Computational fluid dynamic as a feature to understand the heat and mass transfer in a vacuum tower

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Abstract

The understanding of fluid dynamic phenomena in industrial equipment is extremely important for new projects and their optimization. Distillation columns have been used for centuries. Since then many advances have been achieved. The present study shows a methodology to study the heat and mass transfer in empty sections of distillation columns considering the Eulerian-Lagrangian approach. A multiphase model is applied to the vacuum tower, with the vapor-liquid flow being modeled with a Eulerian-Lagrangian approach. The Computational Fluid Dynamic (CFD) technique is adopted as the tool to predict vacuum tower dynamics. The CFD results were validated with real operation behaviour. An ideal multicomponent equilibrium model is adopted to represent the thermodynamics in the heat and mass transfer processes. The characteristic time scales are used in the classification and the understanding of the dominant mechanisms in gas-liquid suspensions. This methodology is general, and therefore can be applicable to any turbulent gas-liquid flow. A discussion on the validity of the models is given, as well as an application to distillation vacuum towers.
Keywords: CFD, thermodynamic equilibrium, multiphase, Lagrangian, spray.

1   Introduction

The heat and mass transfer takes place in a distillation column by vapor and liquid contact. In the vacuum towers wash zones, this contact is promoted by

spray nozzle distributors. This sort of device is widely used in distillation and absorption columns to provide a uniform liquid distribution. One of the challenges in this column section is to reduce the space available for heat and mass transfer, without decreasing process efficiency. The reduction of space between liquid sprays and vapor inlet can bring a couple of advantages:

- minimize column height;
- less maintenance
- lower pressure drop

This potential height reduction was observed in experimental measures, indicated by thermal equilibrium near the vapor entrance.

The literature presents many studies considering spray simulations, each one having its own modeling approach as presented by Mugele and Evans [1], Meyer *et al*. [2], Trompiz and Fair [3] and Beck and Watkins [4], where the heat and mass transfer is modeled considering an Eulerian-Eulerian approach. Authors as Lefebvre [5] and Guet *et al*. [6] argue that an accurate knowledge of drop size distribution as a function of the conditions of the system is an important prerequisite for fundamental analysis of the heat and mass transfer.

Kim [7] and Bozorgi [8] considered a Eulerian-Lagrangian model to represent droplet evaporation. Kim considered phase equilibrium using the fugacities of the liquid and gas phases assuming real gas behavior, and its importance in the calculation of the evaporation of a droplet or spray at high pressures. Bozorgi studied variables effects, such as liquid film, total projected surface area of the droplets and velocity profile of the droplets on the performance of the spray scrubber in the aerosol removing process.

A Lagrangian model has some advantages in comparison to the Eulerian model, such as:

- easy modeling of droplets diameter distribution;
- spatial discretization of spray nozzles (computational mesh) is not required since it is represented by points within the domain

In this study a 4-m diameter vacuum tower was considered with a liquid distributor having 41 spray nozzles.

The vapor-liquid thermodynamic equilibrium is modeled with a "gamma-phi" approach. The model is capable of representing the evaporation and condensation of the droplets. Thus, droplets diameter is variable as a function of system properties. The thermodynamic equilibrium was modeled via FORTRAN subroutines coupled to the commercial CFD code, ANSYS-CFX 11. The main advantage of CFD technique is to allow the user to evaluate conceptual changes in equipment in short-term simulations (compared to experimental measurements) at low computational cost.

Based on these statements, the main target of this work is to gather information on vacuum tower fluid dynamic using an Eulerian-Lagrangian model using Computational Fluid Dynamics (CFD) techniques that represent a powerful tool for better understanding of physical phenomena involved in vacuum towers.

2   Mathematical modelling

The present work applies simplified multicomponent Fick's Law and gamma-phi approach for liquid-vapor equilibrium in a Eulerian-Lagrangean multiphase flow model together with multicomponent heat and mass transfer. This model was applied successfully before by Paladino *et al.* [9] and Ropelato *et al.* [10]. The simplification proposed here is the independence of diffusive mass flux of one component from other components. This implies that each mass flux can be calculated without other fluxes information. In the other hand, thermodynamic equilibrium takes the all components into account. Thus, it is calculated rigorously.

