Assessment of 3D CFD Modeling of W/O Emulsification in Microfluidic Cross-Junctions

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Abstract
This study investigates water-in-oil emulsification in an asymmetric cross-slot microchannel using 3D CFD simulations. Two inlet streams with different cross-sections generate a head-on impinging flow that enhances droplet breakup via recirculation. Simulations are performed using the Volume of Fluid method in ANSYS Fluent, with URANS modeling and Adaptive Mesh Refinement and turbulence closure. Two experimental cases from literature are reproduced to analyze early-phase interface dynamics, velocity fields, and shear rates. Results offer high-resolution insight into emulsion formation mechanisms, supporting experimental design and optimization for high-throughput microfluidic applications.

Introduction
Water-in-oil (W/O) emulsions are gaining traction as alternative fuels for improving combustion and reducing emissions [1]. Water droplets vaporize early during injection, triggering micro-explosions that enhance atomization, improve fuel-air mixing, and lower soot and NOx formation [2]. Emulsion quality depends on droplet size and distribution, which are sensitive to production methods and hydrodynamic conditions [3]. Conventional techniques offer limited control, while microfluidic devices enable precise droplet formation [4]. Belkadi et al. [5] demonstrated high-throughput W/O emulsification in cross-flowing microchannels, highlighting the role of turbulence and asymmetric layouts in improving performance. CFD simulations, particularly using the Volume of Fluid (VOF) method [6], have supported these findings by analysing the effects of geometry and flow on droplet formation [7]. However, 3D simulations of W/O emulsions in high-flowrate cross-slot configurations remain scarce, despite their relevance for scaling up to industrial applications. The aim of this study is to develop a transient 3D CFD model of W/O emulsification in cross-junctions using a Unsteady Reynolds Averaged Navier Stokes (URANS) approach in ANSYS Fluent. The model resolves microsecond-scale interface dynamics, velocity fields, and shear rates, offering insights into early-stage emulsification. The results support experimental validation and can inform process optimization and the design of other multiphase microfluidic systems.

Material and Methods
The investigated microchannel features an asymmetric cross-slot configuration with head-on impinging streams [5]. Two square inlets (300×300 μm and 600×600 μm)

promote emulsification via recirculation-enhanced breakup, while two perpendicular outlets allow emulsion outflow (Figure 1). This study replicates the experimental conditions from [5] for water-in-oil emulsions. Fluid properties and operating conditions for Cases 1 and 2 are summarized in Table 1 and serve as the basis for the 3D CFD simulations.

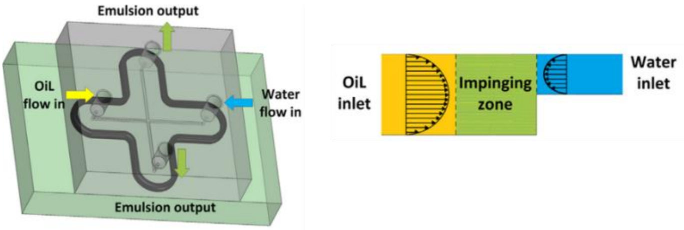

Figure 1. Design of microfluidic device [5].

Table 1. Properties of used fluids and operative conditions [5].

Liquid	Water	Oil
Surface Tension [mN/m]	73.5	33.7
Interfacial Tension [mN/m]	27.6	
Viscosity [mPa s]	0.91	52.2
Density [kg/m^3]	998	865
Flowrate [mL/min] – Pressure [bar] (Case 1)	7.10 – 3.3	64.86 – 7.0
Flowrate [mL/min] – Pressure [bar] (Case 2)	15.17 – 3.7	67.33 – 7.3

Due to flow symmetry, the computational domain includes both inlet channels and a single outlet. Mass flow rate inlets are imposed, along with atmospheric pressure at the outlet. Walls are modeled as adiabatic with no-slip conditions. The mesh consists of hexahedral cells (avg. 25 µm), with a 6-layer boundary refinement (50 µm total, minimum $y^+ = 1$ corresponding to 5 µm on the water side), totaling ~1.08 million cells. Transient simulations are carried out in ANSYS Fluent 2024R2 using a pressure-based solver with absolute velocity formulation. Mass and momentum are solved via an implicit first-order transient scheme, with PRESTO! for pressure and second-order upwind for momentum and turbulence. Pressure-velocity coupling is handled via the PISO algorithm. A 3D Volume of Fluid (VOF) model tracks the water–oil interface using an implicit sharp-capturing strategy. Surface tension is modeled via the CSF approach ($\sigma = 0.0276$ N/m), with wall adhesion and no-slip. Adaptive Mesh Refinement (AMR) based on volume fraction gradient allows up to 6 refinement levels, reaching a minimum cell size of approximately 0.5 µm. In this way, the mesh size can grow to around 20 million cells during the unsteady simulation. Turbulence is modeled using the k-ω SST model [8]. The time step is set to 1 µs to ensure Courant numbers lower than 1 in refined regions. Simulations are initialized via hybrid method, with oil as the base fluid and a water volume fraction patch at the inlet.

