

MATHEMATICAL MODELLING OF MASS TRANSFER  
IN MULTI-STAGE ROTATING DISC CONTACTOR COLUMN

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To  
my beloved husband, Zainidi and  
my loving daughters, Nur Ezzaty and Nur Amira

and

especially my loving  
and supportive parents, Hj. Maan and Hj. Eashah

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## ABSTRACT

In this study, the development of an improved forward and inverse models for the mass transfer process in the Rotating Disc Contactor (RDC) column were carried out. The existing mass transfer model with constant boundary condition does not accurately represent the mass transfer process. Thus, a time-varying boundary condition was formulated and consequently the *new fractional approach to equilibrium* was derived. This derivation initiated the formulation of the modified quadratic driving force, called *Time-dependent Quadratic Driving Force (TQDF)*. Based on this formulation, a Mass Transfer of A Single Drop (MTASD) Algorithm was designed, followed by a more realistic Mass Transfer of Multiple Drops (MTMD) Algorithm which was later refined to become another algorithm named the Mass Transfer Steady State (MTSS) Algorithm. The improved forward models, consisting of a system of multivariate equations, successfully calculate the amount of mass transfer from the continuous phase to the dispersed phase and was validated by the simulation results. The multivariate system is further simplified as the Multiple Input Multiple Output (MIMO) system of a functional from a space of functions to a plane. This system serves as the basis for the inverse models of the mass transfer process in which fuzzy approach was used in solving the problems. In particular, two dimensional fuzzy number concept and the pyramidal membership functions were adopted along with the use of a triangular plane as the induced output parameter. A series of algorithms in solving the inverse problem were then developed corresponding to the forward models. This eventually brought the study to the implementation of the Inverse Single Drop Multi-stage (ISDMS)-2D Fuzzy Algorithm on the Mass Transfer of Multiple Drops in Multi-stage System. This new modelling approach gives useful information and provides a faster tool for decision-makers in determining the optimal input parameter for mass transfer in the RDC column.

## ABSTRAK

Dalam kajian ini, pembentukan model ke depan yang lebih baik dan model songsangan bagi proses peralihan jisim di dalam Turus Pengekstrakan Cakera Berputar (RDC) telah dijalankan. Model yang sedia ada dengan syarat sempadan tetap tidak mewakili proses peralihan jisim dengan tepat. Dengan itu, syarat sempadan yang merupakan suatu fungsi masa berubah telah dirumuskan dan seterusnya *pendekatan pecahan untuk keseimbangan* yang baru diterbitkan. Penerbitan ini telah memulakan perumusan daya pacu kuadratik ubahsuai, yang dipanggil *daya pacu kuadratik bersandaran masa (TQDF)*. Berdasarkan perumusan ini, satu Algoritma Peralihan Jisim untuk Sebutir Titisan (MTASD) telah direkabentuk, diikuti oleh satu algoritma yang lebih realistik algoritma Peralihan Jisim untuk Multi Titisan (MTMD) yang mana kemudiannya, telah diperbaiki dan dinamakan Algoritma Peralihan Jisim Berkeadaan Mantap (MTSS). Model ke depan yang telah diperbaiki, terdiri daripada satu sistem persamaan berbilang pembolehubah yang mana kemudiannya dipermudahkan sebagai sistem berbilang input berbilang output (MIMO) yang merupakan satu rangkap dari satu ruang fungsi-fungsi kepada satu satah. Sistem ini merupakan satu asas pembentukan model songsangan bagi proses peralihan jisim dan pendekatan kabur telah digunakan untuk menyelesaikannya. Secara khususnya, konsep nombor kabur dua matra dan fungsi keahlian piramid digunakan, diikuti dengan penggunaan satu satah segitiga sebagai parameter output teraruh. Satu siri algoritma dalam menyelesaikan masalah songsangan ini kemudiannya telah dibentuk berpadanan dengan model ke depan masing-masing. Kajian ini akhirnya membawa kepada implementasi Algoritma Songsangan Sebutir Titisan Multi-tingkat (ISDMS)-2D Kabur ke atas sistem peralihan jisim Multi Butiran dalam Multi-tingkat. Untuk rumusan yang lebih definitif, pedekatan baru pemodelan ini memberi maklumat yang berguna dan menyediakan suatu alat yang cepat kepada pembuat-keputusan dalam menentukan parameter optimum input untuk peralihan jisim dalam turus RDC.

