Heat Transfer in Adsorption Heat Exchangers between Pellets and Fins

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Abstract: Adsorption heat exchangers (AdHXs) are important components in adsorption heat pumps and chillers, often build as fin-and-tube type heat exchangers with beds of adsorbent pellets. For design and optimization the governing transport phenomena in AdHXs need to be quantified as functions of design parameters like geometry or material properties. In this work the heat transfer between fin surface and adsorbent pellet is analyzed using a three-dimensional COMSOL model. The model is evaluated for generic material combinations with a variation of parameters: pellet size (0.2-4 mm), pellet roughness (20-100 µm) and thermal conductivity of gas (0.01-0.03 W/(m K)) and pellet (0.1-0.3 W/(m K)). The calculated effective heat transfer coefficient is in the range of 16-670 W/(m^2 K). From the simulation results a general Nusselt correlation is deduced allowing a direct calculation of the heat transfer coefficient within the parameter space.

Keywords: Adsorption heat exchanger, heat transfer, pellet, fin, Nusselt number

1 Introduction

Adsorption heat exchangers (AdHXs) are important components in adsorption heat pumps and chillers, a primary energy efficient source of heating and cooling[1,2]. Due to availability and established inexpensive manufacturing, fin-and-tube type heat exchangers with beds of adsorption pellets in the finned space are used in state of the art products. The same design is used for sorption seasonal heat storage with pellets of hydrophilic salt hydrates[3].

For design and optimization the adsorption cycle needs to be modelled with its transient nature[4,5]. Hence, the governing transport phenomena in AdHXs need to be quantified as functions of design parameters like geometry or material properties. This has e.g. been done using complex partial differential equation (PDE) models of the whole AdHX including heat and mass transfer and fluid flows with different level of detail[6–9]. These models allow detailed analyses of geometry and material influences. However, they require high computing times and are e.g. unsuitable to analyze the component's behavior in a system like a building on long time scales.

Simpler transient models are based on ordinary differential equations (ODE)[8] with lumped coefficients for transport resistances and capacitances. They can be parameterized using PDE-models, either by fitting the ODE-model to the PDE-model's results, or by direct deduction of the coefficients from the PDE-model. In this study an example of the latter is presented. For AdHXs ODE-models where shown to reproduce the external behavior of complex PDE-models with high accuracy while demanding orders of magnitude less computing time[10]. However, a variation of design parameters usually requires the complex model to be re-computed.

Some transport resistances can be directly modelled in a lumped form from correlations available in standard literature (e.g. the heat transfer in a pipe flow). These correlations are mostly based on extensive measurements[11]. With them it is possible to include certain design parameters (e.g. the pipe diameter) explicitly in the ODE-model. Parameter variations can then be carried out without re-computing a PDE-model.

In this work a general correlation is deduced from simulation results of a three-dimensional COMSOL model. This is done for the heat transfer between fin surface and adsorbent pellets, an important transport resistance in the described type of AdHX. This heat transfer has been investigated for different configurations[7,12,13]. Here, it is analyzed for the case of a monolayer of pellets on the fin surface. First the model and its implementation in COMSOL will be described, then the results will be presented and a general heat transfer correlation will be deduced.

2 Mathematical Model

The modelled heat exchanger consists of flat fins of metal and spherical porous pellets of adsorp-

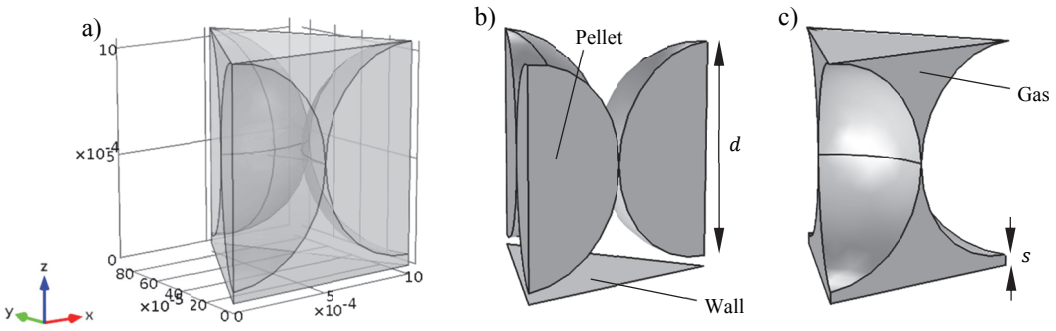

Figure 1: Model geometry implemented in COMSOL: a) complete transparent model, b) pellet domain and wall surface, c) gas domain

tion material. During the adsorption process a gas is adsorbed on the internal surface of the adsorption material. The resulting heat of adsorption leads to a higher pellet temperature and thus a heat transfer to the fin surface (wall) and from there through the fin to some heat exchanger fluid.

To study the heat transfer characteristic between the wall and the pellet a three-dimensional stationary heat conduction model is used. The model will be described in the following.

