DETERMINATION OF EFFECTIVE HEAT TRANSPORT COEFFICIENTS FOR WALL-COOLED PACKED BEDS

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ABSTRACT

THE INFLUENCE IS STUDIED OF SEVERAL ASSUMPTIONS, OFTEN MADE IN LITERATURE, ON THE VALUES FOR THE EFFECTIVE RADIAL HEAT CONDUCTIVITY, WALL HEAT TRANSFER COEFFICIENT AND OVERALL HEAT TRANSFER COEFFICIENT, AS OBTAINED FROM EXPERIMENTS IN WALL-COOLED PACKED BEDS WITHOUT A CHEMICAL REACTION. ESPECIALLY THE CHOICE OF THE INLET BOUNDARY CONDITION CAN HAVE A LARGE IMPACT ON THE VALUES OBTAINED. THE INFLUENCE OF THE PRESENCE OF A RADIAL VELOCITY PROFILE AND ALSO THE CROSS-CORRELATION OF THE PARAMETERS OBTAINED IS STUDIED.

INTRODUCTION

For performing highly exothermic, catalytic reactions in industry often a cooled tubular reactor is used. A major problem with such a reactor is runaway to very high temperatures. It is important to prevent this and to study the behaviour of such a reactor a-priori by computer simulation. For this purpose a good mathematical reactor model is needed, capable of predicting the temperature and concentration profiles in the reactor, given a certain reactor design and operating conditions. Here the description of heat transport in wall-cooled packed beds at a low tube-to-particle diameter ratio, using the pseudo-homogeneous one- and two-dimensional continuum models, is discussed.

MODEL EQUATIONS

The system studied is a hot gas, cooled down in a wall-cooled packed tube with a small number of particles on a diameter. For modelling the heat transport, the following assumptions are made; 1- the system is at steady state and no reaction is carried out, 2- the system is considered to be pseudo-homogeneous, 3- there is no axial dispersion of heat, 4- there is no free convection of heat, 5- there is no radiation, 6- the superficial velocity is constant over the radius, 7- the pressure is constant in the packed bed, 8- the wall temperature is constant, 9- the physical properties of the gas and the solid are independent of the temperature and 10- the inlet temperature profile can be described by a parabola.

A heat balance for an infinitesimally small disc, assuming constant radial temperature, yields the following dimensionless, pseudo-homogeneous one-dimensional model:

$$\frac{\partial \theta^{MC}}{\partial \omega} = -4\,St^{P}\,\theta^{MC}, \quad \text{with the inlet condition:} \quad \omega = 0, \quad \theta^{MC} = \theta_0^{MC} \qquad (1,2)$$

Solving eq. (1) together with eq. (2) yields:

$$\theta^{MC} = \theta_0^{MC}\,\exp\{-4\,St^{P}\,\omega\} \qquad (3)$$

Equation (3) describes the axial temperature profile with only one model parameter St^{P}, containing the overall heat transfer coefficient U_{ov}.

A heat balance for an infinitesimally small ring yields the following dimensionless, pseudo-ho-

mogeneous two-dimensional model:

$$\frac{\partial \theta}{\partial \omega} = \frac{1}{Bo_{h,r}^{\Theta}} \frac{1}{\rho} \frac{\partial}{\partial \rho} \left[\rho \frac{\partial \theta}{\partial \rho} \right]$$ (4)

Subject to:

$$\omega = 0, \quad all \ \rho, \qquad \theta = 1 - A \rho^2$$ (5a)

$$\rho = 0, \quad all \ \omega, \qquad \frac{\partial \theta}{\partial \rho} = 0$$ (5b)

$$\rho = 1, \quad all \ \omega, \qquad \frac{\partial \theta}{\partial \rho} = - Bi_t \theta$$ (5c)

Equation (4) together with eqs. (5a)-(5c) can be solved to yield:

$$\theta(\rho,\omega) = 2 \sum_{i=1}^{\infty} \left\{ \left[\frac{(Bi_t \beta_i^2 + 4 A Bi_t - 2 A \beta_i^2 - A Bi_t \beta_i^2) J_0(\beta_i \rho)}{\beta_i^3 \left[\beta_i J_0(\beta_i) + Bi_t J_1(\beta_i) \right]} \right] \exp \left[\frac{- \beta_i^2 \omega}{Bo_{h,r}^{\Theta}} \right] \right\}$$ (6)

in which β_i is found from:

$$\beta_i J_1(\beta_i) - Bi_t J_0(\beta_i) = 0$$ (7)

Equation (6) describes the axial and radial temperature profiles with two model parameters $Bo_{h,r}^{\Theta}$ and Bi_t, containing the effective radial heat conductivity $\lambda_{e,r}$ and the wall heat transfer coefficient h_w, respectively.

