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Hydrodynamics and mixing in continuous oscillatory flow reactors—Part I: Effect of baffle geometry

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ABSTRACT

Time-dependent laminar flow in a continuous oscillatory baffled reactor has been studied using Computational Fluid Dynamics. The effect of baffle geometry on pressure drop, energy dissipation as well as the instantaneous flow and shear strain rate fields has been investigated for five different geometries, namely single orifice baffles, disc-and-donut baffles and three novel variations of helical blades. All designs show complex flow behaviour and the formations of vortices due to both flow blockage and flow reversal with various amounts of pressure drop and energy dissipation. However, it is clearly difficult to conclude on the impact of baffle design on the performance of the reactor with velocity, shear strain rates and vorticity alone. Part II of the paper therefore presents and exploits alternative quantitative measures to better quantify reactor performance.

1. Introduction

Amongst the different technologies for process intensification, continuous oscillatory baffled reactors (OBRs) have been shown to be highly efficient for a number of different operations, including solids transport [1], crystallisation [2,3], polymerisation [4,5], heat transfer [6,7], as well as liquid-liquid [8,9] and gas-liquid [10] contacting and/or reaction. Examples of application include the production of solid active pharmaceutical ingredients [3], polymers [4,5] and biofuels [8,9].

The continuous oscillatory baffled reactor typically consists of a pipe with sharp-edged baffles along its length and it operates with an oscillatory or pulsed flow rate, which creates recirculating flow and eddies. This unique flow enables the creation of a series of well-mixed volumes, allowing efficient mixing and mass and heat transfer, and also provides reasonable plug flow with long residence times [11–13]. Amongst the numerous works dedicated to oscillatory baffled reactors or columns (OBC), several studies have focused on the observation of flow patterns experimentally, using Particle Image Velocimetry (PIV), and/or numerically with Computational Fluid Dynamics (CFD). The majority of these works study the flow generated in OBRs or OBCs equipped with single orifice (or ring) baffles and the hydrodynamics are generally described in a qualitative manner using planar velocity fields and velocity profiles (e.g. [14–17]). These flow fields show the generation of a non-negligible radial velocity component and the formation of vortices near the baffles that are then transported into the bulk flow. It is this repeating mechanism of vortex generation with flow oscillation that promotes uniform mixing in each cell (i.e. the zone between successive baffles) [18,19]. In order to quantify the importance of the radial flow component that is closely related to the vortices and mixing, Ni and co-workers proposed the use of a dimensionless velocity ratio, R_v, that compares the plane-average axial and radial velocities [20]. Systems displaying lower values of R_v are more effective in enhancing mixing and decreasing axial dispersion. Fitch et al. [20] identified an empirical critical value of R_v equal to 3.5 that is required to sufficiently mix Newtonian and non-Newtonian fluids within an OBC. R_v has also been used to evaluate the effect of viscosity [13,20] and scaling-up [21] on the flow performance of oscillatory baffled reactors.

An obvious way of evaluating the strength of the vortices in the flow is via the calculation of vorticity. Indeed, Nogueira et al. [22] showed that zones of high vorticity are generated in the form of vortex rings as the fluid moves through the orifice plate; these rings are then broken up and reoriented into thread-like structures as the flow direction changes. However, although vorticity is a fundamental characteristic of fluid flow and high levels are present

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Nomenclature

A	Amplitude (m)
d	Channel diameter (m)
f	Frequency of pulsation (Hz)
p	Pressure (Pa)
R	Radius of tube (m)
Re_{net}	net Reynolds number ($u_{net}d\rho/\mu$)
Re_o	Oscillatory Reynolds number ($2\pi f\,Ad\rho/\mu$)
r	Radial coordinate (m)
t	Time (s)
T	Oscillation period (s)
u	Velocity vector ($\mathrm{m\,s^{-1}}$)
u	Axial velocity ($\mathrm{m\,s^{-1}}$)

Greek symbols

μ	Dynamic viscosity (Pa s)
ρ	Fluid density ($\mathrm{kg\,m^{-3}}$)
ω	Angular frequency (=$2\pi f$) ($\mathrm{s^{-1}}$)

Subscripts

0	Constant component
in	Inlet
net	Net
o	Oscillatory

in these oscillating flow devices, its importance for characterising OBR applications is not explicit. Vortices and shear flow are of course closely related, and the analysis of shear strain rates therefore may be more practical when evaluating the performance of OBRs. Characterising mean and maximum strain rates in this type of equipment is of interest for applications involving dispersed liquid-liquid or gas-liquid flow, as well as biochemical processes that suspend and transport cells or other cultures. Ni et al. [23] used PIV to determine instantaneous and average strain rates in an OBC equipped with orifice plates for a range of Reynolds numbers. They showed that the mean strain rates generated in OBCs are lower than those observed in conventional stirred tanks, thereby suggesting the interest of this equipment for applications that require low shear.

