Chemical Engineering Journal 200–202 (2012) 380–390

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Journal

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

Modeling the diffusion-free liquid phase residence time distribution of Taylor flow by the unit cell concept: Progress and limitations

Sercan Erdogan [a,b], Martin Wörner [a,*], Hakan Serhad Soyhan [c]

[a] Karlsruhe Institute of Technology (KIT), Institute for Nuclear and Energy Technologies, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
[b] Mechanical Engineering Department, Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya, Turkey
[c] Mechanical Engineering Department, Faculty of Engineering, Sakarya University, Esentepe Campus, 54187 Sakarya, Turkey

HIGHLIGHTS

- The diffusion-free liquid RTD in Taylor flow is studied analytically and numerically.
- A model for the unit cell RTD is developed which agrees well with the numerical RTD.
- Determining the multiple unit cell RTD by convolution is shown to be inappropriate.
- This is related to the separation of the liquid in a recirculation and bypass region.
- In absence of diffusion both regions are independent which invalidates the convolution.

ARTICLE INFO

Article history:
Received 1 April 2011
Received in revised form 4 April 2012
Accepted 16 June 2012
Available online 23 June 2012

Keywords:
Residence time distribution
Taylor flow
Bubble train flow
Numerical simulation
Unit cell
Compartment model
Convolution

ABSTRACT

In this paper we study the diffusion-free liquid phase residence time distribution (RTD) of laminar Taylor flow in square mini-channels numerically and analytically. We evaluate the RTD caused by the non-uniform laminar velocity field for co-current upward and downward Taylor flow from detailed numerical simulations obtained with a volume-of-fluid method by diffusion-free Lagrangian tracking of a set of virtual particles. The numerical RTD curves are used to develop a compartment model for the RTD of a Taylor flow unit cell (which consists of one gas bubble and one liquid slug) in the fixed frame of reference. While the new model is conceptually similar to models from literature, it is refined with respect to (i) the delay time (i.e. the residence time of the fastest liquid elements, modeled by a plug flow reactor) and (ii) the difference in slope of the RTD at small and large residence times (modeled by two parallel continuous stirred tank reactors with different mean residence time). It is shown that the refined model fits the numerical unit cell RTD reasonably well for different flow conditions. From the unit cell RTD model, the RTD for two and three unit cells in series is computed by a convolution procedure. The agreement between the numerical and the convolution-based RTD for multiple unit cells is not satisfactory and indicates the inappropriateness of the convolution procedure for computing the diffusion-free RTD of multiple unit cells in Taylor flow. The failure of the convolution procedure is attributed to the dividing streamline, which separates in Taylor flow the liquid phase in two regions, one with recirculating and one with bypass flow. In the absence of diffusion, the diving streamline is never crossed. As a consequence, locations of tracer particles in neighboring unit cells are not independent which invalidates the unit cell convolution approach.

1. Introduction

Segmented gas–liquid flow is a common two-phase flow pattern in narrow channels. It is also denoted as Taylor flow or bubble train flow and consists of a sequence of elongated gas bubbles which almost fill the entire channel cross section (Taylor bubbles). The individual bubbles move along the channel while they are separated by liquid slugs. Taylor flow is of technical relevance e.g. for miniaturized multiphase reactors [1–5] and multiphase monolith reactors [6–8]. It has been considered for production of H_2O_2 [9] and is finding increasing interest for potential use in Fischer–Tropsch synthesis [10–13].

In Taylor flow, the length of the liquid slugs and the size of individual bubbles underlie variations. The variation of the bubble size results in a variation of the translational velocity of individual bubbles. This may lead to coalescence and thus a further change of the bubble size and slug length distribution. A useful abstraction of

* Corresponding author. Tel.: +49 721 608 24477; fax: +49 721 608 24837.
E-mail address: martin.woerner@kit.edu (M. Wörner).