With the liquid-vapor equilibrium considering a "gamma-phi" approach, an equation of state is applied to calculate fugacity coefficient (which provides a measure of non-ideality of vapor phase), while an excess Gibbs free energy model is applied to predict the behavior and non-idealities of liquid phase by calculation of an activity coefficient.

The considered equilibrium is a traditional approach and can be applied to many different mixtures cases. It is adequate for systems at low or moderate pressure, as the vacuum tower, for example. This model cannot be applied in systems at high pressures. This limitation can be explained because the excess Gibbs free energy models are determined at low pressures. Moreover, the "gamma-phi" equilibrium model is one of the most used equilibrium approach in Petroleum Industry.

The conservation equations calculated in CFD code are presented below for the Eulerian phase. The mass conservation of the continuous (Eulerian) phase is:

$$\frac{\partial}{\partial t}(\rho_C) + \nabla \cdot (\rho_C \mathbf{v}_C) = \sum_{D=1}^{N_P} \Gamma_{CD} \tag{1}$$

The Γ_{CD} represents each component mass flux through the interface. The subscripts C and D are the continuous and dispersed phase respectively.

The momentum equation is:

$$\frac{\partial(\rho_C \mathbf{v}_C)}{\partial t} + \nabla .(\rho_C \mathbf{v}_C \mathbf{v}_C) = -\nabla p + \nabla .\mathbf{T} + \mathbf{M}_C + \rho_c \mathbf{g} \tag{2}$$

The Mc represents the interfacial momentum transfer terms, turbulent stress tensors and **T** is the viscous stress tensor. For Newtonian fluid, viscous stress can be expressed via Stokes equation:

$$\mathbf{T} = \mu_C \left[\nabla \mathbf{v}_C + (\nabla \mathbf{v}_C)^T \right] \tag{3}$$

Where μ_C is the fluid dynamic viscosity.

The conservation equation for component "i" in the continuous phase is:

$$\frac{\partial}{\partial t}(\rho_C y_{iC}) + \nabla \cdot (\mathbf{v}_C y_{iC}) - \nabla \cdot (\rho_C D_{iC}(\nabla y_{iC})) = \Gamma_{i,mC} \tag{4}$$

The term $\rho_C D_{iC}$ represents the mass diffusion coefficient, D_{iC} represents the kinematic diffusivity and $\Gamma_{i,mC}$ the source term due to mass transfer to/from dispersed phase.

The energy equation can be represented as follows:

$$\frac{\partial}{\partial t}(\rho_C h_C) + \nabla \cdot (\rho_C \mathbf{v}_C h_C) - \nabla \cdot (\lambda_C \nabla T_C) =$$

$$\sum_{i=1}^{Ncomp} \Gamma_{i,mC} h_C + Q_C + S_e \tag{5}$$

where h_C is the enthalpy, T_C is the temperature and λ_C is the convective heat transfer from/to liquid phase.

Evaporation and condensation rates in the Lagrangian model will be indicated by the droplet mass conservation equation:

$$\frac{dm_D}{dt} = \Gamma_{i,mC} = -\pi d_p \rho D Sh(w_L K_e - w_V) \tag{6}$$

The dp is the droplet diameter; D represents the mass diffusivity term; Sh, the droplet Sherwood number; K_e, equilibrium ratio; and w_L and w_V, the component of mass fraction at the interface of the dispersed and the continuous phases, respectively.

The simulation considered a *two-way coupling*. The coupling concept is very important in a multiphase flow. If the flow of one phase affects the other while there is no reverse effect, the flow is said to be *one-way coupled*. If there is a mutual effect between the flow of both phases, the flow is *two-way coupled*. Therefore, the effects of the presence of droplets on the turbulent motion of the continuous phase can be observed. A schematic diagram of coupling is shown in fig 1. The carrier phase is described by density, temperature, pressure and velocity field. The droplet phase is described by concentration, size, temperature and velocity field. Coupling can take place through mass, momentum and energy transfer between phases. Mass coupling is the addition of mass through evaporation or the removal of mass from the carrier phase stream by condensation. Momentum coupling is the result of the drag force on the dispersed and continuous phases. Momentum coupling can also occur with momentum addition or depletion due to mass transfer. Energy coupling occurs through heat transfer between phases.
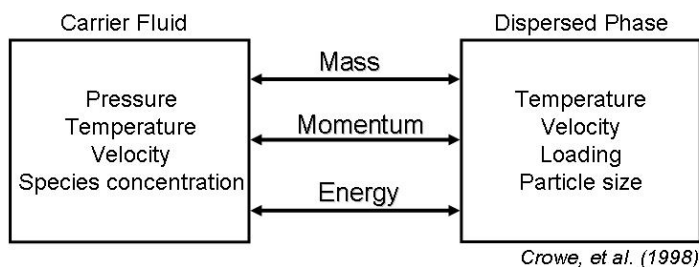

Crowe, et al. (1998)

Figure 1:   Schematic diagram of coupling effects.

