Investigating the Effects of Mass Transfer and Mixture Non-Ideality on Multiphase Flow Hydrodynamics Using CFD Methods

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ABSTRACT: *A numerical framework has been proposed to model the interacting effects of mixture non-ideality and mass transfer on hydrodynamics of a multiphase system using CFD methods. Mass transfer during condensation and vaporization is modeled by chemical potential at the liquid-vapor interface. Species mass transfers are related to the diffusion at the interface which in turn is related to the concentration gradients at the interface. A finite volume scheme is used to solve the equations of motion. Since the thermodynamic non-ideality of the system has been taken into account, the equilibrium calculations were performed using the fugacity coefficient definition for both the liquid and gas phases. The obtained results and their comparison against experimental data show that the proposed framework can simulate the hydrodynamic behavior of multi-component multi-phase systems with thermodynamic non-ideality.*

KEY WORDS: *Multiphase flow, VOF, Mass transfer, Flash calculation, Non-ideal thermodynamic behavior, CFD.*

INTRODUCTION

In the chemical and petrochemical industries, multi-component phases commonly undergo composition changes due to various phenomena resulting in the transfer of species from one phase to another, or conversion of species through chemical reactions. On the other hand, the thermo-physical properties of a multi-component system are strongly dependant on its compositions. This is due to the fact that the properties of a multi-component mixture are not necessarily equal to the weighted average of the corresponding properties of its constituting pure components.

This results in a severe interaction between hydrodynamic and thermodynamic behavior of a multi-component system. This interaction seems to have more effects on the hydrodynamic behavior of multi-component multiphase systems.

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Despite the widespread research efforts devoted to understand the hydrodynamic behavior of multi-component multiphase system, it seems that nobody has focused on the study of the interaction of hydrodynamic and thermodynamic behaviors of multi-component multiphase systems [1].

In the past decade, in most of the studies, mass transfer and non-ideal behavior of various mixtures and chemical reactions between them were ignored due to excessive memory and computational demand requirements.

By employing a so-called hybrid method, some authors tried to solve the problem by decoupling the interaction between hydrodynamics, mass transfer, thermodynamic behavior, and chemical reactions and solve each sub-problem with a separate model. In those models, CFD is employed only for the hydrodynamic simulation, while the chemical reactions are accounted for in a c ustom-built compartmental model [2- 4]. It should be noted that decoupling approach cannot be used in cases where the coupling between hydrodynamics and chemical reactions and/or non-ideal thermodynamic behavior of the mixture is very strong. Combustion and various multiphase systems in which the fluid consists of various types of components whose mixture has a non-ideal behavior can be mentioned as instances of these cases. Since these methods essentially offer a compromise to cope with the necessity to get information on the mass transfer and chemical reaction process and the prohibitively expensive direct CFD calculation, it does not necessarily account for the interaction between hydrodynamics, mass transfer, and non-ideal behavior of the mixture. *Krishna*, has studied the interphase mass transfer without thermodynamic non-idealities. In his study, densities were constant and he estimated equilibrium constants with Henry's coefficients. He has also neglected the effect of mass transfer on hydrodynamics behavior of the system [5]. In another work, *Krishna & van Baten* studied the interphase mass transfer and chemical reaction (with a first order reaction rate) for species whose mixture does not have deviation from ideal mixture. They assumed that the densities were constant and neglected the effect of mass transfer on hydrodynamics behavior of the system [6].

Bezzo, Macchietto & Pantelides developed a framework in which gPROMS, as a modeling software and a commercial CFD code has been linked together; [7]. *Zauner & Jones* [8] used a segregated feed model in conjunction with CFD to study precipitation in a stirred tank. However, the major shortcoming of all multi-zone models is the difficulty of characterizing the mass and energy fluxes between adjacent zones. A priori estimate of these may be obtained by means of preliminary CFD calculations. However, this fails to take into account the fact that the fluid properties are functions of system conditions (e.g. composition, temperature and pressure) which are not known. This framework is applicable to systems whose physical properties are relatively weak functions of intensive properties.

Later *Breach* has modeled non-ideal vapor–liquid phase equilibrium, mass and energy transfer in a binary system (H_2O, H_2O_2). He has neglected non-idealities in liquid density and equilibrium calculations. He has also ignored the effect of thermodynamic non-idealities on the calculation of gas and liquid phase internal energies [9].

In this paper the effects of the non-ideal behavior of phases on their hydrodynamic behaviors, have been studied based on a CFD framework in which the properties of each phase are rigorously modeled as a function of temperature, pressure and concentration of phase constituting components. The CFD framework is developed based on *Eulerian - Eulerian* model. The proposed framework can be used in modeling and simulation of multiphase flow of non-ideal mixtures.

