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Numerical Simulation on Micromixing of Non-Newtonian Fluids in a Stirred-Tank Reactor by Using Parallel Reactions

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ABSTRACT

Micromixing of Non-newtonian fluid in a stirred-tank reactor with Rushton turbine is investigated numerically by using E model. It is characterized by the product selectivity of parallel competitive reactions. Model is implemented and is validated using experimental data in the literature. The simulations show that a higher agitation speed, and a feeding location closer to the discharge area of the impeller favor micromixing and the reaction rate. These results provide useful guidelines for the scale-up of industrial reactors of non-Newtonian fluid with parallel chemical reactions, and the comparison between the experimental and numerical results confirms the accuracy of the simulations.

KEY WORDS: *Mixing; Non-Newtonian fluids; E model*

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1. INTRODUCTION:

Today's consumer society requires more, better quality and innovative products from a wide variety of industries, such as the production of plastics and synthetic resins, man-made fibers, polymers, paints and varnishes, drugs and pharmaceuticals, agricultural chemicals, food and drinks. All of these industries have one point in common: the raw materials are converted into final products by means of chemical reactions in an environment that involves fluid flow. mixing plays very important role in achieving the desired products and reducing unwanted by-products, which is very important from environmental and economic points of view. If mixing to a certain degree lets more materials react to form the wanted products, and reduces the amount of by-products, as a result there will be less amounts of waste to be treated and disposed to the environment. On the other hand, increasing the mixing speed or the fluid viscosity, increases the power needed to rotate the mixer, which would be more expensive and energy related to pollution will be caused. The use of non-Newtonian fluids is very frequent in many industrial operations, particularly in mixing processes. Such fluids often have complex rheological properties, which can increase operating costs and can create other problems during the mixing process. The viscosity, as one of the most important property of the fluid, has a great significance in processes, in which the rheological properties of the fluid are changing with time. Due to a close relation of the viscosity to torque on the impeller in the mixing vessel[1]. To achieve the desired degree of mixing with high efficiency and less by-products more research has to be carried out and that also will be beneficial for the environment. Much modelling as well as experimental work has been done to understand mixing and especially for micro-mixing [2, 3, 4, 5, 6]. The hydrodynamics of non-Newtonian flows at broad range Reynolds number generated by an axial impeller (A310) in a single-phase using CFD modeling and PIV measurement to validate results. The authors demonstrate that the flow field below the impeller is highly dependent on the rheological behaviour of the fluid [8]. Similar impact assessment studies of hydrodynamic conditions on mixing process [9,10], concerning the stability of Pickering emulsion (oil-water mixture with hydrophilic glass beads) in the baffled tank with Rushton turbine (RT) or pitched blade turbine (PBT). The authors found that the energy dissipated and the size of the high shear zone around the impeller are key information to create the emulsion with the desired droplet sizes. The heat transfer data for agitated Newtonian and non-Newtonian fluids related to Nusselt number depends on impeller diameter in the agitated vessel [11]. The authors, by using experimental data, correlated viscosity with of Reynold, Prandtl number and Nusselt Number, which were evaluated at the impeller tip. But still not enough to understand the mixing process of non-Newtonian. More studies will to be able to give better picture and understanding of mixing. Since mixing is connected to the environment through industry and it is a global concern to protect the environment; this work is concerned with mixing, especially micro-mixing of Non-Newtonian fluid in a stirred tank reactor with Rushton turbine which is investigated numerically by using E model and compared with experimental data in the literature[7].

2. Engulfment models

Mass balance for reaction zone:

$$\frac{d(Vc_i)}{dt} = EV < c_i > + Vr_i ,$$

$$\frac{d(Vc_i)}{dt} = V\frac{d(Vc_i)}{dt} + c_i\frac{dV}{dt}$$

$$\frac{dc_i}{dt} = E(\le c_i \ge -c_i) + r_i$$

For irreversible, second order parallel reactions

$$A + B \xrightarrow{K_1} P \quad (2.1)$$

$$A + C \xrightarrow{K_2} Q \quad (2.2)$$

A is the limiting reagent. The integral product distribution with respect to Q may be generally defined as.

$$X_Q = \frac{mole\ of\ Q\ yielded}{mole\ of\ A\ reacted} \quad (2.3)$$

The states of mixing influence the product distributions in different ways for different sequences of adding reagents.

