,z) - T_e$ can be expressed as the product of the inlet temperature and the response to the delta function input, the convolution theorem requires that

$$T(t,z) - T_e = \int_0^t [T_0(t-t') - T_e] \exp(-x'^2) \sum_{n=0}^{\infty} a_n(z) H_n(x')\,dt' \quad (39)$$

where for x', the integration variable t' replaces t in equation (37). Equation (39) permits the evaluation of the temperature profile history in the packed bed, when the moments are available for a particular model, provided the expansion converges. For $\mu'_1/(2\mu_2)^{1/2} \gtrsim 2.5$, i.e. for longer columns and lower fluid velocities [1], the Gaussian profile is sufficiently accurate to represent the impulse response; then

$$T - T_e = \frac{1}{(2\pi\mu_2)^{1/2}} \int_0^t [T_0(t-t') - T_e] \exp[-(t' - \mu'_1)^2/2\mu_2]\,dt'. \quad (40)$$

For the special case of the step input,

$$T_0(t) - T_e = \begin{cases} 0, & t < 0 \\ T_0 - T_e, & t > 0 \end{cases} \quad (41)$$

and equation (40) gives

$$T - T_e = \frac{1}{2}(T_0 - T_e) \times \{\mathrm{erf}[(t - \mu')/(2\mu_2)^{1/2}] + \mathrm{erf}[\mu'_1/(2\mu_2)^{1/2}]\}. \quad (42)$$

The accuracy of this equation has been discussed in the earlier work on breakthrough curves [1].

For a step down in temperature in the adiabatic column, we may interpret T_e as the initial temperature and T_0 as the lower new inlet fluid temperature, i.e. we have $T_0 < T_e$, giving us an inverted "break through curve".

The response to the delta function as an expansion in Laguerre polynomials [2, 8] is

$$T - T_e = \frac{m_0}{(\lambda - 1)!}(\lambda t/a)\exp(-\lambda t/a) \sum_{n=0}^{\infty} k_n L_n(\lambda t/a) \quad (43)$$

where if

$$\lambda = \mu_1'^2/\mu_2 \quad (44)$$

and

$$a = \mu'_1$$

we have the following expansion coefficients [8]

$$k_0 = 1, \quad (45)$$
$$k_1 = 0,$$
$$k_2 = 0,$$
$$k_3 = (\lambda^2\mu_3 - 6\lambda\mu'_1\mu_2 + 4\mu_1'^3)/[6(\lambda+2) \times (\lambda+1)\mu_1'^3].$$

The required Laguerre polynomials are

$$L_0(x) = 1, \quad (46)$$
$$L_3(x) = x^3 - 3(\lambda+2)x^2 + 3(\lambda+2)(\lambda+1)x - (\lambda+2)(\lambda+1)\lambda.$$

When third and higher-order terms are rejected, the convolution theorem yields the solution

$$T(t,z) - T_e = \int_0^t \frac{T_0(t-t')}{(\lambda-1)!} \times (\lambda t/a)^{\lambda-1} \exp(-\lambda t'/a)\,dt'. \quad (47)$$

For a step input equation (47) becomes

$$T - T_e = \frac{(T_0 - T_e)}{(\lambda - 1)!}\Gamma(\lambda, \mu'_1 t/\mu_2) \quad (48)$$

where the incomplete gamma function is the integral

Table 1. Influence of axial dispersion and intraparticle effects on the accuracy of the polynomial expansions

h_c ($J\,m^{-2}s^{-1}{}^\circ C^{-1}$)	k_{zz} ($J\,m^{-1}s^{-1}{}^\circ C^{-1}$)	$100\Delta_3/(T_0 - T_e)$ Hermite	Laguerre
150	0	0.3	1.5
150	9.2	0.9	1.2
4200	9.2	3.1	0.6

$$\Gamma(x, y) = \int_0^y \zeta^{x-1} e^{-\zeta} d\zeta. \quad (49)$$

EFFECT OF THIRD-ORDER TERMS

To determine the quantitative effect of truncating the expansion, we have calculated the magnitude of the third-order term for the step input. For the Hermite polynomial this term has the expression,

$$\Delta_3 = \frac{\mu_3}{12\mu_2^2}(2\mu_2/\pi)^{\lambda}\{[\exp - (t - \mu_1')/2\mu_2] \times [1 - (t - \mu_1')^2/\mu_2] - \exp[-\mu_1'^2/(2\mu_2)] \times (1 - \mu_1'/\mu_2)^2\} \quad (50)$$

and for the Laguerre polynomial,

$$\Delta_3 = \frac{k_3}{(\lambda - 1)!}[-(\mu_1' t/\mu_2)^{\lambda} \exp(-\mu_1' t/\mu_2)] \times [(-\mu_1' t/\mu_2)^2 - 2(\lambda + 2)(\mu_1' t/\mu_2) + (\lambda + 2)(\lambda + 1)]. \quad (51)$$

It is worthwhile to note that for a step input, the third-order terms are algebraic expressions; that is, there is no need to evaluate additional integrals numerically.