Values for θ_0^{MC}, U_{ov}, A, $\lambda_{e,r}$ and h_w for the two models are obtained by fitting eqs (2), (3), (5a) and (6) to experimentally determined temperature profiles.

EXPERIMENTAL SET-UP

The set-up to measure radial and axial temperature profiles contains three stainless steel wall-cooled tubes, with a length of 1.33 m and inner diameters of 49.9, 63.5 and 99.0 mm, respectively. The tubes are filled with a packing and cooled at the wall with water of about 283 K, flowing through a jacket. Hot air with a temperature of about 333 K, flows upwards through the tubes and is cooled down at the wall. In the steady state, the radial temperature profile is measured in the packed bed near the top with 7 to 15 K-type thermocouples of 0.5 mm diameter, fixed in a non-conducting rectangular rod of 2×2 mm, which is placed radially through the centre of the packed bed. The temperature of the gas at the inlet of the packed bed, the coolant temperature at the inlet and outlet, the pressure before and after the bed and the gas flow rate are also measured. During the measurements, the bed can easily be repacked by fluidizing the packing. In Fig. 1 an example of a set of measured radial temperature profiles is given, after repacking the bed only. Radial temperature profiles at different axial positions are obtai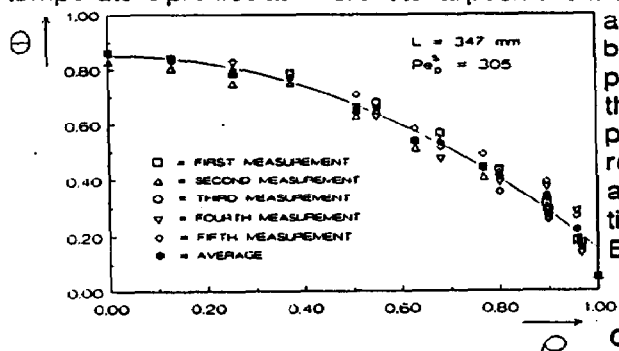ned by lowering the bed support in the tubes and adding extra packing material at the top. Combination of the averaged radial temperature profiles, as obtained for different axial positions at the same experimental conditions, yields a temperature field for the whole tube. All experiments reported here have been performed with air at atmospheric pressure. For a more detailed description of the set-up and the measuring procedure, see Borkink (1991).

Figure 1; Experimentally determined radial temperatures and fitted parabolic profile for glass spheres with $d_p^v = 7.2$ mm. Results for a tube with $D_t = 99.0$ mm and for a certain bed length and gas flow rate.

CORRELATIONS FOR THE EFFECTIVE TRANSPORT COEFFICIENTS

Experimental values for $\lambda_{e,r}$, h_w and U_{ov} are obtained for different gas flow rates, tube diameters and packings. In Figs 2 and 3 experimental values
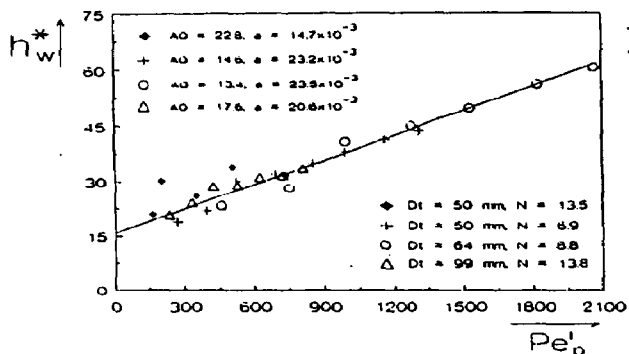
Figure 2;   Best fit values for $\lambda_{e,r}$ as a function of the gas flow rate for glass spheres with $d_p^e = 3.7$ or 7.2 mm.
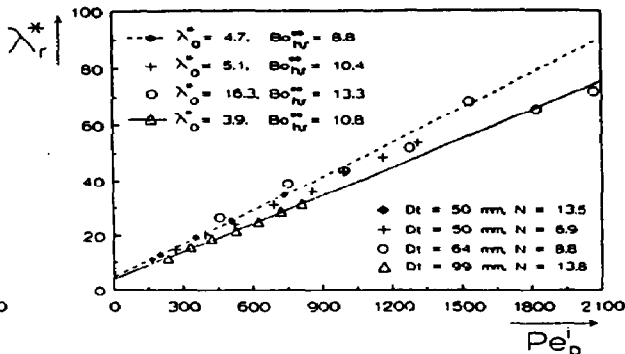
Figure 3;   Best fit values for h_w as a function of the gas flow rate for glass spheres with $d_p^e = 3.7$ or 7.2 mm.