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## LIST OF SYMBOLS/NOTATIONS

$a$	-	radius of a sphere
$A$	-	Column cross sectional area ( $m^2$ )
$C$	-	Concentration ( $kg/m^3$ )
$d$	-	Drop diameter ( $m$ )
$d_c$	-	Column diameter ( $m$ )
$d_{cr}$	-	Critical drop diameter for breakage ( $m$ )
$d_{max}$	-	Maximum stable drop diameter ( $m$ )
$d_o$	-	Initial drop diameter ( $m$ )
$d_{32}$	-	Sauter mean drop size ( $m$ )
$d_{av}$	-	Average diameter of drop ( $m$ )
$D_c$	-	Molecular diffusivity in continuous phase ( $m^2/s$ )
$D_d$	-	Molecular diffusivity in dispersed phase ( $m^2/s$ )
$D_e$	-	Eddy diffusivity ( $m^2/s$ )
$D_{oe}$	-	Overall effective diffusivity ( $m^2/s$ )
$D_r$	-	Rotor diameter ( $m$ )
$D_s$	-	Stator diameter ( $m$ )
$e$	-	Back-flow ratio
$E$	-	Power consumption per unit mass (Eq. (2.9)) ( $w/kg$ )
$E_{am}$	-	Axial mixing coefficient ( $m^2/s$ )
$E_c$	-	Continuous phase axial mixing coefficient ( $m^2/s$ )
$E_o$	-	Eotvos number
$F_d$	-	Flowrate of dispersed ( $cm^3/s$ )
$fr$	-	Fraction of daughter drop
$g$	-	Acceleration due to gravity ( $m^2/s$ )
$g_i$	-	Dynamic volume fraction of drops with size $d_i$
$h$	-	Height of column ( $m$ )
$h_c$	-	Height of an element of compartment ( $m$ )
$H$	-	Column height ( $m$ )
$k_d$	-	Drop film mass transfer coefficient ( $m/s$ )
$K_{od_i}$	-	Overall dispersed phase based mass transfer coefficient for drop with size $d_i$ ( $m/s$ )
$m$	-	Exponent in the equation of slip velocity
$M$	-	Morton number in terminal velocity
$N_r$	-	Rotor speed ( $s^{-1}$ )
$N_{cr}$	-	Critical rotor speed for drop breakage ( $s_{-1}$ )
$N_{cl}$	-	Number of classes

$N_{st}$	-	Number of stages
$P$	-	Probability of breakage
$P_R$	-	Power consumption per disc ( $w/m^3$ )
$Re$	-	Drop Reynolds number
$Re_k$	-	Drop Reynolds number using $V_k$
$Re_{D,\omega}$	-	Disc Reynolds number based on angular velocity
$Sc$	-	Schmidt number
$Sh$	-	Sherwood number
$t_{r,i}$	-	Resident time of drops with size $d_i$ in a stage (s)
$V$	-	Drop volume ( $m^3$ )
$V_c$	-	Continuous phase superficial velocity ( $m/s$ )
$V_d$	-	Dispersed phase superficial velocity ( $m/s$ )
$V_k$	-	Drop characteristic velocity ( $m/s$ )
$V_s$	-	Slip velocity ( $m/s$ )
$V_t$	-	Drop terminal velocity ( $m/s$ )
$We$	-	Weber number for drop
$We_{D,\omega}$	-	Disc angular Weber number
$x_m$	-	Mean number of daughter drops
$X$	-	Hold-up