2.1 Characteristics time scales

In the formulation of the transport equations, several characteristic time scales can be defined. These time scales are of fundamental importance in the classification and understanding of the dominant mechanisms in suspensions. (Elgobashi [11]; Peirano and Leckner [12]).

Time scales are fundamental to understand the vapor and liquid behavior, and also the effects of phase interaction.

The characteristic time scale of the large eddies in the continuous phase (τ_c^t) is defined in accordance with the k-ε model as eqn (7)

$$\tau_c^t = 0.09 \frac{k}{\varepsilon} \tag{7}$$

Where k is the turbulent kinetic energy and ε its dissipation. The Kolmogorov scale dissipative (τ_k) is the characteristic time scale of the smallest scales.

$$\tau_k = \left(\frac{\upsilon_c}{\varepsilon}\right)^{0.5} \tag{8}$$

The time of interaction between particle motion and continuous phase fluctuations is defined by eqn (9)

$$\tau_{cd}^t = \frac{\tau_c^t}{1 + 0.45 \frac{3}{2} \frac{|V_r|^2}{k}} \tag{9}$$

τ_{cd}^t is the Lagrangian integral time scale seen by the particles (computed along the trajectory of the particle). This means that the time spent by a virtual fluid particle in an eddy is not the same as the time experienced by a liquid particle, due to the mean relative velocity between the two phases.

Eqn (10) represents the droplet relaxation time (τ_d^t).

$$\tau_d^t = \frac{4 d_p \rho_d}{3 \rho_c C_D |V_r|} \tag{10}$$

The ratio τ_d^t / τ_k represents the Stokes number in Kolmogorov scale (S_{tk}), which indicates the probability of coalescence in the region of study. The Stokes number is a very important parameter in fluid-particle flows. If $S_{tk} \ll 1$, the response time of the droplets is much less than the characteristic time associated with the flow field. Thus the particle will have ample time to respond to changes in flow velocity. Thus the droplets and fluid velocities will be nearly equal. If $S_{tk} \gg 1$, then the droplets will have essentially no time respond to the fluid velocity changes and the droplets velocity will be little affected in the equipment, Crowe et al. [13].

2.2 Numerical method and geometry details

Element based finite volume method (EbFVM) with unstructured is used by ANSYS CFX solver to solve the set of equations. The pressure-velocity coupling formulation is similar to the Rhie-Chow method where the solution of velocity and pressure is in the same node of element in the numerical mesh.

A computational mesh study was conducted to obtain mesh independent results. A mesh with approximately 1.106 nodes was considered good for the simulations. The independency of mesh and particle tracking was analyzed considering all characteristics of the model (multiphase, heat and mass transfer).

Fig. 2(a) shows the boundary conditions imposed in this study: red color indicates de vapor inlet; yellow indicates the demister pad; blue color, the spray section; and green color represents the bottom of equipment. Fig 2(b) shows the numerical grid details. The vapor inlet doesn't present symmetrical characteristics, thus the whole geometry was taken into account.

The spray distributor with 42 sprays is showed in fig. 3. Each of it with 200 particle tracks being used.

Each spray nozzle was modeled as a full cone with 60º. The droplet diameter distribution used in the simulations was obtained from the spray nozzle provider which was characterized for water. A Petrobras internal correlation was applied considering the oil properties.

