VOF STUDY OF GAS-LIQUID MULTIPHASE FLOW IN STRUCTURED SEPARATION COLUMNS PACKING

MARTIN ISOZ¹

¹Institute of Thermomechanics of the Czech Academy of Sciences, isozm@it.cas.cz

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The distillation and absorption are the most widely used techniques for industrial scale mixture separation. Furthermore, in the literature it is estimated that the distillation alone is responsible for approximately 40% of the energy consumption of the whole chemical industry in the United States and Europen Union [1, 2, 3]. However, despite the energy-intensity of the distillation, the design of the separation columns is still mostly empirical [4, 5].

One of the reasons of the current state of the distillation column design is the shear complexity of the involved technology. In order to increase the size of the gas-liquid interface area and consequently the intensity of the mass transfer, the separation columns are usually filled with a geometrically complex packing (see Figure 1). The packing highly increases intricacy of the flow in the column and also makes almost all types of hydrodynamic measurements impossible. Furthermore, the modeling of the processes occurring in the separation columns has long been limited by the lack of both the required computational power and the appropriate models.



Figure 1: Example of a separation column packing – Mellapak 250Y. An overall view of the packing is depicted on the left. On the right, there is shown a detail of one element of a dismantled packing. Structured packing usually consists of curled, perforated and textured steel plates. Standard mode of operation is typically counter-current: liquid phase flows down and gas phase up.

On the other hand, with the recent increase in available computational resources, the methods of computational fluid dynamics (CFD) may be applied directly to resolve the flow in the whole column at once. This development inspired a number of recent studies in this area (see e.g. [6, 7, 8] or [9]).

Still, the performed studies usually follow one of the three paths. First, the authors concentrate on the simulation of the full geometry, but simulate only a single phase (gas) flow through the column [7, 10]. Second, the authors simulate two phase flow but via the Euler-Euler approach with averaged phase fractions [6]. Third, the authors provide a direct, usually volume-of-fluid (VOF)-based, simulation of the two phase flow, but restrict the computational domain to a small representative element unit of the packing [9].

In the present study, we applied a different approach. Leveraging the available computing power and parallel calculation capabilities of the interFoam solver from the OpenFOAM software package [11], we were able to construct a VOF-based simulation of a gas-liquid multiphase flow in a semi-industrial separation column packed with the Mellapak type structured packing.

The main advantage of the proposed model is its complete independence on the availability of the manufactured packing. The packing geometry generation is fully automatic and parameterizable and performed in the Blender software [12]. The generated geometry is exported as STL surface and meshed using the snappyHexMesh utility available in the core OpenFOAM [11] installation. The final mesh for multiphase calculations was bounded by a cylinder of dimensions $0.15 \times 0.22 \text{ m}$ (diameter × height) and consisted of approximatelly 10 millions cells.



Figure 2: Liquid distribution in the Mellapak 250X structured packing for the case of low liquid flow rate. Pressure and velocity fields on selected slices through the given geometry are depicted on the sides of the overall view. The location of the slices in the full geometry is marked by their transparent representation in the overall view.

An example of the results of the simulation performed in the complete computational domain is depicted in Figure 2. The parameter of our study was surface fluid velocity B defined as,

$$B = \frac{Q_L}{S_{\rm col}} \left[\mathrm{m} \, \mathrm{h}^{-1} \right] \,, \tag{1}$$

where Q_L is the liquid volumetric flow rate in m³ h⁻¹ and S_{col} in m² is the column cross-sectional area. The superficial liquid velocity is a widely used measure of the liquid flow intensity through the device. The industrial devices usually operate within the range of $5 \le B \le 30 \,[\text{m h}^{-1}]$ for the case of the distillation and $20 \le B \le 120 \,[\text{m h}^{-1}]$ for the absorption. In the present study, we selected the values of B as $B = \{5, 10, 20, 40\} \,[\text{m h}^{-1}]$.

$$B = 5 \,[\mathrm{m}\,\mathrm{h}^{-1}]$$
 $B = 10 \,[\mathrm{m}\,\mathrm{h}^{-1}]$



Figure 3: Change of the flow structure in the vicinity of the liquid inlet in dependence on the superficial liquid velocity B.

However, to construct the full scale simulation, we had to undertake a number of preparatory calculations. The mesh size independence study as well as the optimization of the boundary conditions and solver settings were performed on a series of smaller meshes corresponding to a fraction of the full computational domain. Example of the outputs of such a preparatory simulation is depicted in Figure 3, where we show the results of the study of the flow properties in the vicinity of the liquid inlet. The shown simulations were performed on a mesh bounded by a block of dimensions $0.15 \times 0.025 \times 0.03$ m (width × depth × height). The front and back sides of the geometry were equipped with a cyclic boundary condition to get a better notion of the liquid behavior in the full mesh.

Together, the preparatory and the full scale simulations give us a tool to shed some light on the liquid behavior in the distillation and absorption columns packed with the Mellapak type structured packing. More specifically, we study the liquid hold up in the device, the liquid distribution on the packing and the size of the gas-liquid interface area. All three of these parameters play an important role in the modeling of the separation columns. A better understanding of their behavior can be used to improve the models currently used in the engineering practice.

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