Available online at www.sciencedirect.com
SCIENCE DIRECT®
International Journal of Heat and Mass Transfer 47 (2004) 1325–1334
International Journal of HEAT and MASS TRANSFER
www.elsevier.com/locate/ijhmt

Population balance model for particle-to-particle heat transfer in gas–solid systems

Cs. Mihálykó [a,*], B.G. Lakatos [b], A. Matejdesz [a], T. Blickle [c]

[a] Department of Mathematics and Computing, University of Veszprém, P.O. Box 158, H-8201 Veszprém, Hungary
[b] Department of Process Engineering, University of Veszprém, P.O. Box 158, H-8201 Veszprém, Hungary
[c] Research Institute of Chemical and Process Engineering, University of Kaposvár, P.O. Box 125, H-8201 Veszprém, Hungary

Received 20 September 2002; received in revised form 11 August 2003

Abstract

A mathematical model is presented for particle-to-particle heat transfer in gas–solid systems. In developing the model, simple kinetic equations are assumed to describe the inter-particle heat transfer process, and the particle–particle interactions are considered stochastic. A stochastic approach is used to derive the population balance equation describing the variation of the density function of temperature distribution of the particulate phase. The moment equations and numerical solution of the partial integro-differential equation of the population balance model are derived and used to analyse the behaviour of a batch gas–solid system. The results indicate that the population balance approach, used for developing the model describing the inter-particle contact heat conduction during collision capable to take into account a number of parameters affecting the process, can be applied also for predicting heat transfer in gas–solid processing systems.

Keywords: Gas–solid system; Inter-particle collisions; Particle-to-particle heat transfer; Population balance model; Simulation

1. Introduction

In modelling heat transfer in gas–solid processing systems, three inter-phase thermal processes are to be considered: wall-to-bed, gas-to-particle and particle-to-particle heat transfer. In systems with intensive motion of particles, such as fluidised and spouted beds or pneumatic conveying, the particle-to-particle heat transfer occurs through inter-particle collisions. Extensive experimental and theoretical work has been published on wall-to-bed and gas-to-particle heat transfer processes, but the studies of the effects of the inter-particle collisions on the heat transfer processes in multi-phase systems, especially examinations of the direct particle-to-particle heat transfer, are rather scarce.

Dense particulate systems usually are modelled using the Eulerian–Eulerian formulation [1–7] in which all particle interactions are aggregated into some parameters of the particle phase treated also as a continuum. Here, collisions are too frequent to consider those separately, and they influence the gas and particle temperature profiles and the rate of heat transfer.

The Eulerian–Lagrangian approach handles the continuous phase with the help of Eulerian variables, whereas the equations of the particulate phase motion, formulated by Lagrangian variables, are integrated along the separate particle trajectories [8–13]. This method allows to simulate the particle–particle collisions as well, studying their influence on both the hydrodynamic and thermal processes. Whilst simulation results indicated that the inter-particle collisions may affect the heat transfer processes significantly [3,14–18], the direct particle-to-particle heat transfer during collisions has

* Corresponding author. Tel.: +36-88-423239; fax: +36-88-421693.
E-mail address: mihalyko@almos.vein.hu (Cs. Mihálykó).

0017-9310/$ - see front matter © 2003 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ijheatmasstransfer.2003.09.003

Nomenclature

A	surface area, m^2, random event
a	variable $[= 1/(mC)]$ J^{-1} K
a_k	quadrature coefficient (Eq. (18))
b_l	quadrature coefficient (Eq. (18))
C	specific heat J kg^{-1} K^{-1}
f	density function
F	distribution function
h	temperature increment, K
k	frequency coefficient, s^{-1}
m	expected value
m	mass, kg
M_I	I^{th} order moment of the temperature
n	population density function
N	population distribution function, number of particles
P	probability
T	temperature, K
t	time, s
1_A	characteristic function of A

Greek symbols

α	product of parameters β, A and θ
β	heat transfer coefficient, W m^{-2} K^{-1}
ω	random parameter of particle-to-particle heat transfer
η	random variable $(= \xi_{1,t} + (\xi_{2,t} - \xi_{1,t})(\omega/2))$, K
ξ	random variable, °C
τ	time, time increment, s
θ	contact time, s
σ^2	variance

Subscripts

0	initial condition, before collision
J	joint distribution
max	maximal value
min	minimal value
ω	random parameter
β	heat transfer coefficient
θ	contact time
A	random event

been taken into consideration only by Mansoori et al. [18].

In a four-way interaction Eulerian–Lagrangian model, Mansoori et al. [18] computed the inter-particle contact heat conduction in turbulent heat transfer in gas–solid flows by using a deterministic kinetic model. Delvosalle and Vanderschuren [19,20] developed this model for describing heat transfer between particles by conduction through the gas lens in fluidised bed dryers. Recently, Blickle et al. [21,23] and Mihálykó et al. [22] have applied a different approach, deriving a stochastic model for particle-to-particle heat transfer, applying a simple kinetic model with random parameter [23]. On the basis of this stochastic approach, a population balance equation was developed, treating the solid phase as a large population of particles exhibiting temperature distribution.

In this paper, an extension of this stochastic model of particle-to-particle heat transfer is presented. The direct heat transfer between particles is modelled by applying a simple kinetic, characterised by a random variable aggregated from different random physical variables of the process. Using this kinetics, a population balance model is developed for describing the variation of the temperature distribution of particles. The moment equations and numerical solution of the population balance equation are derived, and the properties of the model are analysed by simulation.

2. Heat transfer kinetics with random parameter

Consider a gas–solid system through which the gas flow is continuous while the solid phase, consisted of a large population of particles having identical sizes and physical properties, is assumed to be of batch mode, i.e. the number of particles in the system is constant. Let us assume that this material system is mixed perfectly, through the wall is isolated from the environment, and the properties of particles can be considered constant during the process except their temperature. Furthermore, let us assume that the temperature inside each particle can be considered homogeneous, and the population of particles exhibit significant differences in their temperature that can be described by some distribution function of appropriate properties. If now, in some moment of time heating of particles is started with the gas having constant temperature, then the gas-to-particle and particle-to-particle heat transfer processes are the only changes in the system. Since, however, in the present study we are interested only in modelling the direct particle-to-particle heat transfer in the following we consider only this process.

Let us track two particles having, according to the former conditions, identical mass m and heat capacity C, but different temperatures T_{10} and T_{20}, respectively. If these particles collide at moment of time $t = 0$ and remain in contact for some time θ, then, provided that

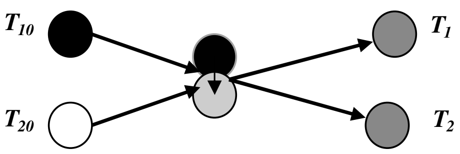

Fig. 1. Heat transfer between two colliding particles.

