TWO-PHASE FLOW IN PACKED ABSORPTION COLUMNS : CFD CONTRIBUTIONS AND CHALLENGES

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Context and Objectives

In the context of climate change and CO_2 mitigation, it is considered that Carbon Capture and Storage, CCS, is one important solution to develop[1]. On the one hand, the development of this technology must go fast enough to meet environmental targets; on the other hand, the captured CO_2, if not used as a raw material or for CO_2 Enhanced Oil Recovery, will not have any direct added-value and capture costs must be as low as possible. Most of the studies dedicated to the development of post-combustion CO_2 capture processes focus on the solvent, from which good performances first in terms of thermodynamic properties and second in terms of kinetics are expected[2,3], with also respecting other criteria concerning degradations, emissions, cost... From the thermodynamic properties, one determines in particular the cyclic loading and the reaction enthalpy which directly impact the energy consumption of the process and further the operational costs. From the kinetics properties, one determines the height of the packed tower in which CO_2 contained in the flue gas is absorbed and reacts with the liquid solvent. The sizing of these columns, equipped with packings and various internals for gas/liquid distribution and collect purposes, is of course of main impact on the investment cost of the process. The sizing of packed columns is also strongly related to hydrodynamic and mass transfer characteristics of the two-phase flow within the packings[4]. Developing our knowledge in terms of pressure drop, liquid hold-up, mass transfer parameters, liquid dispersion of this complex counter-current two-phase flow is thus of great importance. This can be done via intensive experimental work, which is time and cost consuming, but more importantly which cannot address all issues due to the complexity of the problem. To complement experiments, CFD can be of great help to develop knowledge at local scales and intermediate scales, as experiments with laboratory facilities can do, but also to develop scale-up knowledge which is mostly determined from qualitative industrial feedback not always well understood.
In this context of CO_2 capture columns design optimization, this paper presents and discuss how various CFD approaches can be used at different scales and combined in a two-way coupling approach, from local gas-liquid interaction at film scale, to large column design scale.

CFD simulations results

From VOF simulations performed at local scale, it is possible to determine the local contours of the liquid film, further enabling liquid hold-up determination but also mass transfer characteristics. One can indeed determine the liquid side mass transfer parameter, k_L, either with the use of the Higbie theory via the calculation of the velocity at the interface from 2D simulations as shown in Fig.1.a[5], or by more complete simulations solving a transport equation including reaction and diffusion in the liquid film[6]. As shown in Fig.1.b, one can also determine the interfacial area, or effective area, via full 3D simulations taking into account wetting properties (surface tension, contact angle)[7,8]. These types of calculation are CPU demanding and are thus limited to small volumes corresponding to one or a few smallest periodic elements of a packing.

From simulations performed at intermediate scale, that is at the scale of a packing element, one can determine more macroscopic characteristics such as pressure drop or liquid dispersion in the packing channels. This has first been done with gas only simulations for dry pressure drop determination[9,5] and has been extended to gas/liquid simulations via the use of k-ε models with a two-phase flow Euler/Euler approach[10]. Such simulations requires gas/liquid/solid interaction closure laws which can be either developed from experimental results or from CFD results obtained at local scale.

Last from simulations performed at large scale, that is the scale of the whole packed column, involving a macro-porous approach of the packing, one can determine the packed bed / internals interaction in terms of pressure drop and fluid flow dispersion[8,11,12] as can be seen from results of Fig.2.

In the recent years, CFD tools have been more and more used for the determination of the two phase flow within packed columns and very interesting and promising results have been obtained. However, it is also discussed that still work is needed, both in terms of modeling and in terms of experimental

work required for validation purposes. It would be in particular interesting to propose models that could take into account the type of packings walls influence on wetting as observed in experiments[13], or to develop closure laws for Eulerian/Eulerian approaches dedicated to gas/liquid/solid interactions in packing for liquid dispersion determination purposes.

