MOLARITY MODEL OF MASS TRANSFER PROCESS FOR EXTRACTION IN ROTATING DISC CONTACTOR COLUMN

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DEDICATION

TO:
Nurul Sabihah Kadir, Mastura Ab Wahid, Siti Noorhani Jehad,
Nor Syaida Ibrahim, Noratiqah Mohd Ariff

Thank you for your encouragements and helps.

TO:
My beloved parent
Abu Hassan bin Ibrahim & Bedah bt Hj Reduan
terbayang ketenangan yang selalu kau pamerkan,
bagaikan tiada keresahan,
walau hatimu sering terluka tika diriku terlanjur kata,
tak pernah sekali kau tinggalkan diriku sendirian,
ketika ku dalam kedukaan,
kau mendakap penuh pengertian,
di saat diriku kehampaan,
kau setia mengajarku erti kekuatan,
terpancar kebanggan dalam senyumu melihat ku berjaya,
bilaku kegagalan tak kau biarkan aku terus kecewa,
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restu dan doa kau iringkan.

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ABSTRACT

In the rotating disc contactor (RDC) column, liquid-liquid extraction process occurs when one of the liquid phase (drops) is dispersed into another liquid phase (continuous phase). The mass transfer process occurs when the drops flows countercurrent to the continuous phase. In this study, a new mass transfer model will be presented. A number of mass transfer models have been developed. These models are Initial Approach of Mass Transfer (IAMT) model, Boundary Approach of Mass Transfer (BAMT) model and Simultaneous Discrete Mass Transfer (S-DMT) model. IAMT model is a model for mass transfer when the drops first enter the column and move upward the column. BAMT model is a model of mass transfer where the drops already exist in the whole column initially. Meanwhile S-DMT model is a modification of the BAMT model where the concentration of drops in S-DMT model is being determined by using number of particle. In this study, the S-DMT model will be modified in order to develop the Molarity Model of Mass Transfer (MM-MT). In MM-MT, the method to determine the concentration of drops and continuous phase is being substitute with molarity. Molarity is a method in chemistry to determine the concentration of a chemical solution. Since the system that involves in this study is cumene/ water/ acid isobutiric, molarity is used to improve the S-DMT model. A program for MM-MT was developed by using software C++ 6.0. After the program was test, the real simulation of mass transfer process that occurs in the RDC column has been run. The simulation took 500 iterations to complete. The results obtained from the MM-MT simulation were being compared with the result obtained from Separation Process System (SPS). The error for concentration of drops and continuous phase has been determined and this error showed whether the MM-MT model is better than the S-DMT model.

ABSTRAK

Dalam turus pengekstrakan cakera berputar (RDC), pengekstrakan cecair-cecair akan berlaku apabila salah satu cecair (titisan) tersebut diserakan ke dalam cecair (fasa selanjar) yang lain. Titisan ini akan bergerak dalam arah yang bertentangan dengan medium tersebut di dalam turus RDC dan ini akan menyebabkan proses peralihan jisim berlaku. Kajian ini akan menunjukkan satu model baru untuk proses peralihan jisim tersebut. Banyak model yang telah dibina untuk proses peralihan jisim ini. Antaranya ialah model pendekatan nilai awal bagi peralihan jisim (IAMT), pendekatan nilai sempadan bagi peralihan jisim (BAMT) dan juga model peralihan jisim dikret serentak (S-DMT). Model IAMT adalah model peralihan jisim apabila titisan mula masuk ke dalam turus RDC dan bergerak ke bahagian atas turus. Model BAMT pula adalah model peralihan jisim di mana titisan telah bertabur di keseluruhan turus RDC tersebut. Model S-DMT adalah hasil daripada penambahbaikan model BAMT di mana kepekatan titisan di dalam turus akan ditentukan dengan menggunakan jumlah bilangan partikel. Dalam kajian ini pula, penambahbaikan akan dilakukan ke atas model S-DMT untuk menghasilkan Model Molariti Peralihan Jisim (MM-MT). Dalam MM-MT, cara untuk menentukan kepekatan bagi titisan dan juga medium adalah dengan menggunakan molariti. Molariti adalah satu kaedah kimia untuk menentukan kepekatan satu larutan kimia. Disebabkan kajian ini menggunakan sistem kumen/ air/ asid isobutirik, molariti boleh digunakan untuk menambahbaikan model S-DMT. Program untuk MM-MT dihasilkan dengan menggunakan perisian C++ 6.0. Selepas program ini dihasilkan, program ini telah diuji dan simulasi sebenar untuk proses peralihan jisim yang berlaku dalam turus RDC ini dijalankan. Simulasi ini telah mengambil 500 iterasi untuk selesai. Keputusan yang diperolehi daripada simulasi MM-MT ini telah dibandingkan dengan keputusan yang diperolehi melalui Sistem Proses Pemisahan (SPS). Ralat bagi kepekatan titisan dan medium dikira dan hasilnya menunjukkan bahawa model MM-MT adalah lebih baik daripada model S-DMT.

