A CFD model for the washing zone in coker fractionators

Paladino, E. E.(1); Ribeiro, D.(1);Reis, M. V. (1); Geraldelli, W. O.(2), Barros, F. C. C.(2)

(1) ESSS – Engineering Simulation and Scientific Software
CELTA - Rod SC-401, Km01 - Florianopolis - SC – Brazil. CEP: 88030-000
(2) CENPES – PETROBRAS Research and Development Center
Cidade Universitaria Q.7 - Ilha do Fundao - Rio de Janeiro - RJ - Brazil. CEP: 21949-900

Prepared for Presentation at AIChE 2005 Annual Meeting, October 30 - November 3, Cincinnati, Ohio, at the session: Fundamental Research in Transport Processes (01D01)

Unpublished

ABSTRACT

The washing zone region in coker fractionators plays a fundamental role avoiding the undesirable coke formation. This project aims to develop an accurate CFD model for the washing zone, including the vapor (feed) and the washing liquid, taking into account the heat and mass transfer between phases. The main goal when developing this model is to be able to predict the necessary height for the vapor to reach the required temperature and to avoid the coke formation in this region.

The model allows the evaluation of not applying internal baffles, which are normally used to increase the interfacial area and improve vapor distribution. The use of an empty spray section could improve the efficiency of this region reducing the required height, and increasing the fractionation space.

To predict the liquid phase behavior, a Lagrangian approach was used together with a non-ideal Soave-Redlich-Kwong equation of state to model the phase equilibrium and fluid properties calculation within the condensation and evaporation models. The hydrocarbon mixture was represented using five pseudo-components. Mass transfer was modeled to represent mass exchange between liquid and vapor for all the components involved. The model was capable to reproduce the complex phenomena of interfacial heat and mass transfer on multi-component multiphase flow, providing interesting input to help engineering decisions.

Key words: Coker fractionators, washing zone, empty spay section, CFD, Lagrangian model, heat and mass transfer.

Introduction

Empty spray sections, are becoming widely used on fractionation columns due to its low pressure drop. This characteristic is always required in vacuum columns in order to allow the vaporization of heavier oil fractions (Hanson *et al.* (1999), Waintraub *et al.* (2003)). Additionally, in coker fractionators where coke formation on internals is a shortcoming, the use of an empty spray section could be a very good alternative to avoid the use of internal baffles.

This work presents the development of a CFD model for an empty spray section and its application on the analysis of the heat and mass transfer process in the washing zone of a coker fractionator column. The main objective of this study was to determine the required height to cool the vapor to temperatures low enough to avoid coke formation.

Nevertheless, the model developed takes into account the evaporation and condensation of complex hydrocarbon mixtures as well as the phase equilibrium in the interface mass transfer process. Thus, it can be extended to study any empty spray section in fractionation columns.

Currently the washing process is made using baffles, as showed on Figure 1. Through the use of an empty spray section, besides the minimization of the coke formation, a considerable reduction in column height could be achieved and used for fractionation. Moreover, the model built here was used to obtain additional information regarding other design parameters such as the type of spray used (hollow x full cone, spray angle, etc) as well as the influence of the vapor distribution on the heat and mass transfer process.

