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Liquid-phase mass transfer within KATAPAK-S® structures studied using computational fluid dynamics simulations

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Abstract

The liquid-phase mass transfer within the catalyst-packed criss-crossing sandwich structures of KATAPAK-S has been studied with the use of computational fluid dynamics. Due to the "upheaval" caused by the flow splitting at the crossovers, the mass transfer coefficient is about 40% times larger than for fully developed laminar flow in a single, packed tube.

Keywords: Structured packing; Mass transfer; Computational fluid dynamics

1. Introduction

For heterogeneously catalysed reactive distillation processes, hardware design poses considerable challenges [1]. The catalyst particle sizes used in such operations are usually in the 1–3 mm range. Larger particle sizes lead to intra-particle diffusion limitations. To overcome the limitations of flooding during counter-current vapour–liquid contacting, the catalyst particles have to be enveloped within wire gauze structures. Two commonly used structures in industry are:

1. Catalyst particles enclosed in cloth wrapped in the form of bales [2];
2. Catalyst particles sandwiched between corrugated sheets of wire gauze [3–7] (see Fig. 1). Such structures are being licensed by Sulzer, called KATAPAK-S, and Koch-Glitsch, called KATAMAX. They consist of two pieces of rectangular crimped wire gauze sealed around the edge, thereby forming a pocket of the order of 1–5 cm wide between the two screens. These catalyst "sandwiches" or "wafers" are then bound together.

An important claimed advantage of the structured criss-crossing catalyst sandwich structures shown in Fig. 1 over alternative configurations is with respect to radial distribution of liquid through the packed catalyst channels. Our earlier study, using both experiments and computational fluid dynamics (CFD) techniques [3–5], has shown that KATAPAK-S has excellent radial dispersion characteristics, which is a desirable feature in chemical reactors. The primary objective of the present communication is to extend our earlier work to the study of liquid-phase mass transfer within the sandwich structures. There is practically no published work in this area. In view of the success of our earlier CFD approach to describe radial dispersion [7], we have extended this methodology to study mass transfer.

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Nomenclature

A	wall area (m^2)
$\mathbf{B}$	body force (N/m^3)
d	diameter (m)
d_H	hydraulic diameter (m)
D	diffusion coefficient of tracer in liquid (m^2/s)
Gz	Graetz number, DL/d_H^2U
k	mass transfer coefficient (m/s)
L	length (m)
n	normal
p	pressure (Pa)
r	radius (m)
Sh	Sherwood number, kd_H/D
t	time (s)
u	interstitial velocity (m/s)
$\mathbf{u}$	velocity vector (m/s)
U	superficial velocity (m/s)

Greek letters

ε	porosity of packing (–)
μ	viscosity (Pa s)
ρ	density (kg/m^3)
ϕ_{tracer}	flux of tracer (m^3/s)
ω	tracer concentration (–)

Subscripts

bulk	away from the wall, in the bulk
H	hydraulic
L	liquid phase
p	particle
wall	at the wall
$\perp$	perpendicular

2. CFD model development

The computational space for the CFD simulations of the liquid flow in a single sandwich structure of KATAPAK-S is shown in Fig. 2; this corresponds to our experimental set up (see: http://ct-cr4.chem.uva.nl/strucsim/). The sandwich exists of 16 triangular channels, with a total of 32 crossovers. A single triangular channel has a base of 36×10^{-3} m, and a height of 18×10^{-3} m. There is a 2×10^{-3} m gap between the bases of adjoining channels. The liquid flow inside these channels is simulated. In order to study mass transfer, we introduce a tracer component on all the external surfaces of the sandwich with a mass fraction $\omega = 1$, except on inlets and outlets. The liquid flowing into the system does not contain the tracer component. The liquid picks up tracer during its flow through the system. The amount of tracer that has been taken up by the liquid when the liquid leaves the system can be used to calculate a mass transfer coefficient.