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LIST OF SYMBOLS

a	-	Radius of a sphere
C	-	Concentration of a sphere
C_x, C_y	-	Concentration for both X and Y phases
d	-	Diameter of sphere
d_0	-	Initial drop diameter of drop
d_{av}	-	Average diameter of drop
D	-	Molecular diffusivity of dispersed phase
D_R	-	Diameter of rotor disc
D_S	-	Diameter of stator ring
g	-	Gravity
h	-	Height of a stage
i	-	Number of stages
j	-	Number of cells
J_x, J_y	-	Flux or the rate of the mass transfer for both X and Y phases
k_x, k_y	-	Mass transfer coefficient for both X and Yphases
l	-	Radius of the column
m	-	Cell number
n	-	Stage number
$n_{i,j}$	-	Number of drops
N_{Pd}	-	Number of particle of drops
N_{mBal}	-	Balance number of mole for the continuous phase
N_M	-	Number of mole
N_R	-	Rotor speed

r	-	Radius of sphere
t	-	Time of drop to travel along the column
u_{av}	-	Average concentration of sphere
u_i	-	Total concentration of drops
v_c	-	Characteristic velocity of drop
v_t	-	Terminal velocity of drop
V	-	Volume of drops
V_{av}	-	Average volume of drop
V_f	-	Volume fraction
V_m	-	Volume of continuous phase in a stage
x_b, x_i	-	Bulk and interface concentration of X phase
x_{in}, y_{in}	-	Initial concentration of continuous and dispersed phase
X, Y	-	Liquid phases
X_{Bal}	-	Balance concentration of continuous phase
y_b, y_i	-	Bulk and interface concentration of Y phase
z	-	Stator ring number

Greek Symbols

$\Delta\rho$	-	Density difference between the continuous phase and the dispersed phase
γ	-	Interfacial tension
μ_c	-	The viscosity of the continuous phase
ρ_c	-	Continuous phase density
ω_{CR}	-	Critical angular velocity
$\mathcal{E}_Y, \mathcal{E}_X$	-	Relative error for concentration of drops and continuous phase.

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Introductions

Liquid-liquid extraction has become a common subject to be discussed not just among chemical engineers, but mathematicians as well. Liquid-liquid extraction is a process with many applications in pharmaceuticals, petrochemicals processing, industrial chemical production and metals extraction and recovery [1]. This process is a technique to separate two liquids product. The principle of liquid-liquid extraction process entails the transfer of one elements of a solution to another liquid phase which is relatively immiscible in the first solution [2].

There are many types of equipments used for the processes of liquid-liquid extraction. The one that will be considered in this research is the column extractor type called Rotating Disc Contactor (RDC) column. In the RDC column, there are two phases that were involved in extraction process which called the dispersed phase (drops) and the continuous phase. Mathematical model on the mass transfer process that occurred in RDC column were already completed by previous researchers. However, there are still some weaknesses on the latest mass transfer model that can be improved.

In RDC column, chemical substances will be used in order to complete the extraction process. Therefore, molarity is a proper method to determine the concentrations on the chemical substances. Molarity will be embedded in the former model in order to reform it. Then, the suitable algorithm is determined so that the solutions of the improved model can be achieved.

1.2 Problem Statement

Quite a lot of models on RDC column have been developed. The modeling in drops distributions and mass transfer process are the most important factors for the column performance [3]. Therefore, a more realistic mathematical model is presented.

There are a number of researchers in this field such as Ghalehchian [3], Talib [4], Arshad [5], Mohamed [6] and Maan[3]. Talib [4] has presented the mass transfer models which are Initial Approach of Mass Transfer (IAMT) and Boundary Approach of Mass Transfer (BAMT). These two models were said unsteady-state model. According to Maan [3], Ghalehchian has developed a new model by applying the idea of axial mixing into the simulation of the mass transfer process. Arshad [5] also has developed a steady state model for hydrodynamics process. Then, Mohamed [6] has modified a model developed by Talib which is the BAMT model which is called Simultaneous Discrete Mass Transfer (S-DMT) model. Meanwhile Maan [3] has developed an inverse model of mass transfer where it can determine the value of the input while the value of output is known.