The third-order terms were evaluated for a packed-bed (assumed adiabatic) of steel spheres described by Vanden Broek and Clark [9]. The results for the third-order terms appear in Table 1. We observe that Hermite and Laguerre polynomial expansions are influenced differently by the band-spreading effects in the bed. It is expected that cases with low axial dispersion or small intraparticle effects are better described by Hermite expansions, because of the symmetrical nature of the Gaussian term. Cases with large axial dispersion, or large particle conductivities and heat transfer coefficients, on the other hand, are better represented by the Laguerre expansions. These effects are illustrated in Table 1, where $\Delta_3/(T_0 - T_e)$ is less than 5%, showing that the truncation is quite accurate.

CONCLUSION

We have presented a mathematical model for predicting dynamic temperature responses for a packed bed of spheres subject to arbitrary temperature of entering fluid. Longitudinal thermal dispersion and intraparticle heat conduction are included in the governing equations. The model gives the fluid and average particle temperatures as functions of time and axial distance for either adiabatic or non-adiabatic packed beds.

The model is based on the use of Hermite and Laguerre polynomial expansions for expressing the dynamic response to a temperature impulse input. Hermite expansion gives better results for the case of low axial thermal dispersion or large intraparticle effects, namely, low values for the fluid-to-particle heat transfer coefficients or large values of the particle thermal conductivity. Laguerre expansion is better in the opposite case. Owing to the complicated nature of the dependence of the response on these parameters, the limits of the applicability of the criteria described above are specific for each situation so that a general rule cannot be obtained. However, the small differences observed for the results given by each of the expansions indicate that for practical purposes, either approach can be applied with a high degree of confidence.

Acknowledgements — This research was supported by the U. C. Appropriate Technology Program under project No. 80-126se-3998. We thank Mr. O. Maaliou for confirming the calculations of the moment expressions in this paper by using the computer algebra program REDUCE.

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ANALYSE TRANSITOIRE DES SYSTEMES DE STOCKAGE THERMIQUE PAR LIT FIXE

Résumé—On développe un modèle, incluant la dispersion thermique longitudinale et la conduction interparticulaire, pour décrire la réponse transitoire d'une colonne fixe avec température de fluide variable à l'entrée Le modèle peut être appliqué à une colonne diabatique avec une température ambiante uniforme et constante, ou un système parfaitement isolé. L'expression pour la réponse en température dans la colonne, en fonction du temps et de la position axiale, est obtenue en développant la solution d'une impulsion thermique à l'entrée en fonction de polynomes de Hermitte et de Laguerre. La réponse à une température d'entrée arbitraire, trouvée à partir d'une intégrale de convolution, est exprimée par une seule quadrature. La réponse à une entrée échelon est une expression algébrique.

INSTATIONÄRES VERHALTEN VON FESTBETTEN-SPEICHERSYSTEMEN

Zusammenfassung—Ein Modell, das die Wärmeausbreitung in Längsrichtung und die Wärmeleitung zwischen den Partikeln berücksichtigt, wurde entwickelt, um das instätionäre Verhalten einer Festbettsäule-mit zeitlich veränderlicher Temperatur der eintretenden Flüssigkeit zu beschreiben. Das Modell kann auf eine adiabate Säule mit gleichförmiger und konstanter Umgebungstemperatur oder auf ein ideal isoliertes System angewendet werden. Der Ausdruck für den Temperaturverlauf innerhalb der Säule als Funktion von Zeit und axialier Koordinate wird erhalten, indem man die Lösung für eine Impulsfunktion am Eintritt in Form von Hermite'schen oder Laguerre'schen Polynomen entwickelt. Die Lösing für eine willkürliche zeitliche Eintrittstemperatur-Funktion, die mit Hilfe einer Integralfaltung gefunden wird, läßt sich als einfache Quadratur ausdrücken. Die Lösungsfunktion für eine Sprungfunktion am Eintritt ist en algenraischer Ausdruck.

НЕСТАЦИОНАРНЫЙ АНАЛИЗ АККУМУЛИРОВАНИЯ ТЕПЛА В ПЛОТНОМ СЛОЕ

Аннотация—Разработана модель, включающая продольную дисперсию тепла и теплопроводность частиц, для описания функции отклика системы на изменяющуюся во времени температуру жидкости на входе. Модель может быть использована для адиабатической или хорошо изолированной колонны при одинаковой и постоянной начальной температуре. Выражение для температурного отклика системы как функция времени и продольной координаты получено, используя решение отклика на импульс тепла на входе в виде либо полиномов Эрмита, либо Лагерра. Отклик на произвольное изменение входной температуры, полученный с помощью интеграла свертки, выражен как простая квадратура, а для ступенчатого импульса—в виде алгебраического выражения.