Enhanced mass transfer rates of a novel oscillatory flow screening reactor

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A novel continuous small-scale reactor based on the oscillatory flow technology (Harvey et al 2001) is being developed for application to specialist chemical manufacture and high throughput continuous screening (Harvey et al 2003). This novel reactor is able to perform continuous multiphase reactions, including those involving the suspension of catalyst beads. Extensive potential use in chemistry, biological and pharmaceutical laboratories is envisaged.

Optimum operation conditions for applications in the bioengineering field depend on at least four parameters: *1)* fluid mixing, *2)* residence time characteristics, *3)* particle suspension and *4)* (oxygen) mass transfer rates. This work particularly concerns the establishment of the operation conditions in relation to oxygen mass transfer rates, $K_L.a$. Furthermore, $K_L.a$ values are correlated with the fluid mixing, axial dispersion coefficients and finally with the fluid mechanics observed experimentally by particle image velocimetry (PIV) technique and numerically simulated using Fluent® software.

The screening reactor is composed of a 35 cm length glass jacketed tubes (Figure 1), provided with smooth periodic constrictions (SPCs). The internal diameter of the tube is 4.4 mm. The diameter in the constricted zone (the baffle internal diameter) is about 1.6 mm, representing an 87 % reduction in the cross-sectional area. Mixing intensity is controlled by setting up the frequency and the amplitude (centre-to-peak) of the fluid oscillations. Typical oscillation frequencies and amplitudes are from 0 to 20 Hz and from 0 to 4 mm, respectively. A screening arrangement based on some SPC tubes (say 10 to 20) placed at different configurations (serial or parallel) makes this novel reactor suitable for parallel processing and/or for sequential reactions procedures.

State-of-the-art fibre-optical technology was used for on-line monitoring of the oxygen concentration inside the screening reactor by using a special fibre optical micro-probe. The working tip of the probe was dip-coated with a ruthenium complex immobilised in a sol-gel matrix. This complex was excited to fluorescence by a blue led (≈ 470 nm output peak) and the level of such fluorescence is inversely related with the concentration of the oxygen through the Stern-Volmer equation (Wang *et al.*, 1999). Continuous fluorescence levels are accurately measured by an UV/VIS/NIR multi-channel spectrometer.

Numerical simulations by the computational fluid dynamics (CFD) technique, using Fluent ® software, permitted us to conclude that either near plug flow or stirred tank behaviour can be approached in a single SPC tube, by controlling the fluid oscillation conditions, i.e. the oscillation frequency and/or amplitude. For oscillatory Reynolds numbers (Re_o) between 10 and 100, the formation of axisymmetric vortex rings leads to a good radial mixing of the fluid and to low axial dispersions, which suggests that a performance near a plug flow reactor is achieved. For Re_o above 100 the high intensity and asymmetry of the vortex rings leads to an increase of the axial dispersion and the fluid behaviour approach that of a stirred tank. All these results were experimentally validated by PIV observations.

High radial rates of flow exchange were numerically simulated and experimentally observed during a complete oscillation cycle, coupled with a high degree of velocity gradients. Thus, enhancements of heat and mass transfer rates are expectable within this novel screening reactor. Further, an increase of bubbles breakage is also expected (leading to a decrease of bubble diameter, i.e. an increase of the specific bubble area, *a*, and also of the gas hold-up), conducting to a significant improvement of oxygen mass transfer. This will be demonstrated with the present work.

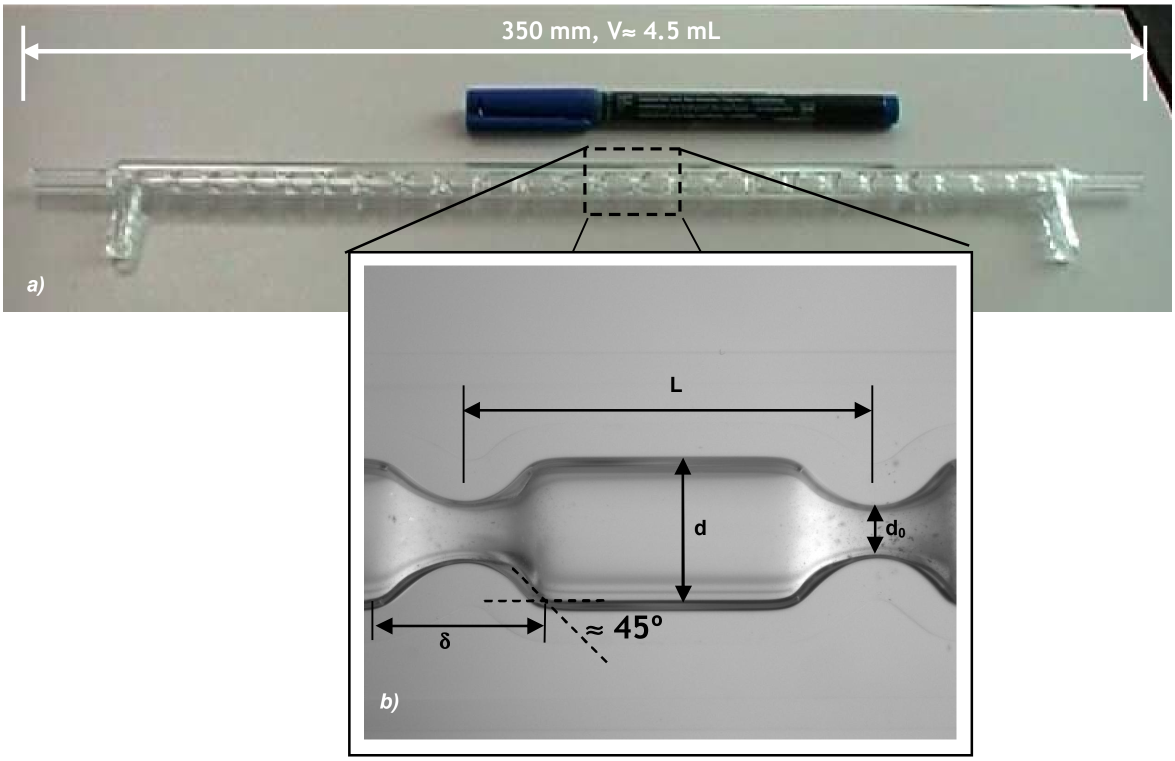

Figure 1. Geometry of a single SPC tube: L = 13.0 mm; d = 4.4 mm; d_0 = 1.6 mm; δ = 6.0 mm.

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