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Impact of Thermodynamic Non-idealities and Mass Transfer on Multi-phase Hydrodynamics

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Abstract. *Considering the non-ideal behavior of fluids and their effects on hydrodynamic and mass transfer in multiphase flow is very essential. Simulations were performed that take into account the effects of mass transfer and mixture non-ideality on the hydrodynamics reported by Bozorgmehry et al. In this paper, by assuming the density of phases to be constant and using Raoult's law instead of EOS and the fugacity coefficient definition, respectively, for both liquid and gas phases, the importance of non-ideality effects on mass transfer and hydrodynamic behavior was studied. The results for a system of octane/propane ($T = 323$ K and $P = 445$ kPa) also indicated that the assumption of constant density in simulation had a major role to diverse from experimental data. Furthermore, comparison between obtained results and previous reports indicated significant differences between experimental data and simulation results with more ideal assumptions.*

Keywords: *Multiphase flow; VOF; Mass transfer; Raoult's law; Non-ideal thermodynamics; CFD.*

INTRODUCTION

Many processes in chemical and petrochemical industries involve gas-liquid mass transfer in the gas or the liquid phase. Despite this fact and substantial research efforts devoted to understanding detailed knowledge on fluid flow, mass and heat transfer and thermodynamic behavior, as well as their interactions, are still lacking. In the past decade, the engineering community has been active in exploring the possibilities of utilizing Computational Fluid Dynamics (CFD) in the modeling of multiphase flow phenomena. However, in most of the studies, mixture non-ideality and mass transfer are not considered simultaneously.

The direct application of CFD to chemical processes faces several problems, however, even in single phase flow, flow and mass transfer are described by highly non-linear terms that often cause numerical instabilities. More complex phenomena, such as multiphase flow and interfacial mass transfer with rigorous non-ideal behavior, are encountered in multiphase flow in chemical processes [1].

Recently, "hybrid" approaches have emerged as an alternative. In those, CFD is employed only for hydrodynamic simulation, while the chemical phenomena are resolved in a custom-built compartmental model [2]. Bauer and Eigenberger [3,4] used a "zone model" to study a bubble column reactor; Bezzo, Macchietto and Pantelides [5] developed an interface of communication between the gPROMS modeling software and a commercial CFD code. Zauer and Jones [6] used a segregated feed model, in conjunction with CFD, to study precipitation in a stirred tank.

A fundamental weakness of all multi-zonal models is the difficulty of characterizing the mass and energy fluxes between adjacent zones. This is the case because the fluid properties are functions of system conditions (e.g. composition, temperature and pressure). However, this framework is only applicable to systems of which their physical properties are relatively weak functions of intensive properties [6].

Krishna and van Baten [7] have studied the interphase mass transfer and reaction (first order reaction rate) for one species without considering mixture non-idealities. In their study, densities were constant and they had estimated equilibrium constants with Henry's

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coefficients. They had also neglected the effect of mass transfer on the hydrodynamics behavior of the system.

Later, Breach [8] modeled non-ideal vapor-liquid phase equilibrium and mass and energy transfer in a binary system (H_2O, H_2O_2). Because of operating conditions in his work, ($P = 100$ kPa and $T = 433$ K) he neglected non-idealities in calculations of liquid density and gas phase equilibrium calculations. He also ignored the effect of non-idealities on the calculation of gas and liquid phase internal energies.

Also, Banerjee modeled the evaporation of a binary mixture of ethanol and iso-octane into air flowing in an inclined 2D channel. Simulation has been carried out at atmospheric pressure, and temperatures ranging from 300 to 340 K. The liquid phase density was calculated based on the averaged mass fraction of individual components, and the gas phase has been considered as ideal gas. He considered two-phase cells as an interface in which the gas and the liquid are in equilibrium. Therefore, the size of meshes should have been very fine around the interface [9].

Recently, the effects of non-idealities on hydrodynamic behavior have been studied based on a CFD framework [10]. The properties of each phase have been rigorously modeled as a function of temperature, pressure and concentrations. The VOF interface tracking method has been used for multiphase flow considerations. Mass transfer during condensation and vaporization was modeled by chemical potential at the liquid-vapor interface. Mass transfer resulting from the chemical potential field is determined by $T - P$ flash calculation at the liquid-vapor interface. The equilibrium calculations were performed using the fugacity coefficient definition for both the liquid and gas phases through an equation of state.

In the present article, two comparative cases (Cases 1 and 2) were considered. The obtained results were compared with a case (Case 0) presented by Irani et al [10]. In the first case (Case 1), the densities of phases were assumed to be constant, and in the second case (Case 2), they were calculated by the Peng-Robinson equation of state. In both cases, Rault's law was used instead of a fugacity coefficient definition for both the liquid and gas phases, in order to study the affection intensity of non-ideality on hydrodynamic behavior (Table 1).

The mathematical model of the system is described in the next section (Mathematical Model), and the benchmark used in this study is explained afterwards in the section of "Benchmark for the Validation of Simulation". The last section goes through the comparison between simulations and experimental results.

MATHEMATICAL MODEL

Continuity Equation for the Liquid and Gas Phases

The variation of liquid holdup with time and position is obtained by solving the continuity equations for the liquid and gas phases. The continuity equation for the flowing liquid and gas is written in terms of accumulation and convection terms, balanced by the total mass transferred to and from the other phases.

Since gas and liquid phases do not interpenetrate each other in the reactor, the VOF approach is used. In this approach, the motion of all phases is modeled by formulating local, instantaneous conservation equations for mass and momentum transfer [11].

