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5th International ATALANTE Conference on Nuclear Chemistry for Sustainable Fuel Cycles

Relevance of CFD in the development of separation processes

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Abstract

CEA Marcoule is in charge of the design of separation devices for spent nuclear fuel treatment at both laboratory and industrial scales. In this aim, and in order to supplement large-scale demonstration steps, which are today excluded, small-scale prototypes of the typical apparatus (i.e. flat-tank dissolver, annular centrifugal separator, pulsed column, etc.) are developed and tested and a phenomenological approach, relying computational fluid dynamics (CFD), is implemented to help in the scale-down and scale-up processes. Besides the design of industrial contactors relevant for the nuclear industry, and the scale-reduction of the demonstrators required for R&D studies, the fluid mechanics studies are also helpful in determining the adjustable parameters of the process simulator which predicts the separation performances (PAREX code).

In this contribution, the methodology based on a multiscale approach, and heavily relying on optical measurement techniques is first introduced. The relevance of CFD simulation and the corresponding limitations are then discussed, based on the study of typical gas-liquid, liquid-liquid and solid-liquid flows encountered in nuclear fuel reprocessing process.

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Keywords: Multiphase flow, Euler-Euler, Euler-Lagrange, DNS

1. Introduction

The design and efficiency optimization of apparatus is an important area of study in the spent nuclear fuel cycle treatment. A new strategy, relying on computational fluid dynamics (CFD), is currently implemented in the chemical engineering laboratory of CEA Marcoule (LGCI), aiming at reducing the need for large-scale demonstration steps in R&D. This methodology is based on both the use of small-scale prototypes for implementing the chemical steps¹ and

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a better understanding of the flow and its coupling with the chemical phenomena, that facilitates the scale-up and the scale-down processes (Fig. 1). While in the past, lot of demonstrators, including full scale pilots, were used to validate the PUREX process, now fluid mechanics studies are becoming more and more important in the R&D program dedicated to the nuclear fuel reprocessing. CFD helps to reduce the amount, and the size, of the demonstrators required for integral experiments and process validation. Indeed, most of the flow features relevant for separation processes (*e.g.* axial dispersion, mean drops / bubbles size and holdup, mass transfer resistance, etc.) can be derived from suitable CFD simulations, and related to the apparatus size and operating conditions thanks to numerical parametric studies. Due to the complexity of most of the flows encountered in separation devices, complementing local scales studies are sometimes necessary.

Nomenclature

CFD	Computational fluid dynamics
DNS	Direct Numerical Simulations
IMFT	Institut de mécanique des fluides de Toulouse (Toulouse institute of fluid mechanics)
LGCI	Laboratoire genie chimique et instrumentation (chemical engineering and instrumentation team)
MPPIC	Multi-phase particles in cell
MRF	Multi-reference frames
PUREX	Plutonium and Uranium Refining by EXtraction
PIV	Particle imaging velocimetry
PLIF	Planar laser induced fluorescence
VOF	Volume of fluid

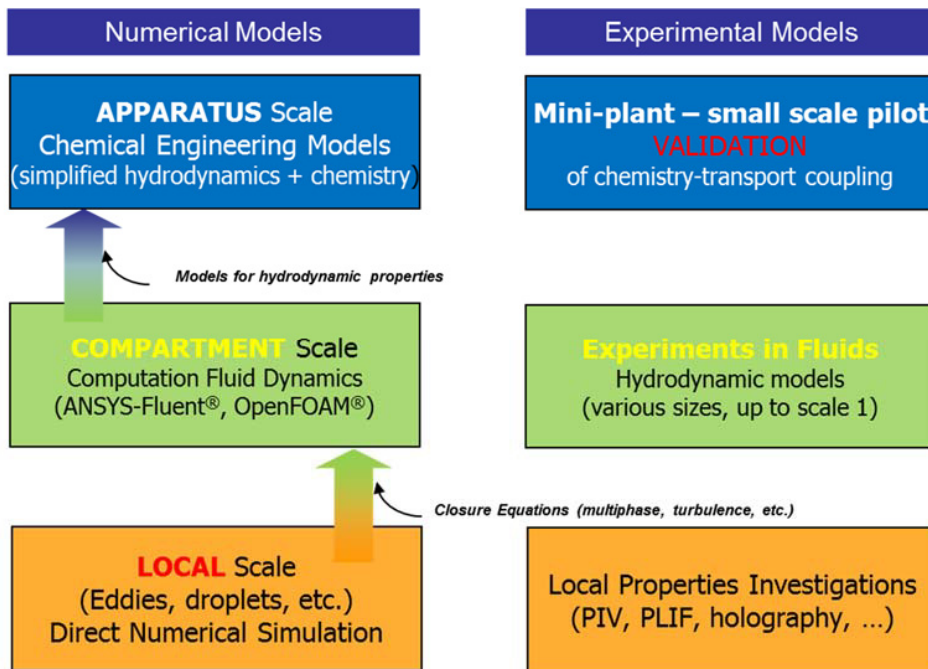


Fig. 1. Schemes of the R&D methodology relying on fluid mechanic studies and simulations

Three examples, highlighting the relevance of CFD for R&D and technological development of nuclear processes, are described in this paper. The experimental tools, complementing the CFD approach, are presented in another paper².