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 the accumulation and convection terms balanced by the total mass transferred to and from the other phases (written in terms of interphase fluxes for gas-liquid equations, discussed in the next section).

Since gas and liquid phases do not interpenetrate into 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 [10].

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

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q\right) + \nabla \cdot \left(\alpha_q \bar{v} \rho_q\right) = S_{pq} \quad \& \quad S_{qp} = S_{pq} \tag{1}$$

The velocity vector $\bar{v}$ comes from solving the Navier-Stokes Equations (NSE).

The left-hand side describes the internal change of mass over time and the convective flux crossing the boundaries of the control volume. 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 Eq. (2).

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

One of the most important characteristics of a multi-phase system is 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. The momentum equations can be written in terms of accumulation and convection terms on the left-hand side, and the gravity, pressure gradient and viscous stresses terms on the right-hand side, as the pressure and velocity are assumed to be equal in both phases. The properties appearing in the transport equations are determined by their averaging based on phase volume-fraction.

$$\frac{\partial}{\partial t}\left(\rho \bar{v}\right) + \nabla \cdot \left(\rho \bar{v} \bar{v}\right) = -\nabla P + \nabla \cdot \left[\mu\left(\nabla \bar{v} + \nabla \bar{v}^T\right)\right] + \rho g_i \tag{3}$$

$$\rho = \sum_{i=0}^{n} \rho_q \alpha_q \qquad \mu = \sum_{i=0}^{n} \mu_q \alpha_q$$

Bulk species transport

The dynamic variation in the liquid and gas phase species concentrations are obtained by solving the unsteady state species mass balance equations, consisting of accumulation, convection, and interphase transport for the gas and liquid phases written as Eqs. (4) and (5), respectively.

$$\frac{\partial}{\partial} \alpha_g C_{ig} + \nabla \cdot \left(\alpha_g \bar{v} C_{gi} - D_{ig} \alpha_g \nabla C_{ig}\right) = \alpha_g N_i^{gl} \tag{4}$$

$$\frac{\partial}{\partial} \alpha_l C_{il} + \nabla \cdot \left(\alpha_l \bar{v} C_{il} - D_{il} \alpha_l \nabla C_{il}\right) = -\alpha_l N_i^{gl} \tag{5}$$

Interphase mass transfer

Observations have indicated that the rates of mass transfers are closely related to the diffusion at the interface that is related to the concentration gradients at the interface, too. In real problems, however, we have usually no direct way to measure the concentration gradients at the interface. One of the approaches that can be used to estimate the concentration gradient is the approximation of various elements of concentration gradient in each phase using Finite Difference approach. In fact mass transfer coefficient based on 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:

$$\frac{\partial C_{iq}}{\partial x_j} \approx \frac{C_{iq} - C_{iq}^*}{\Delta x_j} \tag{6}$$

Where C_{iq} is the concentration of i-th 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. This is based on the fact that in a multiphase system, they are assumed to be at equilibrium right at their interface.

For a mixture containing vapor and liquid the equilibrium concentration of various components can be obtained through isothermal flash calculations which are presented at all chemical engineering thermodynamic text books [11, 12]. Details of flash calculation algorithm and equations were given in appendix.A.

The concentration of various species in vapor and liquid phases are obtained based on Eqs. (4) and (5), respectively. Having obtained equilibrium concentrations, one can obtain the flux of species transfer (N_i^q) and the rate of inter-phase mass transfer (S_{pq}) through Eqs. (8) and (9), respectively, in which M_i is molecular weight for i-th species. Calculated flux or 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.

$$N_i^q = D_i \frac{C_{iq} = C_{iq}^*}{\Delta z_j} \qquad N_i^p = -N_i^q \tag{8}$$