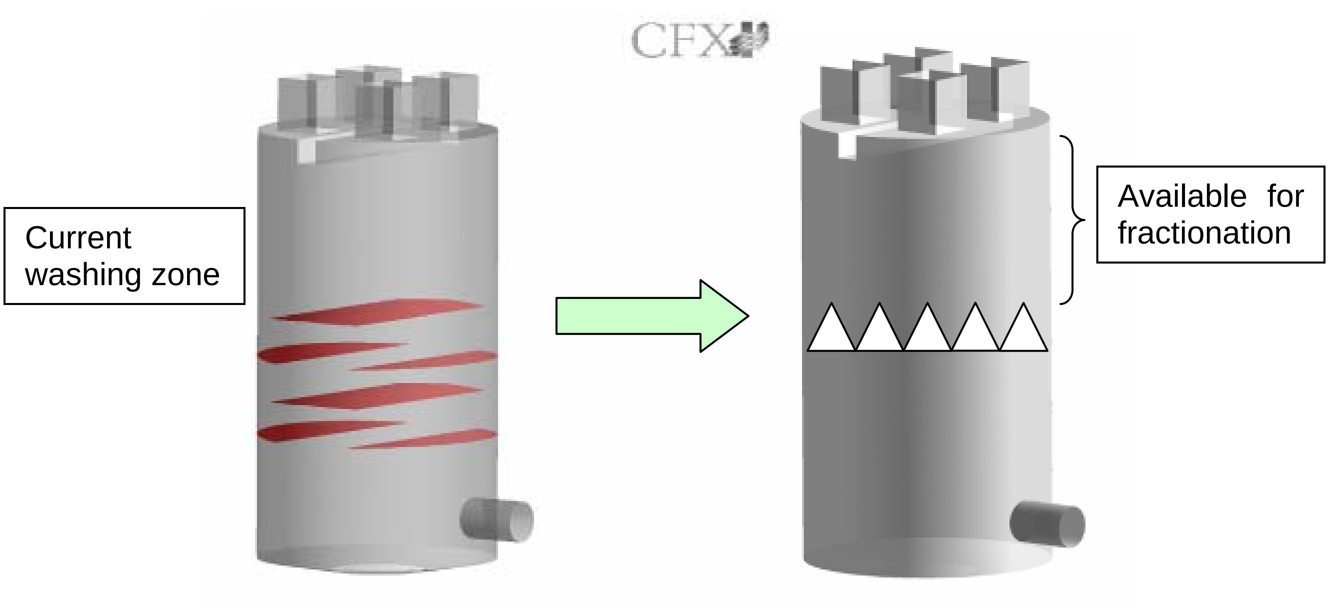


Figure 1 – Coker washing zone

Mathematical modeling

The model implementation is based on the Lagrangian approach (see, for instance, Clift *et al.* (1978)) where each droplet injected has its path traced and the velocity, temperature, composition, diameter and all properties calculated for each droplet position. For each transport equation (momentum, energy and mass) an ordinary differential equation is solved. This reduces substantially the computational time when compared to the Eulerian approach (Drew (1983)). In the Eulerian approach, it is necessary to solve a whole set of transport equations for each droplet size considered. The Lagrangian approach allows a more feasible representation of the droplet size distribution. Thus, it is possible when using the Lagrangian approach, to model the spray injection system using the liquid droplet distribution provided by the spray manufacturer. Another significant advantage of this approach is the representation of the spray injection position and its shape. When the Eulerian approach is used, the spray nozzle shape needs to be represented in the computational domain, increasing the mesh size significantly, especially when representing several spray nozzles, as is in the case of spray chambers. These and other features, make the Lagrangian approach the most used for CFD sprays flow calculations.

This model solves a set of transport equation for the continuous phase and a set of ordinary differential equation for each droplet. The mass and momentum equation for the continuous (vapor) phase are given by,

$$\frac{\partial}{\partial t}\left(\rho_C\right)+\nabla\cdot\left(r_C\rho_C\mathbf{U}_C\right)=\sum_{D=1}^{N_p}\Gamma_{CD} \tag{1}$$

$$\frac{\partial}{\partial t}\left(\rho_C\mathbf{U}_C\right)+\nabla\cdot\left(\rho_C\mathbf{U}_C\mathbf{U}_C\right)=\nabla\cdot\left(\mathbf{T}_C+\mathbf{T}_C{}^{Turb}\right)-\nabla p+\mathbf{f}+\mathbf{M}_C \tag{2}$$

In addition, the energy and mass species transport equation have to be solved in order to compute the inter-phase heat and mass transfer,

$$\frac{\partial}{\partial t}\left(\rho_C h_C\right)+\nabla\bullet\left(\rho_C\mathbf{U}_C h_C-\lambda_C\nabla T_C\right)=\sum_{i=1}^{N_{Comp}}\Gamma_{i,mC}h_{i,L}+Q_C+S_C \tag{3}$$

$$\frac{\partial}{\partial t}\left(\rho_c Y_{iC}\right)+\nabla\cdot\left(\rho_C\mathbf{U}_C Y_{iC}-\Gamma_{i,eff}\nabla Y_{iC}\right)=\Gamma_{i,mC} \tag{4}$$

where *i* represents the component and Γ represents the mass transferred from/to (depending on the conditions, components can evaporate or condensate) the droplets. Equation (4) should be solved for each component in the mixture.
The momentum equation for the dispersed phase (liquid droplets) is given by,

$$m_D\frac{d\mathbf{U}_D}{dt}=\frac{1}{8}\pi\rho d^2C_D\left|U_C-U_D\right|\left(U_C-U_D\right)=\mathbf{M}_D \tag{5}$$

where $\mathbf{M}_D = -\mathbf{M}_C$ represents the momentum transfer to the continuous phase. Integrating the above equation over time, the velocity and path of the droplet can be obtained. In a similar way, the droplet temperature is calculated by an energy balance over its path, given by,

$$m_D C_P \frac{dT}{dt} = \pi d \lambda Nu \left(T_C - T\right) - \sum_{i=1}^{N_C} \frac{dm_D}{dt} h_L \qquad (6)$$

The first term on the right side of equation (6) represents the sensible heat and the second term is the latent heat due to liquid evaporation and condensation. For the specific application in the washing zone of a coker fractionator, some heavy components from the vapor stream will condensate as the light components of liquid will evaporate. The evaporation and condensation rates for the dispersed (liquid) phase are defined by the mass transfer equation:

$$\frac{dm_{i,D}}{dt} = \Gamma_{i,D} = \pi d \rho D Sh \left(m_{i,I\,L} - m_{iG}\right) \qquad (7)$$

In the above equation, m_{iI} represents the component concentration at the interface, which is predicted by the equilibrium conditions. From the liquid phase, it is assumed that the component concentration is constant within the droplet.

Model set-up

Once the governing equations have been defined for both phases, including the interfacial mass, momentum and heat transfer, a brief description of the computational model implementation is presented. This model was implemented in the commercial CFD package ANSYS CFX-5.7.