2. Examples of CFD applications

2.1. Gas-liquid process

A subcritical tank liquid-gas contactor is currently developed for the advanced separation processes of nuclear fuels. This batch reactor has to be i) secure, to mitigate criticality hazard, ii) efficient, exhibiting high reaction yield and short operating times, and iii) flexible, due to the many kinds of possible fuels to be treated. Accompanying the design of the industrial reactor, and complementing the dissolution kinetic study achieved at lab-scale in the ATALANTE facility, a comprehensive hydrodynamic study and modelling of a 10-Liter pilot-scale reactor is currently led. The biphasic flow is modelled thanks to a Volume of Fluid approach (VOF) that enables the evaluation of the main hydrodynamic parameters relevant for the dissolution process, mainly: the drops size, their residence time in the tank, and the mixing efficiency. Moreover, by giving access to temporal and spatial evolutions of all these properties (see Fig. 2), numerical simulation is a powerful tool to optimize the reactor design and the position of sampling and control points. The simulations are implemented in ANSYS-Fluent[®].

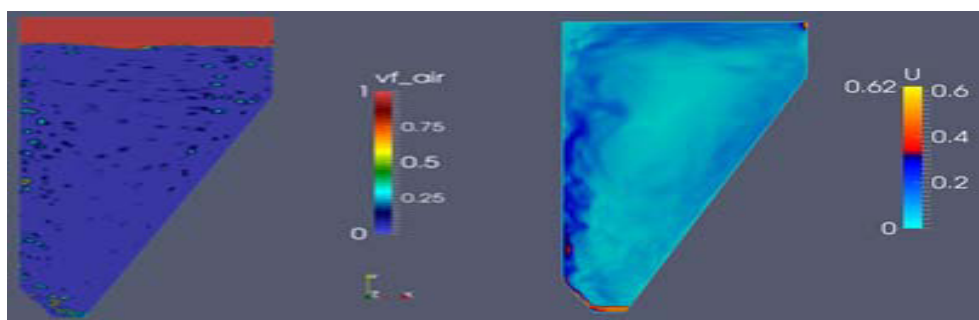


Fig. 2. Example of instantaneous contours of gas fraction (left) and velocity (right) in the flat tank reactor at pilot scale.

2.2. Liquid-liquid separation process

Liquid-liquid extraction processes are efficiently implemented in continuous, multi-stage, counter-current columns. While pulsed columns are intensively used at industrial scale, miniaturized Taylor-Couette columns, which exhibit smaller drops size and lower axial dispersion, are preferred for R&D studies^{1,3}. As in gas liquid contactor, the performances of either type of columns are strongly related to their operating parameters, respectively: the pulsation intensity and the rotation rate, which determine the flow properties. Besides the design and scale-up purposes, a good understanding of the flow features in both kinds of column is therefore mandatory in order to be able to transpose the separation performances achieved in a given column to the other kind. In this aim, because multi-physics phenomena, occurring at different scales, are involved in the turbulent flow and the emulsification process, different models, of increasing complexity are developed. Fig. 3 shows an example of Direct Numerical Simulation (DNS) of local mixing features in a Taylor-Couette column³. A comprehensive experimental and numerical study was led in collaboration with the Fluid Mechanic Institute of Toulouse (IMFT). The simulations were performed with JADIM, the DNS code developed by IMFT.

2.3. Liquid-solid separation process

In the nuclear spent fuel recycling process, liquid-solid separation is carried out through centrifuge devices. For a long time, this technology has proven itself reliable in preventing liquid-liquid separators from fouling by small particles. In the future, the variety of nuclear spent fuel to recycle is expected to increase, and the specifications of the centrifuges will be revised to ensure their efficiency in future recycling process. In this aim, CFD simulations are performed prior, and complementary, to experimental validation.

A numerical centrifuge model was developed helping to finely understand and to gradually improve the design of a device which performances will meet the expected efficiency. An example of results is presented on Fig. 4. The gas-liquid-solid flow in the equipment was modeled using a multi-phase particles in cell (MPPIC) solver coupled with a VOF method. Rotation was handled through the wide-spread multi-reference frames (MRF) method. The multiphase solver was implemented in OpenFOAM, open source software allowing free massive parallelization.

