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Abu Bakr Salem[a]
[a] CHEMICAL ENGINEERING DEPARTMENT, QATAR UNIVERSITY, DOHA, QATAR

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Modeling Phase Inversion in a Mixer-Settler

ABU BAKR SALEM

CHEMICAL ENGINEERING DEPARTMENT
QATAR UNIVERSITY
DOHA, QATAR

Abstract

A mathematical model has been developed to simulate the phase inversion criteria from which the area of a mixer-settler unit can be obtained. The general slip velocity correlation used for continuous differential contactors design has been used for the stagewise units. However, a new functional relationship between the slip velocity and the ratio of the fractional holdups of both phases has been found to fit the stagewise cases. Some published data have been used to check the validity of the model, and excellent agreement has been realized.

INTRODUCTION

Although mixer-settlers are widely used in many liquid-liquid extraction applications for their high capacity and efficiency, many areas in the design of mixers and settlers have not yet been thoroughly investigated.

The Kremser-Brown equation is usually used to estimate the number of units required for a certain extraction duty. However, the size of the unit suitable for certain flow rates is still debatable.

Design of continuous contact column extractors is usually based on the flooding criteria. A similar phenomenon which can take place in most contactors is phase inversion. Trials have been made to make use of this criterion in designing mixer-settlers (*5*), but probably without appreciable success.

The objective of this work was to analyze the phase inversion phenomenon to determine the limiting capacity of a mixer-settler unit.

PHASE INVERSION

The properties of an oil-in-water emulsion are different from those of a water-in-oil emulsion of the same chemical composition. Dickinson (*3*) stated that in over 70 years of colloid literature there have been many rules of thumb for predicting what type of emulsion or micro-emulsion will result from agitating equal volumes of oil and water in the presence of an emulsifying agent or a solute.

In a stirred tank, agitation breaks up one of the phases into droplets suspended in the continuum of the other. The droplet liquid phase is known as the dispersed phase and the other is the continuous one.

Clarke and Sawistowski (*2*) noted that if more dispersed phase is added to a fixed volume of continuous phase, a significant increase in interfacial area occurs. However, a point is eventually reached at which the addition of more dispersed phase causes inversion to take place. The continuous phase suddenly becomes dispersed and the previously dispersed one becomes continuous.

Phase inversion is therefore the transition from one phase dispersed to the other. Such an inversion demonstrates clearly the existence of a hysteresis effect. This effect defines a metastable area called the ambivalence range and shown in Fig. 1. This range has not been

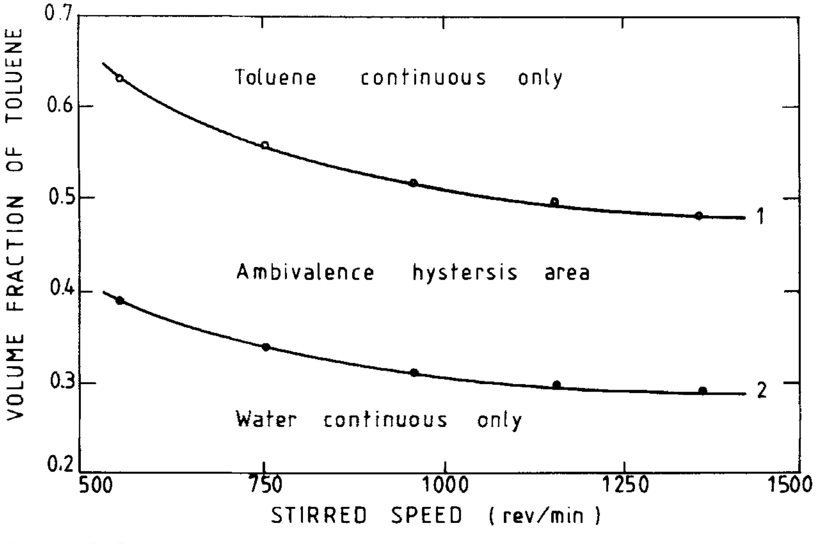

FIG. 1. Inversion characteristics for the toluene-water system. 1: Inversion from o/w to w/o. 2: Inversion from w/o to o/w (*7*).

thoroughly investigated. McClarey and Mansoori (*7*) wrote that the factors established to be effective on the ambivalence range are temperature, density difference, and viscosity difference between the mixed phases. Clarke and Sawistowski (*2*) indicated that the width of the hysteresis gap was critically affected by the interfacial tension; the lower the interfacial tension, the wider was the hystersis gap, i.e., the greater was the resistance of the system to inversion. The presence of solute in phase equilibrium lowers the interfacial tension of the system and thus widens the gap.