2.1 Geometry

The modelled geometry shown in Figure 1 is a three-dimensional symmetrical section consisting of a pellet and a gas domain. A three-dimensional model is necessary to take into account the spherical pellet shape. The pellets are assumed to be a monolayer of close-packing of equal spheres with diameter d. The surface of the fin is only modelled as boundary to the gas domain. The usually rough surface of adsorption pellets is taken into account by a gap s between the wall and the pellets.

2.2 General assumptions

The model is based on the following general assumptions that are similar to those used by other authors[12]:

1. The heat transfer in the gas domain is dominated by conduction.
2. The gas domain can be treated as a continuum (Knudsen number $\ll 1$).
3. Material properties are constant throughout each domain.
4. Gas is adsorbed homogeneously throughout the pellet volume.
5. The heat conductivity of the fin in x and y is high compared to all other heat conductivities.

The first assumption may especially be made for monolayer pellet beds that are openly exposed to a gas volume on the upper side. For densely filled fin-and-tube heat exchangers this assumption is a simplification that requires to be revised if for a specific configuration information on the gas flow are available.

The second assumption reduces the model's validity for small geometries and low gas pressures. When the heat transfer distances are close to the mean free path of the gas molecules the continuum gas model is not valid anymore and the thermal conductivity decreases dramatically[14]. E.g. for the case of water vapor at common working conditions (p = 1-10 kPa, T = 280-370 K) the mean free path is in the range of 0.4-5 µm.

To allow for this effect a geometry dependent heat transfer would need to be implemented which is beyond the scope of the present work.

2.3 Governing equations

In both domains the stationary heat transfer is described by the heat equation

$$0 = \nabla(\lambda \nabla T) + \dot{q}_{\mathrm{ad}} \qquad (1)$$

with the heat conductivity λ_g or λ_p of the gas or pellet domain. The heat source from adsorption $\dot{q}_{ad}$ only applies to the pellet domain and is omitted for the gas domain.

2.4 Boundary conditions

As the fin's conductivity is high, compared to all other conductivities, a uniform wall temperature T_w is assumed. In the pellet volume the assumed homogenous adsorption results in a constant heat source $\dot{q}_{ad}$. All other boundaries are planes of symmetry with no-flux boundary conditions.

3 Implementation

The model has been implemented in COMSOL Multiphysics 4.4 as a "heat transfer in solids" problem.

Values used for geometry parameters, material properties and boundary conditions are given in Table 1. Though absolute values of the boundary conditions do not matter for the analysis used (temperature independent material properties, fully linear equations), the chosen values are within a realistic range for adsorption heat exchangers.

Standard meshing settings ("normal") were used. The mesh was refined to check for mesh invariance. The relative deviations of the results were in the order of the solver tolerance (0.001). No changes to standard solver settings where necessary.

Material properties in adsorption heat exchangers depend on actual materials (e.g. silica gel, zeolite, water vapor, methanol vapor), their properties (e.g. porosity) and state (pressure, temperature, loading). Pellet size and roughness depend on the manufacturing process. In order to analyze the heat transfer characteristic for this broad range of conditions a parametric sweep on pellet diameter d, pellet roughness s, gas conductivity λ_g and pellet conductivity λ_p was employed. The range of values covered is indicated in Table 1.

Table 1: Values used for simulation

Parameter		Value
pellet diameter	d	0.2-4 mm
pellet roughness	s	20-100 µm
gas conductivity	λ_g	0.01-0.03 W/(m K)
pellet conductivity	λ_p	0.1-0.5 W/(m K)
wall temperature	T_w	20 °C
heat source from adsorption	$\dot{q}_{ad}$	100 kW/m³

3.1 Post processing

To evaluate the overall heat transfer characteristic the average wall heat flux (W/m^2)

$$\bar{\dot{q}}_w = \frac{1}{A_{wall}} \int_{wall} \dot{q}_w \, dA \qquad (2)$$

and the average pellet temperature

$$\bar{T}_p = \frac{1}{V_{pellet}} \int_{pellet} T \, dV \qquad (3)$$

are computed. Thereby, a heat transfer coefficient between wall and pellet can be defined (W/(m^{2}K)):

$$\alpha_p = \frac{\bar{\dot{q}}_w}{\bar{T}_p - T_w} \qquad (4)$$

For the given linear model the heat transfer α_p is independent of the actual values of both wall temperature T_w and heat source $\dot{q}_{ad}$.

4 Results

An exemplary result of the temperature field is given in Figure 2.

The heat transfer coefficient α_p depends on the parameters d, s, λ_g and λ_p in a non-obvious way. For the parameter space given in Table 1 α_p is in the range of 16-670 W/(m^{2}K).