$$S_{pq} = \sum_{i=0}^{n} N_i^q M_i \tag{9}$$

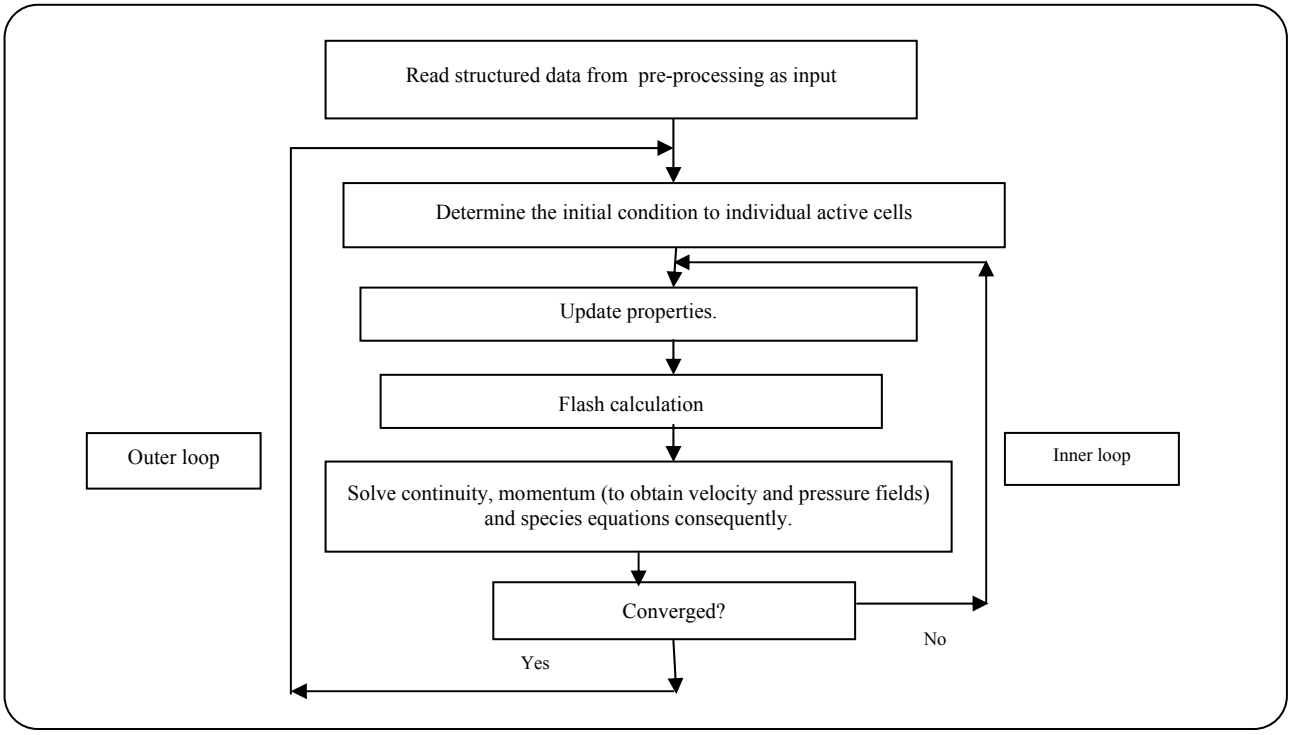


Fig. 1: Schematic illustration of program code structure.

Simulation procedure

The transport equations (Eqs. (1), (3), (4), and (5)) were discretized by control volume formulation [13]. UPWIND scheme 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 the application of the first-order upwind scheme on Eq. (3), and for the pressure velocity coupling, the SIMPLE scheme has been used [13]. For the pressure equation, the pressure staggering option (PRESTO) scheme was used [13].

The structure of the program code is outlined in Fig. 1 and explained below. The program first reads the structured data from 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 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 is 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 the 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 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. Due to the nonlinearity and interactions of various equations, the convergence is usually achieved after several iterations at each time step.

In order to get stable and meaningful results the time step must be very small (in the order of 10^{-4} s). However, as time goes on, and various states of the system (e.g., velocities and species concentration) obtain their corresponding smooth profile throughout the system, the time step can be gradually increased. This is due to

the fact that dependence of various physical properties (e.g., density, specific heat…) on species concentration increases the amount of interaction and coupling of equations. It should also be noted that, in this mechanism the time step could not get values beyond 10^{-3}s. In general, the time-stepping strategy depends on the number of iterations by time step needed to ensure very low residuals values (less than 10^{-7} for concentration and 10^{-5} for momentum and continuity). Computational time is within 7–8 weeks for the two dimensional simulations. Calculations have been carried out on a 3.2 GHz computer with 4GB of RAM,.

A BENCHMARK FOR VALIDATION OF SIMULATION

A cylindrical vessel filled with vapor and liquid hydrocarbons is selected as the benchmark. The liquid hydrocarbon is chosen to be pure octane and the hydrocarbon in the gas phase is assumed to be Propane. It is assumed that the amounts of propane in the liquid phase and octane in the gas phase are initially negligible. As time goes on due to the difference between the chemical potentials of propane and octane in liquid and gas phases, there would be mass transfer between gas and liquid phases which leads to the transfer of propane to the liquid and octane to the gas phase. The mass transfer between gas and liquid phases leads to a spatial and temporal variation of the phase density. Furthermore, there would be a velocity field due to mass transfer occurring between the phases. The objective is to find the concentration profile of various species at each phase and the established velocity field.

