Chemical Engineering & Processing: Process Intensification 126 (2018) 178–189

Contents lists available at ScienceDirect

Chemical Engineering & Processing: Process Intensification

journal homepage: www.elsevier.com/locate/cep

Periodic open cellular structures (POCS) for intensification of multiphase reactors: Liquid holdup and two-phase pressure drop

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A R T I C L E I N F O

Keywords:
Two-phase pressure drop
Liquid holdup
Structured catalysts
Relative permeability model
Additive manufacturing

A B S T R A C T

Structuring concepts for catalytic reactors provide promising options for process intensification on the process unit level [1,2] as they offer a better control on the occurring transport processes, e.g. on the fluid flow, species distribution, pressure drop and heat transfer. Process intensification aims at the realization of processes that are only limited by reaction kinetics, but not anymore on hydrodynamics [3]. For this reason, in multiphase reactors it is desirable to achieve good liquid distribution, advanced heat transport and low pressure drop, just to mention a few transport characteristics. In this regards, the use of periodic open cellular structures (POCS) is a recent and very promising structuring concept, as packings of these structures offer superior and adjustable properties (e.g. low pressure drop, high surface area, good liquid distribution, advanced heat transfer) [4–8].

In this contribution, static and dynamic liquid holdup as well as single- and two-phase pressure drop was measured in POCS. These kinds of structures can be used as catalyst support in packed bed reactors, and also as liquid distributor for trickle-bed applications. The POCS investigated in this study were fabricated with different additive manufacturing methods (fused deposition modeling, stereolithography and selective electron beam melting) to study the influence of different materials (ABS, resin, Ti6Al/4V). For the description of the static liquid holdup, a modified Eötvös correlation, which takes the contact angle of the different materials into account, is proposed. Dynamic liquid holdup and two-phase pressure drop was modelled using an extension of the concept of hydrodynamic tortuosity proposed by Inayat et al. [8], and a modification of the relative permeability model introduced by Saez et al. [9]. Furthermore, equations for the geometric characterization of POCS consisting of different unit cell types, namely Diamond, Kelvin and the recently presented DiaKel hybrid cell [5] were derived. The window diameter of the used unit cells as well as the porosity has a strong influence on the liquid holdup and the pressure drop. By taking the contact angle into account the static liquid holdup can be calculated with good precision (errors smaller than 20%). The concept of geometric tortuosity and the relative permeability model also is applicable to predict the (two-) phase pressure drop and the dynamic liquid holdup in stacked packings of POCS segments of different unit cells and materials. Both, pressure drop and liquid holdup can be predicted a priori (i.e., without further fitting) with good precision using the correlations established in this work solely based on geometric properties of the packing.

1. Introduction

Multiphase reactions (e.g. involving a gas – liquid – solid system) are often carried out in trickle-bed reactors, where gas and liquid are flowing in co- or countercurrent operation mode through a randomly packed particle bed [10,11]. In the trickle flow regime – also referred to as low interaction regime – the gas phase is the continuous phase while the liquid phase rinses down in rivulets or films around the particles [12]. Associated with the flow regime are the characteristics for heat and mass transfer, liquid holdup, liquid distribution and two-phase pressure drop [5,13–15]. Due to the complex hydrodynamic phenomena well-defined geometric properties are of particular importance for multiphase reaction systems [16] for both, the systematic analysis and the structural optimization. For this reason, the development of

Abbreviations: ABS, Acrylonitrile butadiene styrene; CAD, Computer aided drawing; cpi, Cells per inch; CT, Computer tomography; Eö, Eötvös number; FDM, Fused deposition modeling; Ga, ,Galileo number; MAPE, mean average percentage error; POCS, Periodic open cellular structures; Re, Reynolds number; SEBM, Selective electron beam melting; SLA, Stereolithography

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https://doi.org/10.1016/j.cep.2018.02.027
Received 4 September 2017; Received in revised form 15 February 2018; Accepted 26 February 2018
Available online 21 March 2018
0255-2701/

