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Generalized correlations for mass transfer and pressure drop in fiber-based catalyst supports

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HIGHLIGHTS

- Mass transfer in fiber-based supports can be described by a packed bed correlation.
- The Ergun equation can be applied to fiber-based supports.
- The Sauter diameter allows the applicability of the correlations to both structures.
- The correlations are validated for Re = 0.01–10,000.

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ABSTRACT

Fiber-based catalyst supports are of increasing interest for different catalytic applications. So far, no reliable correlations for mass transfer and pressure drop with a wide range of applicability are available. The paper shows that in both cases correlations for packed beds of spheres can be applied if the Sauter diameter is used as characteristic length. The findings are confirmed with help of a comparison to literature data and own experimental results on mass transfer and pressure drop. The generalized correlations simplify the design of novel fiber-based supports and of the corresponding reactors.

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1. Introduction

Due to the shortage of important resources and an increasing competition on the world market, process intensification is of increasing importance for the chemical industry. The major goal is the development of cleaner, smaller and more efficient novel processes or the improvement of established processes. Therefore, several process-intensifying technologies have been developed in industry as well as in academia. Very often these developments are focused on the minimization of mass and heat transfer limitations in different process units. Due to the high importance of heterogeneous catalysis and the great potential for process intensification in this field, several novel reactor concepts and catalyst support structures have been proposed in the last decades. A large number of these concepts are based on structures built from fibers or cylinders. These structures can be summarized by the term fiber-based catalyst supports, including well-known structures like wire meshes, but also metallic fiber filters, glass fiber fabrics, ceramic mats and microfibrous entrapped catalysts [1–3]. In recent years additive manufacturing is becoming increasingly interesting in different fields of application, also for the preparation of catalyst supports. Thus, techniques like robocasting [4,5] and selective electron beam melting [6,7] were applied for the manufacturing of fiber-based catalyst supports. Besides these novel structures also foams [8] can be regarded as fiber-based catalyst supports, with the struts being the basic structure.

Except for wire meshes and to a limited extent foams, most of the fiber-based catalyst support structures proposed in literature are not industrially applied. A step in this direction could be the availability of reliable correlations for mass transfer and pressure drop. So far no generalized correlations for fiber-based catalyst support structures exist, as Section 2 shows. The aim of this work is to show that the mass transfer correlation developed by Reichelt et al. [9] for packed beds can be applied to fiber-based catalyst supports if the Sauter diameter is used as the characteristic length. Following the same approach, the well-known Ergun

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Nomenclature

d	diameter (m)
d_h	hydraulic diameter (m)
d_S	Sauter diameter (m)
D	diffusion coefficient ($m^2\ s^{-1}$)
D_{ax}	axial dispersion coefficient ($m^2\ s^{-1}$)
f	Fanning friction factor (–)
f_S	Fanning friction factor with d_S as characteristic length (–)
Hg	Hagen number $= 2fRe^2$ (–)
Hg_S	Hagen number with d_S as characteristic length $= 2f_S Re_S^2$ (–)
k_m	mass transfer coefficient ($m\ s^{-1}$)
L	length (m)
M	mesh number (m^{-1})
NRMSD	normalized route-mean-square deviation (–)
p	pressure (Pa)
Pe	Péclet number $= \frac{ud}{D}$ (–)
Pe_S	Péclet number with d_S as characteristic length $= \frac{ud_S}{D}$ (–)
Pe_{ax}	axial Péclet number $= \frac{ud}{D_{ax}}$ (–)
$Pe_{ax,S}$	axial Péclet number with d_S as characteristic length $= \frac{ud_S}{D_{ax}}$ (–)
Re	Reynolds number $= \frac{ud\rho}{\eta}$ (–)
Re_S	Reynolds number with d_S as characteristic length $= \frac{ud_S\rho}{\eta}$ (–)
Sc	Schmidt number $= \frac{\eta}{D\rho}$ (–)
Sh	Sherwood number $= \frac{k_m d}{D}$ (–)
Sh_S	Sherwood number with d_S as characteristic length $= \frac{k_m d_S}{D}$ (–)
S_V	geometric surface area (m^{-1})
t	time (s)
u	superficial velocity ($m\ s^{-1}$)
$\dot{V}$	volumetric flow rate ($m^3\ s^{-1}$)