4.1 Data reduction

For use in simplified ODE-models the function

$$\alpha_p = f(d, s, \lambda_p, \lambda_g) \qquad (5)$$

is needed. This four dimensional function could not be deduced directly from the simulation results. However, using the Buckingham π theorem[15,16], Eq. (5) can be reduced to the two dimensional relationship

$$Nu_p = f(\epsilon_p, r_\lambda) \qquad (6)$$

Table 2: Example of simulation results for different geometrical parameters (first three lines) and different material parameters (last three lines) but equal dimensionless parameters

d	s	λ_g	λ_p	$\bar{q}_w$	$\bar{T}_p$	α_p	ϵ_p	r_λ	Nu
mm	µm	W/(m K)	W/(m K)	W/m²	°C	W/(m² K)	-	-	-
0.4	20	0.02	0.2	24.2	20.09	273.6	0.05	10	5.471
0.8	40	0.02	0.2	48.4	20.35	136.8	0.05	10	5.472
2	100	0.02	0.2	120.9	22.21	54.7	0.05	10	5.472
2	100	0.01	0.1	120.9	24.42	27.4	0.05	10	5.472
2	100	0.02	0.2	120.9	22.21	54.7	0.05	10	5.472
2	100	0.03	0.3	120.9	21.47	82.1	0.05	10	5.472

where $\mathrm{Nu_p} = \frac{\alpha_p d}{\lambda_g}$ is the Nusselt number of the fin-pellet heat transfer, $\epsilon_p = \frac{s}{d}$ the specific pellet roughness and $r_\lambda = \frac{\lambda_p}{\lambda_g}$ the ratio of thermal conductivities. All three quantities are dimensionless. This reduction yields a considerably simpler relationship shown in Figure 3.

In Table 2 the effect of data reduction is illustrated: In the first three lines results for different pellet sizes are given. Obviously the heat transfer coefficient α_p is higher for smaller pellets. Also, as the last three lines in the same table show, α_p increases with the heat conductivity of the gas. However, all shown combinations have the same dimensionless input parameters ϵ_p and r_λ and thus the same dimensionless result $\mathrm{Nu_p}$.

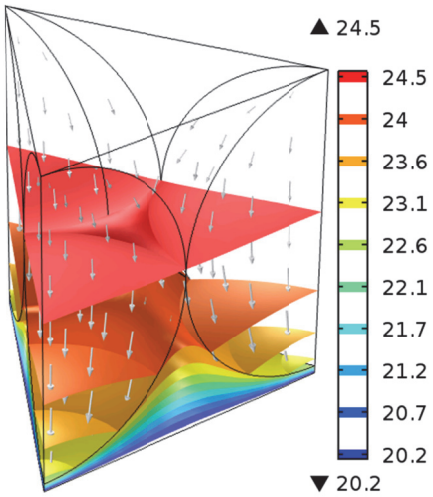

Figure 2: Resulting isotherms (scale in °C) and qualitative representation of heat flux (arrows) for $d = 4\ \mathrm{mm}$, $s = 100\ \mu\mathrm{m}$, $\lambda_g = 0.03\,\frac{\mathrm{W}}{\mathrm{m\,K}}$ and $\lambda_p = 0.5\,\frac{\mathrm{W}}{\mathrm{m\,K}}$ ($\epsilon_p = 0.025$, $r_\lambda = 16.7$)

They all reduce to one data point in Figure 3.

As for experimental results, curve fitting methods[17] can be applied to deduce an approximation of Eq. (6):

$$\mathrm{Nu_p} \approx \left(0.896\epsilon_p^{0.817} + 0.268 r_\lambda^{-0.374}\right)^{-1}. \quad (7)$$

Within the parameter range of $0.005 \le \epsilon_p \le 0.3$ and $3 \le r_\lambda \le 40$ this approximation represents the simulation results with a maximum relative error of 10%. Given the simplifying modelling assumption this is an acceptable value.

5 Conclusion

A three-dimensional COMSOL model of the heat transfer from a monolayer pellet bed to a fin wall was presented. It was shown that the effective heat transfer is highly dependent on pellet size and roughness as well as thermal conductivities of gas and pellet. The relatively simple model proved to be robust and easily meshed also in

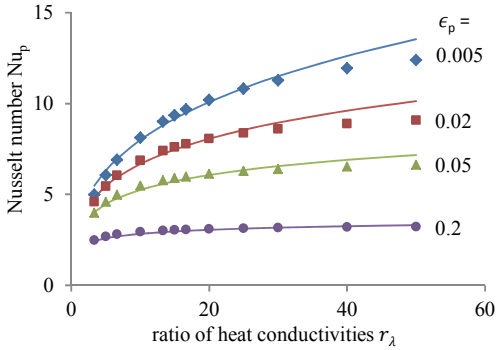

Figure 3: Reduced results of the simulation (points) and the fitted approximation Eq. (7) (lines) as Nusselt number of the fin-pellet heat transfer $\mathrm{Nu_p}$ over the ratio of conductivities r_λ for different values of the relative pellet roughness ϵ_p

extensive parameter sweeps.

The model is based on several assumptions. To prove that the models results are coherent with real physical behavior experimental verification is desirable. Especially the simplified modelling of the roughness as gap should be verified. However, the presented results may serve as a first indication.

For further work should focus on the extension to multilayer beds, the inclusion of non-continuum heat conduction and convective heat transfer.

The method of deducing general non-dimensional correlation from dimension-full data proved to be applicable to COMSOL models. It might have been possible to directly formulate the problem in dimension-less form. This would possibly have reduced the number of parameter combination in a parameter sweep. However, the economy in modelling time by using a model with predefined dimension-full equations overweight drastically.

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