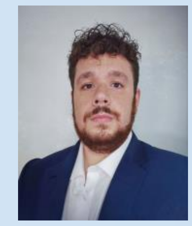
Modelling and Simulation of multiphase and supercritical fluid systems



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Multiphase Fluid Dynamics

Concept

Research on multiphase flows encompasses diverse technological contexts, scales of application, engineering disciplines, and modeling approaches. In my Ph.D. project, Computational Fluid Dynamics (CFD) supports experimental work to advance our comprehension of this field. Three industrial applications were explored*:* ***liquid-liquid extraction with supercritical fluid (a)***, ***mixing in stirred vessels (b)***, and ***vibromixing (c)*** for biodiesel production.

In the first phase, I focused on enriching Omega-3 in fish oil using a liquid-liquid extraction structured packing tower with supercritical-CO_2. Experimental groundwork at the University of Palermo were followed by ANSYS® software-based computational modeling, in order to optimize the column fluid dynamics with the *Volume of Fluid* method.

The second phase studied an Uncovered Unbaffled Stirred Tank (UUST), analyzing power number variations under subcritical and supercritical conditions at different speeds. What was obtained through CFD simulations has been confirmed by results present in literature, demonstrating its industrial feasibility.

Lastly, at INP-ENSIACET, Toulouse, research delved into vibromixing computational modeling challenges, aiming to deeply understand an unexplored domain. Simulation outcomes facilitated the evaluation of flow patterns with different configuration.

Scientific approach

The computational fluid dynamics simulations conducted for this study have focused on capturing the interface between the involved phases, with particular attention to the use of the Volume of Fluid (VOF) model. ANSYS Fluent® software were used as solver using VOF to model the interaction of two immiscible phases:

- Supercritical-CO_2 and transesterified fish oil for liquid-liquid extraction;
- Air and water for mixing;
- Water and glass beads for vibromixing using an Eulerian-Eulerian approach.

The use of the explicit method improved numerical precision, while meticulous geometry and mesh construction using ANSYS WORKBENCH® ensured the accuracy of the simulations. The use of *Dynamic mesh* for mixing modeling guaranteed simulations that closely matched observations.

All simulations conducted included a grid independence study. Turbulence models used involved k-ω SST, RSM, and k-ω SST-SBES. Simulations were conducted in transient state with time step sizes ranging from $1{\cdot}10^{-4}$ to $5{\cdot}10^{-5}$ sec.

Research objectives

- ❑ Investigating multiphase flows across various industrial applications using CFD alongside experimental approaches;
- ❑ Studying the flooding conditions of a supercritical liquid-fluid extraction system within a structured packing column and optimizing operational conditions;
- ❑ Analyzing variations in power consumption and vortex shape in uncovered unbaffled stirred vessels with varying agitation speed and fluid viscosity;
- ❑ Investigating the velocity profile established within a vibromixer with an oscillating plate frequency of 100 Hz.