for the first two parameters are given, for a packing consisting of glass spheres. Other packings investigated consisted of alumina cylinders and Raschig rings. From these figures it can be seen that the tube diameter does not seem to have any influence on the values for $\lambda_{e,r}$ and h_w. The effective radial heat conductivity, as obtained from the experimental set-up, could best be correlated as a function of the gas flow rate by;

$$\lambda_r^* = \lambda_o^* + \frac{Pe_p^s}{Bo_{h,r}^{\infty}}$$ (8)

in which:

$\lambda_0^* = 4.7$ and $Bo_{h,r}^{\infty} = 8.8$ for *glass spheres with* $d_p^e = 3.7$ *mm*

$\lambda_0^* = 6.2$ and $Bo_{h,r}^{\infty} = 10.9$ for *glass spheres with* $d_p^e = 7.2$ *mm*

$\lambda_0^* = 4.0$ and $Bo_{h,r}^{\infty} = 7.6$ for *alumina cylinders with* $d_p^e = 5.9$ *mm*

$\lambda_0^* = 4.5$ and $Bo_{h,r}^{\infty} = 4.2$ for *alumina Raschig rings with* $d_p^e = 6.2$ *mm*

The wall heat transfer could best be correlated by;

$$h_w^* = A0 + a\, Pe_p^j$$ (9)

in which:

$A0 = 16.3$ and $a = 0.022$ for *glass spheres*
$A0 = 10.1$ and $a = 0.021$ for *alumina cylinders*
$A0 = 17.9$ and $a = 0.018$ for *alumina Raschig rings*

The overall heat transfer coefficient could best be correlated by:

$$\frac{1}{U_{ov}^*} = \frac{1}{h_w^*} + \frac{N}{\beta\, \lambda_{e,r}^*}$$ (10)

together with the correlations for $\lambda_{e,r}^*$ and h_w^* as given above. The best fit value for the so called "lump factor" β was 7.4, for all the available data. For a more general discussion of these and other results see Borkink and Westerterp (1992a).

CONFIDENCE INTERVALS

It is important to know the confidence intervals for the effective heat transport coefficients, as obtained from cold-flow experiments. Also it is important to know if, and to what extent, the parameters as used in a model description are cross-correlated. It is possible to show how the fit parameters $\lambda_{e,r}$ and h_w are cross-correlated by looking at the shape of the target function for different values of the parameters. A contour of the target function in a $\lambda_{e,r}$ - h_w plain, containing 68% of the probability distribution for the best fit values, is given in Fig. 4. In this figure also the value is given for the parameter γ, which is used in the following equation:
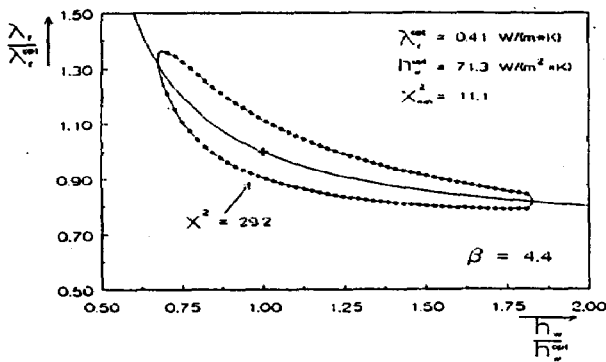
Figure 4;   Confidence region for a tube with D_t = 49.9 mm, filled with glass spheres of d_p^s = 7.2 mm and for Pe_p^s = 105.

$$\frac{\lambda_{e,r}}{\lambda_{e,r}^{opt}} = \cfrac{1}{\left[1 + \cfrac{\gamma\,\lambda_{e,r}^{opt}}{D_t\,h_w^{opt}}\left\{1 - \left(\cfrac{h_w^{opt}}{h_w}\right)\right\}\right]} \qquad (11)$$

to describe the line through the minimum in the target function χ^2. Equation (11) is derived from the lump equation, as given by Eq. (10), assuming U_{ov} is constant. The factor γ, as used in eq. (11), should not be confused with the lump factor as given in literature, see e.g. Crider and Foss (1965). Eq. (11) is only used to show that the cross-correlation of $\lambda_{e,r}$ and h_w can be described by an equation that is very close - but not equal - to the lump equation.

CHOICE OF THE INLET BOUNDARY CONDITION.