2.1. Addition of A to premixed B and C:

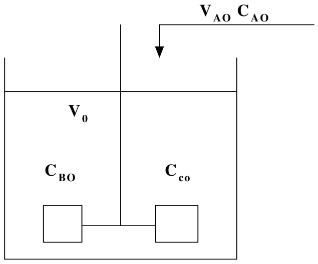

Fig.2.1 Addition of A to premixed B and C

When mixing is perfect, no molecular-scale concentration gradients (or segregation) exist; the product distribution is determined by chemical kinetics. When segregation is complete, the product distribution does not depend on the kinetics, but on the relative frequency with which A comes in to contact with B and C, i.e., on the ratio of initial concentrations of C and B. Suppose that reaction (2.1) is instantaneous and the B and C is initially equimolar. X_Q is written as

$$X_Q = \frac{V_0 C_{C0} - (V_0 + AM\, V_{A0}) C_C}{V_{A0} C_{A0}} \quad (2.4)$$

When partial segregation exists, product distribution may be analyzed in terms of the E model of micromixing. When self-engulfment is negligible, according to E model, the mass balances of substances A, B, and C give

$$\frac{dc_A}{d\alpha} = E(< c_A > - c_A) - k_1 c_A c_B - k_2 c_A c_C \quad (2.5)$$

$$\frac{dc_B}{d\alpha} = E(< c_B > - c_B) - k_1 c_A c_B \quad (2.6)$$

$$\frac{dc_C}{d\alpha} = E(< c_C > - c_C) - k_2 c_A c_C \quad (2.7)$$

if the first reaction can be treated as instantaneous A and B cannot coexist at a given point and a new composition variable u may be introduced:

$$u = c_A - c_B \quad (2.8)$$

It follows that. $C_A = \frac{|u| + u}{2}$ (2.9)

$$C_B = \frac{|u| - u}{2} \quad (2.10)$$

Eqs (2.5) and (2.6) then simplify to a single equation

$$\frac{du}{d\alpha} = E(< u > - u) - k_2 c_C \frac{|u| + u}{2} \quad (2.11)$$

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Whilst Eq (2.7) becomes

$$\frac{dc_C}{d\alpha} = E(c_C > -c_C) - k_2 c_C \frac{|u|+u}{2} \quad (2.12)$$

Dimensionless variables for the solution of Eqs (2.11) and (2.12) may be introduced

using C_{A0} as reference concentration:

$$C_i = c_i / c_{A0} \quad U = u / c_{A0} \quad (2.13)$$

$$T = \alpha E_{av} \, (2.14)$$

Eqs (2.11) and (2.12) written in dimensionless form become

$$\frac{dU}{dT} = \sqrt{\Phi}(<U> - U) - D_a \frac{|U|+U}{2} Cc \quad (2.15)$$

$$\frac{dC_C}{dT} = \sqrt{\Phi}(<C_C> - C_C) - D_a \frac{|U|+U}{2} Cc \, (2.16)$$

$$Da = \frac{k_2 c_{A0}}{E_{av}} \quad (2.17)$$

$$E_{av} = 0.058\sqrt{\frac{\varepsilon_{av}}{\upsilon}} \quad (2.18)$$

$$\varepsilon_{av} = \frac{Npd^5 N^3}{\nu} \quad (2.19)$$

$$\Phi = \varepsilon / \varepsilon_{av} \quad (2.20)$$

Where the ϕ is the specific local energy dissipation rate. Da is the ratio of characteristic times for micromixing by engulfment and chemical reaction. This dimensionless number can also be written in terms of the concentration which the reagent A would have if it had all been added to the reactor and well mixed before reacting. Average Damkohler number Da_{av} can then be used instead of Da:

$$\overline{Da} = \frac{k_2 c_{A0}}{(1+a) AM \, E_{av}} \quad (2.21)$$

$$a = \frac{V_0 (1-f)}{AM \, V_{A0}} \quad (2.22)$$

The initial conditions for the reaction zone and the surroundings are given by Eqs (2.23) and (2.24) respectively.

$$U(0) = 1 \quad C_C(0) = 0 \quad (2.23)$$

$$<U> = -c_{B0} / c_{A0} = -1/a \qquad <C_C> = c_{C0} / c_{A0} = 1/a$$

(2.24)

$X_Q = 1 - (a+1) AM \, C_C$ (2.25) The mass balance to update the concentration in the surroundings is

$$\text{therefore.} <C_{i.j}> = \frac{\left[a\sigma + j - \exp(\theta \Phi^{0.5}) / AM\right] <C_{i.j-1}> + C_{i.j}(\theta) \exp(\theta \Phi^{0.5}) / AM}{a\sigma + j} \quad (2.26)$$

Where j = 0 corresponds to the known concentrations in Eq. (2.24).