$T_{10} \neq T_{20}$, some exchange of heat occurs between them as it shown in Fig. 1.

Assuming that this heat transfer can be described by an overall heat transfer coefficient β, then the equations describing the variation of temperatures of particles are

$$mC\frac{\mathrm{d}T_1(t)}{\mathrm{d}t} = \beta A[T_1(t) - T_2(t)] \tag{1}$$

and

$$mC\frac{\mathrm{d}T_2(t)}{\mathrm{d}t} = -\beta A[T_1(t) - T_2(t)] \tag{2}$$

subject to the initial conditions $T_1(0) = T_{10}$, $T_2(0) = T_{20}$, where A is the contact area of heat transfer between the particles. Adding the two sides of Eqs. (1) and (2), we obtain

$$mC\left(\frac{\mathrm{d}T_1}{\mathrm{d}t} + \frac{\mathrm{d}T_2}{\mathrm{d}t}\right) = 0 \tag{3}$$

expressing the conservation of energy in the process.

From Eq. (3)

$$mC([T_1(t) - T_{10}] + [T_2(t) - T_{20}]) = 0$$

and

$$T_2(t) = T_{10} + T_{20} - T_1(t)$$

and substituting it into Eq. (1) we get the following equation

$$\begin{aligned}\frac{\mathrm{d}T_1(t)}{\mathrm{d}t} &= \frac{\beta A}{mC}[T_{10} + T_{20} - 2 \cdot T_1(t)] \\ &= a\beta A[T_{10} + T_{20} - 2T_1(t)]\end{aligned} \tag{4}$$

where $a = \frac{1}{mC}$.

If the particles remain in contact to time θ, then we get from Eqs. (2) and (4)

$$T_1(\theta) = T_{10} + \frac{T_{20} - T_{10}}{2}(1 - \exp(-2a\beta A\theta)) \tag{5}$$

and

$$T_2(\theta) = T_{20} - \frac{T_{20} - T_{10}}{2}(1 - \exp(-2a\beta A\theta)) \tag{6}$$

In Eqs. (5) and (6) parameters β, A, θ are, in essence, random quantities since the quality and area of contact, as well as the contact time in such system may depend on a number of random conditions [24,25]. As a result, parameter $\omega = 1 - \exp(-2a\beta A\theta)$ is a random function of parameters β, A and θ. These parameters, however, form in this functional dependence a product $\alpha = \beta A\theta$, therefore, since it is difficult to separate their effects and, in addition, the stochastic dependence between the contact time and contact area may be significant it seems to be reasonable to characterise those by means of their joint probability distribution. As a consequence, denoting the density function of α by f_α, the density function f_ω of the distribution of ω can be determined by the following way:

$$f_\omega(z) = \begin{cases} \dfrac{1}{2a(1-z)} f_\alpha\left(-\dfrac{\ln(1-z)}{2a}\right), & \text{if } z \in [0,1) \\ 0, & \text{if } z \notin [0,1) \end{cases}$$

We suppose that the density function f_ω, either from measurement or simulation experiments, is known.

3. The population balance model

Next we will present a stochastic approach to setup the partial integro-differential equation of the population balance model of a gas–solid system with pure particle-to-particle heat transfer. Let us assume that the total number of particles in the system is N, and $N(.,.)$ denotes the population distribution function of the particles. Here, $N(T,t)$ gives the number of particles at time t with a temperature which is less than T. As a consequence, $F_N(T,t) = N(T,t)/N$ is the normalised number distribution function of the particle population. Let N be such a large number, that $F_N(T,t)$ can be approximated satisfactorily (in T and t uniformly) by a family of distribution functions $F(T,t)$ the members of which are differentiable with respect to T and t. Let $f(T,t)$ be $\partial F(T,t)/\partial T$. If now ξ_t denotes the temperature of a randomly chosen particle of the population at time t, then the distribution function of ξ_t is $F_N(T,t)$, and the function $F(T,t)$, as a consequence of the former assumptions, can be substituted for it. Furthermore, we consider the difference between the functions $F_N(T,t)$ and $F(T,t)$ negligible, so that $F(.,t)$ and $f(.,t)$ can be taken as the distribution and density functions of ξ_t, respectively.

Since, as it was assumed, the heat transfer between particles occurs only by inter-particle contact heat conduction during collisions, the changes in the temperature of a particle depend only on two conditions: what is the temperature of the other particle the given particle is contacted with, and what are the actual values of the parameters characterising the heat transfer process. Now, let us assume that the probability that the temperature T_1 of a particle changes in the interval of time $(t, t+\tau)$ in such a way that it meets only one particle of temperature $T_2 \neq T_1$ and the heat transfer process proceeds with parameter ω is $k\tau + o(\tau)$, independently of t, T_1, T_2 and ω, where $k \in [0,\infty($. Further, we suppose that the probability that one particle takes part in more than one heat transfer process during this time is $o(\tau)$.

Let we choose randomly one particle at time $t+\tau$ from the population. If it is such a particle that collided with exactly one other particle in the interval of time $(t, t+\tau)$, the second particle did not meet any other particle during that time, and the temperature of the first particle was changed in this collision, then this event is denoted by A_1. If it is such a particle that collided at most with one other particle in the interval of time $(t, t+\tau)$ and its temperature did not change during this collision, then this event is denoted by A_2. Finally, let A_3 stand for the complement of $A_1 \cup A_2$. It can be easily seen that $P(A_1) = k\tau + o(\tau)$, $P(A_2) = 1 - k\tau - o(\tau)$ and $P(A_3) = 2o(\tau)$.

Now, using Eq. (5), we can determine the temperature $\xi_{t+\tau}$ of the observed particle. If event A_1 occurs, then we have $\xi_{t+\tau} = \eta = \xi_{1,t} + (\xi_{2,t} - \xi_{1,t})(\omega/2)$, but in the case of occurring of the event A_2 the temperature becomes $\xi_{t+\tau} = \xi_{1,t}$. Finally, we do not need the explicit form of $\xi_{t+\tau}$ when A_3 occurs since $P(A_3) = o(\tau)$. Therefore, we denote it simply by $\xi^{(3)}_{t+\tau}$. Let the temperature of the observed particle at time t be denoted by $\xi_{1,t}$. Similarly, let $\xi_{2,t}$ denote the temperature at time t of the particle with which the observed particle collided, and let ω denote the aggregated random parameter characterising the heat transfer process in collision between the particles. We suppose that N is large enough to treat $\xi_{1,t}$ and $\xi_{2,t}$ as independent, identically distributed random variables and their distributions are the same as the distribution of ξ_t. Finally, we suppose that ω is also independent of $\xi_{1,t}$ and $\xi_{2,t}$, the density function of which is $f_\omega(.)$.