However, the research that was being concentrated on this study is the S-DMT model [6]. Some weaknesses have been detected in this model. As mention before, the concentration of a chemical substance is better being determined by using molarity. Molarity is a method used by chemists to calculate the molar concentration of the chemical substances by using the volume and the number of mole for the substances. Therefore, molarity will be embedded into some of the steps in the S-DMT model. Improvements of this model will be explained further in Chapter 4. Then, the concentration for both dispersed and continuous phases obtained in this research will be compared with the SSPS data as cited in Talib [4].

1.3 Objective of the Research

The main goals of the research are to model a mass transfer process by using molarity that happen in the RDC column and compare the data obtained from this model with the experimental data obtained in SSPS as cited in Talib [4]. To achieve these goals, the following objectives are the working strategies. The objectives of the study are:

1. To formulate a new model for the mass transfer process for drops and continuous phase in the RDC column.
2. To incorporate the new mass transfer model in the existing algorithm.
3. To develop a programming to simulate the concentration of drops and continuous phase in the new mass transfer model.

1.4 Scope of Study

In this study, the geometrical properties for RDC column with the height 1.75 meters will be used. The RDC column is modeled into 23 stages. Each stage is between two consecutive stator rings. Let say the stage and stator ring are labeled as i where $i = 1,2,\ldots,23$. Then, the stage i is between the ith stator ring and $i+1$th stator ring. This situation continues along the column. However, stage 23 will be between 23rd stator ring and the top of the column. This is as given in Figure 1.1 below.

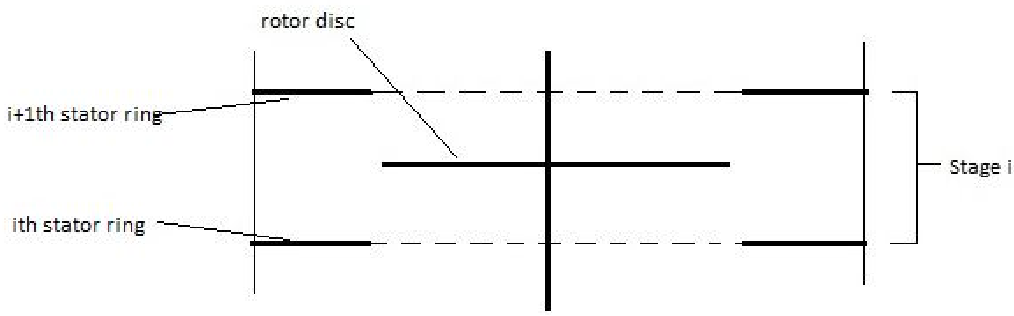

Figure 1.1 : The illustration for stage i located between 2 stator rings next to each other.

Then, each stage is also modeled into 10 cells with the same width. The cell is labeled as j where $j = 1,2, \dots ,10$. Each cell is said to have its own range of drops diameter where this range will be explain further in Chapter 2. The cells can be illustrated as in Figure 1.2. Figure 1.3 shows an RDC column being modeled into 23 stages and 10 cells in every stage.

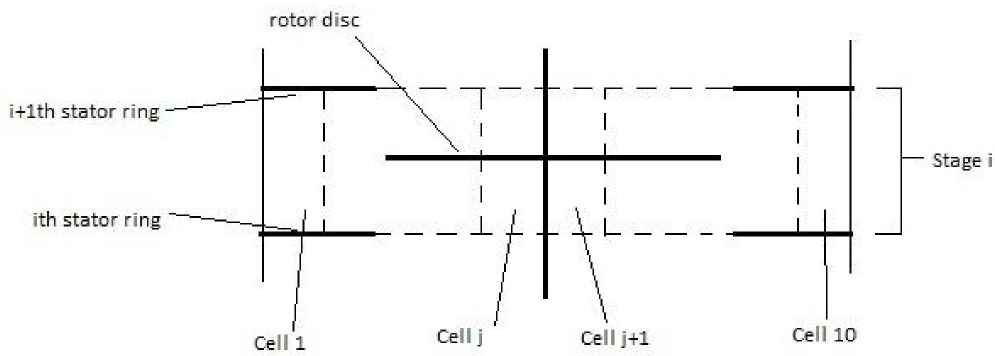

Figure 1.2 : Illustration of stage i being divided into cell with the same width.

The chemical substances that were taken into consideration are cumene in isobutiric acid as the dispersed phase and isobutiric acid in water as continuous phase. The physical properties for the system are obtained from the experiments done by Bahmanyar as cited by Talib[4]. The same applies to the geometrical properties of the RDC column. Both the geometrical properties and the physical properties are given in Appendix A.