The continuity equation for phase, 'q', in a multiphase flow problem is as follows:

$$\frac{\partial}{\partial t}(\alpha_q \rho_q) + \nabla.(\alpha_q \vec{v} \rho_q) = S_{pq},$$

$$S_{qp} = -S_{pq}. \tag{1}$$

The velocity vector, $\vec{v}$, comes from solving the Navier-Stokes Equations (NSE). The right-hand (S_{pq}) side describes mass transfer from phase p to q where α_q is the volume fraction of phase q, which needs to satisfy the following relation:

$$\sum_{q=1}^{n} \alpha_q = 1. \tag{2}$$

One of the most important characteristics of a multiphase system is the fractions of various phases. Thus, it is necessary to know the volume fraction, α_q of each phase, q, in the entire computational domain.

Momentum Transfer Equations

The variation of velocity with time and position is calculated by solving the momentum balance equation.

Table 1. Comparison between case studies considered in this work.

Case Studies	Phase Density	Phase Equilibrium Calculation Method	Comments
Case 0	EOS	Fugacity coefficient for gas & liquid phases	The most non-ideal case
Case 1	Constant	Rault's law	Case with the least non-ideality
Case 2	EOS	Rault's law	Medium non-ideal case

The properties appearing in the transport equations are determined by their averaging based on a phase volume-fraction [11].

$$\frac{\partial}{\partial t}(\rho\vec{v})+\frac{\partial}{\partial x_j}(\rho\vec{v}\vec{v})=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\mu\left(\frac{\partial\vec{v}}{\partial x_j}+\frac{\partial\vec{v}}{\partial x_j}\right)+\rho g_i,$$

$$\rho=\sum_{q=1}^{n}\rho_q\alpha_q, \qquad \mu=\sum_{q=1}^{n}\mu_q\alpha_q. \tag{3}$$

Bulk Species Transport

Dynamic variations in the gas and liquid phase species concentrations are obtained by solving the unsteady state species mass balance equations written as Equations 4 and 5, respectively:

$$\frac{\partial}{\partial t}\alpha_g C_{ig}+\nabla.(\alpha_g\vec{v}C_{ig}-D_{ig}\alpha_g\nabla C_{ig})=\alpha_g N_i^{gl}, \tag{4}$$

$$\frac{\partial}{\partial t}\alpha_l C_{il}+\nabla.(\alpha_l\vec{v}C_{il}-D_{il}\alpha_g\nabla C_{il})=-\alpha_l N_i^{gl}. \tag{5}$$

Interphase Mass Transfer

The interphase mass transfer is related to the diffusion at the interface that is related to the concentration gradients at the interface, too [12]. The concentration gradient of species in each phase was approximated using a Finite Difference approach. In fact, the mass transfer coefficient, based on the Film theory, is originally obtained through this approach. According to this approach, various elements of concentration gradients of phase 'q' can be obtained as follows:

$$\frac{\partial C_{iq}}{\partial x_j}\approx\frac{C_{iq}-C_{iq}^*}{\Delta x_j},$$

where C_{iq} is the concentration of the ith component in phase q right at the interface and C_{iq}^* is the concentration of this component when phase q is at equilibrium with the other phase in the mixture (Figure 1). This is based on the fact that in a multiphase system, they are assumed to be at equilibrium right at their interface. Some authors assumed that vapor and liquid at the interface do not reach saturation and, hence, an efficiency term (between 0.2 and 0.7) has been introduced. As good experimental results are lacking for the present study, the efficiency term has been assumed to be 1 [9].

For a mixture containing vapor and liquid, the equilibrium concentration of various components can be obtained through isothermal flash calculations [13,14]. Details of flash calculation algorithms and equations are given in Appendix.

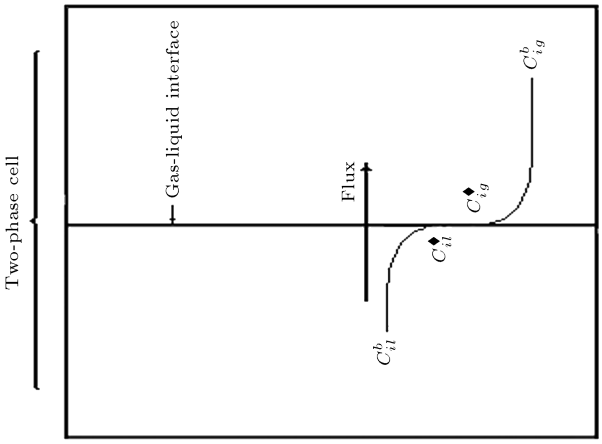


Figure 1. Schematic of two-phase cell and equilibrium at the interface.

The concentrations of various species in vapor and liquid phases are obtained based on Equations 4 and 5, respectively. Having obtained equilibrium concentrations, one can calculate the flux of species transfer (N_i^q) and the rate of inter-phase mass transfer (S_{pq}, which is the source term of Equation 1), through Equations 6 to 8, respectively, in which M_i is the molecular weight for the ith species. The calculated flux for component 'i' (N_i^q) in one phase is a source or sink for the same component in the other phase, because there is no accumulation at the interface.

$$N_i^q=D_{im}\frac{C_{iq}-C_{iq}^*}{\Delta z_j}, \tag{6}$$

$$N_i^p=-N_i^q, \tag{7}$$

$$S_{pq}=\sum_{i=0}^{n}N_i^q M_i. \tag{8}$$

Simulation Procedure

The transport equations (Equations 1 and 3-5) were discretized by a control volume formulation [15]. The UPWIND method was used for discretization. A segregated implicit solver method with implicit linearization was used to solve discretized momentum equations. These equations have been obtained through application of the first-order upwind method on Equation 3, and for pressure velocity coupling, the SIMPLE method has been used [15]. For the pressure equation, the pressure staggering option (PRESTO) method was used [15].