Fluid representation

For a coker fractionator washing zone, the vapor stream was represented, using five pseudo-components, and the washing liquid using two pseudo-components. Other heavy components can appear in the liquid phase because of condensation. Nevertheless, the model can be applied using any number of pseudo-components, depending only on the computational resources. Obviously, the trade-off of the fluid representation should be taken into account. For this case, the fluid representation was defined in order to represent effectively the equilibrium conditions observed by the distillation curve. The pseudo-components were calculated using the process simulator PRO/II by SIMSCI (2002).

All vaporized / condensed components (at the washing zone conditions) were split into four pseudo-components. A fifth pseudo-component called "lights" was included in the vapor stream to represent all other components which might not condensate at the washing zone conditions. The pseudo-components used to represent the fluids and its properties are presented on Table 1:

Components	*Mol. Weight*	*Tc (^{O}C)*	*Pc (atm)*	*Zc*	*Omega*
Lights	88.0	444.8	36.8	0.26	0.229
NBP 447	368.0	920.1	16.0	0.22	0.892
NBP 462	387.5	932.4	15.3	0.22	0.933
NBP 518	461.7	977.5	13.1	0.20	1.089
NBP 558	502.3	1018.4	12.6	0.20	1.176

Table 1 – Properties of the pseudo-components used to represent the fluids

The vapor stream composition based on the selected pseudo-components is showed on Figure 6.

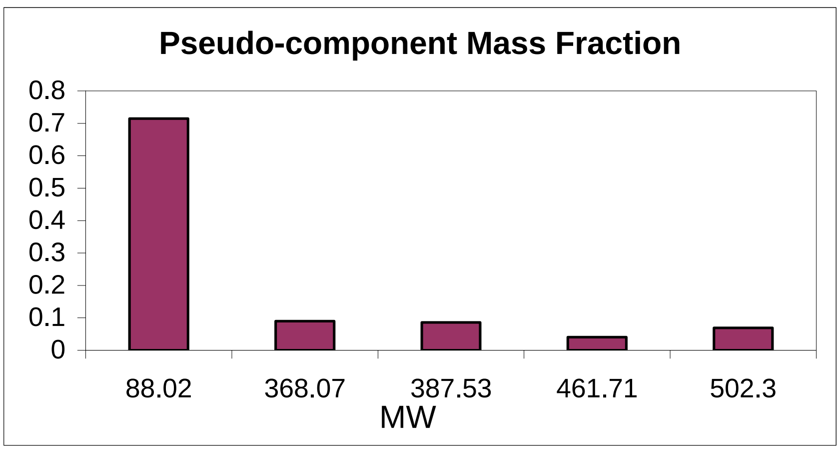


Figure 2 – Vapor stream composition

The washing liquid was modeled by two pseudo-components, presented on Table 2.

Component	Mass Fraction
NBP 447	0,516
NBP 462	0,484

Table 2 – Washing liquid composition

The model takes into account both evaporation and condensation phenomena and the equilibrium condition for the mixture was calculated using the Soave-Redlich-Kwong equation (Walas (1985), Poling *et al.* (2000)). Correlations for transport properties of the mixture were calculated using molecular weight fraction average.

Fluid Domain and Computational Mesh

Two cases were analyzed. Initially, a spray chamber with an ideal vapor distribution was studied. After that, the real geometry of the coker fractionator washing zone was included in the model in order to understand the influence of the vapor distribution in the heat and mass transfer process. The domain and computational mesh for the first model is presented on Figure 3:

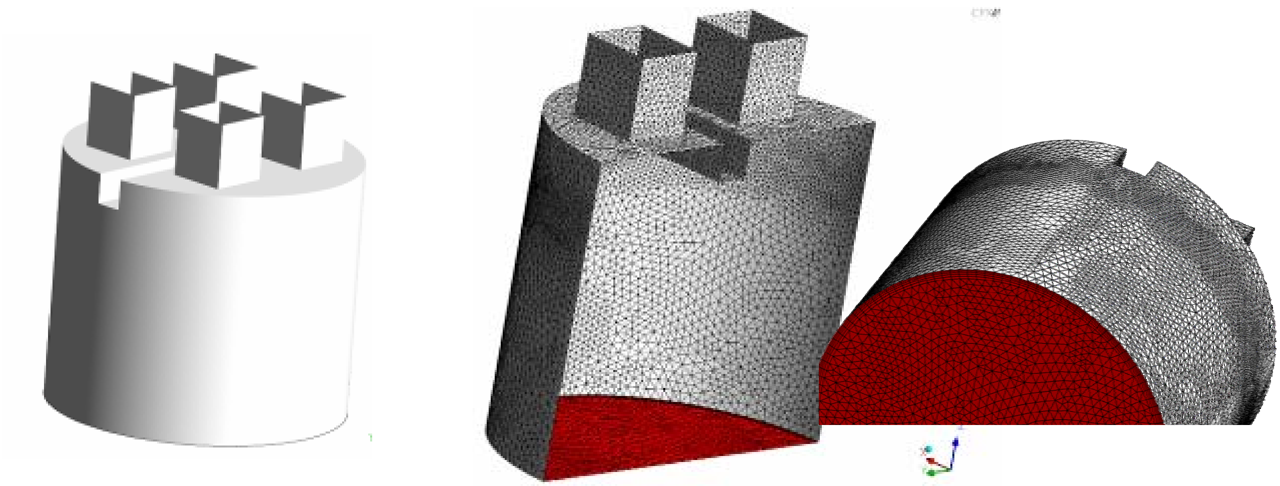


Figure 3 – Computational grid for the model assuming the "ideal vapor" distribution