Then, using the theorem of the total probability, we can write

$$\xi_{t+\tau} = \eta \cdot 1_{A_1} + \xi_{1,t} \cdot 1_{A_2} + \xi^{(3)}_{t+\tau} \cdot 1_{A_3} \tag{7}$$

where 1_{A_k}, $k = 1, 2, 3$ are the characteristic functions of the sets A_k, $k = 1, 2, 3$. From Eq. (7), we conclude that the density function of $\xi_{t+\tau}$ can be derived as

$$\begin{aligned} f(T, t+\tau) = {} & f_\eta(T, t) \cdot (k\tau + o(\tau)) \\ & + f(T, t) \cdot (1 - o(\tau)) + 2o(\tau) \end{aligned} \tag{8}$$

In order to determine the density function $f_\eta(T, t)$, first we determine the joint probability density function $f_J(T, S, t)$ of variables $(\eta, \xi_{2,t}, \omega)$ as

$$f_J(T, S, z) = f\left(\frac{2(T-S)}{z} + S, t\right) \cdot f(S, t) \cdot f_\omega(z) \cdot \frac{2}{z}$$

where it was utilised that $\xi_{1,t}$, $\xi_{2,t}$ and ω are independent random variables. Then, expressing the marginal probability density function $f_\eta(T, t)$ of the variable η, which has the property $f(T, .) = 0$ when $T \notin [T_{\min}, T_{\max}]$, we obtain the following equation for $f_\eta(T, t)$

$$\begin{aligned} f_\eta(T, t) = {} & \int_{T_{\min}}^{T_{\max}} \int_0^1 f\left(\frac{2(T-S)}{z} + S, t\right) f(S, t) f_\omega(z) \\ & \times \frac{2}{z} \, dz \, dS \end{aligned}$$

Substituting this expression into Eq. (8) we obtain

$$\begin{aligned} f(T, t+\tau) = {} & k\tau \cdot \int_{T_{\min}}^{T_{\max}} \int_0^1 f\left(\frac{2(T-S)}{z} + S, t\right) \\ & \times f(S, t) f_\omega(z) \frac{2}{z} \, dz \, dS \\ & + (1 - k\tau) \cdot f(T, t) + o(\tau) \end{aligned}$$

Now, after some mathematical manipulations, we obtain the following integro-differential equation as $\tau \to 0$:

$$\begin{aligned} \frac{\partial f}{\partial t}(T, t) = {} & k\Bigg(- f(T, t) + \int_{T_{\min}}^{T_{\max}} \int_0^1 f\left(\frac{2(T-S)}{z} + S, t\right) \\ & \times f(S, t) f_\omega(z) \frac{2}{z} \, dz \, dS \Bigg), \quad t > 0 \\ f(T, 0) = {} & f_0(T), \quad T \in [T_{\min}, T_{\max}] \end{aligned} \tag{9}$$

where $f_0(T)$ denotes the initial probability density function at time 0.

Introducing the notation $n(T, t) = N f(T, t)$, where $n(T, t)\,dT$ expresses the number of particles in the system having temperature from the interval $(T, T + dT)$ at time t, finally we get the equation

$$\begin{aligned} \frac{\partial n(T, t)}{\partial t} = {} & k\Bigg(- f(T, t) + \frac{1}{N} \int_{T_{\min}}^{T_{\max}} \int_0^1 f\left(\frac{2(T-S)}{z} + S, t\right) \\ & \times f(S, t) f_\omega(z) \frac{2}{z} \, dz \, dS \Bigg), \quad t > 0 \\ f(T, 0) = {} & f_0(T), \quad T \in [T_{\min}, T_{\max}] \end{aligned} \tag{10}$$

This equation is, in essence, the population balance equation of the heat transfer process under the conditions specified previously, and it describes the time evolution of the population density function $n(., .)$ characterising the temperature distribution of the population of particles. Note, that, since N is constant, Eqs. (9) and (10) are equivalent. Also, it is worth to mention that, as it was expected, the population density function is symmetrical to the point $\frac{T_{\min} + T_{\max}}{2}$ for any value of $t > 0$ supposing the symmetry holds for the function $n_0(T)$.

4. Analysis of the moment equations

The moments of the population density function $n(., .)$, expressed as

$$M_I(t) = \int_{T_{\min}}^{T_{\max}} T^I n(T, t) \, dT, \quad I = 0, 1, 2, \ldots \tag{11}$$

often provide very useful information about the system, especially when the integro-differential equation (10) may not be solved explicitly.

Multiplying both sides of Eq. (10) by T^I and integrating from $T_{\min}$ to $T_{\max}$, after some transformations (the details see in Appendix A), we obtain the following system of ordinary differential equations:

$$\frac{\mathrm{d}M_I(t)}{\mathrm{d}t} = k\left(-M_I(t) + \frac{1}{N}\sum_{i=0}^{I} M_i(t)M_{I-i}(t)f_{i,I}\right),$$
$$I = 0,1,2,\ldots \quad t>0$$
$$M_I(0) = M_{I,0} \tag{12}$$

where

$$f_{i,I} = \int_0^1 \binom{I}{i}\left(\frac{z}{2}\right)^i\left(1-\frac{z}{2}\right)^{I-i} f_\omega(z)\,\mathrm{d}z \tag{13}$$

We note that $\sum_{i=0}^{I} f_{i,I} = 1$ and $f_{i,I} \geqslant 0$. Furthermore, in the case of $i \geqslant 1$ $f_{i,I} = 0$ if and only if $f_\omega(z)$ is Dirac-delta function at $z=0$. Eq. (12) forms a recursive set of ordinary equations, i.e. if we know $M_0(t), M_1(t), \ldots, M_{I-1}(t)$, then Eq. (12) is a linear inhomogeneous differential equation for $M_I(t)$.