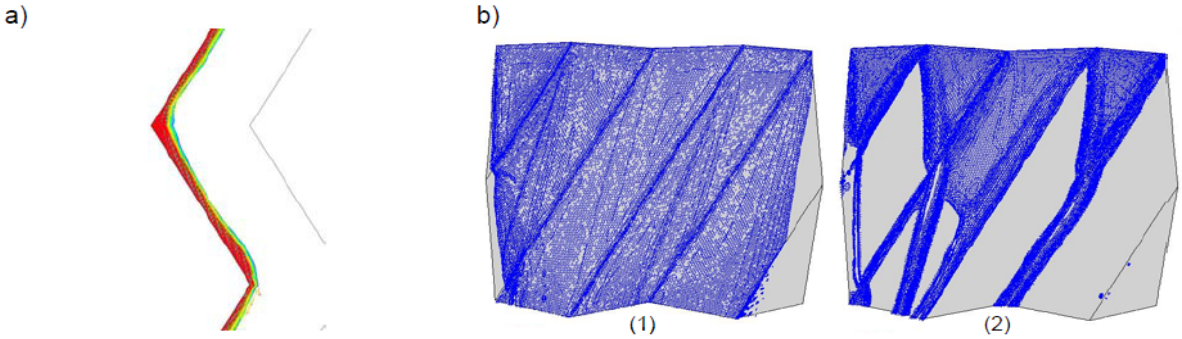

Figure 1 : Results from local VOF simulations for the determination of the liquid film flowing over a structured packing. a) side view corresponding to a 2D calculation; b) front view corresponding to a 3D calculation, the two results 1 and 2 corresponding to identical calculation parameters, only the wetting properties being changed.

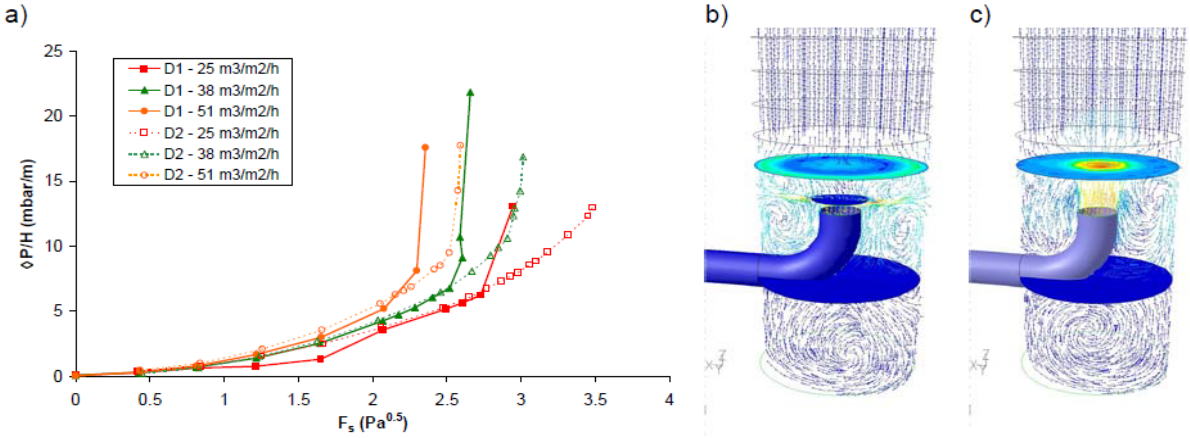

Figure 2 : Influence of the gas distributor. a) Experimental pressure drop curves versus gas load for three values of liquid load for two types of R&D gas distributor, column of 1 m in diameter at ambient pressure, gas is air liquid is water (distributor D1 : curved pipe with baffles – closed symbols with continuous lines; D2 curved pipe without baffles – open symbols with dotted lines). b and c) corresponding CFD calculations results with pressure contours at bed inlet and velocity field in the y=0 plane with respectively gas distributor D1 and D2.

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