On the other hand, inversion is accompanied by a corresponding increase in the mean drop diameter of the dispersion and hence decreases the interfacial area and the mass transfer rate.

Dickinson (*3*) postulated that there exists a relationship between the mixture thermodynamics and the phase volume at which inversion occurs.

However, phase inversion produces a different configuration of the phases which might lead to a different effective viscosity and also to a change in the total energy content of the system.

Hossain et al. (*5*), in investigating the hydrodynamics of a mixer-settler, found that inversion of phases in the mixer affects the geometry of the wedge in the settler.

Inversion of phases is accompanied either by a decrease or by an increase in wedge length and hence affects the effective length of the settler. However, the dimensions of the wedge similarly depend on the coalescence rate and the continuous phase viscosity. On the other hand, phase stability ensures minimum entrainment. Mutual phase entrainment occurs when the dispersion wedge extends across the entire length of the settler. This usually happens in industrial settlers, which seldom operate under steady-state conditions.

Sarker et al. (*10*) pointed out the importance of phase inversion in defining the limiting volumetric capacity of agitated vessels.

MODELING OF PHASE INVERSION

The area of a continuous contact extractor can be obtained using the slip velocity V_s concept, which is the relative velocity of the two liquids and for countercurrent flow (*8*):

$$\frac{V_d}{X} + \frac{V_c}{(1 - X)} = V_s A \tag{1}$$

$$V_s = V_0(1 - X) \tag{2}$$

For very dilute dispersion, i.e., for dispersed phase holdups, $X \rightarrow 0$ and $V_s \rightarrow V_0$, which is the velocity of a single droplet relative to the continuous phase. This is termed the droplet characteristic velocity. On the other hand, as the fractional holdup increases, the relative velocity decreases due to interactions between the droplets.

Equation (*1*) relates the holdup to the flow rates of the phases V_d and V_c and to the contactor diameter through the characteristic velocity V_0. This equation therefore affords a method of calculating the holdup X for a given set of flow rates if V_0 is known. Moreover, this equation can be used to estimate the diameter of a contactor for certain flow rates. Treybal (*13*) and Perry and Chilton (*8*) stated that Eq. (1) was found to be valid up to the flood point for spray, rotary annular and rotary disk columns, and also for conventional pulsed columns. Buoyatiotis and Thornton (*1*) used the same relationship to describe cocurrent flow in a stirred tank but used a negative sign as follows:

$$\frac{V_d}{X} - \frac{V_c}{(1-X)} = V_s A \tag{3}$$

They found that the slip velocity V_s was approximately proportional to the square of the drop size, and that drop size was proportional to holdup. They also correlated the characteristic velocity to the power input per unit volume:

$$V_0 = \frac{K(P_v)^{-0.62}}{(1-X)} \tag{4}$$

Longsdail et al. (*6*) related the slip velocity to the holdup by

$$V_s = KX^n \tag{5}$$

where K is a constant that accounts for the physical properties of the liquids and agitator speed.

Hossain et al. (*5*) used the following modified relationship to represent the multistage countercurrent extractor, assuming $n = 2$, for the system they were investigating,

$$\frac{V_d}{X} + \frac{V_c}{1-X} = K_1 A X^2 \tag{6}$$

However, they found large differences between the model predictions and their experimental values of holdup at phase inversion for the kerosene–water and toluene–water systems studied, as shown in Fig. 2.

However, since the emperical relation (1) has proved to be valid for different types of extractors, it may be assumed to be generally accepted for all types of extractors including mixer-settlers. It seems that the only problem is to find out a suitable relationship between the slip velocity and the dispersed phase holdup for each type of contactor. Therefore, Eq. (1) can be generally written for countercurrent or cocurrent contactors as

$$\frac{V_d}{X} \pm \frac{V_c}{1-X} = V_0 A f(X) \tag{7}$$

The problem is to try to find out the functional relationship $f(X)$ which can fit each type of contactor.