When $I=0$, then $\mathrm{d}M_0(t)/\mathrm{d}t = 0$, that is $M_0(t) \equiv M_{0,0}(=N)$, as it was expected, since it means that the total number of particles is constant. For $I=1$ we obtain $\mathrm{d}M_1(t)/\mathrm{d}t = 0$ that is $M_1(t) \equiv M_{1,0}$. This means that during the heat transfer process the total amount of heat of the system also remains constant, according to the expectations. This latter consequence, together with the case $I=0$, indicates that our model is an adequate model of the physical process. In the case of $I=2$

$$\frac{\mathrm{d}M_2(t)}{\mathrm{d}t} = -kf_{1,2}\left(M_2(t) - \frac{M_{1,0}^2}{M_{0,0}}\right) \tag{14}$$

from which we obtain

$$M_2(t) = \left(M_{2,0} - \frac{M_{1,0}^2}{M_{0,0}}\right)\mathrm{e}^{-kf_{1,2}t} + \frac{M_{1,0}^2}{M_{0,0}} \tag{15}$$

Using this expression, we can calculate the standard deviation, namely

$$\sigma^2(t) = \frac{M_2(t)}{M_0(t)} - \frac{M_1^2(t)}{M_0^2(t)} = \left(\frac{M_{2,0}}{M_{0,0}} - \frac{M_{1,0}^2}{M_{0,0}^2}\right)\mathrm{e}^{-kf_{1,2}t}$$
$$= \sigma^2(0)\mathrm{e}^{-kf_{1,2}t}. \tag{16}$$

Taking into account our former remark concerning $f_{i,I}$, we see that if $t \to \infty$ then $\sigma^2(t) \to 0$ except when $f_\omega(z)$ is a Dirac-delta function at $z=0$. This is the special case when there is no heat transfer between the particles at all. In general, the model predicts that the temperature distribution of the particle population is equilising with time and becomes uniform as $t \to \infty$.

Since we have the equality

$$f_{1,2} = m_{1,\omega}\left(1 - \frac{m_{1,\omega}}{2}\right) - \frac{\sigma_\omega^2}{2} \tag{17}$$

where $m_{1,\omega} = \int_0^1 z f_\omega(z)\,\mathrm{d}z$ is the expectation of ω and $\sigma_\omega^2 = \int_0^1 (z - m_{1,\omega})^2 f_\omega(z)\,\mathrm{d}z$ is its variance, thus $\sigma^2(t)$ is the function of $m_{1,\omega}$ and σ_ω^2 as it seen from Eq. (16).

Using Eq. (13) it is proved that $0 \leqslant f_{1,2}$. Furthermore, since $0 \leqslant m_{1,\omega} \leqslant 1$ one can conclude that $0 \leqslant m_{1,\omega}(1 - \frac{m_{1,\omega}}{2}) \leqslant \frac{1}{2}$, and the relation $f_{1,2} \leqslant \frac{1}{2}$ follows from Eq. (17). It can be easily seen also that $f_{1,2} = 0$ if and only if $f_\omega(z)$ is a Dirac-delta function at $z=0$, and $f_{1,2} = \frac{1}{2}$ if and only if $f_\omega(z)$ is a Dirac-delta function at $z=1$. As a consequence, $\sigma_0^2 \mathrm{e}^{-\frac{k}{2}t} \leqslant \sigma^2(t) \leqslant \sigma_0^2$ and the equalities hold if and only if $f_\omega(z)$ is a Dirac-delta function at $z=1$ or at $z=0$, respectively.

Analysing Eq. (16) it can be proved that $\sigma^2(t)$ is a monotonic decreasing function of $f_{1,2}$, $\sigma^2(t)$ is a monotonic increasing function of σ_ω^2 for any fixed $m_{1,\omega}$, and for any fixed σ_ω^2 $\sigma^2(t)$ is a monotonic decreasing function of $m_{1,\omega}$. These conclusions correspond to the physical requirements. If the expectation of ω is constant but its dispersion decreases, then the dispersion of the particle temperature becomes smaller, and if the dispersion of ω is constant but the expectation diminishes then the dispersion of the particle temperature increases. These facts indicate as well that our model is adequate to the physical process examined.

5. Numerical solution of the population balance equation

Since analytical solution of the integro-differential equation (10) is not known, thus a numerical procedure has been constructed for solving it, using discretization with respect to both the temperature and time. The temperature interval $[T_{\min}, T_{\max}]$ was transformed into interval $[0,1]$ by means of normalisation $(T - T_{\min})/(T_{\max} - T_{\min})$. This does not restrict the generality of the model, and does not alter the accuracy of simulation results.

Let us divide the time interval $(0,t)$ into M parts of length τ. We introduce mesh points $t_j = j \cdot \tau$, $(j = 0,1,\ldots,M)$. Similarly, let the temperature interval $[0,1]$ and the interval $[0,1]$ of the dummy variable z be divided into N equal parts using the mesh points $T_i = i \cdot h$ and $z_l = l \cdot h$, $i,l = 0,1,\ldots,N$, $h = \frac{1}{N}$. Now, replacing the time derivative in Eq. (10) by the time increment, and by applying a quadrature form to approximate the double integral, we obtain the following difference equation:

$$\frac{n(T_i,t_{j+1}) - n(T_i,t_j)}{\tau} = -kn(T_i,t_j) + \frac{k}{M_{0,0}}\sum_{k=0}^{N} a_k \cdot n(T_k,t_j)$$
$$\cdot \sum_{l=1}^{N} n\left(\frac{2\cdot T_i + (z_l - 2)\cdot T_k}{z_l}, t_j\right)$$
$$\cdot \frac{2}{z_l} \cdot f_l \cdot b_l + \text{error term} \tag{18}$$

where $i = 0,1,\ldots,N$ and $j = 0,1,\ldots,M-1$.

The constants a_k and b_l in Eq. (18) are the coefficients of the quadrature form which depend on N and the type of the quadrature applied, and $f_l = f_\omega(z_l)$. By means of Eq. (18), we approximate the values $n(T_i, t_{j+1})$ belonging to the $(j+1)$st plane of time from the values $n(T_i, t_j)$, i.e. from by the values belonging the jth plane of time.

Since the values $\frac{2\cdot T_i+(z_l-2)\cdot T_k}{z_l}$ in Eq. (18) usually do not meet the mesh points, these are determined additionally in each time step by means of interpolation on the basis of the previously determined values of the actual plane of time. Let the interpolation function be denoted by $\phi(T, t_j)$, then Eq. (18), neglecting the error term, can be written as

$$\tilde{y}_{i,j+1} = y_{i,j} + \tau\cdot\left(-ky_{i,j} + \frac{k}{M_{0,0}}\sum_{k=0}^{N} y_{k,j}\cdot a_k \cdot\sum_{l=1}^{N}\phi\left(\frac{2\cdot T_i+(z_l-2)\cdot T_k}{z_l}, t_j\right)\cdot\frac{2}{z_l}\cdot f_l\cdot b_l\right) \qquad (19)$$

where $i = 0, 1, \ldots, N$, $j = 0, 1, \ldots, M-1$, and $y_{i,0} = M_{0,0}\cdot\frac{n_0(T_i)}{\sum_{k=0}^{N} n_0(T_k)\cdot a_k}$.