The structure of the program code is outlined in Figure 2 and explained below. The program first reads the structured data from the pre-processing section (in which the mesh representing the equipment has been built) before it goes into two nested iteration loops. Inner loop iterations are performed within each

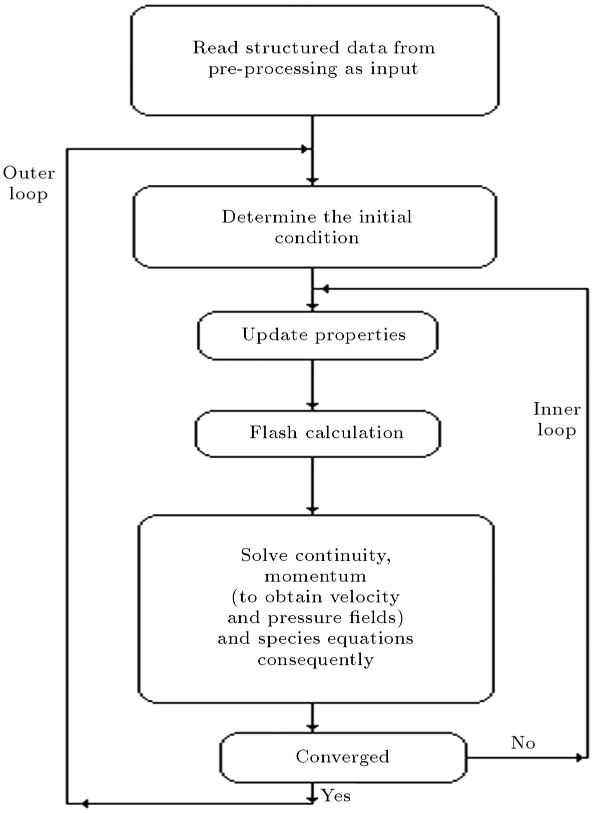


Figure 2. Diagram illustration of program code structure.

time step using the equations corresponding to the discretized version of the proposed model while the outer loop goes through simulation times until it gets to the final time or steady state; whichever happens sooner. At each time step, before going into the inner loop, the fluid properties in each cell are calculated.

In the inner loop, all the discretized equations are solved in three steps. In the first step, the physical properties, such as density, are updated based on the current solution. If the calculation has just begun, the fluid properties will be updated based on the initialized solution. In the second step, the flash calculation is performed in order to obtain equilibrium concentrations based on which the source terms of the species concentrations and continuity equations are obtained. In the third step, equations of continuity and momentum are solved and after obtaining the velocity and pressure fields, equations corresponding to species concentration are solved in order to obtain the profiles of the concentration of various species. In this step, with the help of the Eulerian-Eulerian approach (VOF approach), the trajectory of interface between two phases (liquid and gas) is determined. At the end of this step, convergence checking based on the norm of errors is done [14].

In order to get stable and meaningful results, the time step must be very small (in the order of 10^{-4} s). In general, the time-stepping strategy depends on the number of iterations by time step needed to ensure very low residual values (less than 10^{-7} for concentration and 10^{-6} for momentum and continuity). Computational time is within 3-4 weeks for the two dimensional simulations. Calculations have been carried out on a 4GB RAM, 3.2 GHz CPU computer.

BENCHMARK FOR VALIDATION OF SIMULATION

We used experimental results that were taken for validation of the simulation in the Research Institute of Petroleum Industries (RIPI) [10]. A cylindrical vessel (Figure 3) filled with vapor and liquid hydrocarbon was selected as the benchmark. The liquid hydrocarbon was chosen to be pure Octane and the hydrocarbon in the gas phase was assumed to be Propane. Only the gas concentrations can be measured online due to the impossibility of the liquid phase measurement. The system was connected to a Gas Chromatography (GC) via two lines. Gas sampling is done automatically every 20 minutes. The location of sampling points was 20 cm from the top of the vessel.

RESULTS AND DISCUSSION

Figures 4 and 5 show the initial conditions of the simulations for Cases 1 and 2 at which the concentration of octane in the gas phase and propane in the liquid phase is set to zero. It was also assumed that there is no movement in the system and, hence, the velocity was set to zero for the whole domain.

As time goes on, species are transferred between phases. This leads to a time varying concentration profile in both phases and a general velocity field for

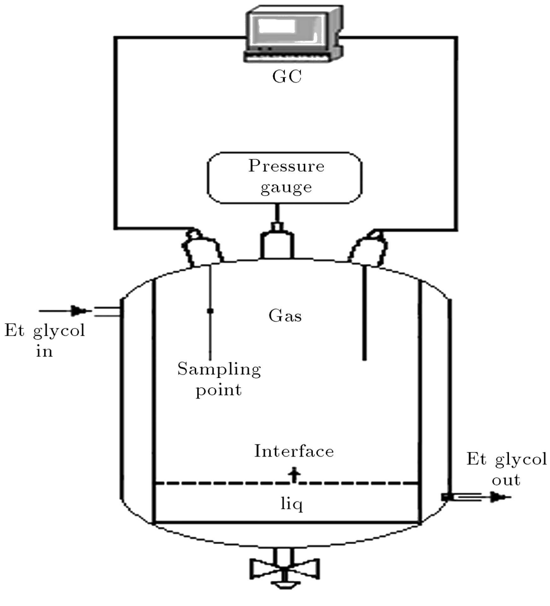


Figure 3. Schematic of experimental set up.

