



Development of Numerical Eulerian-Eulerian Model for Computational Analysis of Potential in Chemical Process Intensification from Trickle Bed Reactors

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Abstract

The computational fluid dynamics techniques keep a paramount role by evaluating a reactor performance. The transitory performance of a Trickle bed reactor is readily monitored from its three phase's flow conditions. This research review study corresponds towards the formation of boundaries in this Trickle bed reactors system to designate its comprehensive methodology with an optimized solution. The main paramount significance of computational fluid dynamics techniques is to observe the validity and an effective significance of the experimental result. The catalyst bed is modelled with the help of dynamic and steady state models by introducing mass and energy conservation equations. The Eulerian-Eulerian multiphase modelling technique is designed for hydro-desulfurization (HDS) and hydro-dearomatization (HDA) chemical process change from interactive momentum models. The effect in bed porosity on the HDS reaction process is observed from interactive mass transfer with solid bed condition in Trickle bed reactor. The congregated results from computational fluid dynamics codes show that wetting efficiency increases with increase in both hydrogen sulphide concentration and HDS conversion. The conversion of HDS reaction decreases with increase in hydrogen disulphide (H₂S) concentration at both partially wetted and wetted bed conditions. On the other hand, there is small decrease in HDS conversion from 72% to 63.75% at H₂S volumetric concentration of 0 to 8%. These observations also indicate that computational fluid dynamics provides random accessibility of liquid flow in Trickle bed reactor. These results also reveal that there is periodic variation in saturated liquid phase. The regions which are close to its wall are less irrigated. These characteristics can be changed and have effect on the reactor performance. Hence, the present review study presents the unprecedented results with high accuracy.

Keywords: Dynamics modelling, Eulerian-Eulerian model, Chemical process intensification and Wire mesh sensing technique

Introduction

The Trickle bed reactor is classified as a bed with fixed catalyst material. The catalyst bed is interconnected with downward flow of gas and liquid phases. They have a paramount role for gas-liquid-solid reactions towards an industrial application. These reactors are widely used in petroleum industry for hydro-

treating, hydro-demetalization and hydrocracking chemical processes [1-2]. The computational fluid dynamics codes demonstrate an effective approach by reducing and developing the experimental effort for industrial sector. The mathematical simulation on Trickle bed reactor governs a paramount

understanding of chemical reactions dynamics and its yield with improved results. These simulation models need experiments to get validated. The computational fluid dynamics mathematical models give developed techniques which are useful by regarding selectivity and yield of chemical processes [3-5].

The hydrodynamics study on Trickle bed reactor is governed from Eulerian–Eulerian mathematical modelling tool. In this technique, a simplified model is being used on porous media by reducing the computational budget. Different models are investigated by demonstrating the porosity effects on its hydrodynamics parameters. The chemical reactions network is interconnected with reactor hydrodynamics. It corresponds to give better conversion of hydro-desulfurization (HDS) and hydro-dearomatization (HDA) chemical processes at constant temperature. Firstly, new chemical kinetics constants are being evaluated for reaction dependency in computational fluid dynamics study. The effects of hydrodynamics parameter on reaction constants are being studied with (Liquid and Gas velocities, Temperature, Pressure and Reactants concentrations) [6-7].

The chemical reaction kinetic effects on process selectivity are being investigated with comparison of actual and experimental results. The chemical conversion in reactant phase solely depends on reactor intrinsic properties by including temperature, pressure and reactants concentration. The simulation codes seem effective by developing new innovative techniques to obtain high process yield. The computational fluid dynamics codes are employed on catalyst bed in the Trickle bed reactors to improve the chemical process intensification. These computational fluid dynamics codes use the functions by including (Forced convection, Phases dispersion, Interactive Diffusion, Adsorptions

and Reaction kinetics) which are occurred in the Trickle bed reactor [8-9].

Literature Review

Turbulent Modelling

The turbulent modelling is a mathematical model which is mainly dependent on Reynold Average Navier Stokes equation (RANS) and Large Eddy simulation methods. It is used to detect the turbulence effects. As, there are occurred this flow in our daily life such as air flow, cardiovascular flow and Jet and rockets flow [10]. On the other side, the major disadvantage of turbulent modelling is that there is not existing proper analytical theory to quantify it with precision [11].

