



# A theoretical model on the effective stagnant thermal conductivity of an adsorbent embedded with a highly thermal conductive material



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## ABSTRACT

The effective stagnant thermal conductivity of an adsorbent bed plays an important role in the system performance of adsorption cooling systems and other applications. It is proposed that embedding the adsorbent with a highly thermal conductive material by forming a coating layer on the adsorbent molecules could increase the overall heat transfer rate resulting in a higher COP and SCP. A theoretical model based on the area-contact approach was developed in this study to predict the effective stagnant thermal conductivity of a surface coated porous material. This modified area-contact model can also be employed in different applications where surface coated porous materials are used. It was found that the coating layer thickness,  $c$ , the solid/fluid thermal conductivity ratio,  $\lambda$ , and the porosity,  $\phi$ , are factors that can affect the effective stagnant thermal conductivity. When  $\lambda = 10^3$ , the effective stagnant thermal conductivity was improved by about 4.3 times for  $\phi = 0.4$  and 9.7 times for  $\phi = 0.8$  with a deformed factor,  $\alpha = 0.002$  and a coating layer thickness,  $c = 0.05$ . An FEM simulation model was built showing that the modified area contact model has better agreement with the simulation result than the area contact model. It is suggested that this modified area contact model can be applied to predict the effective stagnant thermal conductivity of a surface coated porous material.

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## 1. Introduction

With the development of advanced materials, different kinds of surface coated porous materials have been invented and put to use in many areas, including use as additives and adsorbents for thermal storage purposes [1–3], surface catalysts for contaminant control processes [4–6], and adsorbents for dehumidification systems and adsorption cooling systems [7–9]. Thermal storage is used to store the thermal energy produced or gathered during the production of electric power. Thermal storage materials can also reduce the temperature variation of an indoor environment. Surface catalysts decompose contaminant particles into non-hazardous substances. The adsorbents in dehumidification systems adsorb water vapour and reduce the absolute humidity of process air directly. Compared to dehumidification systems, the working principle of an adsorption cooling system is much more indirect. In adsorption cooling systems, the adsorbent and adsorbate (e.g. water) are placed in two evacuated containers which are inter-connected. The adsorbate evaporates and is adsorbed onto the adsorbent. A low pressure is maintained by the adsorption process so

the adsorbate can evaporate at a low temperature. The evaporation of the adsorbate removes latent heat and creates a cooling effect. The adsorption process allows more adsorbate to evaporate, so the cooling effect continues. This process reduces the adsorbate temperature, and thus chilled water is produced. The adsorbent will eventually be saturated with the adsorbed adsorbate. Heat needs to be supplied to the adsorbent to desorb the adsorbate, i.e. a drying process.

Adsorption cooling systems allow energy efficient cooling, but some challenges need to be overcome. It was found that the low thermal conductivity of commercial adsorbents is one of the reasons leading to low a coefficient of performance (COP) and specific cooling power (SCP), COP: 0.15–0.6 and SCP: 10–1000 W/kg, thus increasing the size, energy consumption, and cost. Many adsorbents show good mass transfer characteristics but have low thermal conductivity [10]. Different adsorber designs have made in an attempt to increase the overall thermal conductivity of the adsorber, including the use of extended surfaces such as plate-fin heat exchangers [11,12], adsorbent-coated heat exchangers [13] and embedded composite adsorbents [14]. An extended surface is not applicable for low pressure operation of adsorbents and refrigerant pairs such as zeolite–water, silica gel–water and activated carbon–methanol because of Knudsen effect. The extended surface increases the thermal mass of the adsorber and lowers the COP and SCP of the system [15]. Coating adsorbents on the

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## Nomenclature

$B$	shape factor
$c$	thickness of the coating layer
$k$	thermal conductivity (W/mK)
$R$	radius of unit cell (m)
$V$	volume (m <sup>3</sup> )

### Greek symbols

$\alpha$	deformed factor
$\lambda$	fluid/solid thermal conductivity ratio
$\lambda'$	fluid/coating thermal conductivity ratio
$\lambda''$	coating/solid thermal conductivity ratio
$\phi$	porosity

### Subscripts

$cs$	coating–solid composite layer
$e$	effective stagnant
$f$	fluid phase
$fc$	fluid–coating composite layer
$fcs$	fluid–coating–solid composite layer
$fs$	fluid–solid composite layer
$s$	solid phase

surface of the heat exchanger can decrease the thermal contact resistance between the adsorbent and the wall, but only a thin layer of coated adsorbent, about 1 mm, can be formed [16]. The use of a coated adsorbent results in a very high ratio between the inert mass and the adsorbent mass which limits the COP and SCP of the system [17]. The best solution may be the development of embedded composite adsorbents. Embedding adsorbents with high thermal conductivity material can greatly increase the thermal conductivity of the adsorbent bed. The addition of high thermal conductivity material can form a layer of coating on the adsorbent molecules and fill up the empty spaces between the adsorbent molecules to increase the overall thermal conductivity.