The OBR technology and design are inspired from pulsed and reciprocating plate columns created for liquid-liquid extraction applications since the first patent by Van Dijck in 1935 [24]. Although different baffle designs, such as perforated plates and disc-and-donut internals, have been used in the long history of extraction columns [25], the baffles in OBRs have traditionally been single orifice plates and the effect of baffle design has only become of interest in recent years. Mackley and co-workers investigated the effects multi-orifice plates on hydrodynamics and axial dispersion for the scale-up of OBRs [22,26]. In particular, Smith and Mackley [26] have shown that axial dispersion is affected very little by scale-up when using multi-orifice plates compared with single orifice plates. This means that development studies at lab-scale can be performed in small baffled tubes and the result can be used to estimate the performance of larger scale multi-orifice plate geometries.

With the objective of process intensification via the reduction of equipment size, Harvey and co-workers [12,27–29] have investigated novel designs of mesoscale oscillatory baffled reactors. These reactors that have a diameter of just a few millimetres allow the manipulation of small fluid volumes at low flow rates, thereby reducing reagent use and waste production. Their motivation for exploring the effects of baffle design was to achieve good mixing conditions even at very low net flow rates (down to <1 ml/min). In their papers, they have compared the performance of central baffles and single orifice (or integral) baffles [27] with different types of helical baffles [12,28,29] via residence time distribution (RTD) measurements and analysis. The helical baffle allowed a significantly higher degree of plug flow compared with the other geometries and particularly at higher oscillation amplitudes (2–4 mm). The helical baffles used were coiled wires varying in pitch and diameter. Although the diameter of the wire only had a noticeable effect on RTD at higher oscillatory Reynolds numbers, the authors highlighted the strong relationship between helical pitch and oscillation amplitude. When the pitch is increased, the oscillation amplitude must be increased to achieve plug flow.

Considering the current literature on baffle design and the limited techniques used to characterise the performance of hydrodynamics mixing in OBRs, this work, which is presented in two parts, addresses (i) the flow characteristics of some conventional and novel baffle designs, analysed using data directly accessible from numerical simulations and (ii) alternate post-processing methods for characterisation mixing that are tested using the different baffle designs presented in this paper [30]. The underlying objective of studying different baffle designs is to identify the flow and mixing characteristics generated by each, thereby defining a larger choice of equipment for more varied applications. In this paper, Part I, time-resolved laminar CFD simulations have been performed to study the flow generated in five OBR designs. The flow is assessed by examining instantaneous velocity fields, shear strain rate, vorticity, Q-criterion, velocity ratio, pressure drop and energy dissipation.

2. Geometries

Five OBR geometries with different baffle designs have been studied and are shown in Fig. 1. The first is the conventional single orifice plate, which provides a basis for comparison with the other geometries. The second geometry is the disc-and-donut design that has been used largely in pulsed extraction columns. It consists of alternating disc and single orifice plates; the disc acts as a barrier to the axial flow in the centre of the tube and generates additional radial flow. The remaining three baffle geometries are based on the use of a sharp-edged helical blade, which is inspired from helical ribbon impellers used for mixing viscous fluids in stirred tanks. It is similar to that employed by Hegwill et al. [10] in an open ended vertical tube with flow oscillations for gas-liquid mass transfer. This design also shows some similarity with the helical wire inserts used by Harvey and co-workers [12,28,29,31] except that it consists of a sharp-edged blade, which is oriented such that the blade is normal or oblique to the net flow direction and therefore expected to increase the radial flow component. Harvey and co-workers have also used a sharp-edged helical baffle for biodiesel production [32]; however the blade in their design was parallel to the main flow direction. The other helical blade designs are a double helical ribbon where the blades revolve in opposite directions and an alternating helical ribbon, which consists of a single blade that revolves in different directions every two periods. At first sight these geometries may appear difficult to manufacture, however with the recent advances of additive manufacturing, the cost-effective fabrication of such structures at small scales in now possible [33,34].

The dimensions of the different baffles are such that they fit flush within a 15 mm diameter tube. The distance between orifice plates (or donuts) is 26 mm and the diameter of the orifice is 8 mm. For the disc-and-donut geometry, the discs (8 mm diameter) are positioned midway between the orifice plates. The helical baffles are 3.75 mm wide and have a pitch equal to 26 mm.