The mass and momentum conservation equations are:

$$\frac{\partial \varepsilon \rho_L}{\partial t} + \nabla \cdot (\rho_L \varepsilon \mathbf{u}_L) = 0 \tag{1}$$

$$\frac{\partial \rho_L \varepsilon \mathbf{u}_L}{\partial t} + \nabla \cdot (\rho_L \varepsilon \mathbf{u}_L \mathbf{u}_L - \mu_L \varepsilon (\nabla \mathbf{u}_L + (\nabla \mathbf{u}_L)^T)) = \varepsilon \mathbf{B} - \varepsilon \nabla p \tag{2}$$

The liquid phase was taken to be water with $\rho_L = 998\,kg/m^3$ and $\mu_L = 0.001$ Pa s. In the equation above, $\mathbf{B}$ is the body force resulting from the flow resistance caused by the packing in the system. This flow resistance is assumed to be isotropic, and with uniform porosity $\varepsilon = 0.37$. The Ergun equation [8] has been used to formulate the resistance term

$$\mathbf{B} = \left[150 \frac{\mu_L}{d_p^2} \frac{(1-\varepsilon)^2}{\varepsilon^2} + 1.75 \frac{\rho_L}{d_p} \frac{(1-\varepsilon)}{\varepsilon} |\mathbf{u}_L| \right] \mathbf{u}_L \tag{3}$$

The particle size was taken as 1.1 mm. Diffusion and convection of mass tracer is described by the following equation of continuity:

$$\frac{\partial \varepsilon \rho_L \omega}{\partial t} + \nabla \cdot (\rho_L \varepsilon \omega \mathbf{u}_L) = \nabla \cdot (\rho_L \varepsilon D \nabla \omega) \tag{4}$$

Here, ω is the mass fraction of tracer in the liquid phase. The diffusion coefficient D of tracer in water was taken as $10^{-9}\,m^2/s$.

Velocities are specified at the eight inlets. No-slip boundary conditions are applied to the walls. A Neumann boundary condition was applied to the velocities at the eight outlets:

$$\frac{\partial \mathbf{u}_\perp}{\partial n} = 0 \tag{5}$$

For solving the above set of equations, a commercial CFD package CFX, version 4.2, was used with an algebraic multi-grid (AMG) solver. The simulations were

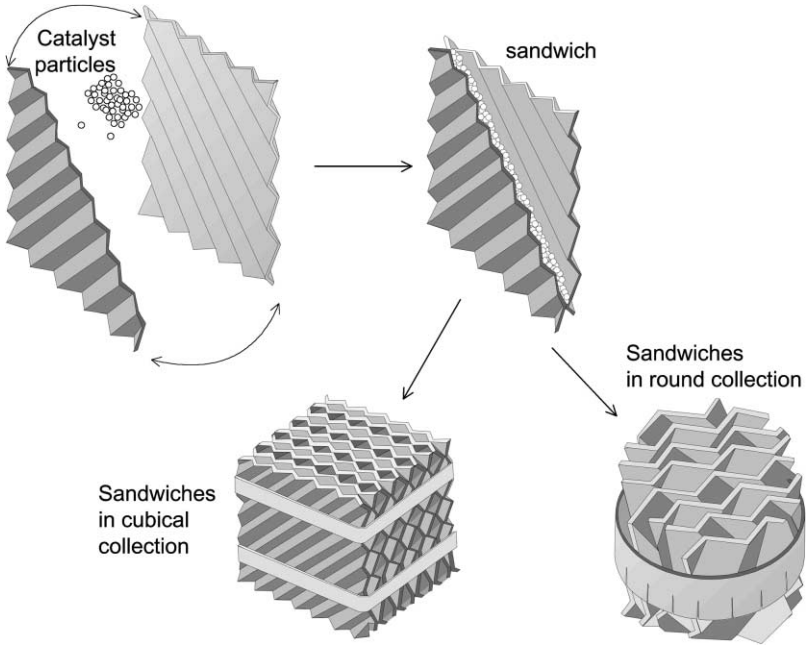

Fig. 1. Structured catalyst sandwiches. Catalyst sandwiched between two corrugated wire gauze sheets, then joined together and sewn on all four sides into a sandwich "configuration", arranged into a cubical collection or round collection.

run on a Silicon Graphics Power Challenge machine with 1 GB RAM and a single R10K 200 MHz processor. Discretisation of the equations is performed using a finite volume method. Velocity vectors are treated as scalar equations, one equation for each of the three velocity components. All scalar variables are discretised and stored at the cell centres. A sample grid view of the triangle face with 10^{-4} m cell size at the wall, 5×10^{-3} m horizontal cell size in the centre and 1.5×10^{-3} m vertical cell size in the centre is shown in Fig. 3. The front plane as shown in the figure contains 595 grid cells.