In the applications of surface coated porous materials, the heat transfer can strongly affect the performance of the systems. Since porous materials consist of more than one material and have different geometries, the overall heat transfer performance of the systems cannot be simply found by the material properties alone. Thus, the effective thermal conductivities of these surface coated porous materials have to be determined in order to design and control the systems. Some generally employed theoretical models have been summarized in the literature [18–20]. However, most models consider solid and fluid phases only [18,21–32] and there are few theoretical models that predict the effective thermal conductivities of multiphase materials [20,33–34]. Among these theoretical models, the most fundamental approach is the limiting (series/parallel) model [35]. The limiting model gives the maximum and minimum limit of the effective thermal conductivity and is used as the building block in other models. Other basic models include the Maxwell-Eucken model [36,37] and the effective medium theory (EMT) model [38] are also used. Some studies directly combine these basic models with weighting functions to calculate the effective thermal conductivity. One of the earliest models, developed by Krischer, consists of series and parallel regions [22]. Raghavan and Martin used dimensionless height,  $h$ , to divide the porous material into sections of parallel, series and Maxwell resistances [22]. Wang et al. further combined all these basic models using structure composition factors and constructed a multi-structure model [23]. Samantray et al. [24] also employed a particle inclusion height, found by averaging over the restrictive bounds proposed by Hashin and Shtrikman [25]. Yang and Nakayama modelled by building a cubic model with different contact areas in all directions [26]. The approach using a direct combination of these basic models can give an approximation of the effective thermal conductivity with good agreement with experimental results. This approach, however, does not have physical meaning and can only provide bounds for the thermal conductivity estimation [27]. A real porous material cannot be divided into different geometries as described in the direct combination approach. An-

other approach is by analytically solving the governing equation of heat transfer. This can provide the most accurate result. Since porous material consists of more than one phase, the heat transfer equations can be directly solved for some specific geometries and arrangements [28,29]. The volume average method is often used but it creates new unknown terms in the equations [30,39]. This requires additional information about the material and measurements have to be conducted.

Besides the combination of basic models and direct equations solving, the unit cell model is another approach. The unit cell representing the repeating unit of the porous material can have many different forms depending on the physical problem. For instance, the structures of metal foam [31] and graphite foam [32] can be modelled by unit cells. The heat transfers in different regions can then be analysed as a thermal circuit. Zehner and Schlunder proposed a unit cell model in which the shape of the solid phase can be adjusted for different situations [40]. This model was further improved by Hsu et al. [21] considering the finite contact area between solid particles, which was assumed to be point contact in Zehner–Schlunder's model. It was also validated that the Zehner–Schlunder's model is applicable for conductivity ratios less than 2000 [18]. For conductivity ratios higher than 2000, the contribution of particle–particle contact becomes significant and the area contact model should be employed [21]. Thus, a theoretical model to predict the effective stagnant thermal conductivity of a surface coated porous material is proposed in this study based on the Zehner–Schlunder's model and area contact model.

## 2. Theoretical models

### 2.1. Zehner–Schlunder's model and area-contact model

Zehner–Schlunder's model is the theoretical model to predict the effective stagnant thermal conductivity of a porous material [40]. The unit cells of Zehner–Schlunder's model and the area-contact model are shown in Figs. 1 and 2, respectively. In the adsorption cooling system, the fluid phase, the adsorbate, is a gas which has very low thermal conductivity compared to the solid phase, the adsorbent. For example, the thermal conductivities of water vapour and ethanol are 0.018 W/mK and 0.014 W/mK, respectively, while that of the adsorbents, e.g., zeolite 13X and activated carbon, are in the order of 0.2 W/mK [41,42]. In the most extreme case, the adsorbent bed is evacuated so that there is no fluid phase, but the thermal conductivity of the adsorbent bed will not decrease to zero because of the direct contact between the adsorbent molecules. Thus, Hsu et al.'s model can better represent reality. In Hsu et al.'s model, the unit cell is a cylinder with a radius of  $R$  and a height of 1. The shape of the solid particle is described by

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