Nomenclature

List of symbols

F_α	Drag force per volume element on the α-phase ($N\ m^{-3}$)
S_g	Gas saturation (-)
S_i	Surface area (mm^2)
a	Length of one unit cell (m)
A	Ergun parameter (-)
$\acute{a}$	Coefficient relative permeability model (-)
B	Ergun parameter (-)
$\acute{c}$	Parameter relative permeability model (-)
d_i	Hydraulic diameter (mm)
G	Total gas flow rate ($m^3\,s^{-1}$)
k_i	Relative permeability (-)
L	Packing length/total liquid flow rate ($mm/m^3\,s^{-1}$)
L_e	Additional length (mm)
l_s	Strut length (mm)
N	Number (-)
S_V	Specific surface area (m^{-1})
V	Volume (m^3)
ΔP	Pressure drop (Pa)
v	Velocity ($m\,s^{-1}$)

Subscripts

a, b	Coefficients Eötvös correlation
b	Bed
d	Dynamic
e	Equivalent
g	Gas
H	Hydrodynamic
l	Liquid
o	Open
p	Particle, packing
s	Static
s	Strut
w	Window

Superscripts

EtOH	Ethanol
in air	Weighing of the packings in air
in EtOH	Weighing of the packings in ethanol

Greek symbols

ε_i	Porosity (-)
ε_{li}	Liquid holdup (-)
Ψ	Dimensionless pressure drop (-)
α	Phase (gas, liquid) (-)
δ	Reduced saturation (-)
μ	Dynamic viscosity ($kg\,m^{-1}\,s^{-1}$)
ρ	Density ($kg\,m^{-3}$)
σ	Surface tension ($mN\,m^{-1}$)
τ	Tortuosity (-)
Θ	Contact angle (°)

new reactor concepts and equipment for process intensification and optimization is one of the main challenges on the agenda of today's chemical reaction engineering. These novel designs aim at safe, sustainable, compact, energy efficient and environmentally friendly processes with reduced investment and capital costs [17].

In order to achieve improved control on the transport processes on

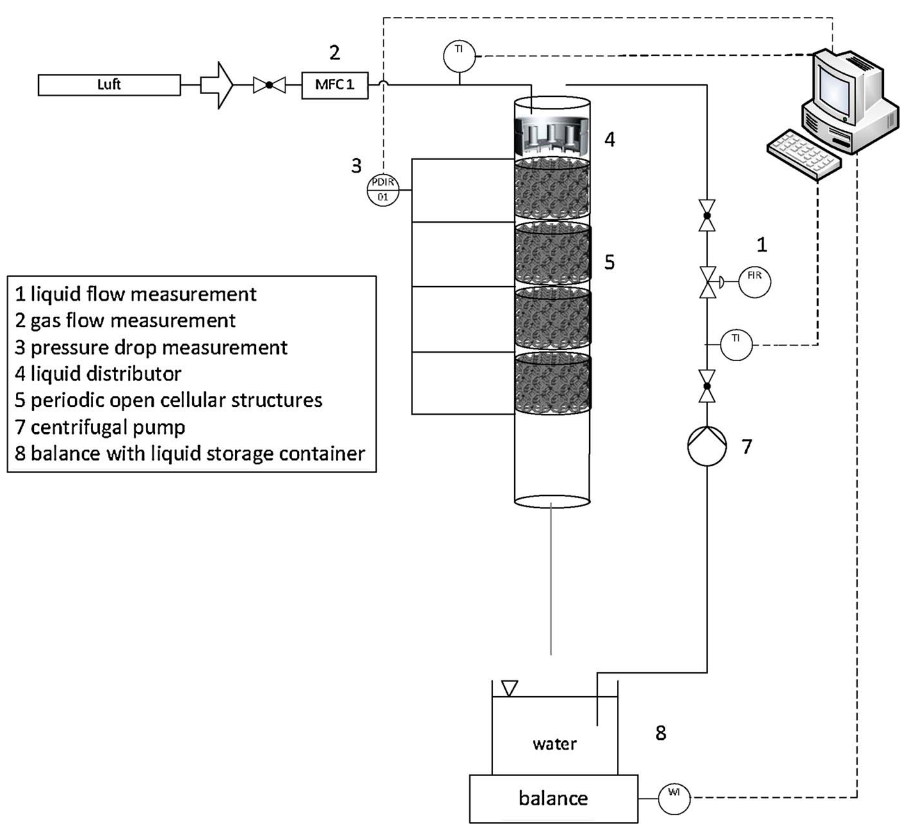

Fig. 1. a) Schematic drawing of the test rig for investigation of liquid holdup and two-phase pressure drop measurements.