Computing $\tilde{y}_{i,j+1}$ we have to take into account that $\phi(\frac{2\cdot T_i+(z_l-2)\cdot T_k}{z_l}, t_j) = 0$ when the value of $\frac{2\cdot T_i+(z_l-2)\cdot T_k}{z_l}$ is out of the interval $[0, 1]$. After determining $\tilde{y}_{i,j+1}$ they are normalised in each time step by using the expression $y_{i,j+1} = M_{0,0}\cdot\frac{\tilde{y}_{i,j+1}}{\sum_{k=0}^{N}\tilde{y}_{k,j+1}\cdot a_k}$, in order to have the conservation law held.

In the numerical experiences, the composite trapezoidal rule and linear spline interpolation was applied. The value of parameter k was chosen 1. Comparing the differences between the analytically and numerically computed moments of the temperature distribution checked the accuracy of the numerical results. The moments determined by numerical method were computed as $m_{0,j} = \sum_{i=0}^{N} y_{i,j}\cdot a_i$; $m_{1,j} = \sum_{i=0}^{N} T_i y_{i,j}\cdot a_i$ and $m_{2,j} = \sum_{i=0}^{N} T_i^2 y_{i,j}\cdot a_i$.

In the case of the zeroth order moment, the differences were zero because of the normalised numerical values, but for first order moment we obtained errors as small as the round errors were.

The absolute values of the differences between the variances computed numerically and analytically for different values of h and τ are shown in Fig. 2. With increasing number of mesh points, the differences tend to zero what indicate the convergence of the method applied.

6. Simulation results and discussion

The behaviour of the population balance model developed was examined by simulation using a computer program written in Visual C++. Since the interval of variation of the temperature and parameter ω is $[0, 1]$, both the initial distribution of temperature and distribution of parameter ω were described with beta distributions. The computations were carried out in the time interval $[0, 7]$ with parameters $\tau = 1/40$ and $h = 1/20$ in all cases.

The time evolution of the population density function of temperature distribution of the particulate phase is presented in Figs. 3–5, starting from different initial density functions $n_0(T)$. In Fig. 3, $n_0(T) \equiv 1$ and $f_\omega(z) \equiv 1$ were chosen. It is seen that the density function $n(T, .)$, remaining symmetrical all time, gradually concentrates around the average value of temperature.

In Figs. 4 and 5, the initial density functions were chosen $90T(1-T)^8$ and $90T^8(1-T)$, respectively, but the density function $f_\omega(z)$ was identically 1 in both cases. It is seen well that the density functions kept the skew shapes of the initial density functions and they concentrate on lower and higher average temperature respectively.

The computational results, obtained for the initial population density function of temperature $n_0(T) \equiv 1$ and presented in Figs. 6–9, illustrate the influence of the density function $f_\omega(z)$ of random parameter ω. The

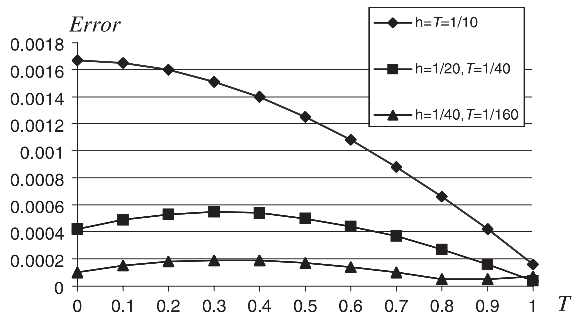

Fig. 2. Differences between the variances computed numerically and analytically.

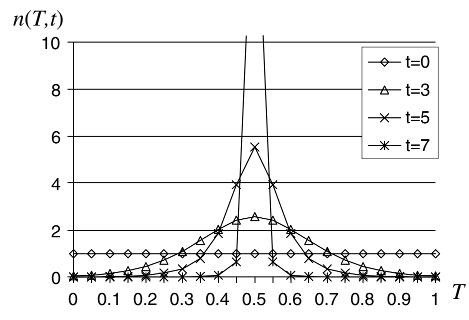

Fig. 3. Time evolution of the population density function of temperature starting from the initial distribution $n_0(T) \equiv 1$.

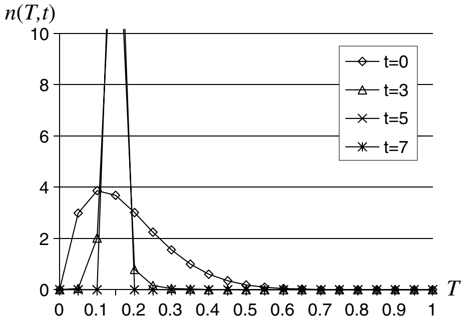

Fig. 4. Time evolution of the population density function of temperature starting from the initial distribution $n_0(T) = 90T(1-T)^8$.

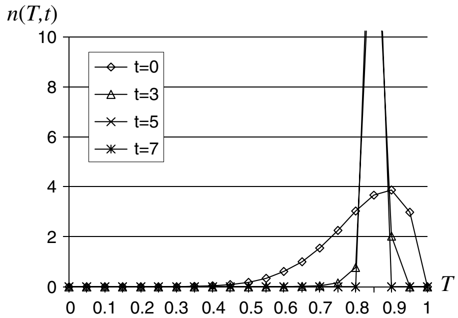

Fig. 5. Time evolution of the population density function of temperature starting from the initial distribution $n_0(T) = 90T^8(1-T)$.

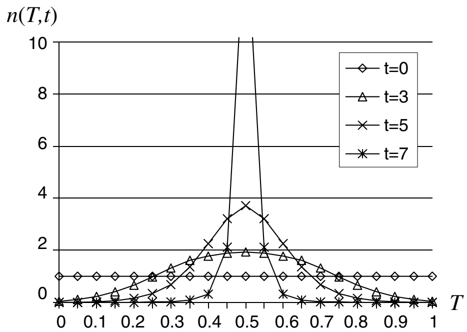

Fig. 6. The population density function at different moments of time obtained for the density function $f_\omega(z) = 2(1-z)$.

results shown in Fig. 6 were computed for $f_\omega(z) = 2(1-z)$, while results shown in Fig. 7 were obtained for the case $f_\omega(z) = 2z$. The population density functions of temperature at different moments of time are similar as regards the symmetry but the rates of equalisation of temperature differ from each other. This follows

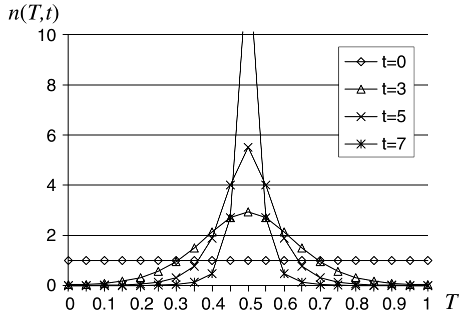

Fig. 7. The population density function at different moments of time obtained for the density function $f_\omega(z) = 2z$.