#### Greek symbols

$\Phi$	-	Equilibrium curve slope ( $dC_d/dC_c$ )
$\gamma$	-	Interfacial tension (N/m)
$\beta_n$	-	Eigenvalues
$\mu_c, \mu_d$	-	Continuous and dispersed phase viscosities ( $mPas$ )
$\rho_c, \rho_d$	-	Continuous and dispersed phase densities ( $kg/m^3$ )
$\Delta\rho$	-	densities differences ( $kg/m^3$ )
$\kappa$	-	Viscosity ratio
$\omega$	-	Angular velocity ( $s^{-1}$ )
$\omega_{cr}$	-	Critical angular velocity ( $s^{-1}$ )

#### Superscripts

*	-	dimensional variables
'	-	differentiation with respect to $\bar{\eta}$
$s$	-	denotes steady part of the solution
$u$	-	denotes unsteady part of the solution

#### Subscripts

$c, d$	-	Continuous and dispersed phase
$i$	-	drop size classes
$n$	-	Stage number
$av$	-	average value

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## CHAPTER 1

### INTRODUCTION

#### 1.1 Preface

The study of liquid-liquid extraction has become a very important subject to be discussed not just amongst chemical engineers but mathematicians as well. This type of extraction is one of the important separation technology in the process industries and is widely used in the chemical, biochemical and environmental fields. The principle of liquid-liquid extraction process is the separation of components from a homogeneous solution by using another solution which is known as a solvent [1, 2]. Normally, it is used when separation by distillation is ineffective or very difficult. This is due to the fact that certain liquids cannot withstand the high temperature of distillation.

There are many types of equipments used for the processes of liquid-liquid extraction. The concern of this research is only with the column extractor type, namely the Rotating Disc Contactor Column (RDC). Modelling the extraction processes involved in the RDC column is the major interest in this work. Modelling can be divided into two categories. One is the forward modelling and the other is the inverse modelling.

From mathematical and physical point of view, it is generally easier to calculate the “effect of a cause” or the outputs of the process than to estimate the “cause of an effect” or the input of the process. In other words, we usually know how to use mathematical and physical reasoning to describe what would be measured if conditions were well posed. This type of calculation is called a forward problem. The resulting

mathematical expressions can be used as a model and we call the process in obtaining the values of outputs as forward modelling.

On the other hand, inverse problems are problems where the causes for a desired or an observed effect are to be determined. Inverse problem come paired with direct problems and of course the choice of which problem is called direct and which is called inverse is, strictly speaking, arbitrary [3]. Before an inverse problem can be solved, we first need to know how to solve the forward problem. Then the appropriate steps or algorithms need to be determined in order to get the solution of the inverse model.

Apart from producing an improved mathematical model for the mass transfer process, another concern of this research is to develop the inverse models that can determine the value of the input parameters for a desired value of the output parameters of the mass transfer process in the multi-stage RDC column.

## 1.2 Motivation

Several models have been developed for the modelling of RDC columns. The modelling shows that the drop size distribution and the mass transfer processes are important factors for the column performances. Since the behavior of the drop breakage and the mass transfer process involve complex interactions between relevant parameters, the need to get as close as possible to the reality of the processes is evident.

Several researchers namely Korchinsky and Azimzadih[4], Talib[5], Ghalehchian[6] and Arshad[7] had been working in this area. Korchinsky and Azimzadih[4] introduced a stage wise model for mass transfer process, which was furthered by Talib[5] and Ghalehchian[6]. The unsteady-state models developed by Talib[5] are referred to as the IAMT (Initial Approach of Mass Transfer) and BAMT (Boundary Approach of Mass Transfer). To get closer to reality, Ghalehchian[6] had developed a new steady-state model of mass transfer by including the idea of axial mixing into the simulation of the mass transfer process. Then Arshad[7] developed a new steady state model for hydrodynamic process, which updates the current hold up and drops velocities in every stage after certain time intervals until the system reaches steady state.