Velocities required at the cell faces are evaluated by applying improved Rhie–Chow [9] interpolation. Transport variables such as diffusion coefficients are evaluated and stored at the cell faces. The SIMPLEC [10] pressure correction method is applied. The equations are solved for steady-state conditions. Differencing of the diffusion terms is performed by central differencing. Various schemes have been tested for differencing of the advection terms in the various equations.

At steady state, the volumetric rate of transfer of tracer into the liquid-phase ϕ_{tracer} can be determined and the mass transfer coefficient k is obtained from

$$k = \frac{\phi_{\text{tracer}}}{A(\omega_{\text{wall}} - \omega_{\text{bulk}})} \tag{6}$$

where A is the total external surface area of the sandwich structure expressed in m^2 and ω_{bulk} the mass fraction of tracer in the bulk liquid leaving the system at the outlets under steady state. We can also determine the Sherwood number Sh defined by

$$Sh = \frac{kd_{\text{H}}}{D} \tag{7}$$

where the hydraulic diameter of the system is denoted by d_{H}.

3. Simulation results

For comparison purposes, we also determined the mass transfer in simpler structures, in addition

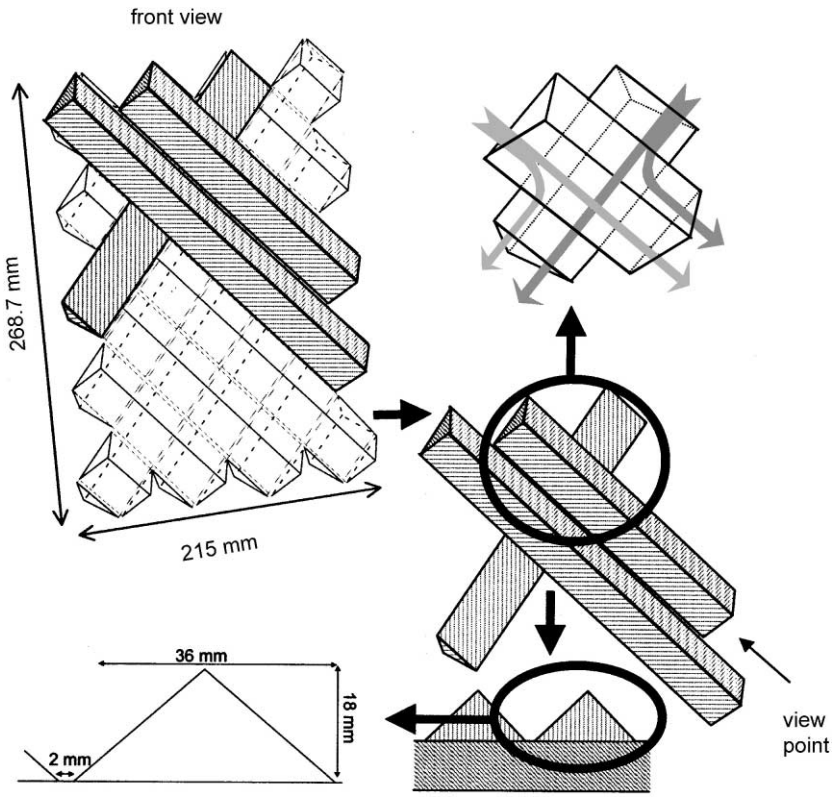

Fig. 2. Reconstruction of KATAPAK-S structure as a set of intersecting triangular tubes. A single sandwich consists of 16 triangular channels with 32 crossovers. A single triangle is 0.036 m high, 0.018 m wide. A space of 0.002 m is present between two adjoining channels.

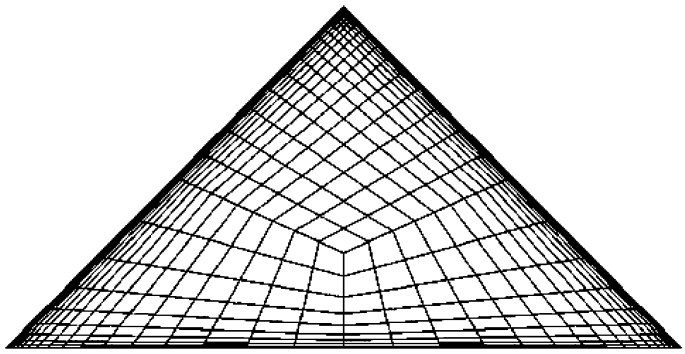

Fig. 3. Schematic overview of meshing of a triangular face. Front view of meshed triangle with 10^{-4} m cell size at the wall, 5×10^{-3} m horizontal cell size in the centre and 1.5×10^{-3} m vertical cell size in the centre, using quadratic seeding. The face contains 595 grid cells.