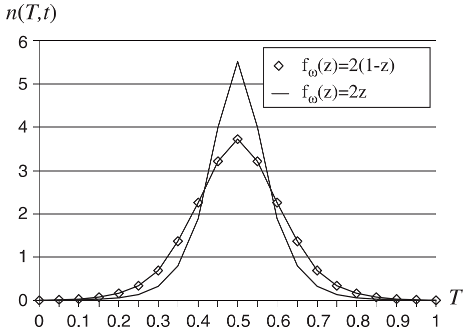

Fig. 8. Comparison of the population density functions obtained at time 5 for $f_\omega(z) = 2(1-z)$ and $f_\omega(z) = 2z$.

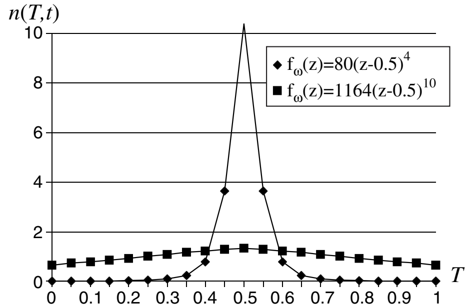

Fig. 9. Comparison of the population density functions at time 5 for $f_\omega(z) = 80(z-0.5)^4$ and $f_\omega(z) = 11,264(z-0.5)^{10}$.

from the fact that when $f_\omega(z) = 2(1-z)$ then $m_{1,\omega} = \frac{1}{3}$ and $\sigma_\omega^2 = \frac{1}{18}$, but when $f_\omega(z) = 2z$ then $m_{1,\omega} = \frac{2}{3}$ and $\sigma_\omega^2 = \frac{1}{18}$.

The population density functions in Figs. 6 and 7 obtained at time 5 are compared in Fig. 8. It illustrates well that the density function in the case of $f_\omega(z) = 2(1-z)$ is wider than that computed for $f_\omega(z) = 2z$ at the same time. It indicates also that the model corresponds to the physical requirements, as for fixed value of

σ^2_ω equalisation of the temperature proceeds with higher rate when the expectation of heat transfer parameter ω is larger. This also fits the results obtained with the aid of the moment analysis.

Also, as it was established analysing the moment equations, for fixed value of $m_{1,\omega}$, the rate of equalisation of the temperature is higher when σ^2_ω is smaller. Illustration of this statement is presented in Fig. 9. Here, the density functions obtained for $f_\omega(z) = 80(z-0.5)^4$ and $f_\omega(z) = 11,264(z-0.5)^{10}$ at time $t=5$, computed for value $m_{1,\omega} = 0.5$ and initial density function $n_0(T) \equiv 1$, are presented. In the first case $\sigma^2_\omega = 5/28$ was chosen, but in the second case we had $\sigma^2_\omega = 11/52$. Fig. 9 shows that, as it is expected, in the case of $f_\omega(z) = 80(z-0.5)^4$ the population density function concentrates around the expectation more quickly.

7. Conclusions

Using a simple kinetic model with random parameters, a population balance model was developed for describing particle-to-particle heat transfer during collisions in fluid–solid processing systems. Using a stochastic approach for treating the events of particle population derived the population balance equation. The moment equations, describing the time evolution of the moments of the temperature distribution, were derived from the population balance equation that proved to be closed for any order.

The simulation results, obtained by solving the integro-differential equation using the finite difference technique combined with linear spline interpolation, indicate that the model developed provides a good tool for describing the temperature inhomogeneities of the population of particles in gas–solid systems. The model in the present form describes, as the simulation results also show quite well, the behaviour of a batch gas–solid system satisfactorily, and it allows taking into account a number of parameters affecting the process.

In further development of the model, the fluid-particle and wall-to-particle heat transfer processes will also be considered, and by means of such generalisation we will obtain population balance-based models for describing heat transfer processes in a number of fluid–solid processing systems. This is especially important in the case of the highly exothermic processes in which hot spots may appear because of the not satisfactory mixing of the particulate phase.

Acknowledgements

The work was supported by the Hungarian Research Foundation under Grants *T26228* and *T034406*. The financial support is gratefully acknowledged. Csaba Mi-hálykó is grateful for the financial support of the János Bolyai Research Fellowship of the Hungarian Academy of Science.

Appendix A

Derivation of the moment equations.

Taking into account that the interval $[T_{\min}, T_{\max}]$ can be transformed into interval $[0,1]$ by means of the transformation $x = \frac{T-T_{\min}}{T_{\max}-T_{\min}}$ and $y = \frac{S-T_{\min}}{T_{\max}-T_{\min}}$, we can use in our consideration interval $[0,1]$ instead of $[T_{\min}, T_{\max}]$ without any restriction.

Since $n(x,t) = 0$, if $x \notin [0,1]$, and $f_\omega(z) = 0$, if $\omega \notin [0,1]$ from Eq. (10), after determining the bounds, we obtain the following equations

$$\frac{\partial n(x,t)}{\partial t} = k\cdot\left[-n(x,t) + \frac{1}{N}\cdot\int_0^{2x}\frac{2}{z}f_\omega(z) \times \int_{\frac{2(x-1)}{2-z}+1}^{\frac{2x}{2-z}} n(y,t)\cdot n\left(\frac{2(x-y)}{z}. + y,t\right)\mathrm{d}y\,\mathrm{d}z + \frac{1}{N}\int_{2x}^{1}\frac{2}{z}f_\omega(z)\int_0^{\frac{2x}{2-z}} n(y,t)\cdot n\left(\frac{2(x-y)}{z} + y,t\right)\mathrm{d}y\,\mathrm{d}z\right],\quad \text{if } x\in[0,0.5]$$

and

$$\frac{\partial n(x,t)}{\partial t} = k\cdot\left[-n(x,t) + \frac{1}{N}\int_0^{2(1-x)}\frac{2}{z}f_\omega(z) \times \int_{\frac{2(x-1)}{2-z}+1}^{\frac{2x}{2-z}} n(y,t)\cdot n\left(\frac{2(x-y)}{z} + y,t\right)\mathrm{d}y\,\mathrm{d}z + \frac{1}{N}\int_{2(1-x)}^{1}\frac{2}{z}f_\omega(z) \times \int_{\frac{2(x-1)}{2-z}+1}^{1} n(y,t)\cdot n\left(\frac{2(x-y)}{z} + y,t\right)\mathrm{d}y\,\mathrm{d}z\right],$$

if $x \in]0.5, 1]$.