Greek letters

γ	coefficient from Eq. (9)
ε	porosity (–)
η	dynamic viscosity (Pa s)
ϑ	temperature (K)
ρ	density ($kg\ m^{-3}$)
τ	tortuosity (–)
φ	volume fraction (–)
χ	trade-off index (–)
ω	mass fraction (–)

Subscripts

AP	active particle
app	apparent
B	bed
corr	calculated by a correlation
F	fiber
i	inner
max	maximum value
meas	measured value
min	minimum value
Re = 0	at stagnant conditions
SC	single cylinder
Sph	sphere
SS	single sphere
St	strut
Str	structure

equation [10] can be applied for the description of pressure drop characteristics.

2. Literature review

Considering the large number of publications on different fiber-based catalyst supports [3], the amount of works on mass transfer is rather low. Nevertheless, some correlations were reported [3]. A drawback is that the applicability of these correlations is most often only confirmed for a limited range of Reynolds number. A summary of experimental results on mass transfer at different fiber-based catalyst supports is given in Fig. 1. As characteristic lengths for Sherwood and Reynolds number the fiber or strut diameter (d_F, d_{St}) were chosen. The results are not corrected for the influence of bed porosity ε_B on mass transfer. For packed beds of spheres with bed porosities in the range of $\varepsilon_B = 0.26–0.80$ the dependence is known to be about $Sh_{app} \sim \varepsilon_B^{-1}$ [11–14]. However, the influence of porosity on mass transfer at fiber-based catalyst supports is less considered in literature. Bed porosities for fiber-based structures are generally in the range of $\varepsilon_B = 0.70–0.95$ [3]. Considering this rather low range of variation, the results depicted in Fig. 1 indicate the possibility to describe the mass transfer of fiber-based catalyst supports by a single correlation.

The results of Richardson et al. [15] on foams and of Groppi et al. [16] on fiber filters differ from the bulk of experimental results. They show considerably lower apparent Sherwood numbers.

In general, the choice of a suitable characteristic length for foams is difficult. Often pore or window diameters are used [17–19]. However, these lengths are difficult to compare with other foams. Also the application of the strut diameter is problematic, because it is not constant over the whole cell length. It is therefore more reasonable to directly measure or calculate an average strut diameter [20–22]. For the results from Ref. [18] presented in Fig. 1, the average strut diameter was calculated by applying a simple cubic cell model:

$$\bar{d}_{St} = \frac{4(1-\varepsilon_B)}{S_{V_B}}. \tag{1}$$

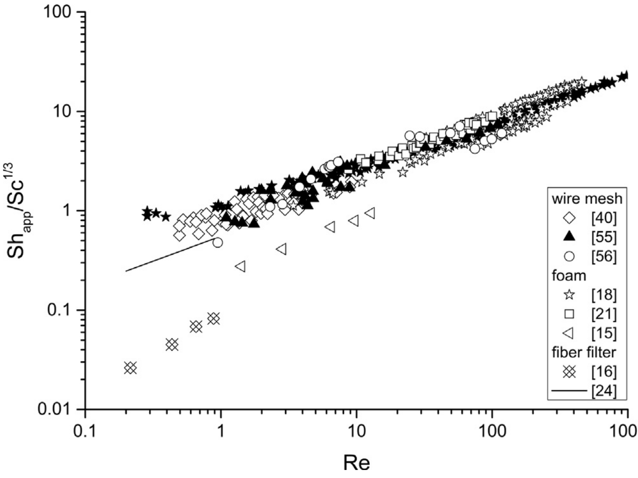

Fig. 1. Literature data on apparent mass transfer in fiber-based catalyst support structures.

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