Methodology

The computational fluid dynamic code such as Eulerian-Eulerian numerical method enables to compute and optimize the chemical process intensification (Yield, Selectivity) of hydrogenation process. The hydrogenation process has an application to produce cooking oil which has prime importance in daily life. In Trickle bed reactor, there is executed hydrogenation process. Hence, it is vitally important to understand the mechanism to acquire upgraded results. The Eulerian-Eulerian numerical method is based on the differential equation which is described as follows;

$$Y_n = Y_{n-1} + hF(X_{n-1}, Y_{n-1}) \text{ Equation 1.}$$

The Ansys-Fluent Software is used to optimize the process dynamics in Trickle bed reactors. It is selected because of its key facets including inexpensive, high precision, safe and low time consuming. Hence, the Eulerian-

Eulerian model in Ansys-Fluent is being selected for its characteristics regarding the optimization of phases dynamics in Trickle bed reactor. The phases dynamics can upgrade the chemical process intensification (yield, selectivity) in Trickle bed reactor [12, 13].

Dynamic Modelling

Silva did the research work on dynamic simulation with laplace transform technique in Trickle bed reactor. In this work, the major focus was to develop innovative model to elaborate the transient behavior in Trickle bed reactor. The dynamic simulation analysis is carried out in all three (Gas-Liquid-Solid) phases. The developed numerical simulation model is interconnected with (Gas residence time, Solid dispersion, Gas-Liquid-Solid mass transfer, Solid particle diffusion, Partial wetting and Reaction kinetics). This correlated model gives results on (Isothermal region, Gas distribution in plug flow region, Liquid phase in dispersion, Wetting on fixed bed, Adsorption equilibrium and Gas concentration). These parameters are studied from (Mass, Energy, Laplace transformation) equations. The basic mass transfer equation describes the dynamic behavior of three (Gas-Liquid-Solid) phases in Trickle bed reactors. Thus, an effective study on transient behavior in Trickle bed reactor has evolved from simulating solid bed [14-16].

Eulerian-eulerian Numerical Simulation

Mousazadeh et al., (2012) research work is based on the heat transfer in Trickle bed reactor by using Eulerian-Eulerian numerical model. The Eulerian-Eulerian numerical model is used to solve problems in fluid dynamics. There is maintained constant wall temperature in this reactor. This multiphase

model uses the (Mass, Energy and Volume of fraction) equations for each phase in Trickle bed reactor. The volume fraction is a function of time. There is achieved coupling from pressure and phases interaction through drag force and heat transfer [12-13].

Liquid Mal Flow Distribution in Trickle Bed Reactor

Bazmi et al., (2012) did the research work on liquid phase flow distribution in Trickle bed reactor. The two fluid model is utilized from Euler-Euler numerical model. The porosity is studied from interphase momentum transfer. The results were validated from the experimental data. The liquid and gas as feed enter in reactor though the same direction. The developed model proves to be an accurate one by comparing with experimental results [17].

The above simulation results in Fig. 1. are obtained by simulating the liquid distribution in Trickle bed reactor. The flow behaviour of liquid phase is being simulated with different gas and liquid velocities. There are two kind of liquid distributor on the bottom of reactor. The obtained results show the liquid volume fraction on different radius and their collector at bottom. There is a flow of liquid on the bed via Ergun's constant as shown in Fig. 1A. It is being demonstrated from Fig. 1B that there is not even distribution of liquid in Trickle bed reactor. The inter-phase momentum transfer could distribute the liquid evenly on the bed surface. The Fig. 2 shows the simulation and experiments results data at variable liquid phase flow rate. It is being showed that uniform distribution is attained by increasing the liquid phase flow rate [18, 19].

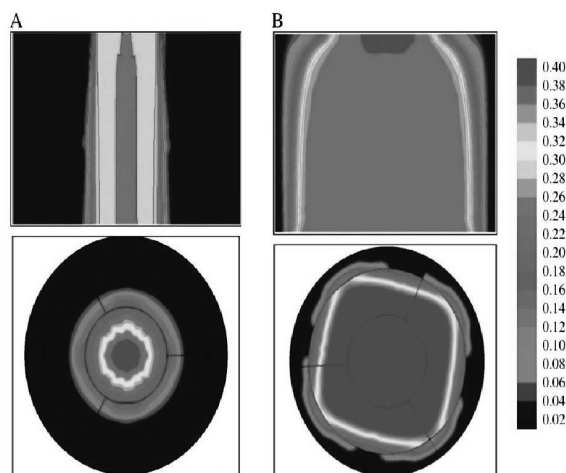


Figure 1. Contour of liquid phase distribution in upper section of the bed (A), A radial view on collector of orifice distributor (B) [17].