Perry and Chilton (*8*) wrote that there is an ill-defined upper limit to the volume fraction which may be maintained in an agitated dispersion. Quinn and Sigloh (*9*) correlated this maximum holdup to the agitation speed and system physical properties and geometry. Thus inversion of a dispersion may occur when the maximum value of the holdup is reached

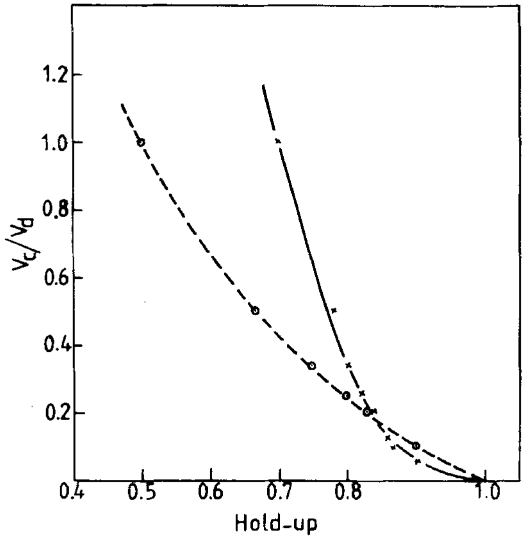

FIG. 2. Phase ratio vs hold-up value. Systems: kerosene—water and toluene—water. (O) Experimental values. (X) Theoretical values (*5*).

due to an increase in the agitator speed or to the flow rate of one of the phases with respect to the other. This might well justifies the assumption that as V_d is increased at constant V_c, X is a continuous function of V_d such that V_d passes through a maximum in the algebraic sense. This maximum value occurs at the point of inversion.

Since X reaches a maximum value at phase inversion and the inversion state represents a stationery point, then the inversion holdup may be obtained in a way similar to that of the limiting flooding condition in extraction towers. Thus, by setting

$$dV_d/dx = 0 \tag{8}$$

the value of V_c at the inversion holdup can be obtained as follows. From Eq. (7):

$$V_d = \pm V_c\left[\frac{X}{(1-X)}\right] + V_0 AXf(X) \tag{9}$$

Therefore, from Eqs. (8) and (9):

$$V_c = \pm V_0 A(1-X)^2[Xf^1(X) + f(X)] \tag{10}$$

Similarly, by arranging Eq. (7) to get

$$V_c = \pm V_d\left(\frac{1-X}{X}\right) + V_0 A(1-X)f(X) \tag{11}$$

and setting

$$dV_c/dX = 0 \tag{12}$$

the value of V_d at the inversion point can be obtained as follows:

$$\frac{dV_c}{dX} = 0 = \pm\frac{V_d}{X^2} + V_0 A[(1-X)f^1(X) - f(X)]$$

$$V_d = \pm V_0 AX^2[(1-X)f^1(X) - f(X)] \tag{13}$$

Dividing Eq. (10) by Eq. (13) gives the phase ratio at the inversion point for both counter and cocurrent flow:

$$R = \left(\frac{1-X}{X}\right)^2 \left[\frac{Xf^1(X) + f(X)}{f(X) - (1-X)f^1(X)}\right] \tag{14}$$

By setting

$$f^1(X)/f(X) = Z \tag{15}$$

then

$$R = \left(\frac{1-X}{X}\right)^2 \left[\frac{1+ZX}{1-Z(1-X)}\right] \tag{16}$$

Rearrangement of Eq. (16) gives

$$R = \left(\frac{1-X}{X}\right)\left[\left(\frac{1}{X} + Z\right)\Big/\left(\frac{1}{1-X} - Z\right)\right] \tag{17}$$

Equation (17) shows that the phase ratio at the inversion point is largely dependent upon the ratio between the fractional holdups of these phases, no matter what the form of the functional relationship $f(X)$ is.

This functional relationship for a mixer-settler can be explored using the data published by Hossain et al. (*5*). Figure 3 represents a plot of the experimental values of R vs the parameter $(1 - X)/X$ on log-log paper. A straight line with a slope of 1 and an intercept at 1 is obtained.

This suggests that the second term of Eq. (17) is

$$\frac{\dfrac{1}{X} + Z}{\dfrac{1}{1-X} - Z} = 1 \tag{18}$$

Therefore, for this mixer-settler data,

$$Z = \frac{2X - 1}{2X(1-X)} \tag{19}$$

Generally, according to the previous analysis, the phase ratio at the inversion point in a mixer-settler contactor can be written as