In the present work, we made some modification to this model to suitable for the calculation of Non-Newtonian fluid. I.e. before they did not consider side reaction when they chose the precipitation reaction as one of the two parallel competing reactions. This is probably because in their case, the limited concentrated sodium hydroxide was fed rapidly into the vessel. The fast injection may reduce the chance of the formation of $[Cu_2(OH)_2]SO_4$. It should be pointed out that in the rapid feed case, it is macro- and meso-mixing rather than the micromixing that determines the distribution of product of complex reactions. But in our case, the limited concentrated sodium hydroxide was fed very slowly in to the vessel. That means, slow injection give the chance for the formation of $[Cu_2(OH)_2]SO_4$, and micromixing is the controlling regime. For that, we added $(1-f)$ to equation (2.22), where f is the factor of copper ion loss due to side reactions.

According to the literature the following assumptions are made for the formation of a flow field generated by a Rushton turbine in a stirred tank. Mean flow is characterized by plug circulation flow along one streamline. The tank can be divided in to 6 characteristic flow regions, that is, region 1: impeller swept volume; region 2: radial flow in turbine discharge; region 3: axial flow along the wall; region 4: radial flow near top or bottom; region 5: axial flow along the shaft and region 6: flow in the center. These regions are shown in fig (2.2).

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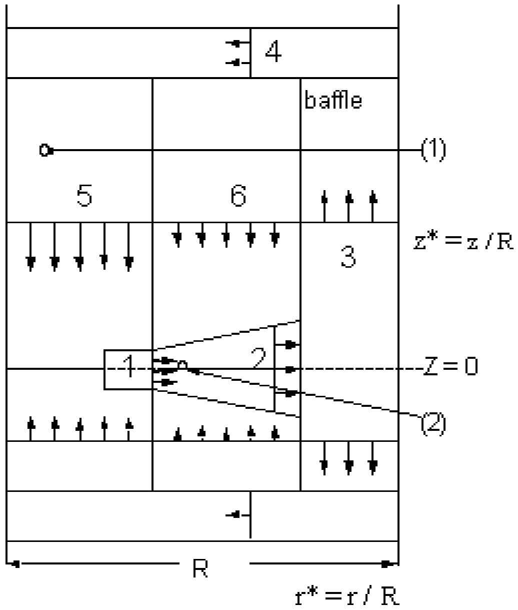

Fig 2.2 Schematic diagram of flow field

Table 2.1 ϕ correlations for each region [12].

Region	ϕ correlations
1	$\phi_1 = 33.8$
2	$\phi_2 = 178.6\ r^* - 55$ for $1/3 < r^* < 0.46$ $\phi_2 = 268.7 \exp(-4.98\ r^*)$ for $0.46 < r^* < 0.8$
3	$\phi_3 = 1.7 \exp(-2.5\ z^*)$ for upper loop $\phi_3 = 1.7 \exp(-6.1\ z^*)$ for lower loop
4	$\phi_4 = 0.02 + 0.08\ r^*$
5	$\phi_5 = 2.23 - 1.95\ z^*$ for upper loop $\phi_5 = 2.45 - 5.21\ z^*$ for lower loop
6	$\phi_6 = 0.08$

In the present work.

$r^* = r/R$ for the feed position (2) $r^* = 0.4075$ that means the feed position at region 2 in this case $\phi_2 = 178.6\ r^* - 55 = 178.6 * 0.4075 - 55 = 17.78$

But the feed position (1) at the region 5 in this case $\phi_5 = 2.23 - 1.95\ z^*$

$z^* = z / R = 0.912$ for position (1), that means $\phi_5 = 2.23 - 1.95 * 0.912 = 0.45$

In this work we use different impeller diameter for that we suppose ϕ at the feed position (1) is 0.4 and 20 at feed position (2) approximately.

3. Results and discussion

The Engulfment model were used to calculate X_Q, and the results compared with experiment [7],were pictured in Fig 3.1~3.3.