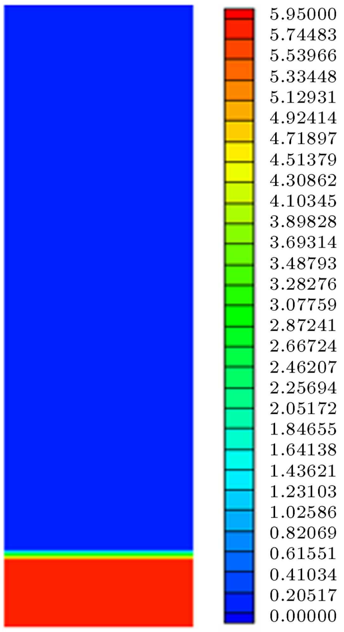


Figure 4. Contour of octane concentration (mol/liter) at $t = 0.0$ second (Cases 1 and 2).

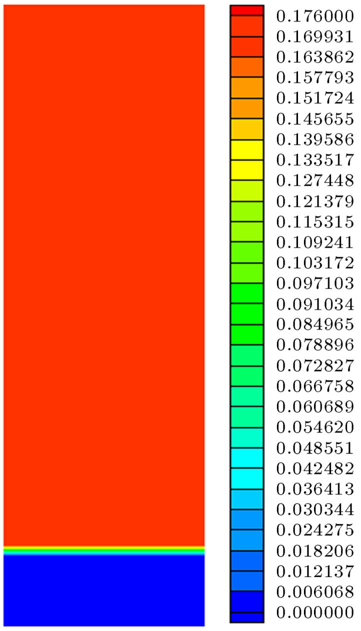


Figure 5. Contour of propane concentration (mol/liter) at $t = 0.0$ second (Cases 1 and 2).

the whole fluid both of which originated from the interphase mass transfer. The simulation results for concentration profiles and velocity fields at certain times, for both cases, are shown in Figures 6 to 11. As seen in these figures, specific colors do not refer to the same levels in Cases 1 and 2 in a particular figure, because the variations of variables are different in the two cases and the colors are generated automatically by software. As Figures 7 and 10 show, octane was transferred from the liquid phase to the gas phase, and

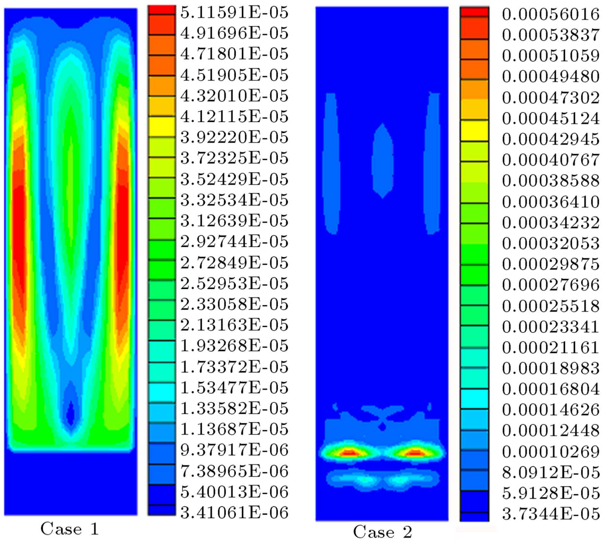


Figure 6. Contours of velocity (m/sec) at $t = 185$ seconds (Cases 1 and 2).

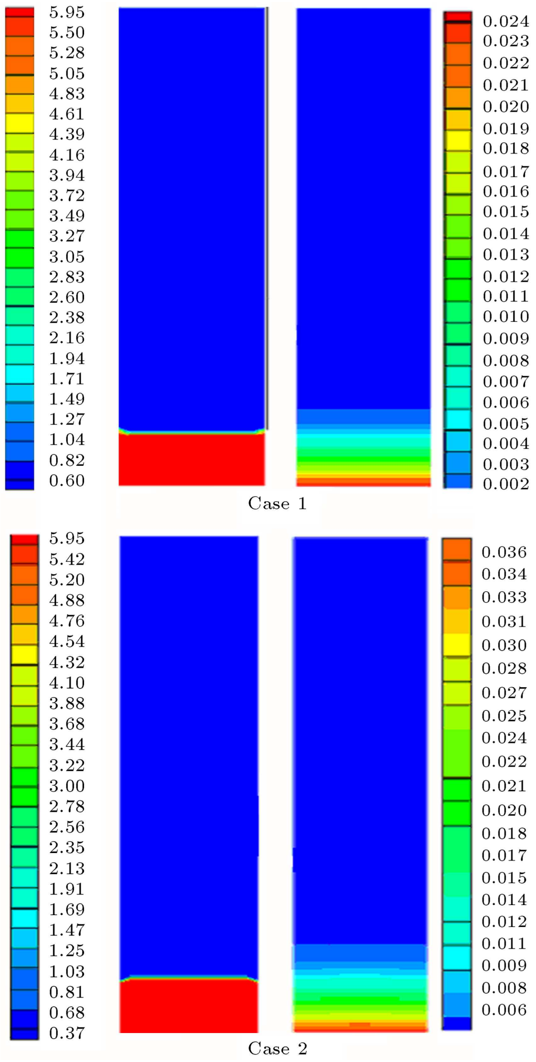


Figure 7. Contour of octane concentration (mol/liter) at $t = 185$ seconds (Cases 1 and 2).