The mass transfer models are based on a radial diffusion equation with a constant boundary condition. However a mass transfer model with varied boundary condition has yet to be developed. The development of the model will enhance the understanding of the real process. This is because in reality the concentration of the drops in each compartment in the RDC column is not constant.

The mathematical simulation models of the processes in the RDC column are very complex and need excessive computer time, particularly in predicting the values of output parameters. The determination by trial and error of the input parameter values in order to produce the desired output need excessive computer time and it will be costly if the actual processes are involved. This type of problem is known as inverse problem. Therefore, to overcome these difficulties, an alternative approach based on fuzzy logic is considered.

Fuzzy logic is a well-known method for modelling such uncertain systems of great complexity. They have been approved and demonstrated by many researchers in other disciplines of study to have the capability of modelling a complicated system as well as predicting the actual behavior of a system. So, this study will adopt this method for assessing inverse modelling of the mass transfer process in the RDC column.

A few researchers for examples Ahmad et.al. [8, 9] and Ismail et. al. [10] have been using this approach in their works. Ahmad developed an algorithm which was used in determining the optimized electrical parameters of microstrip lines. The problem was presented as multiple input single output (MISO) system of some algebraic equations. Whilst, the problem involved in Ismail's work is a multiple input multiple output (MIMO) system of a crisp state-space equation. Both works used a one dimensional fuzzy number concept and a triangular membership function.

The forward model of the mass transfer process in the RDC column consists of Initial Boundary Value Problem (IBVP) of diffusion equation, a nonlinear and a few of linear algebraic equations. The details of the equations will be found in Chapter 3 to 6. Thus the multivariate system modelled by these equations can be simplified as MIMO system. In this work, a two dimensional fuzzy number concept will be used. A pyramidal membership function will be also implemented in this work.

### 1.3 Objectives of the Research

1. To investigate an equation that will be used as the boundary condition of the IBVP.
2. To formulate a new fractional approach to equilibrium based on the IBVP of time-dependent boundary condition.
3. To formulate a modified driving force based on the new fractional approach to equilibrium.
4. To develop an algorithm for the mass transfer of a single drop in the multi-stage RDC column.
5. To develop algorithms for the mass transfer of the multiple drops in the multi-stage RDC column.
6. To establish a technique for assessing the inverse models of the corresponding new forward mass transfer models.

### 1.4 Scope of Study

This study will be based on a radial diffusion equation with varied boundary value problem for mass transfer process and a few algebraic equations governed by experiments carried out by a previous researcher for the process of hydrodynamics in the RDC column. The study will also be based on the experimental data obtained by the researchers at the University of Bradford under contract to Separation Processes Service, AEA Technology, Harwell.

In this study, the development of inverse model will be based on the concept of fuzzy algorithm. In this development, the mathematical equations used in mathematical forward modelling are also being considered. This model is a structure based model.

## 1.5 Significance of the Findings

This study achieves a new development of the forward model which will provide a better simulation and hence get a better control system for the RDC column. This study also give a significant contribution in the form of algorithms. These algorithms are able to calculate the optimal solution of the inverse model for the mass transfer process in the RDC column. The inverse model will give a new paradigm to the decision maker or to the engineer in making decision to decide approximate values of input concentrations of continuous and dispersed phases for desired values of output concentrations of continuous and dispersed phases.

## 1.6 Thesis Organization

Chapter 2 gives a literature review on liquid-liquid extraction in general. It is then followed by a review on the RDC columns including the important processes involved. The theoretical details on the drop distribution, breakage phenomena and the mass transfer process are also included. The existing forward mathematical modelling by the most recent researchers are presented. These reviews are significantly used as a background in order to develop a new mass transfer model; which will be described in Chapter 3.