In order to validate the simulation results, an extensive comparison was made against the experimental data obtained in Research Institute of Petroleum Industry Laboratories.

EXPERIMENTAL SECTION

Material

N-octane was supplied by ACROS ORGANICS New jersey, USA, and was of laboratory grade (an average purity of 97%). Propane is selected as gas phase with 99% purity.

Reactor geometry

The vessel used in this work is a quartz cylinder with radii and lengths of 14 and 57 cm, respectively.

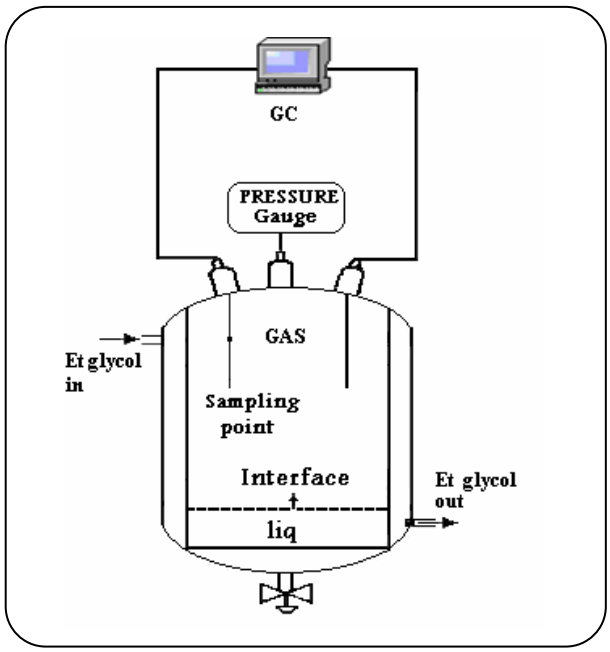


Fig.2: Schematic of Experimental set up.

The system is assumed to be isothermal, therefore, temperature of system was controlled and fixed using a jacketed system around the vessel. A circulator was used for circulation of ethylene glycol in jacket system (Fig.2)

The top of the vessel was closed and in order to be able to get gas and liquid samples, two sampling holes at the top and one in the bottom of cylindrical vessel were made.

Experimental methodologies

The experiments as well as simulation were conducted at P= 445 kpa and T=50 ºC. The pressure of system was supplied using pressurized propane gas. Because of isothermal assumption , experimental run started by heating of octane liquid up to 50 °C in the oven and then filling the column with the appropriate heated octane (50 ºC) up to 7 cm. Then the gas phase was preheated and injected slowly from top of the vessel. The system was connected to a Gas Chromatography (GC) via two lines. Gas sampling is done automatically every 20 minutes. This would lead to minimum sampling error.

RESULTS AND DISCUSSION

Fig. 3 to 5 show initial condition of the simulation at which the liquid height measured from bottom was 7cm. At the same time, the concentration of octane in gas

phase and propane in liquid phase were 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 profiles in both phases and a general velocity field for the whole fluid. The simulation results for concentration profiles and velocity field at various times are shown in Figs. 6 to 15. As Figs. 7 and 12 show, octane was transferred from liquid phase to gas phase and concentration of octane in liquid was decreased whereas concentration of octane in gas was increased. On the other hand, Propane dissolved in liquid phase which leads to its concentration decrease in gas phase, can be seen right at the interface. The propane concentration has its least value for gas phase and the largest value for the liquid phase (Figs. 8, 13). As a result of mass transfer in the interface, velocity in this region is higher than others (Figs. 6, 14). Density of gas phase was increased near the interface because concentration of octane was increased (Figs. 10, 15). In contrast, density of liquid phase was decreased near interface because concentration of propane was increased (Figs. 10, 15).