The model has been generated as three-dimensional (3D), steady-state and the continuous phase (vapor) was model using the k-ε turbulence model. The k-ε
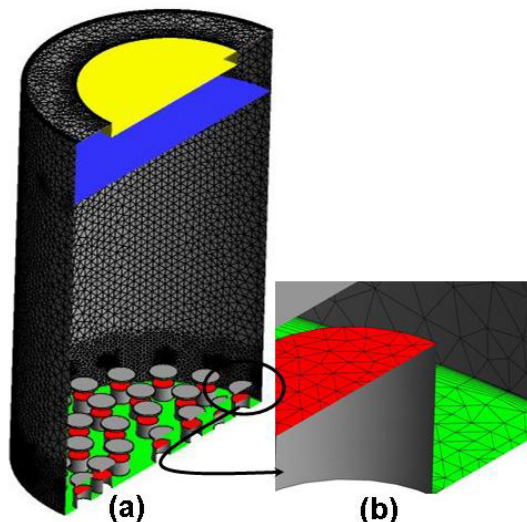

Figure 2:   Vacuum tower. (a) Physical geometry with and boundary conditions; (b) Numerical grid details.
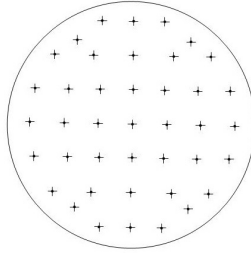
Figure 3:   Spray section distributor.

turbulence model is the most prominent turbulence models has been implemented in most general purpose CFD codes and is considered the industry standard model. It has proven to be stable and numerically robust and has a well established regime of predictive capability. For general purpose simulations, the k-ε model offers a good compromise in terms of accuracy and robustness (Wilcox [14]). A high resolution scheme (a bounded second order upwind) was used to model the advection terms of the momentum equation.

2.3 Boundary conditions

The vapor flows upwards through the vacuum tower and the light gas oil liquid phase flows downwards counter-courant to the vapor phase. The case analyzed is considered a large vacuum tower with high capacity; the vapor/liquid flow ratio is 0.43.

3   Results and discussions

The analysis of time scales was considered in the whole domain in two orthogonal slice planes. The vapor and liquid contact considering the effects of vapor inlet was evaluated by time scales. The characteristic time scale of the large eddies in the continuous phase (τ_c), fig. 4(a), considered the rate of effects of turbulent kinetic energy and the rate of dissipation of turbulent kinetic energy. Regions of high values of dissipation energy represent the low values of τ_c. These regions are close to the spray section.

The Kolmogorov scales (τ_k) indicates regions of smallest vortices in the domain, hence these regions show the highest values of turbulent energy dissipation fig. 4(b).

Fig. 5 considered the effects of vapor velocities in droplets behavior. Regions closed to the vapor inlet indicates low values of droplet relaxation time (τ_d^t), fig. 5(a), which means that these are regions of low droplets inertia. Thus phases are well mixed. Drag values are high in these regions.

The time of interaction between particle motion and continuous phase fluctuations is defined by the Lagrangian integral time scale (τ_{cd}^t), fig. 5(b). The
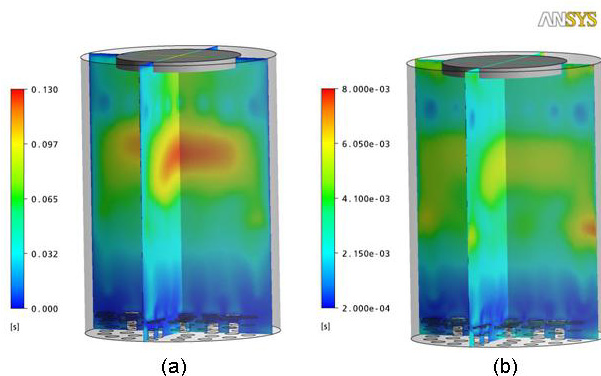
Figure 4:   Vapor fluid dynamics behavior (a) characteristic time scale of the large eddies in the continuous phase (τ_c), (b) characteristic time scale of the Kolmogorov scales (τ_k).
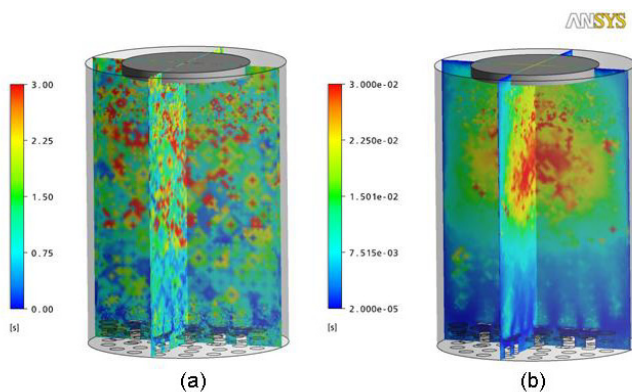

Figure 5:   Droplets flow properties, (a) droplet relaxation time (τ_d^t), (b) Lagrangian integral time scale (τ_{cd}^t).

red color indicates regions where low values of heat and mass transfer occurs, these regions are close to spray section.