$$R = a\left(\frac{1-X}{X}\right)^b \tag{20}$$

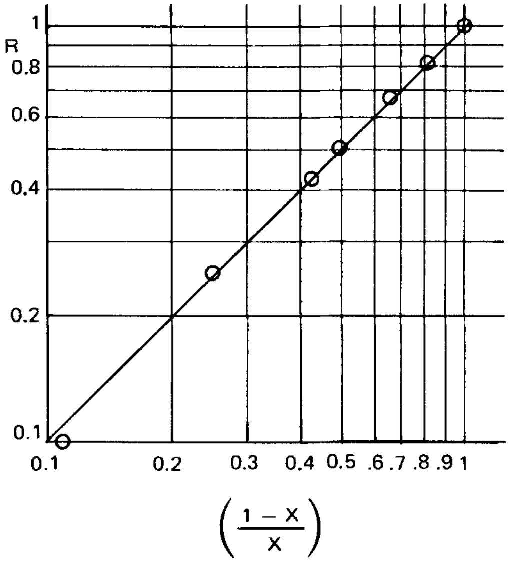

FIG. 3. Phase ratio vs $(1 - X)/X$.

where a and b are constants that depend on the system's properties and contactor design. However, fitting this model to the published data gave values of $a = 1$ and $b = 1$, so this may justify assuming that

$$f(X) = \left(\frac{1 - X}{X}\right)^{-C} \tag{21}$$

where C is a constant that depends on the system and the contactor.

$$f^1(X) = \frac{C}{X^2} f(X) \left(\frac{1 - X}{X}\right)^{-1} \tag{22}$$

$$Z = \frac{C}{X^2} \left(\frac{1 - X}{X}\right)^{-1} \tag{23}$$

Then Eq. (16) becomes

$$R = \left(\frac{1 - X}{X}\right)\left[-\frac{(1 - X) + C}{X - C}\right] \tag{24}$$

This equation suggests that C should be positive. It should take values lower than the dispersed phase holdup at the inversion point for any system.

However, Selkers and Sleicher (*11*) introduced a useful correlation for predicting which phase is dispersed. Their correlation has been approximated by Hooper and Jacobs (*4*) in the following form:

$$\frac{V_L}{V_H}\left(\frac{\rho_L \mu_H}{\rho_H \mu_L}\right)^{0.3} = \theta \tag{25}$$

If θ is less than 0.3, then the light phase will always be dispersed. The heavy phase will be the dispersed one if θ exceeds 3.3. Phase inversion is most probable when θ lies between 0.5 and 2.

Assuming in general that the light phase is the dispersed phase, then rearranging Eq. (25) allows calculation of the phase ratio at the ambivalance range where inversion can take place:

$$R = \frac{V_c}{V_d} = \left(\frac{\rho_c}{\rho_d}\frac{\mu_d}{\mu_c}\right)^{0.3}\frac{1}{\theta} \tag{26}$$

where $\theta = 0.5\text{–}2$.

Having determined R from Eq. (26), the value of X at the inversion points can be determined from Eq. (24). By assuming a value for V_c, V_d can be determined and then the area of the contactor can be estimated from Eq. (1), presumably after determination of the characteristic velocity V_0. Once the area of a unit is determined, the mixer and the settler sizes can be determined by the normal methods. The mixer may be taken as representing 20–25% of the total area of the unit according to the degree of agitation.

CONCLUSION

Phase inversion, although not completely similar to flooding phenomena, generally follows the same concepts. The mathematical analysis is sound in respect of flooding, and extensive experimental work has been done to validate such an analysis. The analysis introduced in this work has lead to a semitheoretical model based on the slip velocity concept and can be used for sizing stagewise contactors as well as continuous contactors. An available set of data has been used to test the model, and the agreement between them is excellent. However, the model has to be tested more rigorously with the quantitative results from a number of systems. Unfortunately, data in this area are very scarce. It is hoped that the analysis introduced in this work will open the door for research workers to investigate this important field and furnish experimental data which might well support the hypothesis considered.

SYMBOLS

A	cross-sectional area of the contactor (m^2)
a	constant
b	constant
c	constant
d	droplet diameter (m)
g	acceleration due to gravity = 9.80 m/s^2
K	constant
K_1	constant
K_2	constant
K_3	constant
K_4	constant
P_v	power per unit volume
R	phase ratio = V_c/V_d
V_c	continuous phase flow rate (m^3/min)
V_d	dispersed phase flow rate (m^3/min)
V_H, V_L	heavy and light phase flow rate (m^3/min)
V_0	droplet characteristic velocity (m/min)
V_s	slip velocity of dispersed phase relative to the continuous phase (m/min)
X	dispersed phase holup, volume fraction
Z	$f^1(X)/f(X)$
ρ	density (kg/m^3)
μ	viscosity (cP)
θ	parameter defined by Eq. (23)

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