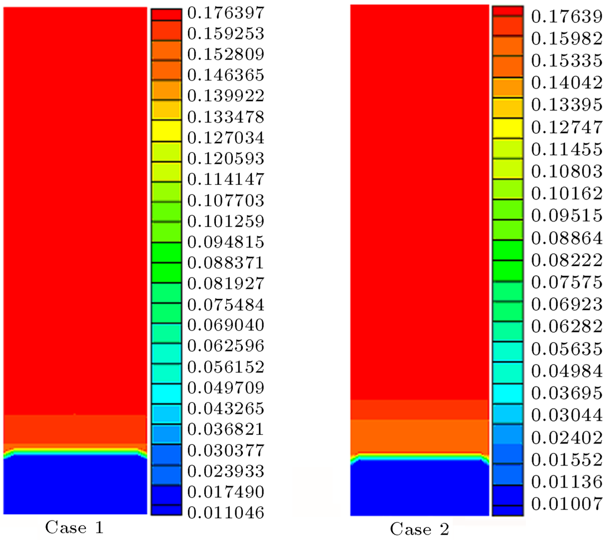


Figure 8. Contour of propane concentration (mol/liter) at $t = 185$ seconds (Cases 1 and 2).

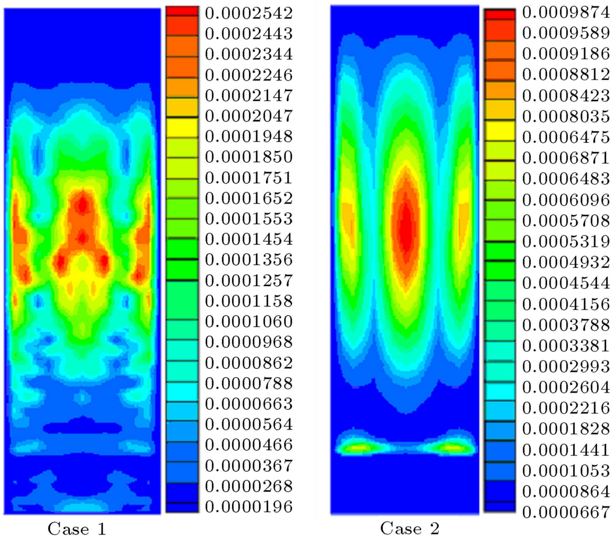


Figure 9. Contour of velocity (m/sec) at $t = 3500$ seconds (Cases 1 and 2).

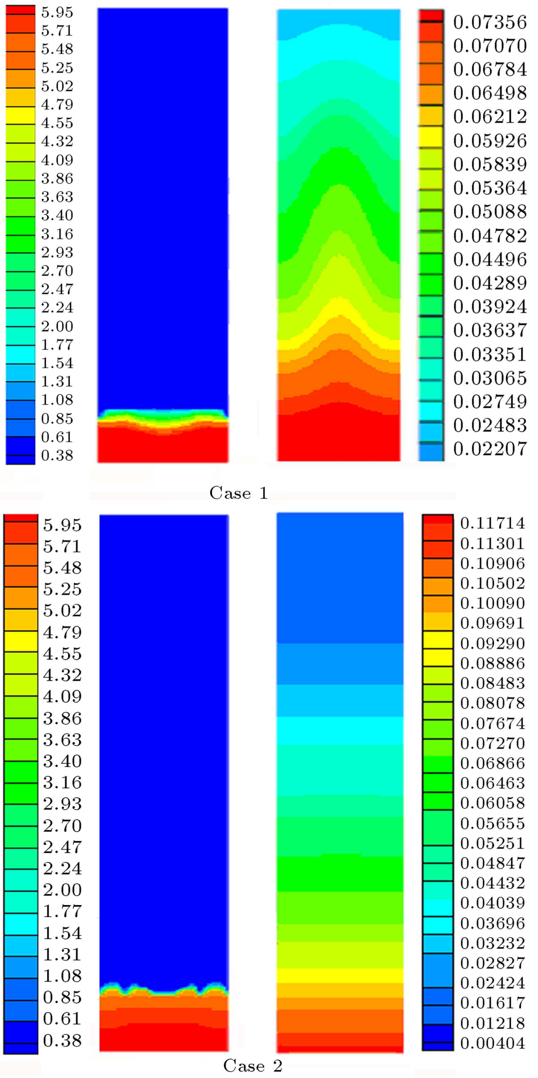


Figure 10. Contour of octane concentration (mol/liter) at $t = 3500$ seconds (Cases 1 and 2).

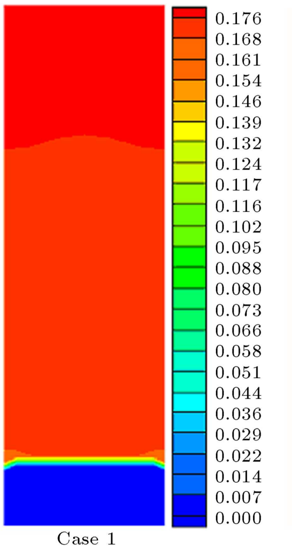
the concentration of octane in the liquid was decreased, whereas the concentration of octane in the gas was increased.