Quantitative validation

Despite the fact that the results shown in Figs. 6 to 15 were used for qualitative validation of the model and the solution procedure, in order to ensure the accuracy of the model, quantitative comparison of experimental data obtained for Octane concentration in gas phase and their corresponding simulated results is shown in Fig. 16. Since it was not possible to use the GC for dynamic measurement of more than one point, only five experimental data have been obtained and compared against their corresponding points obtained by simulation. Only the gas concentrations can be measured online due to impossibility of liquid phase measurement. As illustrated in Fig. 16, the maximum amount of difference between simulation and experimental data would occur at the start of simulation (t=0). The mentioned difference was due to the delay in Gas Chromatograph injection during fixing the system pressure. Table 1 shows the simulated and measured concentration of Octane in gas phase along with their relative difference. As this table shows, the errors in

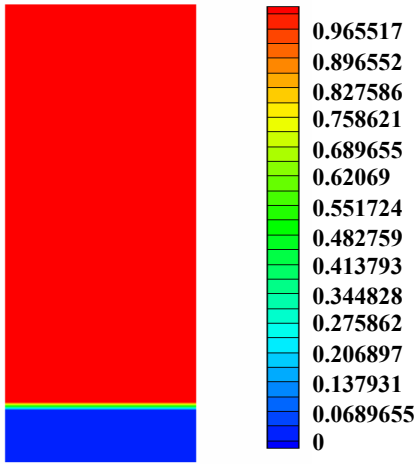


Fig. 3: Contour of gas volume fraction at t=0.0 second.

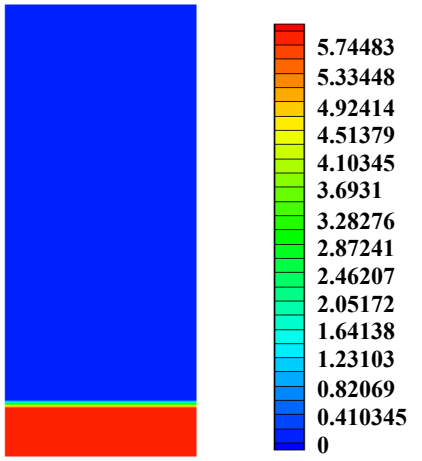


Fig. 4: Contour of octane concentration (mol /liter) at t=0.0 second.

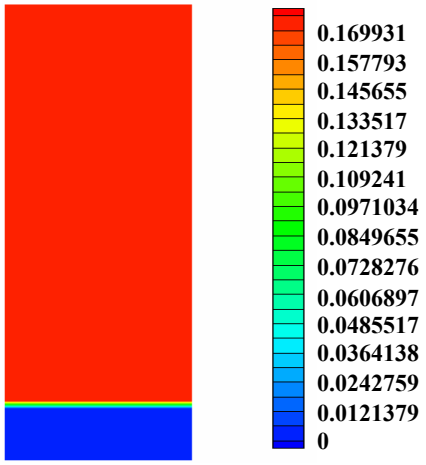


Fig. 5: Contour of propane concentration (mol /liter) at t=0.0 second.

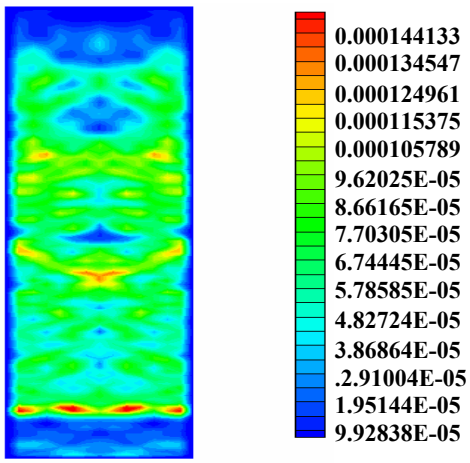


Fig. 6: Contour of velocity (m/sec) at t=2539 seconds.

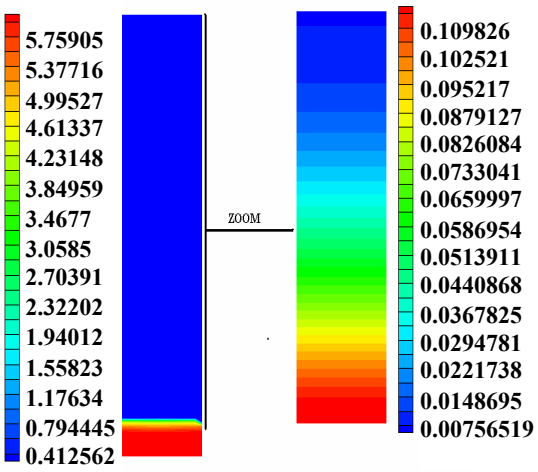


Fig. 7: Contour of octane concentration (mol /liter) at t=2539 seconds.