Figure 4 shows the domain and computational mesh for the real washing zone geometry:

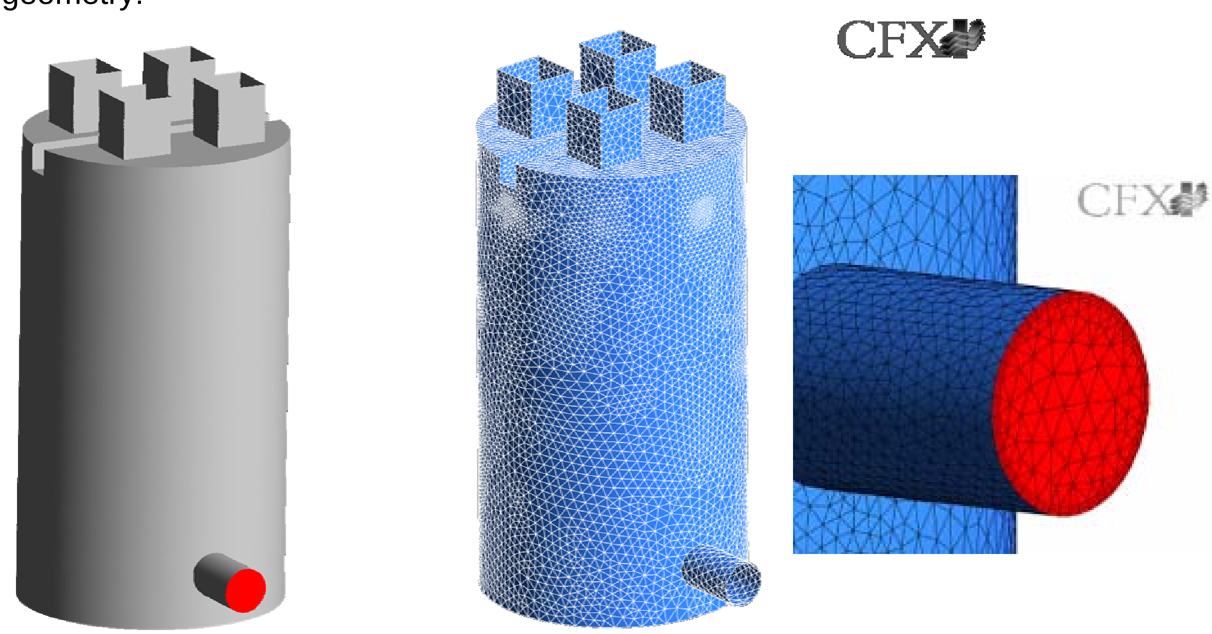
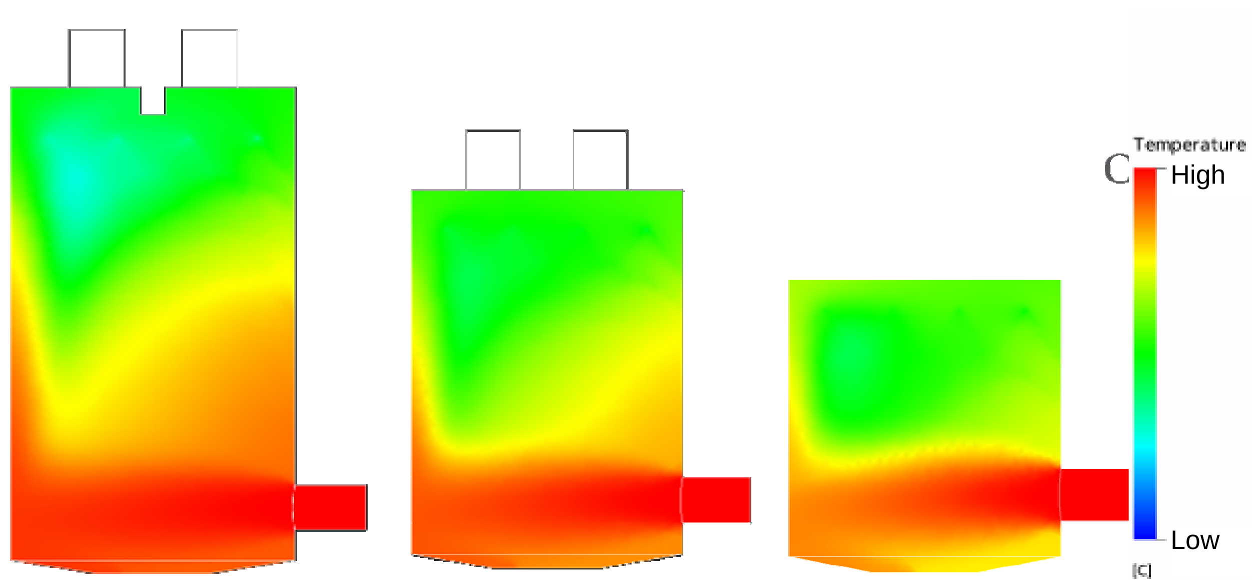


Figure 4 – Computational grid for the real washing zone geometry.
Detail: inlet region showing prism layer near the walls

Results

In this section we will show some results obtained with the described model. As mentioned before, the model was mainly used for the investigation of the required height to cool the vapor. Another issues studied were the spray type to be used, understanding the effects of using hollow and full cone sprays, and the influence of the vapor distribution.