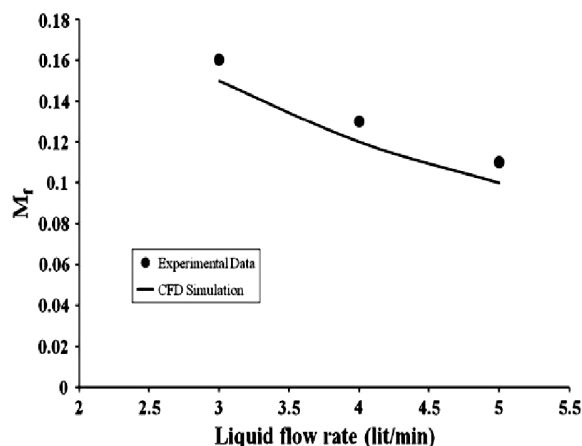


Figure 2. Comparison of experiments results and computational fluid dynamics result with liquid flow rates from orifice distributor [17]

Process Intensification Operability in Trickle Bed Reactor

Heidari and Hashemabadi did the research work to develop an optimum model for HDS and HDA of diesel oil in trickle bed reactor. The computation fluid dynamic model is being utilized to evaluate the optimum process intensification in Trickle bed reactor. The same Eulerian-Eulerian model is used for momentum and mass transfer to demonstrate the reactor performance. The mathematical simulation is being carried out on different parameters by including (Temperature,

Pressure and Liquid and Gas velocities). The HDA and HDS conversion was studied with rate of the reactions. They were dependent on both partially and fully wetted conditions. These reactions take place in Trickle bed reactor, shown in Fig. 3. In Trickle bed reactor; there is (Inert particles and Reactive zone) with definite dimensions. The major investigation was to study HDA conversion with reactor operational pressure and its pressure drop throughout the solid bed. The HDA reaction rate was also investigated from parameters by including (Bed porosity, Phases velocity and Hydrogen mass transfer) [20].

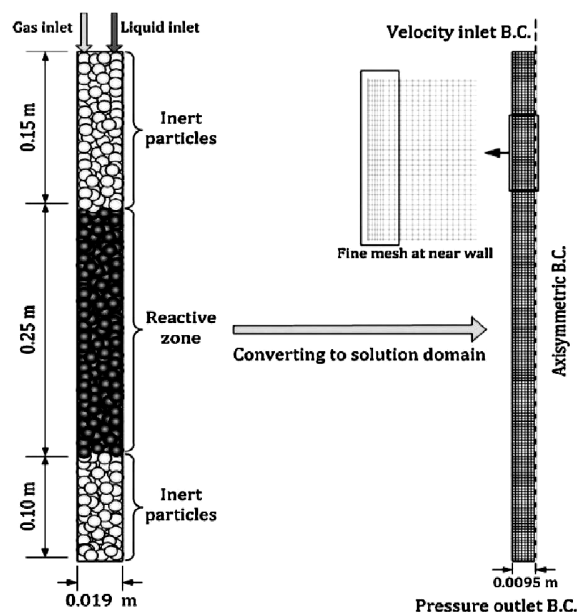


Figure 3. Modelled Trickle bed reactor with dimensions [20]

Figure 4 shows the HDA and HDS reactions rate at partially wetted and fully wetted bed conditions. The line trend demonstrates that there is achieved maximum rate of reaction on reactive region. The Fig. 4A shows that there is a peak at HDS reaction rate in the inner reactive area. This type of trend is not observed in HAD reaction. In Fig. 4bB, the increase in rate of HDS reaction is due to the fact that consumption of hydrogen occurs in liquid phase. After it, the peak damps.