1385-8947/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cej.2012.06.062

Nomenclature

C	tracer concentration (mol/m^3)
C_{cs}	ratio between mean and maximum velocity in laminar channel flow
Ca	capillary number
d_B	bubble diameter at a certain axial position (m)
$d_{B,max}$	maximum bubble diameter (m)
d_h	hydraulic diameter of channel (m)
D	molecular diffusion coefficient of tracer in liquid phase (m^2/s)
E	residence time distribution (1/s)
h_F	thickness of liquid film between gas bubble and channel wall (m)
J	total superficial velocity (m/s)
J_G	superficial velocity of gas phase (m/s)
J_L	superficial velocity of liquid phase (m/s)
L_{ref}	reference length scale (m)
L_S	liquid slug length (m)
L_{travel}	axial traveling distance of particles to determine the RTD (m)
L_{UC}	length of unit cell (m)
n	number of CSTRs or unit cells in series
N_{cross}	number of unit cells particles must travel to obtain the RTD
N_P	number of particles
Pe	Peclet number
Q	volumetric flow rate (m^3/s)
Re_B	bubble Reynolds number
t	time (s)
t_{ref}	reference time scale (s)
Δt	time step width (s)
Δt_{class}	time interval of classes in the RTD (s)
U_B	bubble velocity (m/s)
U_F	mean velocity in liquid film at a certain axial position (m/s)
U_L	mean liquid velocity in the computational domain (m/s)
$U_{L,max}$	maximum axial velocity in the liquid slug (m/s)
$U_{L,max}^{fd}$	maximum axial velocity in fully developed Poiseuille flow (m/s)
U_{ref}	reference velocity scale (m/s)
V	volume (m^3)
Δx	mesh size (m)

Greek symbols

α	weighting factor in PDD model
β	pre-factor of maximum bubble diameter in PDD model
δ	Dirac delta function
ε	gas volume fraction in the unit cell
λ	ratio $U_{L,max}/U_{L,max}^{fd}$
μ	dynamic viscosity (Pa s)
ρ	density (kg/m^3)
σ	coefficient of surface tension (N/m)
τ	mean residence time (s)
τ_B	bubble break through time (s)
τ_D	delay time (s)
τ_F	mean residence time of liquid film/corner flow (s)
τ_h	mean hydrodynamic residence time (s)
τ_S	mean residence time of liquid slug (s)

Subscripts

B	bubble
F	liquid film
G	gas phase
L	liquid phase
p	particle
ref	reference value
S	liquid slug
UC	unit cell

Abbreviations

CSTR	continuous stirred tank reactor
PD	peak-decay
PDD	peak-decay-decay
PFR	plug flow reactor
RTD	residence time distribution

real Taylor flow is *perfect Taylor flow*, where the bubbles are assumed to have identical size, shape and velocity and where the length of all liquid slugs is the same. Then, the hydrodynamics of Taylor flow is fully described by a unit cell (UC) which consists of one bubble and one liquid slug.

For the design and optimization of micro-structured chemical reactors, the ability to reliably predict the RTD is of great importance. In Taylor flow, the RTD of the continuous liquid phase is of major interest, since the variation of the residence time of the gas phase is small and its mean value is given by the ratio between channel length and bubble velocity. Desirable is a plug flow behavior of the liquid phase with a narrow RTD. Sun et al. [14] recently investigated the influence of the RTD on the synthesis of biodiesel in capillary micro-reactors operated with Taylor flow. They found that the RTD in the micro-channel reactor was remarkably decreased compared to the RTD which is required in batch systems to obtain a high yield under the same reaction conditions. However, the RTD of the micro-reactors had to be controlled to avoid the saponification of the biodiesel. While this example demonstrates the practical importance of the RTD, there are, unfortunately, only very few experimental data on the liquid phase RTD available in literature for miniaturized multiphase reactors such as monolith reactors. This may be attributed on one hand to the difficulties of performing local measurements of the RTD in narrow channels and on the other hand to the only recently increasing interest in this topic. As a consequence, reliable and validated general models for the RTD in multi-phase micro-structured reactors are missing. This is in particular true for channels of non-circular cross-section, which are quite common in monoliths and micro-structured reactors. In rectangular channels, the film thickness at the circumference of the bubble is not constant. The resulting so-called corner flow can be significant [15] and makes the application of RTD models for circular channels inappropriate.

In experiments the RTD is often measured by a stimulus–response technique, where a specific quantity of a tracer is introduced at the system inlet as a short duration pulse or a step function and where the time variation of the tracer concentration is recorded at the outlet. This procedure is well suited for macro-reactors, where the reactor volume is much larger than the volume of the tracer measurement device. However, for micro-structured reactors, the reactor volume is usually smaller than the volume of the measuring unit. This means that the response of the tracer may already be influenced by the measurement configuration itself. Therefore, for RTD measurements in small channels optical methods should be preferred which measure directly inside the channel. Measurements of the liquid phase RTD in two-phase flow