Then, introducing the notation

$$M_I^{(1)}(t) = \int_0^{0.5} x^I n(x,t)\,\mathrm{d}x \quad \text{and}$$

$$M_I^{(2)}(t) = \int_{0.5}^{1} x^I n(x,t)\,\mathrm{d}x$$

and taking into account that

$$M_I(t) = \int_0^1 x^I n(x,t)\,\mathrm{d}x = M_I^{(1)}(t) + M_I^{(2)}(t)$$

the moment equations will look like:

$$\frac{\partial M_I^{(1)}(t)}{\partial t} = k\cdot\left[-\int_0^{0.5} x^I n(x,t)\,\mathrm{d}x. + \frac{1}{N}\int_0^{0.5} x^I \int_0^{2x}\frac{2}{z}f_\omega(z) \times \int_{\frac{2(x-1)}{2-z}+1}^{\frac{2x}{2-z}} n(y,t)\cdot n\left(\frac{2(x-y)}{z}y,t\right) \mathrm{d}y\,\mathrm{d}z\,\mathrm{d}x + \frac{1}{N}\int_0^{0.5}x^I\int_{2x}^1 \frac{2}{z}f_\omega(z)\times\int_0^{\frac{2x}{2-z}} n(y,t)\cdot n\left(\frac{2(x-y)}{z}y,t\right)\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}x\right] \tag{A.1}$$

and

$$\frac{\partial M_I^{(2)}(t)}{\partial t} = k\cdot\left[-\int_{0.5}^{1} x^I n(x,t)\,\mathrm{d}x. + \frac{1}{N}\int_{0.5}^{1} x^I \int_0^{2(1-x)}\frac{2}{z}f_\omega(z) \times \int_{\frac{2(x-1)}{2-z}+1}^{\frac{2x}{2-z}} n(y,t)\cdot n\left(\frac{2(x-y)}{z}y,t\right) \mathrm{d}y\mathrm{d}z\mathrm{d}x + \frac{1}{N}\int_{0.5}^{1}x^I\int_{2(1-x)}^1 \frac{2}{z}f_\omega(z)\times\int_{\frac{2(x-1)}{2-z}+1}^{1} n(y,t)\cdot n\left(\frac{2(x-y)}{z}y,t\right)\mathrm{d}y\mathrm{d}z\mathrm{d}x\right] \tag{A.2}$$

Substituting the new variable $u=\frac{2(x-y)}{z}+y$ into Eqs. (A.1) and (A.2), we obtain

$$\frac{\partial M_I^{(1)}(t)}{\partial t} = -kM_I^{(1)}(t)+\frac{k}{N}\cdot\left[\int_0^{0.5}\int_0^{2x}\int_0^1\frac{2f_\omega(z)}{2-z} \times x^I n\left(\frac{2x-zu}{2-z},t\right)n(u,t)\,\mathrm{d}u\,\mathrm{d}z\,\mathrm{d}x + \int_0^{0.5}\int_{2x}^1\int_0^{\frac{2x}{z}}\frac{2f_\omega(z)}{2-z}x^I n\left(\frac{2x-zu}{2-z},t\right)n(u,t)\,\mathrm{d}u\,\mathrm{d}z\,\mathrm{d}x\right] \tag{A.3}$$

and

$$\frac{\partial M_I^{(2)}(t)}{\partial t} = -kM_I^{(2)}(t)+\frac{k}{N}\cdot\left[\int_{0.5}^1\int_0^{2(1-x)}\int_0^1\frac{2f_\omega(z)}{2-z} \times x^I n\left(\frac{2x-zu}{2-z},t\right)n(u,t)\mathrm{d}u\mathrm{d}z\mathrm{d}x + \int_{0.5}^1\int_{2(1-x)}^1\int_{\frac{2(x-1)}{z}+1}^{1}\frac{2f_\omega(z)}{2-z}x^I n\left(\frac{2x-zu}{2-z},t\right)n(u,t)\mathrm{d}u\mathrm{d}z\mathrm{d}x\right] \tag{A.4}$$

Now again, substituting the variable $y=\frac{2x-zu}{2-z}$ into Eqs. (A.3) and (A.4), and changing the order of integration, these equations take the forms

$$\frac{\partial M_I^{(1)}(t)}{\partial t} = -kM_I^{(1)}(t)+\frac{k}{N}\cdot\left[\int_0^1\int_0^1\int_{\frac{z(1-u)}{2-z}}^{\frac{1-zu}{2-z}} f_\omega(z) \times\left(\frac{z}{2}u\left(1-\frac{z}{2}\right)y\right)^I n(y,t)n(u,t)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}u + \int_0^1\int_0^1\int_0^{\frac{z(1-u)}{2-z}} f_\omega(z)\left(\frac{z}{2}u+\left(1-\frac{z}{2}\right)y\right)^I \times n(y,t)n(u,t)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}u\right] \tag{A.5}$$

and

$$\frac{\partial M_I^{(2)}(t)}{\partial t} = -kM_I^{(2)}(t)+\frac{k}{N}\cdot\left[\int_0^1\int_0^1\int_{\frac{1-zu}{2-z}}^{\frac{2-z-zu}{2-z}} f_\omega(z)\left(\frac{z}{2}u + \left(1-\frac{z}{2}\right)y\right)^I n(y,t)n(u,t)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}u + \int_0^1\int_0^1\int_{\frac{2-z-zu}{2-z}}^{1} f_\omega(z)\left(\frac{z}{2}u+\left(1-\frac{z}{2}\right)y\right)^I \times n(y,t)n(u,t)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}u\right] \tag{A.6}$$

Since the sequence inequalities $0\leqslant\frac{z(1-u)}{2-z}\leqslant\frac{1-zu}{2-z}\leqslant\frac{2-z-zu}{2-z}\leqslant 1$ hold, the integrals can be added leading to the equations

$$\frac{\partial M_I^{(1)}(t)}{\partial t} = -kM_I^{(1)}(t)+\frac{k}{N}\cdot\int_0^1\int_0^1\int_0^{\frac{1-zu}{2-z}} f_\omega(z) \times\left(\frac{z}{2}u+\left(1-\frac{z}{2}\right)y\right)^I n(y,t)n(u,t)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}u \tag{A.5$'$}$$

and

$$\frac{\partial M_I^{(2)}(t)}{\partial t} = -kM_I^{(2)}(t)+\frac{k}{N}\cdot\int_0^1\int_0^1\int_{\frac{1-zu}{2-z}}^1 f_\omega(z) \times\left(\frac{z}{2}u+\left(1-\frac{z}{2}\right)y\right)^I n(y,t)n(u,t)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}u \tag{A.6$'$}$$

and the equation governing the variation of the Ith moment of the temperature distribution takes the form

$$\frac{\partial M_I(t)}{\partial t} = -kM_I(t)+\frac{k}{N}\cdot\int_0^1\int_0^1\int_0^1 f_\omega(z) \times\left(\frac{z}{2}u+\left(1-\frac{z}{2}\right)y\right)^I n(y,t)n(u,t)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}u \tag{A.7}$$