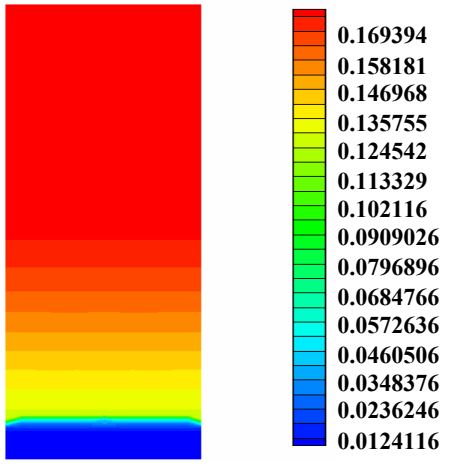


Fig. 8: Contour of propane concentration (mol /liter) at t=2539 seconds.

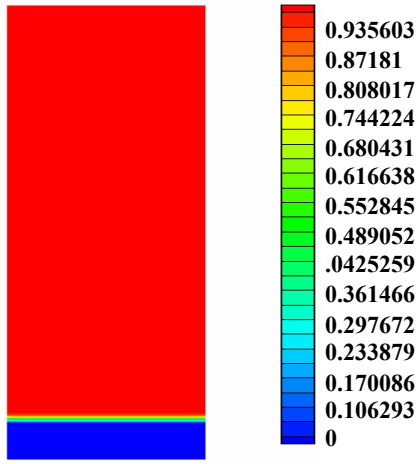


Fig. 9: Contour of volume fraction at t=2539 seconds.

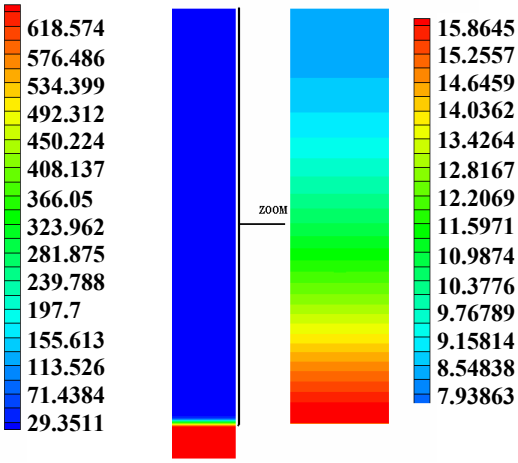


Fig. 10: Contour of density (kg/m^3) at t =2539 seconds.

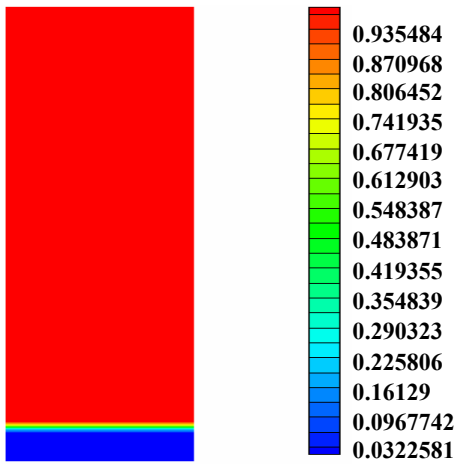


Fig. 11: Contour of gas volume fraction at t=3650 seconds.

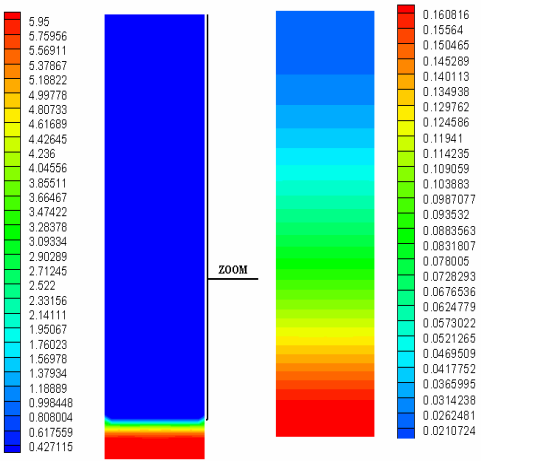


Fig. 12: Contour of octane concentration (mol /liter) at t=3650 seconds.

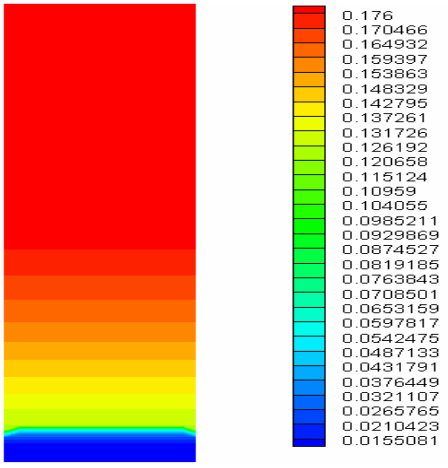


Fig. 13: Contour of propane concentration (mol /liter) at t=3650 seconds.