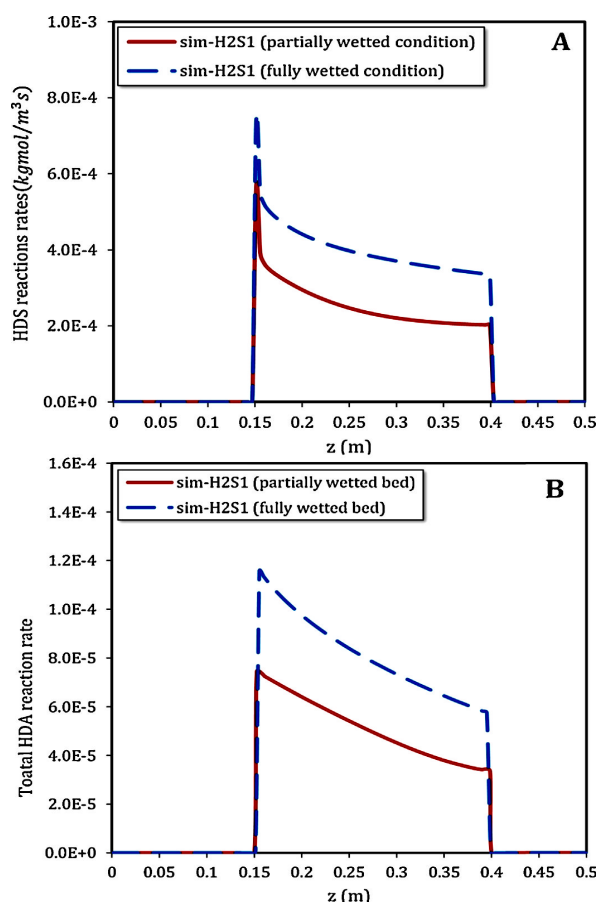


Figure 4. Illustration on variation in velocity of gas and liquid phase in radial direction [20]

In Fig. 5 the simulation in Trickle bed reactor to optimized parameters on HDS and HAD reactions. The HDA conversion was simulated with the factors by including (Bed porosity, Bed wetting, Temperature, Pressure, Liquid and gas velocities).

The simulation results are being obtained with different reaction conversion by regulating porosity factor. In Fig. 5a, it is demonstrated that the reaction conversion and yielded desulfurized products is influenced from velocity near the reactor wall. Thus, total conversion is strongly affected from high velocity near the reactor wall. The low residence time is shown in Fig. 5b which is due to the high velocity effect. The reaction conversion is also low due to small residence time.

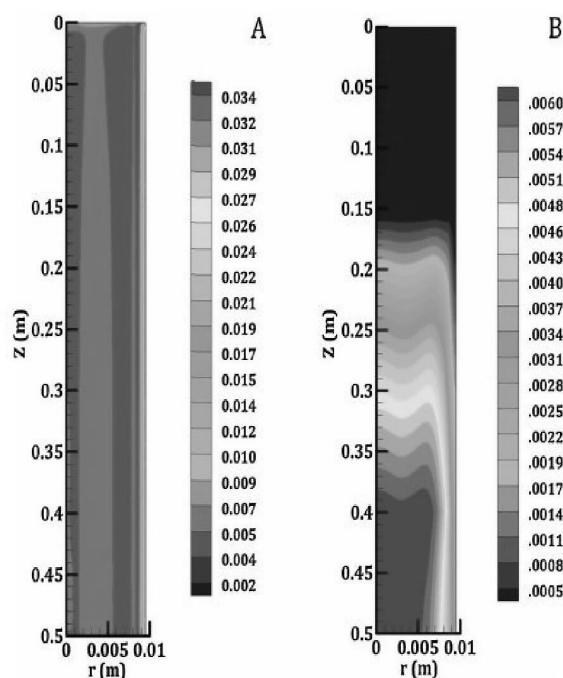


Figure 5. Illustration on gas velocity distribution (m/s) (A) and distribution of mass fraction for desulfurized elements (B) [20]

The Fig. 6A illustrates the interphase momentum of hydrogen. It is inferred from it that there is high amount of mass transfer on inlet region which has no hydrogen in liquid feed. It is being demonstrated that mass transfer rate decreases as reaction proceeds. The mass transfer increases between the liquid and gas phases till the fluid comes to inert zone (Bottom of reactor). The liquid velocity directly effects the process yield. The comparison on average hydrogen interphase mass transfer with Liquid hourly space velocity (LHSV) with partially wetted and fully wetted bed with different values as shown in Fig. 6B. The increase in Liquid hourly space velocity causes increase in interphase mass transfer. The hydrogen concentration becomes lower due to high rate of reaction at fully wetted bed condition. While at partially wetted bed condition, the hydrogen concentration in liquid phase is more. Consequently, the hydrogen mass transfer increases on the conditions which are far from fully wetted bed condition.

