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Coupling experimental and numerical modeling for studying mixing thermo-hydrodynamic phenomena in a microfluidic reactor working under pressure

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In the frame of the SCWO insert development aiming at studying cold combustion process in supercritical water ($T < 600^\circ\text{C}$, $p < 300$ bar) for the recycling and valorization of wastes for long term exploration missions, we focus in here on mixing phenomena occurring within microreactors working in realistic pressure conditions (100 bar). We have considered model fluid mixtures (CO_2 -water diphasic and CO_2 -ethanol monophasic), which are representative of the future thermo-hydrodynamic properties, which will be used in SCWO with supercritical water. We have first identified new jetting mode for coflow injection, mostly driven by inertia. Then, we have determined by numerical simulation the mixing time associated with coflowing fluids inside microchannels for a monophasic system (CO_2 – ethanol) at both laminar and turbulent conditions.

Results

For immiscible fluids (CO_2 and water), a specific focus has been drawn on the effects of inertial forces to the interfacial and viscous forces. Three distinct modes have been identified for jet break-up in confined microfluidic scale: the conventional Rayleigh mode and two additional inertia-driven modes occurring at higher Reynolds numbers, namely: the sinuous wave breakup and an atomization-like mode. All these regimes from dripping to jetting are differentiated by characteristic droplet sizes, size distributions and the evolution of jet length as function of the external fluid velocity. A general phase diagram has been proposed to categorize the jet breakup mechanisms based on the inner and outer fluid inertial forces (Figure 1). These results provide fundamental new insight into the flow behavior of co-flowing jets confined at microscale for two immiscible fluids [1].

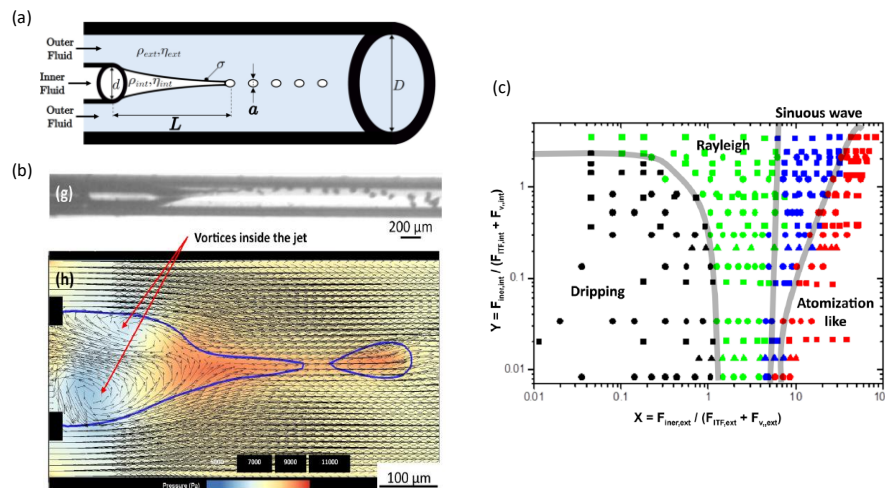


Figure 1: (a) Coflowing setup developed for this study. D and d are the inner diameters of the outer and inner tubing, respectively. L is the jet length, while a is the droplets diameter., (b) Optical image of the atomization-like mode and median plane visualization of the 3D numerical modeling of the atomization-like jetting mechanism displaying the velocity vectors inside the core of the jet, (c) Log-log plot of the ratio ($X:Y$) of the inertial forces over the sum of the viscous and interfacial forces for different investigated systems.

In the case of miscible fluids (CO_2 and ethanol), thermodynamics plays an important role over hydrodynamic behavior. Depending on the considered conditions (p , T , X_{EtOH}) and the location within the EtOH- CO_2 phase diagram, several different behaviors can be observed. In the particular case of monophasic mixture (liquid or supercritical), no obvious interface could be noticed, meaning the mixture velocity plays an essential role to characterize the fluid behavior. By applying a micro Particle Imaging Velocimetry (μPIV) technique to a mixture of ethanol and CO_2 at laminar flow conditions, the fluid mixture velocity field is obtained and compared with numerical simulation in order to provide interesting data and to estimate the micromixing time [2].