On the other hand, Propane dissolved in the liquid phase, which led to its concentration decrease in the gas phase. It can be seen, right at the interface, that the Propane concentration has its least value for the gas phase and the largest value for the liquid phase (Figures 8 and 11).

As seen in Figures 6 and 9, since the dissolution of octane in gas has not been considered in the calculation of the gas phase density (Case 1), velocity fields were different for Cases 1 and 2. Thus, bulk species concentrations in gas and, consequently, gradients in the gas-liquid interface were solved differently. Therefore, mass fluxes of species were different too. Also, in both cases, phase equilibrium calculations were done using Raoult's law, in spite of Case 0. Therefore, the errors are intensified, in comparison with Case 0. The inter-phase mass transfer for Cases 0, 1 and 2 (at $t = 3500$ s) were 0.07, 0.05 and 0.009 kg/m^3.s, respectively.

At $t = 3500$ s, the profiles of species concentrations along with the vessel length for Cases 0, 1 and 2 were presented (Figures 12 and 13). As a result of ideal assumptions, the species mole fraction in Cases 1 and 2 go away from the mole species fraction in Case 0. Due to the difference in the rate of species transfer between the phases for these cases, the distribution of species concentration was different.

In order to see the deviation of the mentioned cases from experimental data, quantitative comparisons were done between data obtained for Octane concentration in the gas phase [10] and the corresponding simulated results shown in Figure 13. Since it was



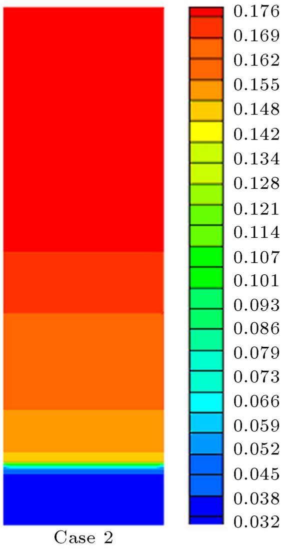


Figure 11. Contour of propane concentration (mol/liter) at $t = 3500$ seconds (Cases 1 and 2).

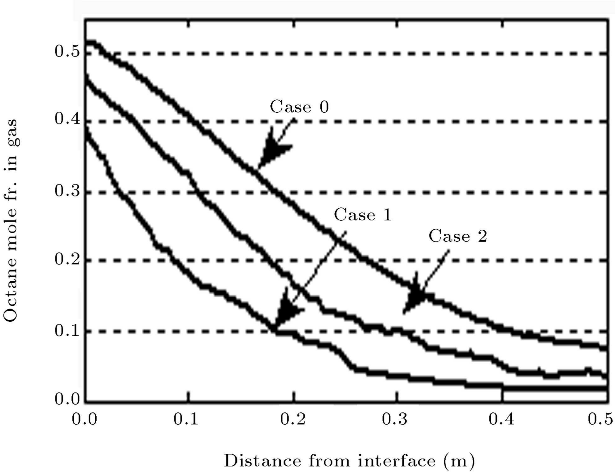


Figure 12. Profile of octane concentration in gas phase (mol/liter) at $t = 3500$ seconds (Cases 1 and 2).

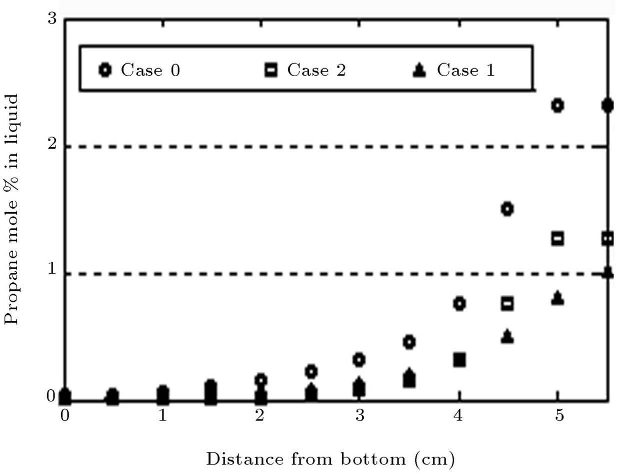


Figure 13. Profile of propane mole fraction in liquid phase at $t = 3500$ s (Cases 0, 1 and 2).

not possible to use the GC for the dynamic measurement of more than one point, only five experimental data have been obtained and compared against their corresponding points obtained by simulation. Only gas concentrations can be measured online due to the impossibility of the measurement liquid phase. As illustrated in Figure 14, the maximum amount of difference between simulations and experimental data would occur at the start of the simulation ($t = 0$). The mentioned difference was due to the delay in the Gas Chromatograph injection during the fixing of the system pressure. Because of using Raults law in equilibrium calculation, instead of the fugacity coefficient definition for the liquid and gas phases, in both cases, the flux of species is calculated incorrectly. As seen in Figure 13, the differences in the cases between simulations and experiments intensified, in comparison with previous studies [10]. In Case 1, since the densities of phases were assumed constant, the effects of dissolved components on the density of phases and the buoyancy effect are not considered. Consequently, incorrect velocity fields and species concentrations, in addition to the mass transfer flux, are predicted.

Table 2 shows the simulated and measured concentration of Octane in the gas phase, along with their relative differences. As this table shows, the errors in the Octane mole fraction in the gas phase at all times are less than five percent, while all non-idealities were considered (Case 0). Since the system is not at equilibrium and the mass transfer is simulated based on the CFD approach, and no empirical correlation has been used in the simulation, these small errors can be used as a rationale for the accuracy of the simulation results including the velocity and gas phase volume fraction profiles. The errors in Cases 2 and 1 were higher: (21-31%) and (38-65%), respectively. These errors show that such simplifications in similar modeling cases lead to wrong predictions.