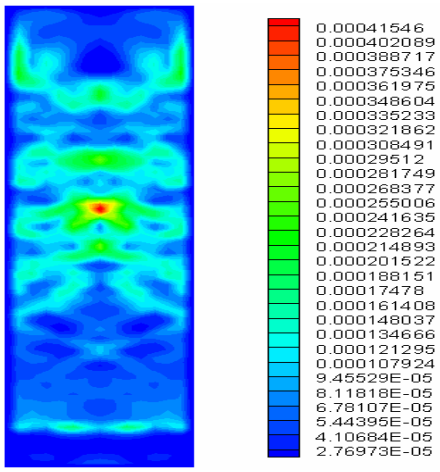


Fig. 14: Contour of velocity (m/s) at t=3650 seconds.

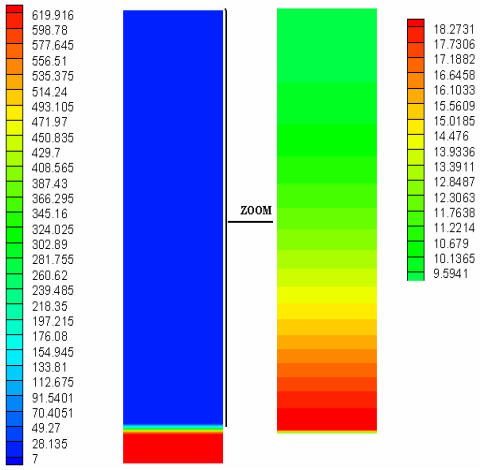


Fig. 15: Contour of density (kg/m^3) at t =3650 seconds.

Octane mole fraction in gas phase at all times are less than five percent. 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 rational for the accuracy of the simulation results including the velocity and gas phase volume fraction profiles.

CONCLUSIONS

In the present work, a CFD framework has been proposed to simulate the multiphase mass transfer problems in chemical processes. For this purpose, a numerical method based on a macroscopic model and the finite volume method was applied. The proposed CFD framework is able to solve multiphase mass transfer problems with high interaction of thermodynamic and hydrodynamic behavior of the system.

Quantitative validation of simulated system with experimental data was based on online analyzing of gas phase flow by Gas Chromatograph. The predictions obtained by proposed framework were compared with the experimental measurements. It was found that the proposed framework predicts the gas species concentrations well. Since the velocities originated from mass transfer were so small, our instrument did not measure them. Due to the correct prediction of gas species concentrations by simulation, it seems that the simulated hydrodynamic is correct. This is due to the

fact that there is a high interaction between mixture non-ideality (composition dependence of the mixture density and fugacity), mass transfer and hydrodynamics of the system.

The proposed framework makes it possible to take into account the interacting effects of mixture non-ideality, mass transfer and hydrodynamics on multiphase system in a more realistic way. None of the analysis and studies that have been done on the hydrodynamic of multiphase systems has covered these effects till now, the major reason why these issues have not been covered till now was the fact that none of the available commercial CFD applications has a ready made frame work for such an analysis.

Appendix.A

The algorithm for calculation of C^*

A.1.In each two-phase cell calculate dew-point (Pdew) and bubble-point (Pbub) pressures

A.2. If pressure of system greater than Pbub then:

$X_i = Z_i$

A.3. If pressure of system less than Pdew then:

$X_i = Z_i/K_i$

A.3. If pressure of system greater than Pdew and less than Pbub then:

Perform flash calculation

$$K_i(x_i, y_i, T_i) = \frac{\hat{\varphi}_i^l(x_i, y_i, T_i)}{\hat{\varphi}_i^g(x_i, y_i, T_i)} \quad \text{A1}$$

$$x_i = \frac{z_i}{1 + V(K_i - 1)} \quad \text{A2}$$

$$y_i = \frac{z_i K_i}{1 + V(K_i - 1)} \quad \text{A3}$$

$$\ln \hat{\varphi}_i (Z-1)\frac{b_i}{b_m} - \ln(Z - \text{beta}) - \quad \text{A4}$$

$$I \times q \times \left(\frac{\partial a_m / \partial X_i}{a_m} - \frac{b_i}{b_m} \right)$$

$$I = \frac{1}{\varepsilon_1 - \varepsilon_2} \ln \left(\frac{Z + \varepsilon_1 \times \text{beta}}{Z + \varepsilon_2 \times \text{beta}} \right)$$

$$\text{beta} = \frac{b_m P}{RT} \quad , \quad q = \frac{a_m}{bRT} \quad , \quad \varepsilon_1 = 1 + \sqrt{2} \quad , \quad \varepsilon_2 = 1 - \sqrt{2}$$

$$F(VF) = \sum y_i - \sum x_i = 0 \quad \text{A5}$$

Table 1: Comparison between simulation and experimental data and relative errors.