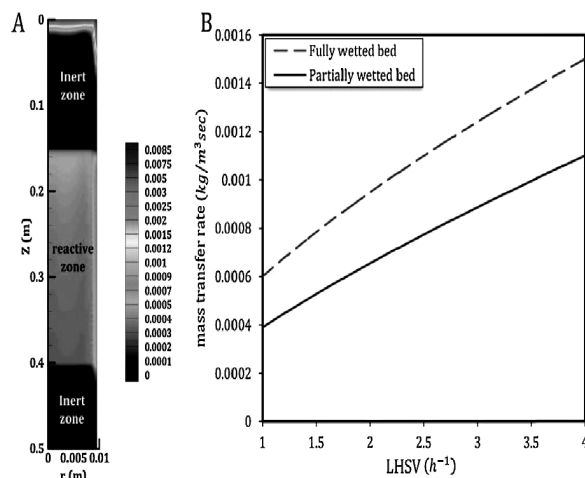


Figure 6. Illustration on distribution of hydrogen interphase with its mass transfer rate ($\text{kg/m}^3\cdot\text{s}$) (A), Effect of liquid hourly space velocity (LHSV) on hydrogen interphase mass transfer rate (B) [20]

The Fig. 7 shows the HAD conversion from as a comparison between experiments and simulation work. In computational fluid dynamics work, the HAD conversion is studied at partial wetted and wetted conditions. There is an observation that the decrease in conversion of HAD comes up to 7 and 2.7 % at partially wetted and fully wetted bed conditions simultaneously. On the other side, the experiment result shows that at minimum Liquid Hourly Space Velocity (LHSV) value of 1, the conversion of HAD goes on 30%.

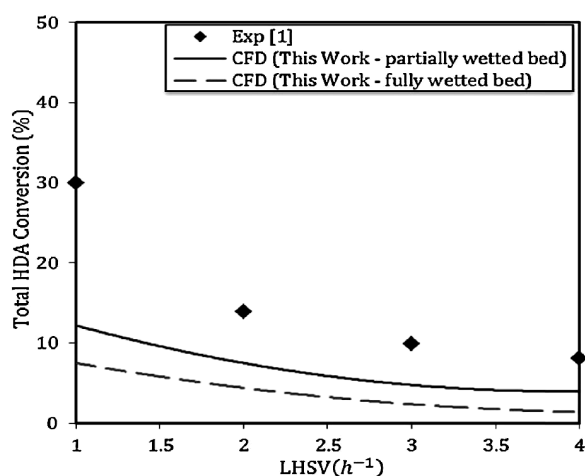


Figure 7. Illustration on liquid hourly space velocity with total HDA reactions [20]

In Fig. 8, there is high deviation between computational fluid dynamics and experimental results at both partially wetted and fully wetted bed conditions. There is an observation that wetting efficiency increases with increase in both hydrogen sulphide concentration and HDS conversion. The conversion of HDS reaction decrease with increase in H_2S concentration at both partially wetted and wetted bed conditions. On the other hand, there is small decrease in HDS conversion from 72 to 63.75% in H_2S volumetric concentration of 0 to 8% [21, 22].

Simulation on Temperature Effect on Chemical Process Intensification in Trickle Bed Reactor

Tohidani et al., (2015) did the research work on hydrogenation of 1,3-butadiene (BD) into n-butane 9 (BA) in Trickle bed reactor. In this research work, a detailed kinetic structure is being developed from reactions. The mathematical modelling is carried out to evaluate the plant output. The effect of temperature on the reactor is studied through mathematical modelling significantly [23].

Fig. 9 shows the molar flow rate variation with increase in its temperature. There is increase in temperature from 322 K to 340 K of the feeding stream with the reactor length. There is attained high inlet temperature of about 340K. At this temperature, BD is consumed readily to 150 % by passing the liquid distributor. The 38% reaction rate is increased between 322 K and base temperature of 332 K. It accounts for decrease in reactor length.

Fig. 10 demonstrates the BA production by increasing the its flow rate on solid bed. The specific yield of BA can be obtained by providing high temperature with a reduction in reactor length. The result shows that with increase in temperature up to 3.7%,

there cause decrease in 36 % of catalyst bed height. There is temperature increase up-to 3.7 % which is suitable for reduction in reactor length.