The first model presents a comparison for different heights for the washing zone. With this target, three cases were analyzed: the original geometry, and two geometries considering 75% and 50% of the original height, respectively. In all cases the same vapor mass flow was prescribed and the same liquid mass flow was injected. Figure 5 presents the temperature distribution at mid plane of the domain for the three heights analyzed.



Aver. temp. drop = 12 °C
Original height

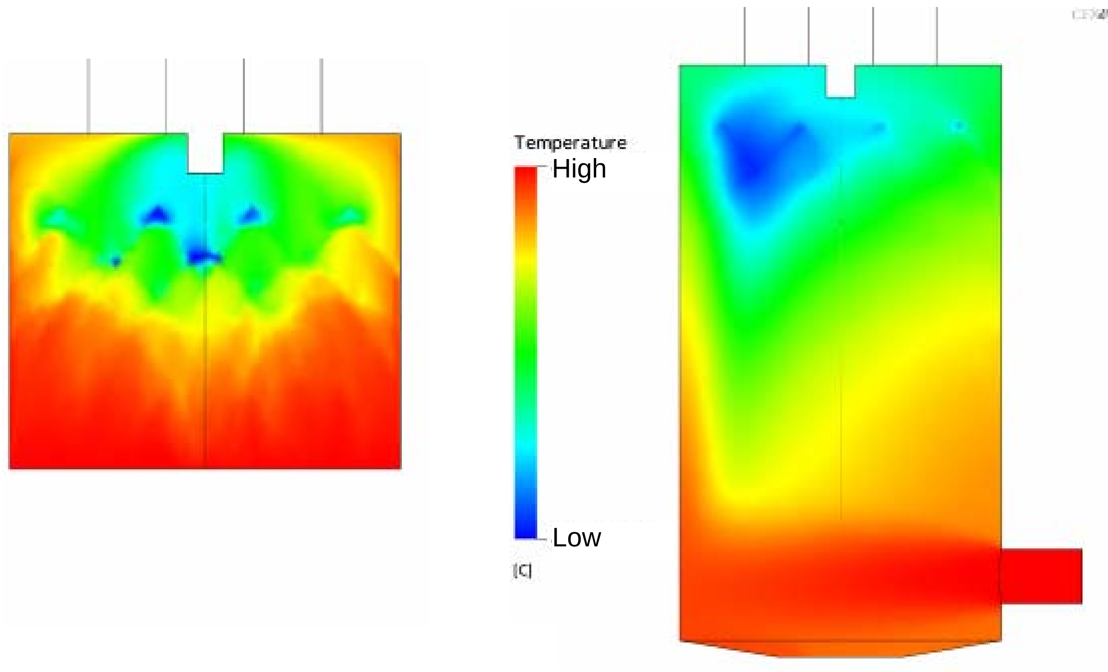
Aver. temp. drop = 10 °C
75 % of original height

Aver. temp. drop = 9 °C
50% of original height

Figure 5 – Comparison of temperature distribution at washing zone mid-plane for three different heights

An interesting point observed from the results presented above is that the average vapor temperature drop for the case considering 50% of the original height was about 75% of the temperature drop for the original height. This indicates that the height can be reduced with a good trade-off in terms of temperature drop.