The Stokes in Kolmogorov scale is a very important parameter in liquid-vapor flows. If Stokes number approaches to zero, the response time of droplets is much less than characteristic time associated with the flow field. Thus the droplets will have enough time to respond to the changes in flow field. In other words, droplets and vapor will be flowing at very close velocities. If the opposite behavior is noticed the droplets velocity is unaffected by vapor phase. Fig. 6 shows the Stokes number in the vacuum tower and the regions with Stokes number close to one represent regions with risk of coalescence.

The studied region doesn't show a strong risk to this phenomenon take place. There are no assumptions in the model with this regard. Problems with large coalescence regions should be treated with a more suitable model.
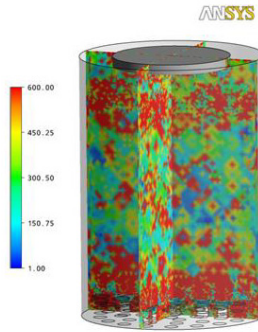

Figure 6:   Stokes in Kolmogorov scale (S_{tk}).

Fig. 7(a) and (b) represent the temperature and volume fraction profile respectively. As the time scale analyses showed, the main region of heat transfer is close to the bottom of equipment. The thermodynamic equilibrium is achieved at half of the height of the equipment. The CFD temperature and thermodynamic equilibrium results were compared with values obtained in a Petrobras` Vacuum Tower with good agreement.
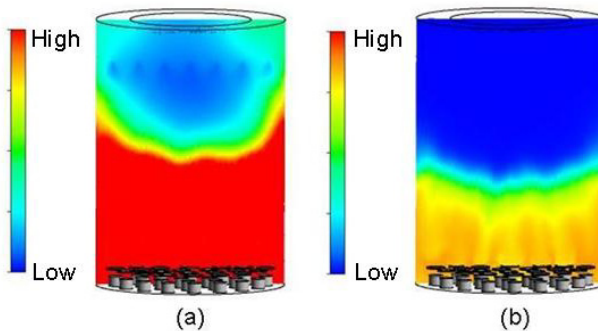

Figure 7:   (a) Temperature profile, (b) Volume fraction profile.

4   Conclusion

The proposed 3D, steady-state, and multiphase model represented adequately the vacuum tower fluid dynamics.

The time scale methodology was presented as a feature for fluid dynamics understanding of a vacuum tower. The continuous phase turbulent behavior and its interaction with the droplets were studied in equipment entrance section. The

more relevant regions of heat transfer and thermodynamic equilibrium was analyzed.

CFD tool proved to be also a powerful tool to predict the fluid dynamic of heat and mass transfer in vacuum towers, and it can be used with success in chemical process optimization to predict critical points of scientific investigation.

A potential height reduction in this case is possible as long as the assumptions taken in this model are suitable for the present case.

Future studies are being carried out, to propose some optimization points in the studied vacuum tower.

5   Nomenclature

C_D drag coefficient, [kg.m^3/s]
dp   droplet diameter [m]
F   diffusion, resistive force
g   gravity acceleration, [m/s^2]
k   turbulent kinetic energy, [m^2/s^2]
p   pressure, [Pa]
S   source term
t   time, [s]
v   velocity vector, [m/s]
V_r slip velocity, [m/s]
x   Cartesian coordinate, [m]
y   Cartesian coordinate, [m]
z   Cartesian coordinate, [m]

Greek letter
Γ   interphase mass flux [kg/m^2/s]
ε   rate of dissipation of "k", [m^2/s^3]
μ   dynamic viscosity, [kg/m s]
ρ   density, [kg/m^3]
τ   characteristic time scale (s)
ν   kinematic viscosity [m^2/s]

Subscript
c   gas phase
d   liquid phase
k   Kolmogorov scale
x   cartesian coordinate
y   cartesian coordinate
z   cartesian coordinate
ϕ   fluid dynamic property

Superscript
t   turbulent

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