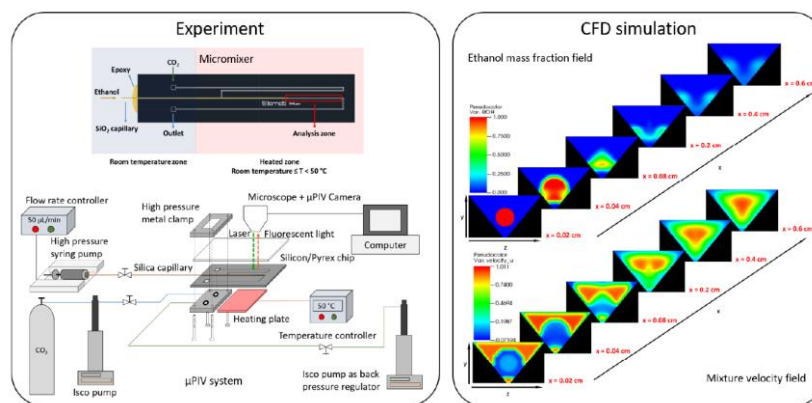


Figure 2: (Left) Experimental setup developed for acquiring the local velocity field in a CO_2 – EtOH mixture coflowing under pressure inside a microreactor. μPIV technique was used to acquire the data. (Right) Numerical modeling of the EtOH mass fraction and the local velocity of fluid for different cross section of the microchannel.

Eventually, we have investigated by numerical modelling the mixing efficiency of such devices configuration under turbulent conditions. We have shown experimentally that the turbulent mixing could be reached in the microchannel thanks to the "high pressure microfluidic" technology developed in the laboratory. The study of the mixing quality is based on two criteria commonly used in the literature. The first is the segregation intensity based on the variance of the ethanol concentration. This can be estimated for all simulation cases, from laminar to turbulent mixing. The second criterion is the micromixing time related to the turbulent kinetic energy dissipation rate directly estimated from the local velocity fluctuations in turbulent flow conditions. One of the major interests of the use of microfluidic reactors lies especially in its small scales of time and space allowing accessing mixing time in the order of magnitude of 10^{-5} second [3].

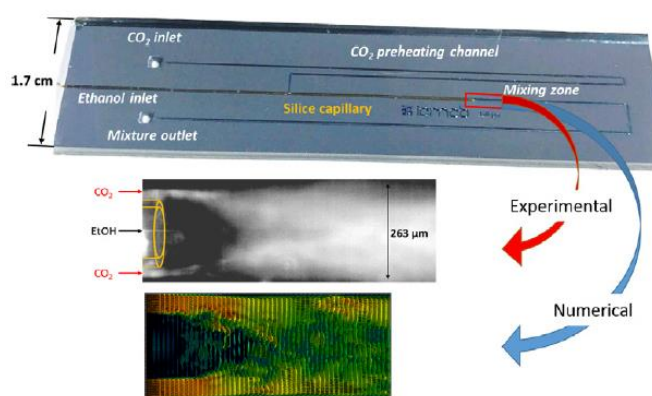


Figure 3: (top) high pressure microreactor for accessing turbulent mixing conditions on chip, (middle) Turbulent mixing of CO_2 -ethanol fluid mixture observed in a microreactor under high pressure and (bottom) 3D CFD is performed for microfluidic turbulent mixing by using direct numerical simulation (DNS).

Perspectives

The obtained results are a first test of the final configuration of mixing, which will be used in the future DECLIC SCWO insert. We are now developing a new microreactor design, made of sapphire, for implementing supercritical water and investigating – in particular the hydrothermal flame behavior (which depends on the thermo-hydrodynamic flow properties, based on the experimental and numerical tools, which have been developed.

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