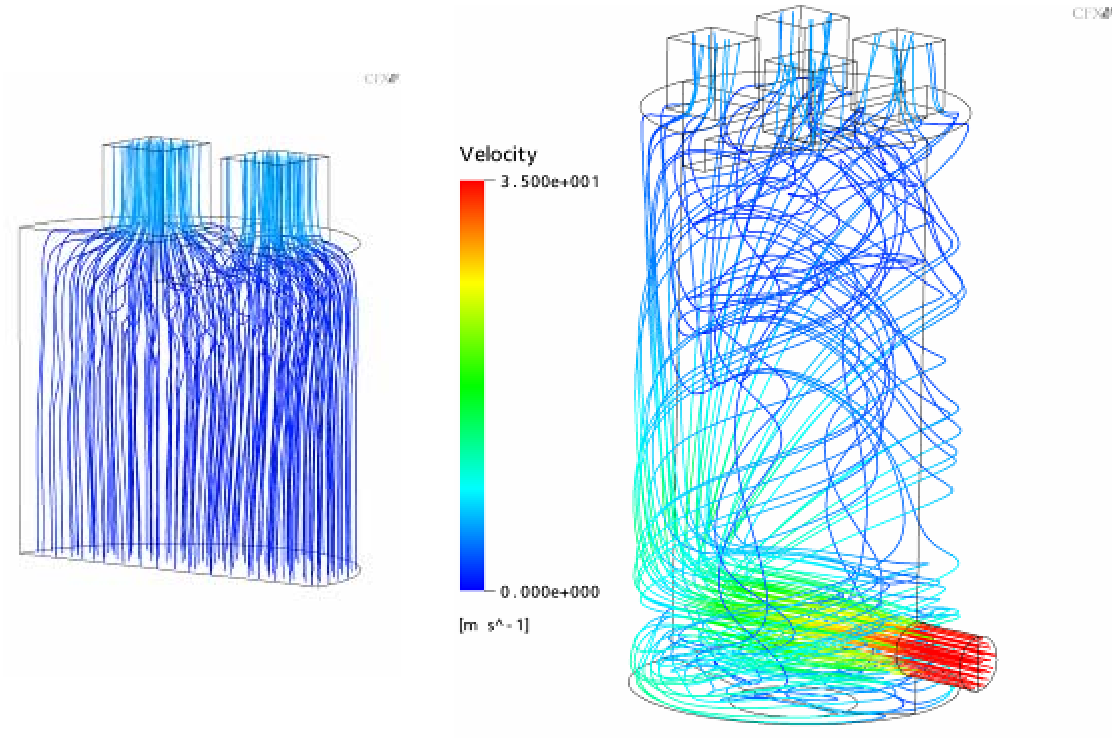
Another study was developed in order to understand the influence of the vapor distribution. Some results obtained considering an ideal vapor distribution are presented and compared with the real vapor distribution case. This model considered the real spray distribution, but assumes that the vapor is ascending homogeneously. Figure 6 shows the temperature profile for the ideal vapor distribution and real geometry models at the column mid-plane.



Ideal vapor distribution Real vapor distribution

Figure 6 – Temperature distribution at washing zone mid-plane

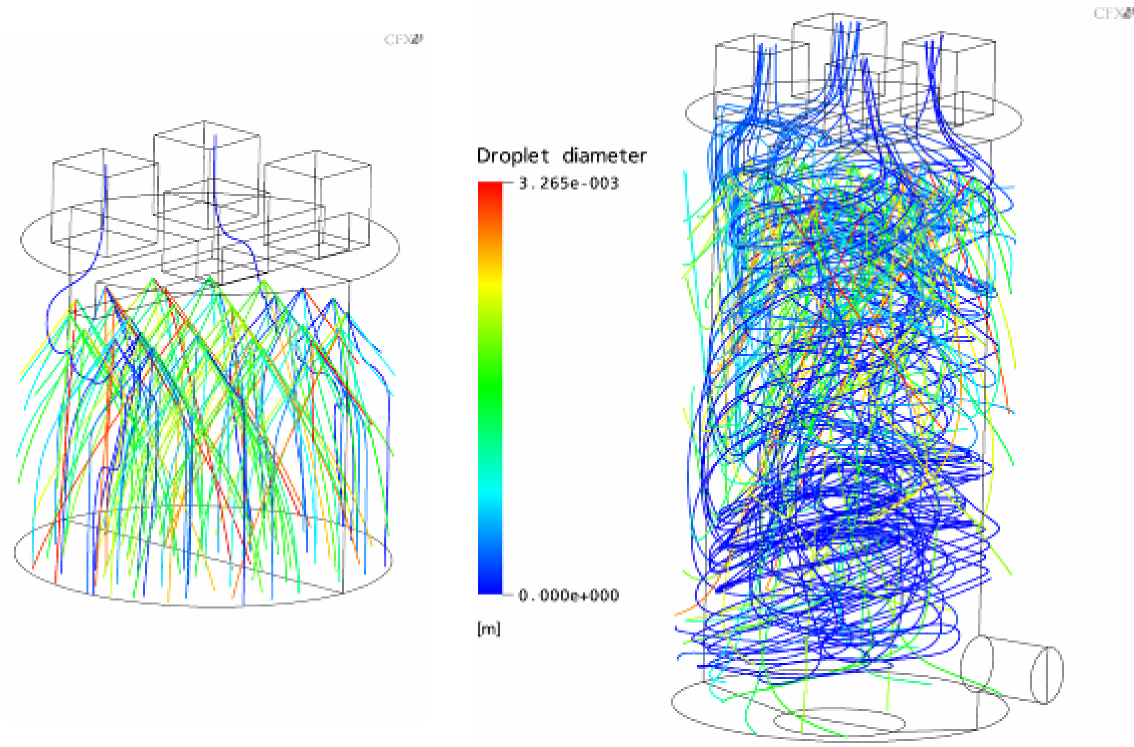
The non uniform flow pattern observed in the real geometry is due to the radial vapor feed, as showed on Figure 7, where the vapor streamlines for both cases can be seen.



Ideal vapor distribution Real vapor distribution

Figure 7 – Vapor streamlines

High vertical velocities can be observed near the wall opposite to the inlet, which generate a large recirculation in the whole washing zone, and consequently the interfacial heat and mass transfer becomes less efficient. Besides, these high velocities substantially increase the liquid entrainment as shown on Figure 8. The liquid droplet path are colored by droplet diameter. As the liquid evaporates and diameter decrease, the droplets are more prone to be dragged by the vapor. It is important to point out that the same vapor superficial velocity was considered in both cases.