Table 1
Details of simulated geometries and the obtained mass transfer coefficients

Geometry	Superficial liquid velocity, U_L	Hydraulic diameter, d_H	Minimum grid size at wall for convergence	Mass transfer coefficient, k_L	Sherwood number, Sh
Single empty tube	0.005	0.024	60×10^{-5}	1.25×10^{-6}	30.1
	0.011	0.024	60×10^{-5}	1.65×10^{-6}	39.3
	0.018	0.024	60×10^{-5}	1.96×10^{-6}	46.7
	0.025	0.024	60×10^{-5}	2.21×10^{-6}	52.6
	0.050	0.024	60×10^{-5}	2.92×10^{-6}	69.5
Single tube, packed with 1.1 mm particles	0.005	0.024	2×10^{-5}	1.87×10^{-6}	44.5
	0.011	0.024	2×10^{-5}	2.63×10^{-6}	62.5
	0.018	0.024	2×10^{-5}	3.26×10^{-6}	77.5
	0.050	0.024	2×10^{-5}	5.16×10^{-6}	122.8
Single triangular tube, packed with 1.1 mm particles	0.007	0.015	1×10^{-5}	3.93×10^{-6}	58.5
	0.011	0.015	1×10^{-5}	4.78×10^{-6}	71.2
	0.015	0.015	1×10^{-5}	5.46×10^{-6}	81.4
	0.011	0.024	1×10^{-5}	3.97×10^{-6}	94.3
	0.0175	0.024	1×10^{-5}	4.86×10^{-6}	115.4
Single crossover, packed with 1.1 mm particles	0.0079	0.017	1×10^{-5}	4.63×10^{-6}	79.4
	0.011	0.017	1×10^{-5}	5.30×10^{-6}	91.0
	0.015	0.017	1×10^{-5}	6.03×10^{-6}	103.4
	0.004	0.024	1×10^{-5}	3.07×10^{-6}	73.0
	0.007	0.024	1×10^{-5}	3.87×10^{-6}	92.0
	0.011	0.024	1×10^{-5}	4.58×10^{-6}	108.9
	0.015	0.024	1×10^{-5}	5.33×10^{-6}	126.8
Sandwich structure, packed with 1.1 mm particles	0.007	0.024	1×10^{-5}	3.61×10^{-6}	85.8
	0.011	0.024	1×10^{-5}	4.45×10^{-6}	105.8
	0.015	0.024	1×10^{-5}	5.16×10^{-6}	122.6

to the sandwich structure: (a) an empty cylindrical tube, (b) a cylindrical tube packed with 1.1 mm particles, (c) single triangular tube packed with 1.1 mm particles, and (d) two triangular, packed tubes with single crossover; the details are given in Table 1 and Fig. 4. For each of the geometries listed in Table 1, grid convergence was checked by varying the grid cell size near the wall. Near the wall, molecular diffusion controls mass transfer; somewhat further from the wall convection is the dominating process. Therefore, the required cell size near the wall for the current problem needs to be examined critically. Details of grid sizes and convergence have been given on our web site: http://ct-cr4.chem.uva.nl/walltracer/; the minimum wall grid size to ensure convergence is also listed in Table 1.

Fig. 5 shows a comparison of the *Sh* numbers for the various packed geometries, all with the hydraulic diameter of 0.024 m, as a function of the interstitial liquid velocity. When we compare mass transfer in a single triangular, packed tube with that of two triangular tubes with a single crossover we note that the crossover geometry leads to a significant increase in the mass transfer coefficient. To rationalise this, we examine the flow streamlines in the crossover geometry in Fig. 6. As can be seen in Fig. 6, a significant exchange of flow between the channels is present at the crossover.

The Sherwood number for the complete structure (shown in Fig. 2) almost coincides with that obtained for two triangular tubes with a single crossover. This leads us to conclude that the phenomena of redistribution of streamlines, shown in Fig. 6 for a single crossover, repeats itself over the whole structure. There are no additional mass transfer effects to be accounted for and a single crossover geometry provides an adequate representation of the flow and mass transfer of the complete structure.