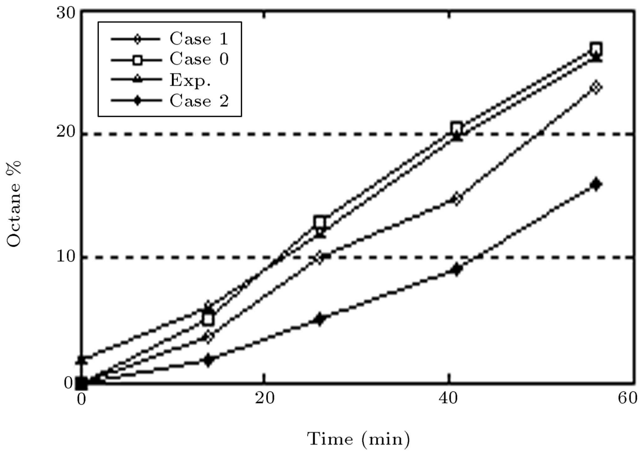


Figure 14. Comparison of experimental and simulations results.

Table 2. Comparison between simulation and experimental data and relative errors.

Time	**Experimental**	**Case 0**	**Case 2**	**Case 1**	**Error (Case 0)**	**Error (Case 2)**	**Error (Case 1)**
0	0.018	0	0	0	100	100	100
14	0.0528	0.0515	0.036	0.018	2.46212121	31.818182	65.909091
26	0.1273	0.128234	0.1	0.05	0.73369992	21.445405	60.722702
41	0.1983	0.2047	0.147	0.09	3.22743318	25.869894	54.614221
56	0.26053	0.2676	0.238	0.16	2.713699	8.6477565	38.586727

CONCLUSIONS

The aim of this paper was to study the importance and effects of considering non-ideal thermodynamics in the simulation, which were presented in previous studies [10].

For this purpose, the benchmark was simulated by using a numerical method based on a macroscopic model and the finite volume method. In this simulation, non-ideality was not considered in the cases. Raoult's law was used in the equilibrium calculation instead of the fugacity coefficient definition for the liquid and gas phases, in both cases, and in Case 1 the density of phases was assumed constant.

Quantitative validation of the simulated system with experimental data was based on the online analysis of gas phase flow by Gas Chromatography. The predictions in both cases were compared with the experimental measurements and the simulation data in our previous work. It was found that the difference between the gas species concentrations in experiment and simulation increased by the assumption of more ideality. The results also indicated that the assumption of constant density in simulation had a major role in diverting from experimental data (Figure 14). It is worth mentioning here that the closure for the mass transfer is not as mature as the closures used for the hydrodynamics. However, we became confident that if a more accurate closure for the mass transfer by considering non-ideality were to be applied, the present model would give a closer comparison with the experimental investigation, as has been shown in this study.

The model in our previous work was based on the Eulerian-Eulerian approach. Also, it combined hydrodynamics, mass transfer and mixture non-ideality. The model and results presented in this work would be useful for extending the application of CFD based models for simulating large multiphase reactors.

NOMENCLATURE

C_{ig}	gas species concentration
C_{il}	liquid species concentration
C_i^*	Equilibrium species concentration
C_{g^T}	total concentration of gas
D_{im}	diffusion coefficient of species i in mixture
K_i	equilibrium constant t
M_i	molecular weight
N_i	flux of species transfer
P	pressure
VF	Equilibrium volume fraction
$\vec{v}$	velocity vector
S_{pq}	rate of interphase transfer
ρ_q	phase density
ρ	mixture density
μ_q	phase viscosity
μ	mixture viscosity
α_q	volume fraction of each phase
P_{dew}	dew point pressure
P_{bub}	bubble point pressure
Z_i	mole fraction of species i in mixture
y_i	gas phase mole fraction
x_i	liquid phase mole fraction

REFERENCES

1. Rigopoulos, S. and Jones, A.G. "A hybrid CFD-reaction engineering framework for multiphase reactor modeling: basic concept and application to bubble column reactors", *Chem. Eng. Sci*, **58**, pp. 3077-3089 (2003).

2. Darmana, D., Henket, R.L.B., Deen, N.G. and Kuipers, J.A.M. "Detailed modeling of hydrodynamics, mass transfer and chemical reactions in a bubble column using a discrete bubble model: Chemisorption of CO_2 into NaOH solution, numerical and experimental study", *Chemical Engineering Science*, **62**, pp. 2556-2575 (2007).

3. Bauer, M. and Eigenberger, G. "A concept for multiscale modeling of bubble columns and loop reactors", *Chem. Eng. Sci.*, **54**, pp. 5109-5117 (1999).

4. Bauer, M. and Eigenberger, G. "Multiscale modeling of hydrodynamics, mass transfer and reaction in bubble column reactors", *Chem. Eng. Sci.*, **56**, pp. 1067-1074 (2001).

5. Bezzo, F., Macchietto, S. and Pantelides, C.C. "A general methodology for hybrid multizonal/CFD models. Part I: Theoretical framework", *Computers and Chemical Engineering*, **28**, pp. 501-511 (2004).

6. Zauner, R. and Jones, A.G. "Scale-up of continuous and batch precipitation processes", *Industrial and Engineering Chemistry Research*, **39**(7), pp. 2392-2403 (2000).

