

# A study on the kinetics of ethanol-activated carbon fiber: Theory and experiments

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## Abstract

An experimental and theoretical study has been conducted on the adsorption kinetics of ethanol onto a pitch-based activated carbon fiber (ACF) of type (A-20). Experiments have been carried out across assorted adsorption temperatures that are useful to the operation of adsorption chillers. The kinetic curve for each isotherm is measured accurately using a thermal-gravimetric analyzer (TGA) from which the diffusion time constant and consequently, the overall mass transfer coefficient could be evaluated. A novel concentration profile, with an exponent parameter  $k$ , has been proposed in the theoretical model which accounts for the effect of meso- and micro-pore structures within the ACF. The proposed concentration profile removes the restrictions between the overall mass transfer coefficient and the diffusion time constant. Using the measured kinetics, the numerical value of  $k$  is evaluated, leading to a new form of the linear driving force (LDF) model for cylindrical adsorbent that could capture the higher ethanol uptake in ACF and this LDF model has been validated experimentally.

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## 1. Introduction

Activated carbon fibers (ACFs) have many intrinsic characteristics that are superior as compared with the pelletized or granular activated carbon, for example, the large surface area, fast inter-particle adsorption kinetics, ease of handling and manufacture into belts or foam components. It could be used in applications such as gas separation, gas storage and catalytic reactions [1–5]. In recent years, several studies have been conducted to investigate the potential types of ACFs–refrigerant pairs in adsorption cooling or heat pump applications [6–8]. The uptake behaviour of ACF (A-20)/ethanol pair seems to be a promising for cooling applications. Besides the high affinity for ethanol, the salient features of ACF (A-20) are (i) a high surface

area of about  $1.95 \times 10^6 \text{ m}^2/\text{kg}$ , (ii) a pore volume of  $10.28 \times 10^{-4} \text{ m}^3/\text{kg}$  and (iii) a suitable average pore diameter of approximately  $21.6 \text{ \AA}$  [9,10].

For design purposes and improving the understanding of adsorption chillers, it is essential to determine accurately the kinetics of adsorbent–adsorbate (refrigerant) pair. Design codes of chiller must be equipped with the correct isotherms, isosteric heat of adsorption and the coefficients for the uptake model. With these key data furnished for the adsorbent–sorbate pair, only then the numerical modeling of the processes of chiller operation can be computed accurately with high level of degree of confidence [11]. Conventionally, the computations time of the code could be optimized using the well-known linear driving force (LDF) correlation.

In the LDF method, the key parameter employed here is the determination of the overall particle mass transfer coefficient. Both the diffusion time constant and the overall

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## Nomenclature

$a_0$	time dependent coefficient of Eq. (7)	$t$	time [s]
$a_2$	time dependent coefficient of Eq. (7)	$v$	elemental volume of fiber ( $2\pi rL$ ) [ $m^3$ ]
$D_s$	surface diffusion coefficient [ $m^2/s$ ]	$v_0$	volume of fiber ( $2\pi RL$ ) [ $m^3$ ]
$F_0$	constant used in Eq. (1)	$\bar{w}$	average amount of adsorbate [ $kg/m^3$ or $kg_{ethanol}/kg_{ACF}$ ]
$k$	constant used in Eq. (7)	$W$	equilibrium adsorption capacity [ $kg/m^3$ or $kg_{ethanol}/kg_{ACF}$ ]
$K_s a_v$	overall mass transfer coefficient [ $s^{-1}$ ]	$D_s/R^2$	diffusion time constant [ $s^{-1}$ ]
$L$	fiber length [m]	$w/W$	fractional uptake [–]
$r$	radial distance in the fiber [m]		
$R$	fiber radius [m]		

mass transfer coefficient are estimated by tracking the experimental vapour-uptake behaviour using the solution of a diffusion equation where the particle mass transfer coefficient ( $K_s a_v$ ) could be determined [12]. Should only the surface diffusion parameter  $D_s$  is used, there exist a constant relationship between the overall mass transfer coefficient to the particle shape (e.g., described by the radius) and local concentration profile within the adsorbent. Liaw et al. [13] showed that a parabolic concentration of the form,  $w(t, r) = a_0(t) + a_2(t)r^2$  as prescribed within the spherical particle, led to the well-known LDF model. Recently, Li and Yang [14] also demonstrated the use of the general profiles of the LDF model but modified with an exponent index  $n$  on  $w(t, r)$ , where  $n$  is an integer  $\geq 2$  and commented that the parabolic profile of Liaw et al. [13] is one of the many possible local solutions. A recent article of Sircar and Hufton [15] highlighted that as long as the local concentration profile of the adsorbent is continuous, a constant relationship exist between  $K_s a_v$  and the diffusional time,  $D_s/R^2$ , which is given by Eq. (1). This relation is originally derived by Gluckauf [16] where  $F_0$  is 15 for spherical shapes of adsorbents:

$$F_0 = \frac{K_s a_v}{\left(\frac{D_s}{R^2}\right)} \quad (1)$$

In this paper, the adsorption rates of ethanol uptake onto the adsorbent ACF (A-20) for an assorted range of temperature have been measured which corresponds to useful temperatures expected of the operation of adsorption chillers, namely between 27 and 60 °C, respectively. Using a thermal-gravimetric analyzer (TGA) unit, instantaneous uptake measurements, as well as the adsorbent temperatures, are accurately recorded at regular time interval of 0.5 s. The chamber pressure of adsorbent is maintained constant during the experiments by a vacuum pump and a pressure-feedback modulating valve. Guided by the experimental measurements, a new concentration profile through the adsorbent is proposed in this paper where the exponent of the function for  $w(t, r)$  has been found to be greater than what has been reported conventionally. The additional vapour-uptake, arising from the effect of the meso-pores within the uniformly distributed

micro-pore structures of adsorbent material, can now be described by a variable  $k$  in the local concentration profile and this effect has been reported by Dubinin et al. [17]. However, they considered a statistical-moment method for the concentration profile that entails an infinite series solution for the kinetic curve.

## 2. Experiments

Fig. 1 shows a pictorial view of the experimental apparatus which comprises the TGA (CAHN TG 2121) unit, a water-heated evaporator, and a vacuum pump with the modulating valve. To measure the adsorption temperature, a thermocouple of type K is inserted into the reacting chamber near the bottom of the adsorbent or sample pan where both the adsorbent and the temperature sensor would be exposed to the same heater. The system pressure is controlled by the MKS pressure controller (type 651C) and a MKS-Baratron pressure sensor (type 631A) records the chamber pressure. The controller then operates the modulating vacuum valve. A diaphragm type vacuum pump is used to evacuate the system continuously, operating in concert with the pressure sensor and controller so as to maintain a pre-set chamber pressure condition. Fine porous meshes are mounted at the inlet and exit of the adsorbent chamber which provide damping for any pressure fluctuations arising from the modulating actions. During testing, the microbalance unit of the TGA is protected from any reactive gas by introducing a small amount of helium gas, which is injected from the top of the dome-shaped cover. As the sorbate is a condensable vapour, condensation is prevented by raising the tube and chamber wall temperatures, using an externally wrapped electric tape-heater.

A series of experimental runs have been carried out at different adsorption temperatures within a range from 27 to 60 °C. The evaporator, containing the liquid ethanol, is kept at a constant temperature of 15 °C by an adjustable temperature bath. Samples of ACF, typically about 71 mg in weight, are inserted into the reactor chamber of the TGA unit. Prior to each adsorption experiment, the sample is first regenerated under vacuum conditions but adsorbent is maintained at a temperature of 140 °C for several hours

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