Time (min.)	Experimental	Simulation	Relative error (%)
0	0.018	0	100
14	0.0528	0.0515	2.462121
26	0.1273	0.128234	0.733504
41	0.1983	0.2047	3.227433
55	0.26053	0.2676	2.713699

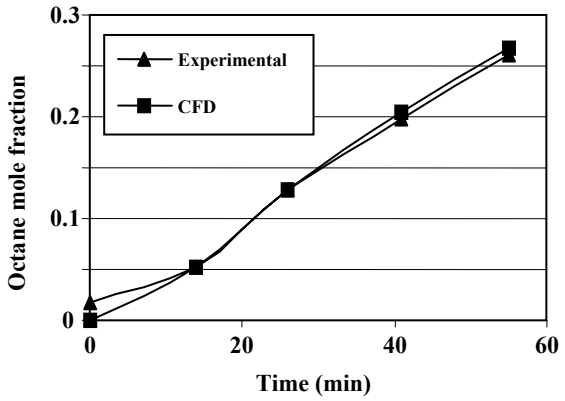


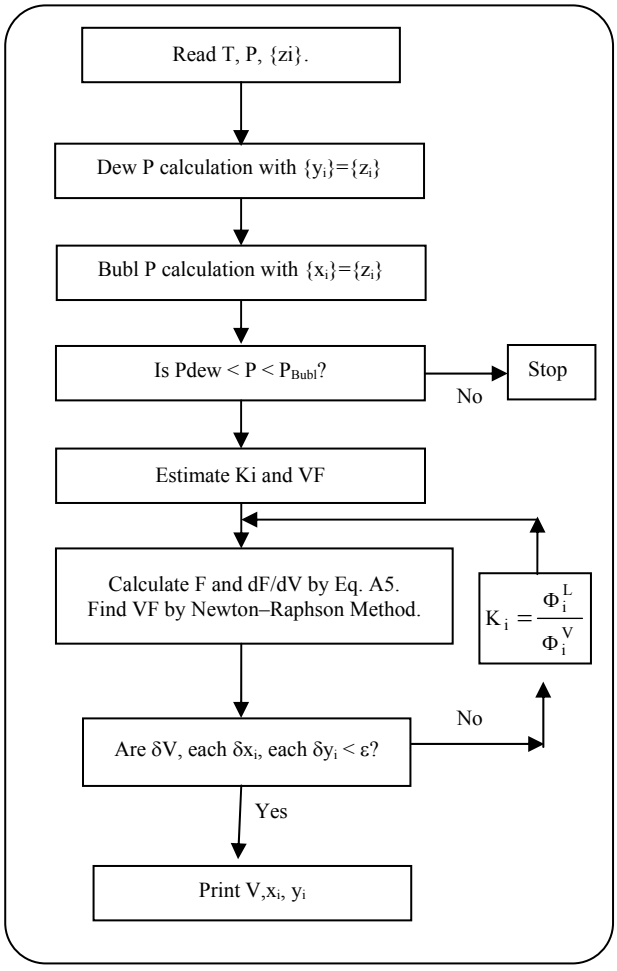
Fig. 16: Comparison of experimental and simulation.

$$C_{Total}^g = \sum_{j=1}^{n} C_j^g \quad \text{A6}$$

$$C_{ig}^* = y_i \times C_{Total}^g \quad \text{A7}$$

Nomenclature

C_{iq}	Gas species concentration
C_{il}	Liquid species concentration
C_i^*	Equilibrium m constant
C_{Total}	Total concentration on of gas phase
D_i	Diffusion coefficient t
f	Fugasity
K_i	Equilibrium m Constant
M_i	Species molecular weight
N_i^q	Flux of species transfer
P	Pressure
$\vec{v}$	Velocity vector
S_{pq}	Rate of mass transfer between p and q phases
ρ_q	Phase density



ϕ_I	Fugacity coefficient t
μ_q	Viscosity of phase q
μ	Viscosity of mixture of phases
α_q	Volume fraction of each phase
Z	Compressibility factor
x_i	liquid phase mole fraction
y_i	Gas phase mole fraction
z_i	Total mole fraction
T	System temperature
P	System pressure
VF	Equilibrium m gas volume fraction

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