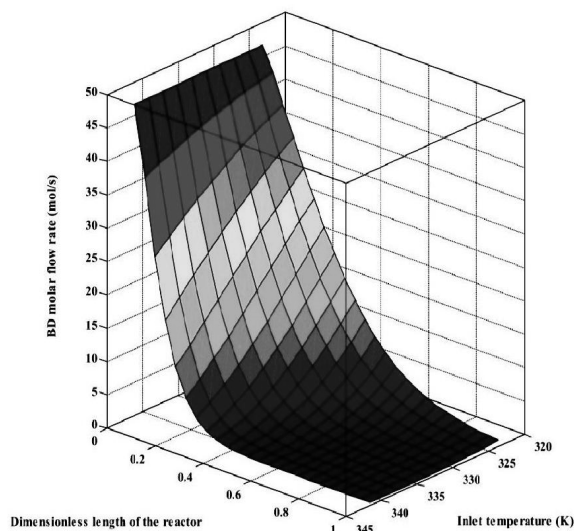


Figure 9. Illustration on effect of the inlet temperature on the Butadiene molar flow rate with length of the reactor [23]

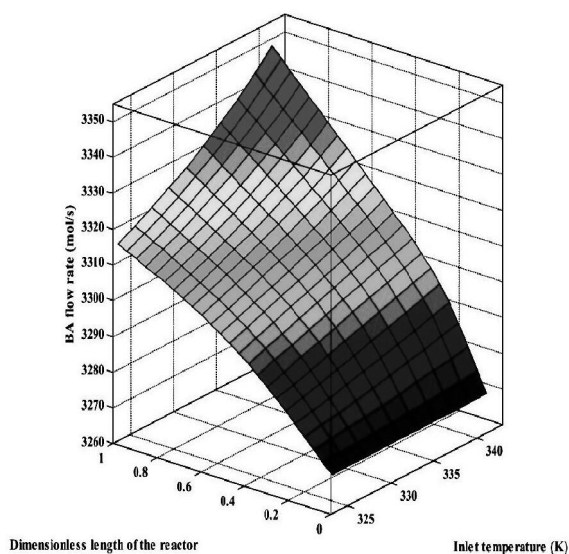


Figure 10. Illustration on effect of the inlet temperature on butane molar flow rate along the length of the reactor [23]

The Fig. 11 shows the effect on temperature and molar flow rate on the BA yield. The maximum yield of BA is obtained to about 32% at inlet flow rate 3500 mol/s and inlet temperature of 320 K. It is due to the fact

that at lower liquid molar flow rate, the reactants have high residence time for conversion and BA yield becomes maximum [24-27].

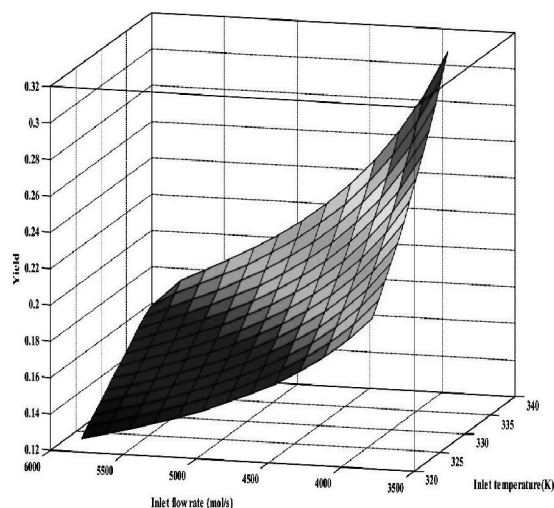


Figure 11. Illustration on effect of butane yield with the inlet temperature and the feed mass flow rate [23]

Simulation of Periodic Hydrodynamic in Trickle Bed Reactor

Schubert et al., research work elaborates the periodic hydrodynamics in Trickle bed reactor. The mesh sensor is used in present research study to measure periodic hydrodynamics. It is being characterized from liquid saturation over reactor length. This technique gives direct access towards liquid pulse break and its cycle's positions. It is measured from four different positions in axial direction. This measurement also results to analyse pulse attenuation and its velocity [28].