Results

Figure 2.a shows the contour of water fraction (blue) in oil (white) at 6 ms from the start, on a plane passing through the center of the inlet channels, highlighting both the grid refinement at the interface between the two fluids and the formation of a recirculation vortex. Moreover, Figure 2.b shows the water iso-surface colored with local values of Capillarity, a non-dimensional number defined as the ratio between the product of dynamic viscosity and velocity, and the interfacial tension. It has been proved [5] how this parameter is inversely proportional to the average emulsion diameter: indeed, as reported in Figure 2.c, it can be seen how Case 2 (characterized by higher velocities) shows higher values of average capillarity in the outlet volume with respect to Case 1.

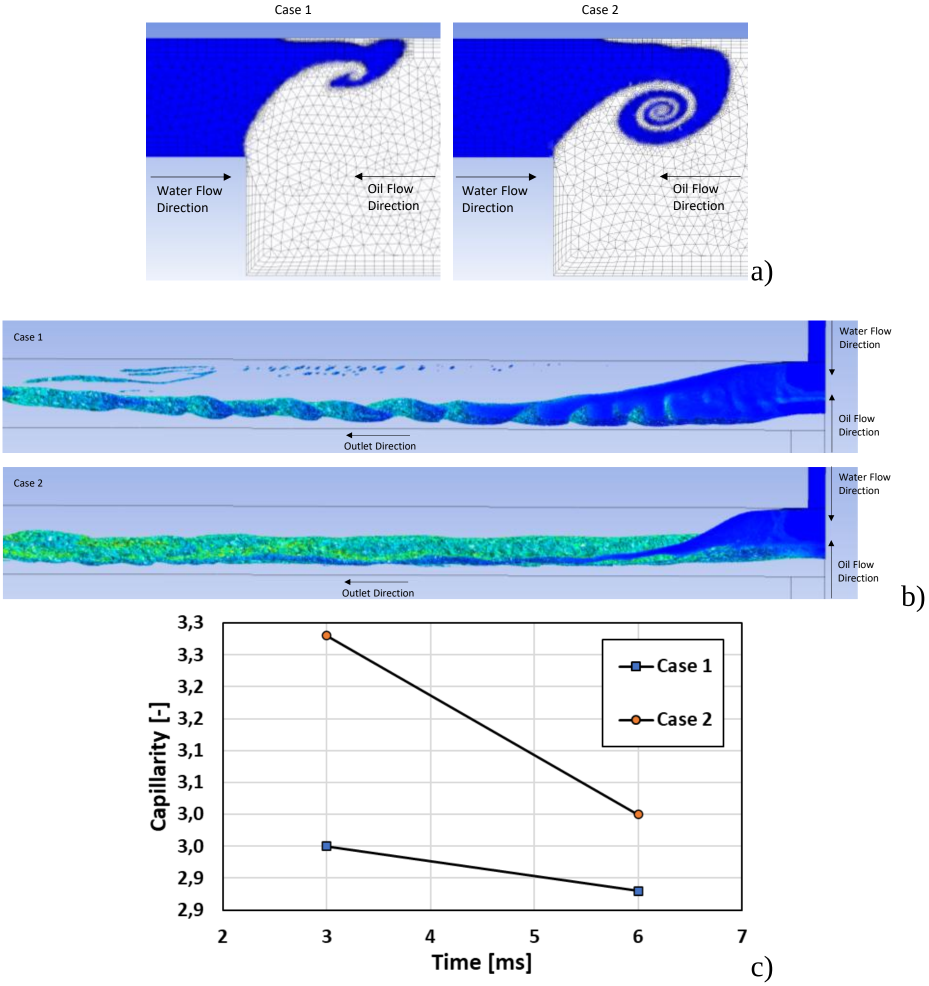

Figure 2. a) Contour of water fraction (blue) in oil (white) on a plane passing through the center of inlet channels; b) water iso-surface colored with capillarity; c) evolution of average capillarity in outlet volume for both cases.

Conclusions

This study presents a 3D CFD analysis of W/O emulsification in asymmetric microfluidic cross-junctions, capturing transient interface dynamics and flow features with high spatial and temporal resolution. The simulations confirm the role of recirculation-enhanced breakup and highlight capillarity as a key indicator of emulsion quality. Results from both investigated cases offer insight into droplet formation mechanisms and lay the groundwork for future experimental validation and optimization of high-throughput microfluidic systems for fuel applications.

Nomenclature

3D Three Dimensional
AMR Adaptive Mesh Refinement
CFD Computational Fluid Dynamics
URANS Unsteady Reynolds Averaged Navier Stokes
VOF Volume of Fluid
W/O Water-in-oil

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