In literature often a length dependence of the heat transport coefficients is observed. In the previous section we assumed the radial gas inlet temperature to be parabolically shaped, see eq. (5a). However, often the following inlet condition is used:

$$\omega = 0, \ all \ \rho, \qquad \theta = 1 \qquad (12)$$

In Fig. 5 best fit values for the overall heat transfer coefficient U_{ov} are given for different values of

Figure 5;   Overall heat transfer coefficients for different bed lengths, for a tube with D_t = 99.0 mm and filled with alumina Raschig rings of d_p^s = 6.2 mm.

the number of particles on the bed height N_l. These figures are calculated for the case a parabolic inlet temperature profile is used, as well as for a radially flat inlet temperature profile, based on the centre temperature at the inlet. From these figures it can be seen that a "length effect" is nearly absent in case a parabolic inlet temperature profile is used. For a more general discussion of the influence of the choice of the inlet boundary condition see Borkink et al. (1992b).
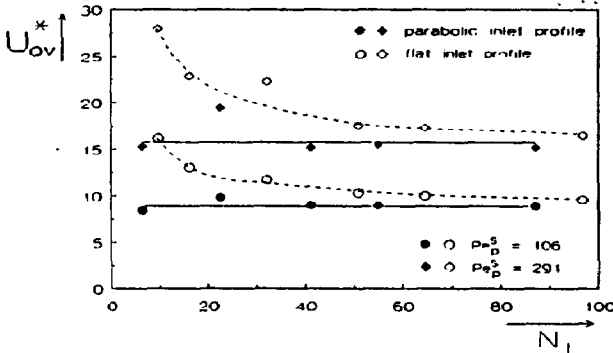
Assuming a radially flat inlet temperature profile, whereas the actual profile is curved, may also lead to an apparent influence of an axial dispersion of heat. An overestimation of the inlet gas temperature - in case of cooling - can be compensated for by a assuming a lower temperature or a "temperature jump" at the inlet, as is done with the Danck-

werts inlet boundary condition:

$$\omega = 0, \qquad \frac{\partial\theta^{MC}}{\partial\omega} = -Pe_{h,a}^{\theta}\left(1 - \theta^{MC}\right) \qquad (13)$$

Because eq. (13) can compensate for the over- or underestimation of the inlet gas temperature, also the apparent length dependence of the transport coefficients seemingly vanishes if axial dispersion of heat is included in the model equations, see Borkink and Westerterp (1992c).

INFLUENCE OF A RADIAL VELOCITY PROFILE.

The influence of a non-constant radial porosity and velocity profile was studied theoretically, as well as experimentally, using a first order approximation for these profiles, see Borkink (1991). In this approximation the packed bed is divided into two regions, each with a different but constant
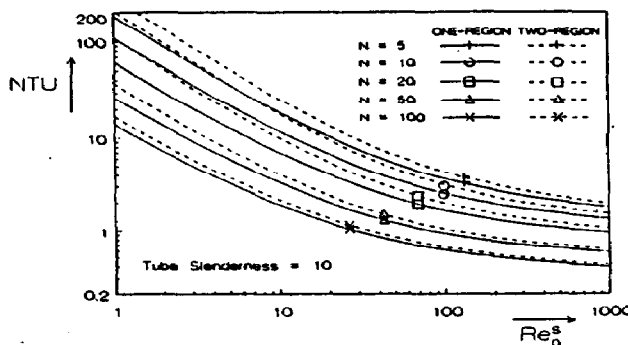
Figure 6; Calculated values for NTU for laboratory conditions with $\Gamma = 10$ and $\lambda_{e,r} \neq f(r)$.

porosity and superficial velocity, called the two-region model. The gas flow rate through the wall region is higher than through the core region and the total gas flow through the two zones is equal to the average. By doing so the heat balance for a wall-cooled packed bed, in which a hot gas is cooled down without reaction, can be solved analytically. The radial superficial velocity profiles on which the calculations were based, were taken from literature [Vortmeyer and Schuster (1983)]. In Fig. 6 the calculated number of heat transfer units NTU is given as a function of the Reynolds number, for different values of the number of particles on a diameter. Literature relations were used for the heat transfer coefficients and $\lambda_{e,r}$ was assumed constant over the radius. As can be seen from Fig. 6, the NTU is always higher in case a a two-region model is used, due to the higher volumetric flow rate near the wall. Also, it can be shown that if best fit values for the heat transport coefficients are obtained from cold-flow experiments, the two-region model yields a lower $\lambda_{e,r}$ compared to the value obtained from the one-region model.

CONCLUSIONS

One should be very careful in choosing the inlet boundary condition, when modelling the heat transport in wall-cooled packed beds. If the inlet temperature profile is assumed to be radially flat, whereas the actual profile is curved, an apparent length dependence of the heat transport coefficients and an apparent influence of an axial dispersion can be found. The presence of a radial superficial velocity profile may lead to a higher overall rate of radial heat transport. The effective radial heat conductivity and the wall heat transfer coefficient are found to be strongly cross-correlated and both parameters are found to be independent of the tube diameter.