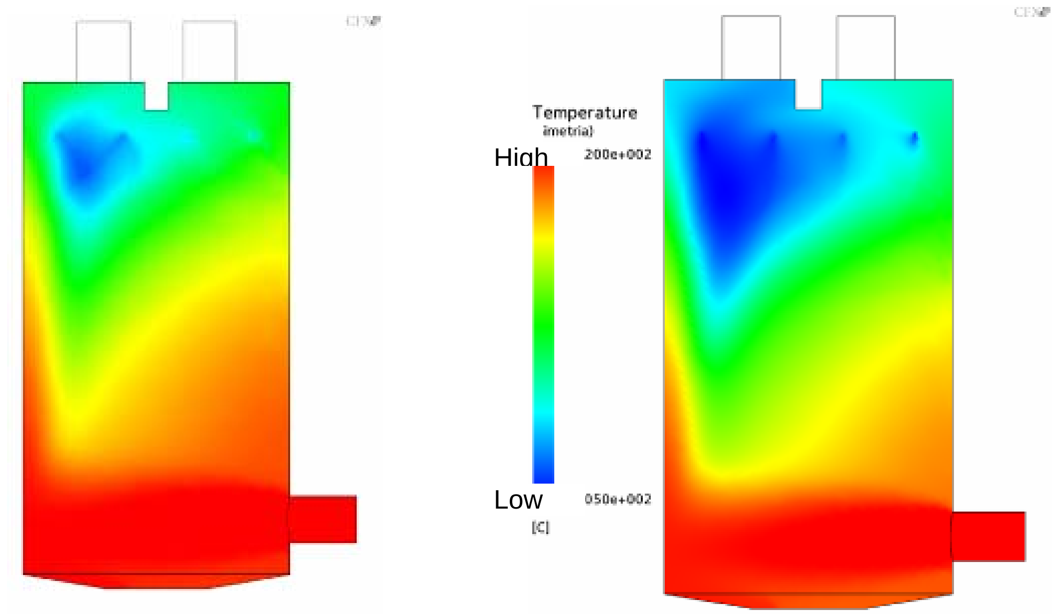


Ideal vapor distribution Real vapor distribution

Figure 8 – Liquid droplets path

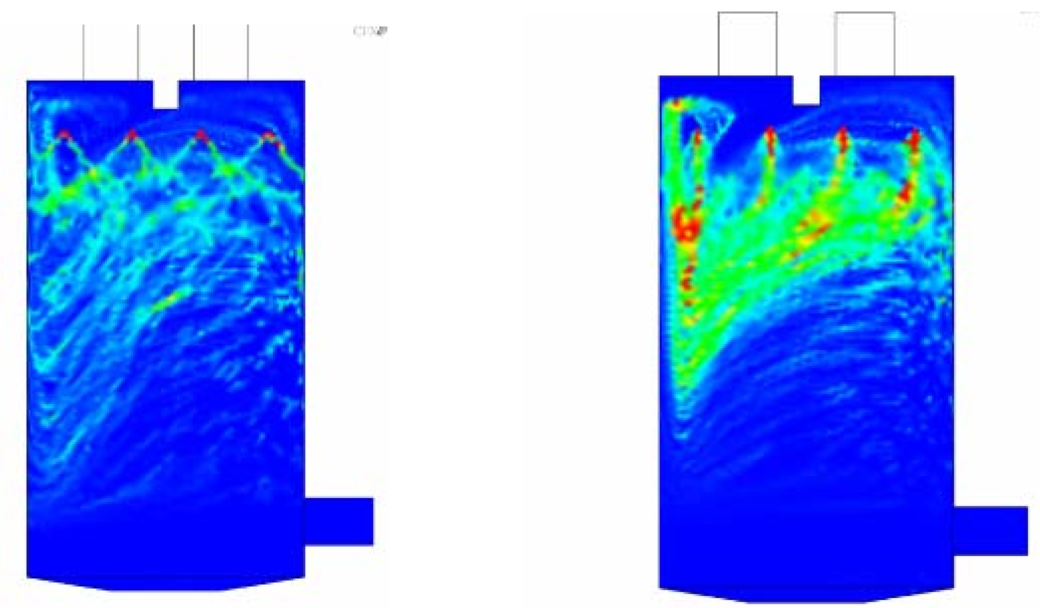
Another feature evaluated, using the real geometry, was the comparison between the hollow cone and full cone spray in terms of heat and mass transfer capacity. These "what if" scenarios at very low costs are one of the main advantages of this Computational Fluid Dynamics tool.

Figure 9 presents the temperature distribution at mid-plane for the hollow cone and full cone cases. In this comparison, the spray manufacturer's parameters were taken into account. The full cone spray presents a smaller mean droplet diameter (increasing the interfacial area) when comparing to the hollow cone spray and the liquid is also better distributed across the transversal section, as it can be seen in Figure 10. On the other hand, a higher injection velocity is used for the hollow cone, increasing the liquid penetration within the chamber (see Figure 11). Some of these features just presented improve and other decreases the heat and mass transfer rates. Hence, each situation needs to be analyzed and this model is very useful to assist the engineer taking the decision of which spray type to use.