The hydrodynamics in Trickle bed reactor is measured from high speed wire mesh sensor and distributed capacitance. The sensors are used to detect the liquid saturation on local area with different positions. The simulation is being run on four different positions in the axial direction of reactor. The wire sensor consists of stainless steel wire of 0.2 mm diameter. The sensor sampling area is

of 0.36 cm^2 . The small area in wire mesh sensor is affected from its wires. The sensing points in sensor have same spatial coordinates, shown in Fig. 12. On the other side, it does not have any effect on hydrodynamic parameter such as liquid holdup. It is due to the fact that porosity height does not account for re-route the liquid flow. The disturbance on the solid bed is being reduced by filling particles in bed free space (Voidage) which is between sensing points and sensor wires. The normalized permittivity distribution is being obtained from wire mesh sensors and electrical tomography demonstrated in Fig. 12. It is measured from capacitance in the reactor region. This shows the hydrodynamics properties of reactor by measuring instantaneous liquid distribution.

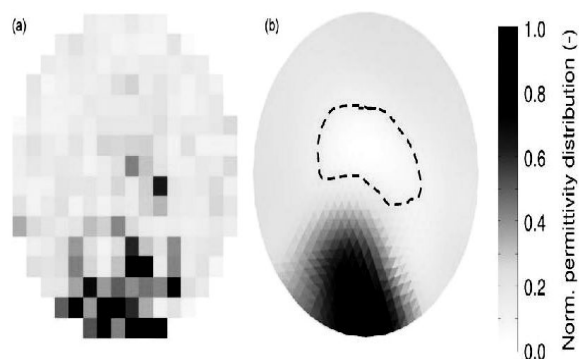


Figure 12. Illustration on permittivity distribution of wire-mesh sensor (A), Electrical capacitance tomography (B) [28]

The flow pattern in liquid phase is being studied by varying time position cycles. The liquid saturation area with its position is demonstrated in time step of 30 s. The flow pattern is obtained with different liquid feeding rate $S=0.7S_3$, $S=0.7S_1$, $S=0.3S_3$ and $S=0.3S_1$ of the time cycles. The flow pattern on liquid distribution is shown in Fig. 13. It demonstrates the random accessibility of liquid flow in Trickle bed reactor. There is an observation that there is periodic variation in saturated liquid phase. The regions which are close to its wall are less irrigated. These characteristics can be change and have effect

on the reactor performance. The accessibility of channels depends in operating conditions on the solid bed area [29-32].

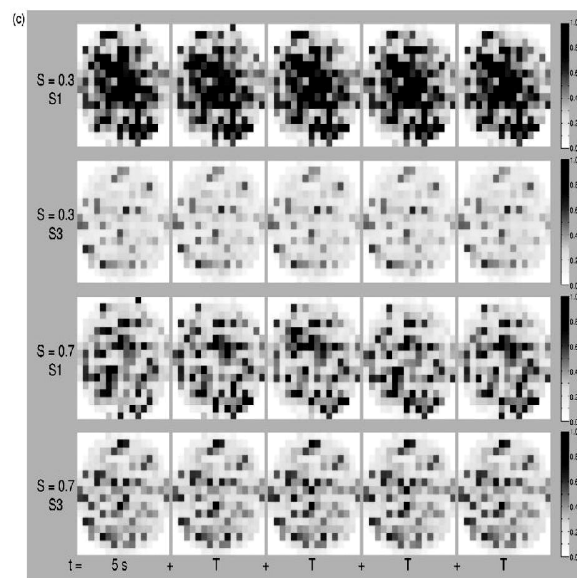


Figure 13. Illustration on liquid distribution (A), Illustration on liquid saturation distribution cross sectional area with different sensors position (B) [28]

Conclusion

The recognized results on transient behavior in Trickle bed reactor are being attained through dynamic and Eulerian-Eulerian mathematical simulation. They are based on intrinsic conditions to simulate problems on fluids dynamic in Trickle bed reactor. Henceforth, they provide the overview on behavior of all three phases with respect to different parameters in reactor.

The chemical process intensification and liquid mal flow studies elaborate the yield of the process and liquid phase distribution by regulating the intrinsic parameters in Trickle bed reactor. The simulation results are well briefed on the reactants conversion by comparing with experimental ones.

The computational fluid dynamics simulation shows the effect of temperature on

the conversion of reactant with its molar flow rate over the reactor length. It demonstrates the novel overview on Trickle bed reactor dynamics and its product yield.

The periodic hydrodynamic demonstrates the liquid saturation over the reactor. It includes the detection of liquid pulse breakage on different positions. Through this novel technique, the liquid flux detection with the most accurate results is being attained.

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