NOTATION

A_p	surface area of a particle [m^2]		Bi_t	$= \dfrac{h_w R_t}{\lambda_{e,r}}$, tube Biot number [-]
$Bo_{h,r}$	$= \dfrac{\rho_g C_{pg} v\, d_p^e}{\lambda_{e,r}}$, Bodenstein number for radial heat dispersion [-]		$Bo_{h,r}^-$	Bodenstein number for heat at fully developed turbulent flow [-]
$Bo_{h,r}^\theta$	$= \dfrac{\rho_g C_{pg} v\, R_t^2}{\lambda_{e,r} L} = \dfrac{Bo_{h,r} N}{4\,\Gamma}$, modified radial Bodenstein number for heat [-]		C_{pg}	specific heat of the gas at constant pressure [$J\,kg^{-1}\,K^{-1}$]
D_t	tube diameter [m]		d_p^e	$= \dfrac{6\,V_p}{A_p}$, equivalent diameter of a sphere [m]
h_w	wall heat transfer coefficient [$W\,m^{-2}\,K^{-1}$]		h_w^*	$= \dfrac{h_w\, d_p^e}{\lambda_g}$, dimensionless wall heat transfer
J_0, J_1	zeroth-order and first-order Bessel functions of the first kind [-]			coefficient [-]
			N	$= \dfrac{D_t}{d_p^e}$, number of particles on a diameter [-]
L	bed length [m]		Pe_p^s	$= \dfrac{\rho_g C_{pg} v\, d_o^e}{\lambda_g} = Re_p^s\, Pr$, molecular Peclet
Pr	$= \dfrac{\eta_g C_{pg}}{\lambda_g}$, Prandtl number for the gas [-]			number based on the superficial velocity [-]
Re_p^s	$= \dfrac{\rho_g v\, d_p^e}{\eta_g}$, Reynolds number based on the superficial velocity [-]		R_t	tube radius [m]
			r	radial coordinate [m]
St	$= \dfrac{U_{ov}}{\rho_g C_{pg} v}$, Stanton number for the overall heat transfer coefficient [-]		St^ρ	$= \dfrac{U_{ov} L}{\rho_g C_{pg} v\, D_t} = St\,\Gamma$, modified Stanton number [-]
			T	temperature [K]
T_0	temperature in the centre of the packed bed		U_{ov}	overall heat transfer coefficient [$W\,m^{-1}\,K^{-1}$

	at the first axial positions [K]	U_{ov}^*	$= \dfrac{U_{ov} d_p^e}{\lambda_g}$, dimensionless overall heat transfer coefficient [-]	u
V_p	volume of a particle [m^3]			
v	superficial gas velocity [$m\,s^{-1}$]	z	axial coordinate [m]	
χ^2	$= \displaystyle\sum_{i=1}^{n}\left(\dfrac{\theta_i - \theta(\rho,\omega,U_{ov},\lambda_{e,r},h_w)}{\sigma_i}\right)^2$, chi-square	ε_b	average porosity of the bed [-]	
	target function [-]	η_g	dynamic viscosity of the gas [$Pa\,s$]	
Γ	$= \dfrac{L}{D_t}$, tube slenderness [-]	λ_g	heat conductivity of the gas [$W\,m^{-1}\,K^{-1}$]	
$\lambda_{e,r}$	effective radial heat conductivity [$W\,m^{-1}\,K^{-1}$]	λ_0	effective heat conductivity of the packed bed with	
λ_r^*	$= \dfrac{\lambda_e}{\lambda_g}$, dimensionless effective radial heat		a stagnant fluid [$W\,m^{-1}\,K^{-1}$]	
	conductivity [-]	ω	$= \dfrac{z}{L}$, dimensionless axial coordinate [-]	
ρ	$= \dfrac{r}{R_t}$, dimensionless radial coordinate [-]	ρ_g	density of the gas [$kg\,m^{-3}$]	
σ	standard deviation [-]	θ	$= \dfrac{(T - T_{cl})}{(T_0 - T_{cl})}$, dimensionless temperature [-]	
θ^{MC}	$= 2\displaystyle\int_0^1 \rho\,\theta(\rho,\omega)\,d\rho$, mean-cup temperature [-]			

Subscripts

cl	coolant
e	effective
g	gas
p	particle
r	radial
t	tube
w	wall

Superscripts

e	equivalent
i	interstitial
s	superficial

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