To achieve Objective 6 of the research, the review on the inverse problem in general, including the definition, the examples of real world problems, the classes of the inverse problem and the steps involved in solving the problem are given. Whilst Section 2.8 will provide the reviews on the Fuzzy Concepts. These concepts will be applied in Chapters 5 and 6 to develop an algorithm for solving the corresponding inverse problem.

Chapter 3 provides the formulation of the varied boundary function from the experimental data in [5]. The details of the exact solution of the IBVP with the time depending function boundary condition will be shown which is then followed by the derivation of the new fractional approach to equilibrium. The comparison between the new fractional approach to equilibrium and the one introduced in [11] will be made in the last section of Chapter 3.



Chapter 4 comprises the development of the forward models of the mass transfer in the multi-stage RDC column. Prior to the development, the formulation of the modified quadratic driving force which is called *Time-dependent Quadratic Driving Force (TQDF)* will be given. Based on this formulation, a Mass Transfer of A Single Drop Algorithm is designed and this is then followed by a more realistic Mass Transfer of Multiple Drops Algorithm. An alternative method for calculating the mass transfer of a Multi-Stage System will also be presented in the form of an algorithm named as the Mass Transfer Steady State Algorithm.

Chapter 5 discusses the formulation of the inverse model for mass transfer process in the RDC column. The mappings which represent the forward model involved will also be given. Basically this chapter introduces an *Inverse Single Drop Single Stage-Fuzzy (ISDSS-Fuzzy)* model which represents the mass transfer process of a single drop in a single stage RDC column. This model is a base for the inverse model of the mass transfer process in the real RDC column.

Chapter 6 provides the theoretical details which become the basis for accomplishing the task of the thesis. The details are about the relation of two crisp sets and this is followed by the relation of two fuzzy sets. We also include some examples which can explain the concept more clearly. From fuzzy relation we extend the concept of fuzzy number of dimension one to dimension two. Section 6.4 discusses the development of the Inverse Model of Mass Transfer Process of a Single Drop in a Single Stage RDC Column based on the two dimensional fuzzy number. We then implement the algorithm to the mass transfer process in the multi-stage RDC column.

We then summarize the findings and suggest areas for further research in Chapter 7.

## 1.7 Summary

In this introductory chapter, a short introduction on the liquid-liquid extraction process particularly on the RDC column has been presented. The deficiency of the existing mass transfer models in the multi-stage RDC column has also briefly discussed. Next, come the research objectives and scope, and the contributions of the work

described in the thesis. Finally, the outline of the thesis is presented.

The current chapter serves as a defining point of the thesis. It gives direction and purpose to the research and the discussions presented here are the basis for the work done in the subsequent chapters.

controlled and adjusted such as that of rotor speed ( $N_r$ ), dispersed phase flow rate ( $F_d$ ) and interfacial tension ( $\gamma$ ). Although interfacial tension could not be controlled directly but at least by varying this value will provide us with some useful information. These three parameters are determined or fixed outside the RDC column, but once they are applied to the modelling, it will give whatever calculated value for the holdup. This is an inverse problem of type *coefficient inverse problem*.

- Development of the intra-stage control system for the RDC column.

In this study the inverse problem in determining the value of the input parameter for the desired value of output of 23-stage RDC column has been successfully solved. Intra-stage control system is the control system inside the RDC column. The inverse algorithm developed in this study only need the information of the input and output parameters outside the RDC column. Whilst for the intra-stage control, more information is needed in particular the information on the concentrations of both liquids at certain stage or if possible at every stage in the RDC column.

- Further investigation and development on the theory of two dimensional fuzzy number in multi-stage systems.
- Development of the integrated model of the hydrodynamic and mass transfer processes.

Parallel processing is suggested to be introduced in order to develop the integrated model of the hydrodynamic and mass transfer processes. This integrated model is hoped to give better simulation and better control system for the RDC column.

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