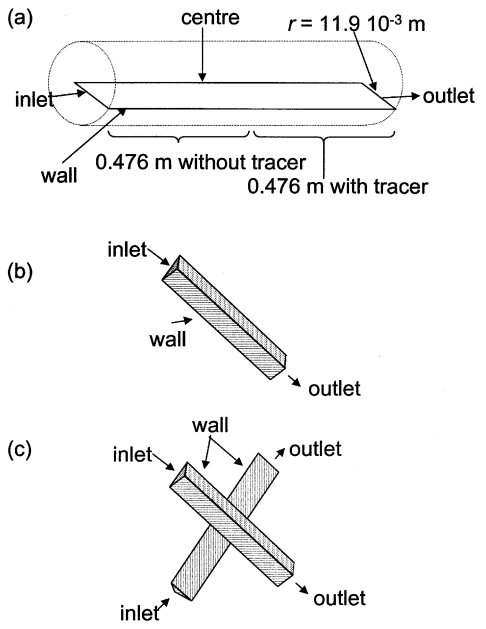

Fig. 4. Three simpler geometries in which simulations have also been performed: (a) circular tube; (b) single triangular channel; (c) single crossover of two triangular channels.

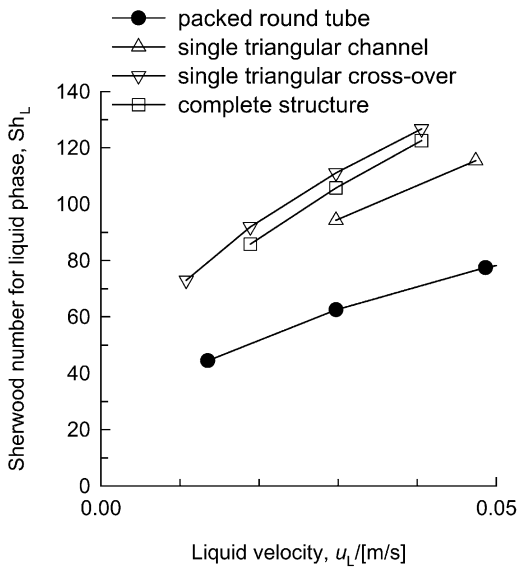

Fig. 5. Sherwood number for various geometries as function of the interstitial liquid velocity.

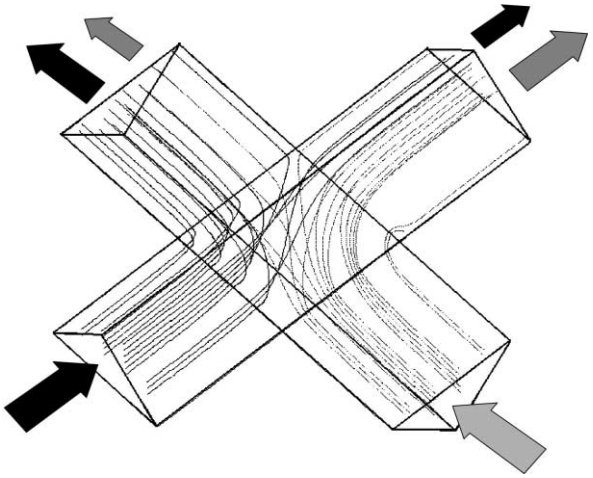

Fig. 6. Streamlines within single crossover of triangular channel. As can be seen, a significant exchange of liquid takes place between the channels.

4. Conclusions

We have used CFD techniques to study mass transfer within the criss-crossing structures of KATAPAK-S. The KATAPAK-S structure is reconstructed as a set of intersecting triangular tubes (Fig. 2). Mass transfer in a packed triangular tube is significantly higher than that of a packed circular tube due to improved convective contribution in the corner regions. Further improvement in mass transfer takes place when the two triangular tubes are made to intersect and exchange mass at the junctions, due to upheaval at the junctions. Mass transfer in a sandwich KATAPAK-S structure consisting of 16 triangular tubes and 32 crossovers gives the same *Sh* values as for a single crossover. Our results offer a simple methodology for scaling up because we could consider the complete structure simply as a repetition of a single crossover geometry.

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