Residence times and mixing of a novel continuous oscillatory flow meso reactor

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A novel meso reactor based on oscillatory flow technology (Harvey et al., 2001) has been recently presented in Harvey et al. (2003) as a new technology for reaction engineering and particle suspension applications. Due to the demonstrated enhanced performances for fluid micro mixing and suspension of catalyst beads and to the small volume of the reactor, this novel miniature reactor is suitable for applications at specialist chemical manufacture and high throughput screening. Furthermore, a high control of environment conditions (e.g. mixing intensity, temperature) coupled with an online monitoring turns this reactor suitable for small-scale applications to the bioengineering field, such as for fast parallel bioprocessing tasks.
This work concerns with the fluid dynamics characterisation of a novel miniature reactor. Experimental results using state-of-art fibre-optic technology is used in order to demonstrate that an accurate control of the residence time distribution (RTD) of liquid and solid phases can be achieved within this reactor as well as enhanced (oxygen) mass transfer rates. Furthermore, numerical simulations using Fluent ® software will be presented where simulated RTDs agrees with the experimental results.
The meso reactor unit consists of 4.4 mm internal diameter and 35 cm long jacketed glass tubes, with a unit volume of 4.5 ml and provided with smooth periodic constrictions (SPCs), with an average baffle spacing of 13 mm. The internal diameter at the constricted zone (baffle internal diameter) is 1.6 mm, leading to a reduction of the baffle free are of 87 %. This unit is able to support batch or continuous operations mode, simply by configuring the tubes in parallel or in series, according to the intended application. Mixing is achieved by oscillating the fluid at the bottom or the top of the reactor by means of a piston pump, using oscillation amplitudes and frequencies ranging from 0 to 4 mm centre-to-peak and 0 to 25 Hz, respectively.
Experimental studies using the Particle Image Velocimetry (PIV) technique (Harvey et al., 2003) showed that different fluid mechanics are originated at different oscillation conditions (oscillation amplitudes and frequencies). A plug flow or a stirred tank behaviour can be obtained just by controlling the oscillation conditions. At low oscillatory Reynolds numbers (Re_o), e.g. 10 to 100, the formation of axisymmetric eddies detached from the constrictions is coupled with low axial velocities and makes it possible to continuously operate the reactor in a plug flow mode. Increasing the Re_o to values higher than 100, the eddy symmetry is broken and a complete mixing state is achieved inside the meso reactor. Low oscillation amplitudes must be used if axial dispersion is intended to be minimized, namely at plug flow setup.
Through an overall oscillation cycle, changes of the location of the main flow stream from near the wall to the centre of each cavity and vice-versa was observed and is expected to lead to high mass and heat transfer rates (Perry, 2002). Due to the observed high radial velocities, narrow residence times distributions are expected to be obtained (Perry, 2002). Also high axial circulation rates were also observed at high Re_os (above 100) and it was proved to lead to an enhanced performance on catalyst beads suspension. The relation of this fluid mechanics with the real performance of this novel meso reactor will be demonstrated.
Tracer injection technique is applied to perform RTD studies inside a single SPC tube of the meso reactor. Spectroscopy UV/VIS technique is used to measure the concentration of a coloured tracer at the inlet and outlet (at continuous mode) or at the bottom and the top of the

tube (at batch mode). A fibre optic apparatus is employed in order to obtain highly accurate online measurements of the UV/VIS absorbance. Mixing times are calculated for experiments at batch mode. Different flow rates are used to determine the effect of the flow rate over the RTD at continuous operation and axial dispersion is presented by the Bodenstein number, B_o. Determination of $K_L.a$ values is achieved by online measurement of the oxygen concentration using a special fibre optic probe. The working tip of the probe was dip-coated with a ruthenium complex immobilised in a sol-gel matrix. This complex is excited to fluorescence by a blue led (470 nm outpuk peak) and the level of the fluorescence is inversely related to the concentration of the oxygen through the Stern-Volmer equation (Wang *et al.*, 1999), which is measured by the fibre-optic apparatus. Retention of solid phases (e.g. catalyst beads and yeast cells) inside the meso reactor will also be tested.

Further studies using the Computation Fluid Dynamics (CFD) technique will be presented where accurate prediction of the distribution of residence times is achieved. The use of the distribution-functions permits to classify the flow behaviour inside this novel meso reactor patterns and to calculate mixing efficiencies and axial dispersion coefficients (expressed by the B_o number) at different oscillation conditions.

A simple 2-D axisymmetric laminar model showed good agreement with flow patterns visualisations using PIV for Re_o below 100 but a 3-D model with a very fine mesh was required to simulate breakage of axisymmetry. Consequently, 3-D models based on laminar and Large Eddy Simulations (LES) will be used to maximize the matching of RTD at higher oscillation conditions. Main intended application of CFDs to this novel meso reactor is the design of a meso reactor unit, which could operate at the best oscillation conditions and flow rate for cell cultures and biocatalyst applications.

References

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