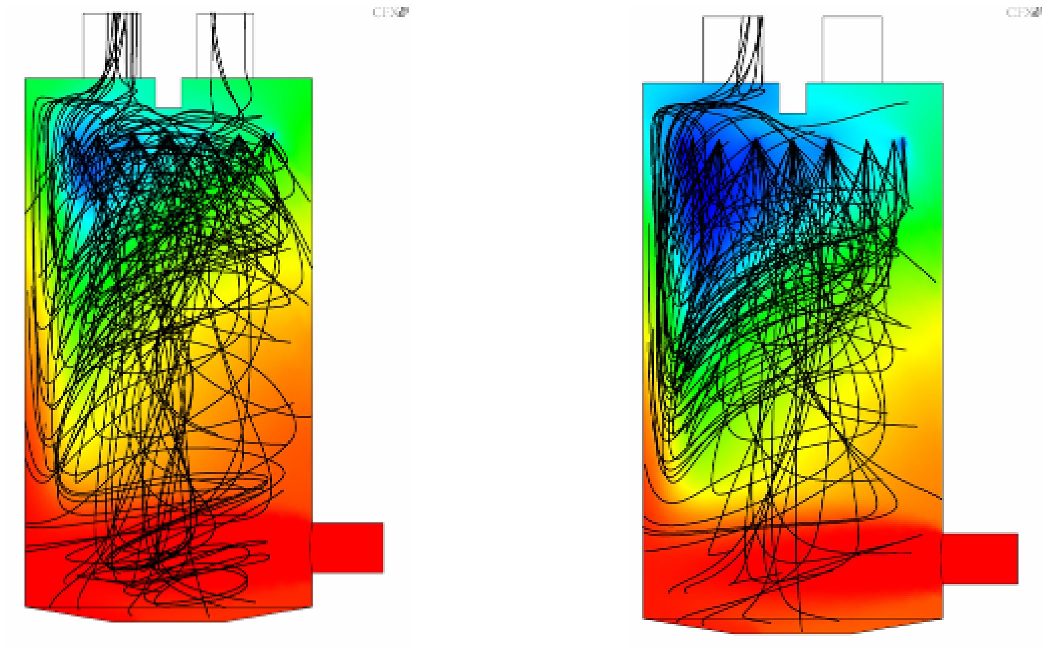
Hollow cone spray Full cone spray

Figure 9 – Temperature distribution at washing zone mid-plane



Hollow cone spray Full cone spray

Figure 10 – Liquid distribution at washing zone mid-plane



Hollow cone spray   Full cone spray

Figure 11 – Liquid droplet path

Conclusions

This paper presented the implementation and a few applications of a CFD model for an empty spray section in fractionating columns. This model is a very valuable tool for the evaluation of these types of devices.

Some parameters for the washing zone of a coker fractionator were studied, such as the required height to meet the vapor cooling requirements to avoid coke formation and also hollow cone versus full cone spray comparison. All of these studies were done taking into consideration the heat and mass transfer process in the spray chamber.

This work is still going on, so that other aspects of the process are now being investigated. Furthermore, the model is being applied to other spray chambers in different fractionating columns, showing the ability and its flexibility to represent these devices.

Acknowledgements

This work was done with financial support of PETROBRAS S.A. First author would like to thank ESSS – Engineering Simulation and Scientific Software for the financial support to attend this meeting.

Nomenclature

$\mathbf{U}_C$	Continuous phase velocity vector
$\mathbf{U}_D$	Continuous phase velocity vector
Nu	Droplet Nusselt number
Sh	Droplet Sherwood number
ρ_C	Continuous phase mass density
m_D	Droplet mass
d	Droplet diameter
$\mathbf{T}_C, \mathbf{T}_C^{Turb}$	Viscous and Turbulent stress tensors
Γ_i	*i* component mass flux through the interface
h_i	*i* component latent heat
$\mathbf{M}_C$; $\mathbf{M}_D$	Interfacial momentum transfer terms
m_i	*i* component mass concentration
m_i; m_{iI}	*i* component mass concentration at the interface

References

- Hanson, D. W., Lieberman, N. P., Lieberman, E. T., (1999), De-entrainment and washing of flash zone vapors in heavy oil fractionators, *Hydrocarbons Processing* pp 55-60.
- Clift, R., Grace, J. R., Weber, M. E., (1978), Bubbles, Drops and Particles, Academic Press, New York, NY, USA
- Drew, D., (1983), Mathematical modeling of two-phase flows, *Annual Review of Fluid Mechanics*, Vol. 15, pp 261-291.
- Waintraub, S., Torres, G.A.S, Guimaraes, F.M.Q., Barbabela, B.A., (2003), Is It Necessary To Use Internals In Heat Transfer Sections Of Refinery Columns?, Petrobras Tech. Bulletin, Rio de Janeiro, 46 (3/4):366 . 382, Jul./Dec.
- PRO/II 5.61 Reference Manual, 2002.
- Walas, S., 1985, Phase Equilibria in Chemical Engineering, Butterworth Pub. EUA
- Poling, B. E., Prausnitz, J. M., O' Çonnel, J. P., (2000), The Properties of Gases and Liquids, McGraw-Hill Professional, 5th Edition.