Introducing the notation $f_{i,I}=\int_0^1\binom{I}{i}\cdot\left(\frac{z}{2}\right)^i\cdot\left(1-\frac{z}{2}\right)^{I-i} f_\omega(z)\,\mathrm{d}z$, Eq. (A.7) can be rewritten into the final form

$$\frac{\partial M_I(t)}{\partial t} = -kM_I(t)+\frac{k}{N}\cdot\int_0^1\int_0^1\sum_{i=0}^{I}u^i\cdot y^{I-i} \cdot n(u,t)n(y,t)\cdot f_{i,I}\,\mathrm{d}u\,\mathrm{d}y = k\left(-M_I(t)+\frac{1}{N}\cdot\sum_{i=0}^{I}M_i(t)\cdot M_{I-i}(t)\cdot f_{i,I}\right) \tag{A.8}$$

References

[1] C.K.K. Lun, S.B. Savage, D.J. Jeffrey, N. Chepurniy, Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flow field, J. Fluid Mech. 140 (4) (1984) 223–256.

[2] O. Simonin, Prediction of the dispersed phase turbulence in particle-laden jets, ASME, FED, Gas–Solid Flows 121 (1991) 197–206.

[3] M. Louge, J.M. Yusof, Heat transfer in the pneumatic transport of massive particles, Int. J. Heat Mass Transfer 36 (2) (1993) 265–275.

[4] D. Gidaspow, Multiphase Flow and Fluidization, Academic Press, San Diego, 1994.

[5] A. Berlemont, O. Simonin, M. Sommerfeld, Validation of inter-particle collision models based on large eddy simulation, ASME, FED, Gas–Solid Flows 228 (1995) 359–369.

[6] L.I. Zaichik, V.A. Pershukov, M.V. Kozelev, A.A. Vinberg, Modeling of dynamics, heat transfer, and combustion in two-phase turbulent flows 1. Isothermal flows, Exp. Thermal Fluid Sci. 15 (4) (1997) 291–310.

[7] M.J.V. Goldschmidt, J.A.M. Kuipers, W.P.M. van Swaaij, Hydrodinamic modelling of dense gas-fluidised beds using the kinetic theory of granular flow: effect of coefficient of restitution on bed dynamics, Chem. Eng. Sci. 56 (2) (2001) 571–578.

[8] A. Berlemont, P. Desjonqueres, G. Gouesbet, Particle Lagrangian simulation in turbulent flows, Int. J. Multiphase Flow 16 (1) (1990) 19–34.

[9] T. Tanaka, Y. Tsuji, Numerical simulation of gas–solid two-phase flow in a vertical pipe: on the effect of interparticle collision, ASME, FED, Gas–Solid Flows 121 (1991) 123–128.

[10] Y. Tsuji, T. Kawaguchi, T. Tanaka, Discrete particle simulation of two-dimensional fluidized bed, Powder Technology 77 (1993) 79–87.

[11] M. Sommerfeld, Modelling of particle-wall collisions in confined gas-particle flows, Int. J. Multiphase Flow 18 (6) (1992) 905–926.

[12] B. Oesterle, A. Petitjean, Simulation of particle-to-particle interactions in gas–solid flows, Int. J. Multiphase Flow 19 (2) (1993) 199–211.

[13] M. Sommerfeld, Modeling and numerical calculation of turbulent gas–solid flows with the Euler/Lagrange approach, Kona 16 (2) (1998) 194–205.

[14] R. Avila, J. Cervantes, Analysis of heat transfer coefficient in a turbulent particle pipe flow, Int. J. Heat Mass Transfer 38 (11) (1995) 1923–1932.

[15] P. Boulet, S. Moissette, R. Andreux, B. Oesterle, Test of an Eulerian–Lagrangian simulation of wall heat transfer in a gas–solid pipe flow, Int. J. Heat Mass Transfer 21 (2) (2000) 381–387.

[16] A. Schmidt, U. Renz, Numerical prediction of heat transfer in fluidized beds by a kinetic theory of granular flows, Int. J. Therm. Sci. 39 (9–11) (2000) 871–885.

[17] Z. Mansoori, M. Saffar-Avval, H. Basirat-Tabrizi, G. Ahmadi, Modeling heat transfer in of turbulent gas–solid flow, Int. J. Heat Mass Transfer 45 (6) (2002) 1173–1184.

[18] Z. Mansoori, M. Saffar-Avval, H. Basirat-Tabrizi, G. Ahmadi, S. Lain, Thermo-mechanical modeling of turbulent heat transfer in gas–solid flows including particle collisions, Int. J. Heat Fluid Flow 23 (6) (2002) 792–806.

[19] C. Delvosalle, J. Vanderschuren, Gas-to-particle and particle-to-particle heat transfer in fluidized beds of large particles, Chem. Eng. Sci. 40 (5) (1985) 769–779.

[20] J. Vanderschuren, C. Delvosalle, Particle-to-particle heat transfer in fluidized bed drying, Chem. Eng. Sci. 35 (8) (1980) 1741–1748.

[21] T. Blickle, B.G. Lakatos, Cs. Mihálykó, Modeling interactive populations of solid particles, Bulg. Chem. Commun. 31 (2) (2000) 378–391.

[22] Cs. Mihálykó, B.G. Lakatos, T. Blickle, Modelling heat transfer between solid particles, Math. Comp. Simul. 53 (3) (2000) 403–408.

[23] T. Blickle, B.G. Lakatos, Cs. Mihálykó, Mathematical Models of Particulate Systems, A kémia újabb eredményei-89, Akadémiai Kiadó, 2001, pp. 173–348 (in Hungarian).

[24] M.L. Hunt, Discrete element simulations for granular material flows: effective thermal conductivity and self-diffusivity, Int. J. Heat Mass Transfer 40 (13) (1997) 3059–3068.

[25] M. Sommerfeld, Validation of a stochastic Lagrangian modelling approach for inter-particle collisions in homogeneous isotropic turbulence, Int. J. Multiphase flow 27 (12) (2001) 1829–1858.