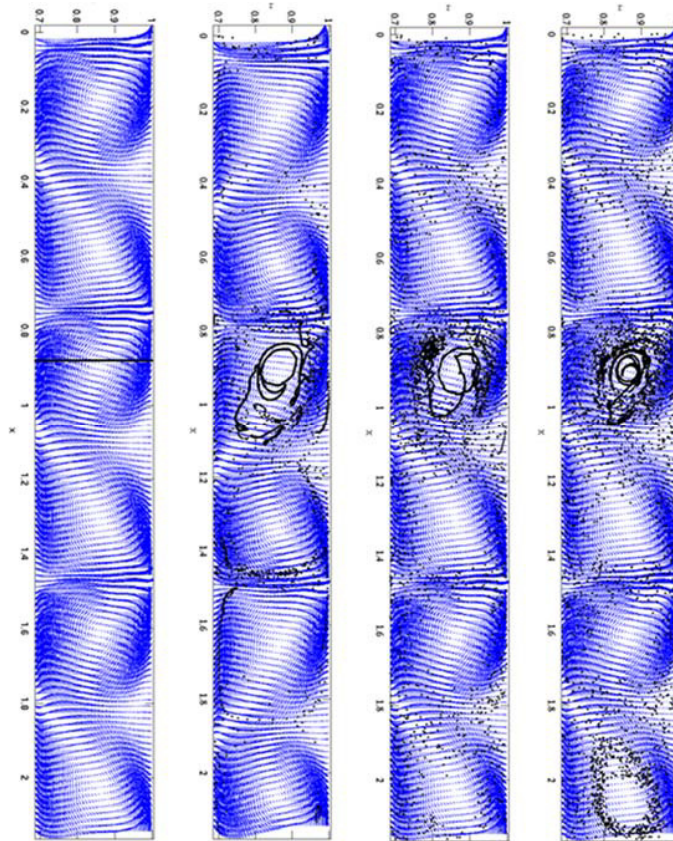


Fig. 3. DNS of instantaneous velocity fields and weightless particles dispersion in Taylor-Vortex flow. From left to right: after 0 (seeding), 2, 4 and 8 rotations of the cylinder

As in the first example, the numerical model is part of the development methodology of new prototypes. Besides the three-phase flow properties calculation at local scale, the numerical tool allows the prediction of the grade efficiency of the equipment. The experimental study recently highlighted a good agreement between the measured and predicted values of this macroscopic parameter.

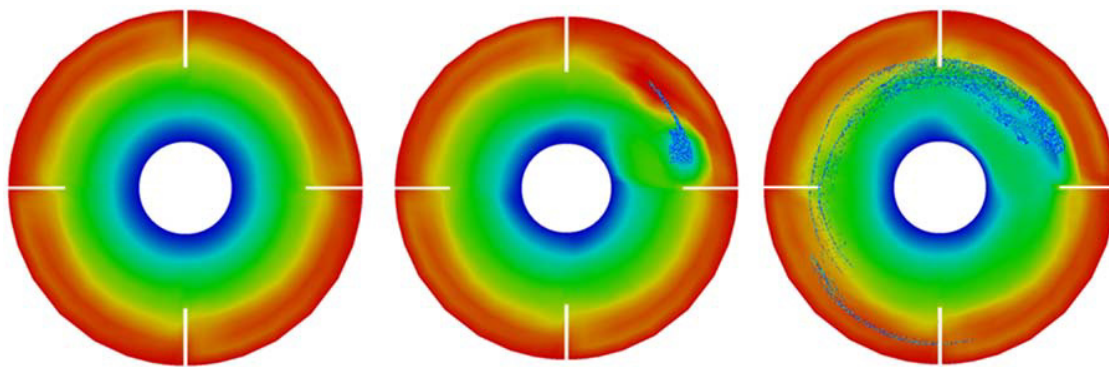


Fig. 4. Example of centrifugation of a particles cloud in a lab-scale centrifuge with the MPPIC-VOF multiphase solver.

3. Conclusions

The input of CFD in R&D studies devoted to nuclear fuel reprocessing is currently increasing in order to reduce the volume (in number, size and nuclear effluents) of experiments. This new methodology provides also a better understanding of the flow issues in separation processes. Moreover, besides the design of industrial contactors relevant for the nuclear industry, and the scale-reduction of the demonstrators required for R&D studies, the fluid mechanics studies are also helpful in determining the adjustable parameters of the process simulator which predicts the separation performances (the PAREX code, developed at CEA Marcoule⁶), such as the axial dispersion coefficient⁴, drop size distribution and holdup⁵, mass transfer resistance, etc.

Acknowledgements

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