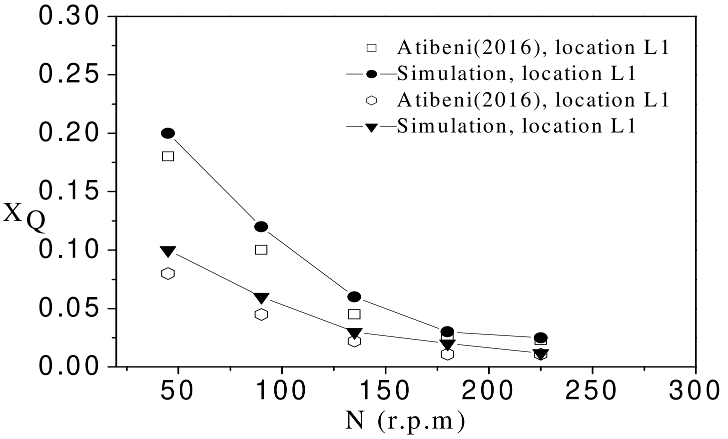

Fig (3.1) X_Q vs. N Exp and Cal for 0% HEC and two feed position

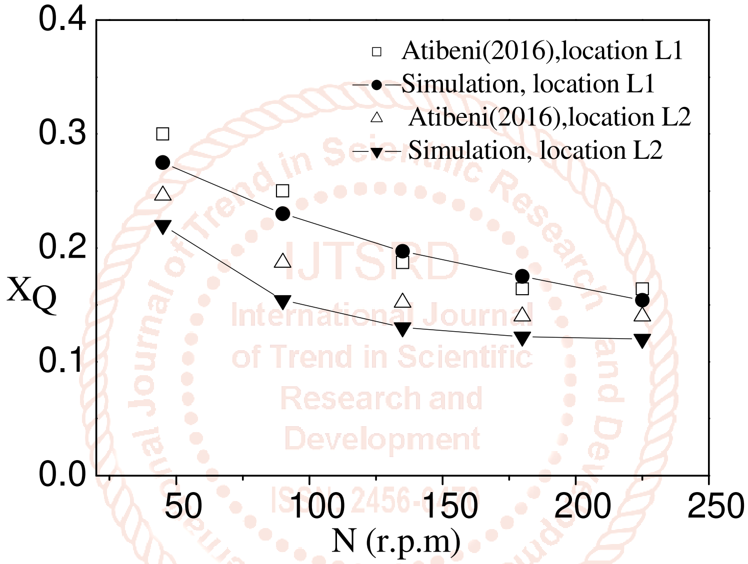

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Fig (3.2) X_Q vs. N Exp and Cal for 0.1% HEC and two feed position

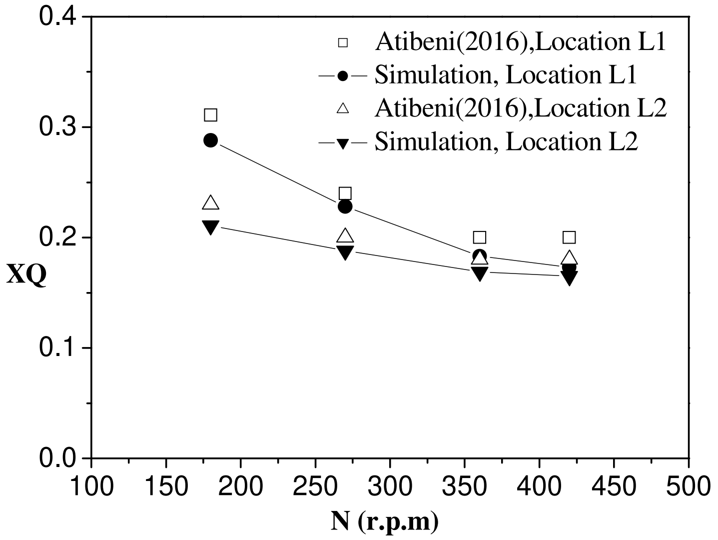

Fig (3.3) XQ vs. N Exp and Cal for 0.5% HEC and two feed position

The data obtained when the NaOH solution was added just below the free surface of the liquid and in the impeller discharge flow. Higher selectivity when the feed located at the surface. This can be explained by the widely varying energy dissipation rates throughout a stirred tank reactor with the local energy dissipation rates near the liquid surface much smaller than the impeller discharge. This leads to the segregation between reactants being greater offering a larger chance for the side reaction to occur. Thus, for each speed, X_Q decreases in going from position (1) to position (2), i.e. from position of low to high local energy dissipation rates, position (2) in the impeller discharge, This feed position has very good micromixing. Figure (1,2,3) shows that X_Q different for different feed position. And the same observation for different HEC concentration. also shows that the comparison between experimental results and E model is good especially the trend of the curve is very well for all HEC concentrations also the relation between the by-product and the speed for different feed position and different viscosity is very well for experimental results and also E model.

4. CONCLUSION

The effects of impeller speed, feed position and viscosity on the yields of by-product (X_Q) were investigated. The experiments results show that X_Q as a measure of the amount of by product was strongly depends on the viscosity of the liquid. X_Q increases greatly as the viscosity of HEC increases, and decreases with increasing impeller speed. As we may expect, feeding at the impeller region has a lower X_Q than feeding at the liquid surface due to the difference of local energy dissipation. the engulfment model (E-model) was modified to suit the working reactions in this work. The product distributions predicted by modified E-model were in reasonable agreement with the experimental data. The results are of importance to the design and scale-up of industry stirred reactors with fast complex reactions.

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