7. Krishna, R. and Van Baten, J.M. "CFD modeling of bubble column reactor carrying out consecutive reaction ($A \rightarrow B \rightarrow C$)", *Chem. Eng. Thechnol.*, **27**, pp. 67-75 (2004).

8. Breach, M.R. and Ansari, N. "Modeling non-ideal vapor-liquid phase equilibrium, mass and energy transfer in a binary system via augmentation of computational fluid dynamical methods", *Comput. Chem. Eng.*, **31**, pp. 1047-1054 (2007).

9. Banerjee, R. "Turbulent conjugate heat and mass transfer from the surface of a binary mixture of ethanol/iso-octane in a countercurrent stratified two-phase flow system", *International Journal of Heat and Mass Transfer*, **51**, pp. 5958-5974 (2008).

10. Irani, M., Bozorgmehry, R.B., Pishvaie, M.R. and Tavasoli, A. "Investigating the effects of mass transfer and mixture non-ideality on multiphase flow hydrodynamics using CFD methods", *IJCCE* (2009).

11. Hirt, C.W. and Nichols, B.D. "Volume of Fluid (VOF) method for the dynamics of free boundaries", *J. Comp. Phys.*, **201**, p. 39 (1981).

12. Treybal, R.E., *Mass Transfer Operation*, Third Edition, McGraw-Hill (2001).

13. Smith, J.M. and Van Ness, H.C., *Introduction to Chemical Engineering Thermodynamics*, 6th Edition, McGraw-Hill (2001).

14. Walas, S.M, *Phase Equilibria in Chemical Engineering*, Butterworth, Storeham, USA (1985).

15. Patankar, S.V., *Numerical Heat Transfer and Fluid Flow*, Taylor and Francis (1980).

16. Poling, B.E., Prausnitz, J.M. and O'Connell, J.P., *The Properties of Gases & Liquids*, 5th Ed., McGraw-Hill, New York (2000).

APPENDIX

Algorithm for Calculation of C^*

A flow chart has been sketched to describe the algorithm graphically (Figure A1). However, the routine for calculation of C^* is as follows:

1. In each two-phase cell, calculate dew-point (P_{dew}) and bubble-point (P_{bub}) pressures.
2. If pressure of system is greater than P_{bub} then:

$$X_i = Z_i.$$

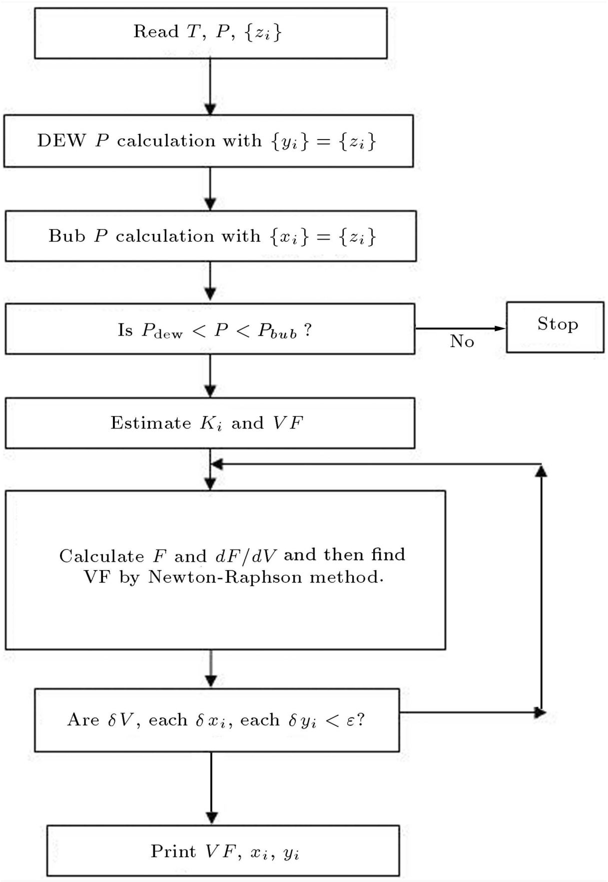


Figure A1. Flow chart of equilibrium calculation.

3. If pressure of system is less than P_{dew} then:

   $X_i = Z_i/K_i$.

4. If pressure of system is greater than P_{dew} and less than P_{bub} then perform flash calculation (the Antoine vapor pressure correlation was was used in equilibrium calculation):

$$\ln P^{\text{sat}} = a + \frac{b}{T+c} + d\ln(T) + eT^f,$$

$$K_i(T_i) = \frac{P_i^{\text{sat}}(T)}{P},$$

$$x_i = \frac{z_i}{1+VF(K_i-1)},$$

$$y_i = \frac{z_iK_i}{1+VF(K_i-1)},$$

$$F(V) = \sum y_i - \sum x_i = 0,$$

$$C_{\text{Total}}^g = \sum_{j=1}^{n} C_j^g,$$

$$C_{ig}^* = y_i \times C_{\text{Total}}^g.$$

Binary Diffusivity

Fuller's method was used to determine diffusivity:

$$D_{AB}=\frac{0.0143\,T^{1.75}}{PM_{AB}^{0.5}\left[(\sum v)_A^{\frac{1}{3}}+(\sum v)_B^{\frac{1}{3}}\right]^2},$$

$$\frac{2}{M_{AB}}=\frac{1}{M_A}+\frac{1}{M_B}.$$

$\sum v$ is found for each component by summing atomic diffusion volumes given in [16].

BIOGRAPHIES

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