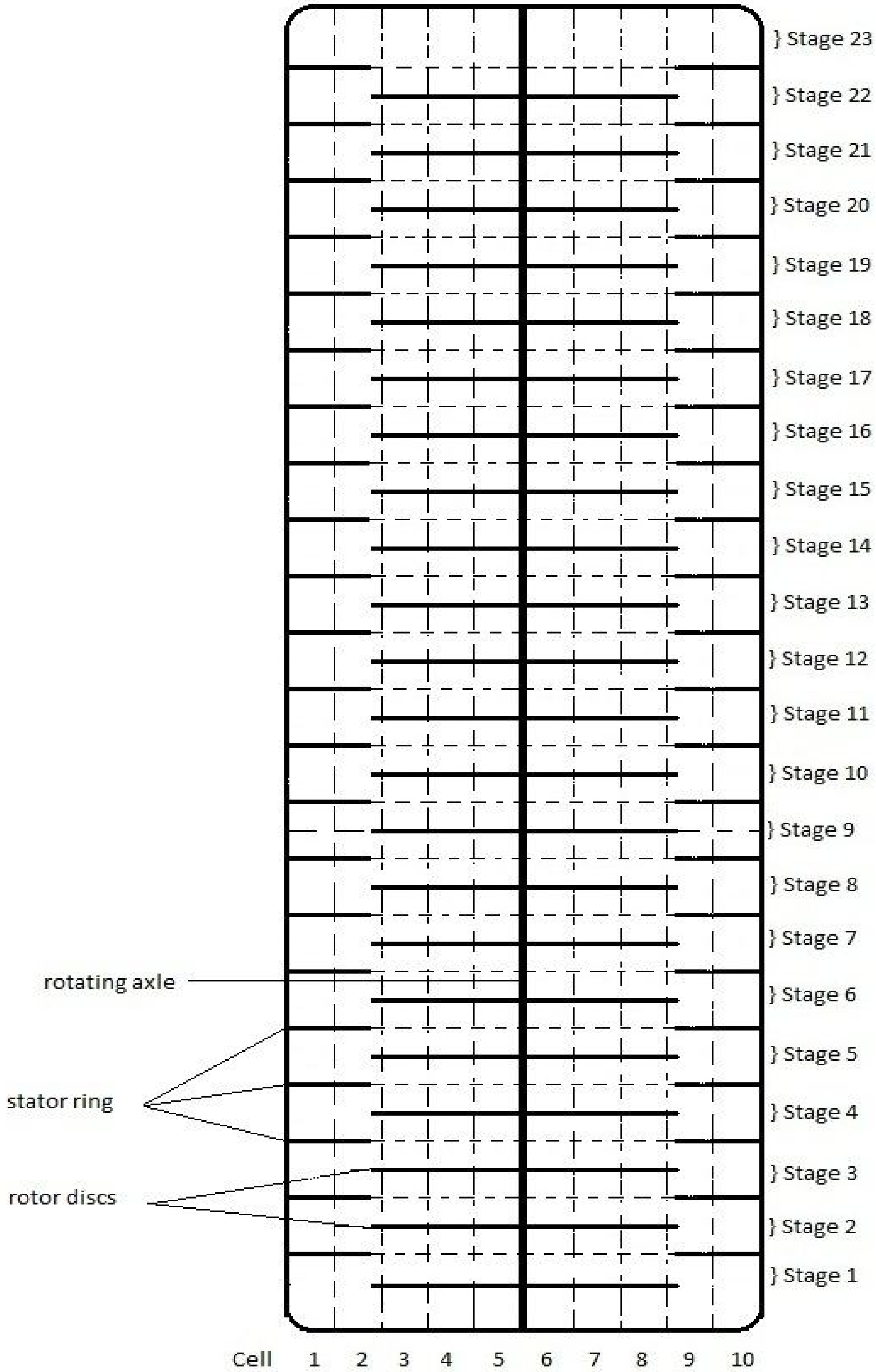

Figure 1.3 : The RDC column that was modeled into 23 stages and 10 cells in each stage.

Next, the hydrodynamics of drops, the drops distribution, the range of drops diameter and average of drops diameter that are used in order to achieve the objectives above has been obtained by Talib [4]. The hydrodynamic of drops is used to determine the time taken for drops to travel along the column. The drops distribution is used to calculate the number of drops in every cell in every stage. All these data are used to determine the concentration of dispersed and continuous phases. These data are used in simulating the mass transfer process by using C++ 6.0 software.

1.5 Significant of Study

The purpose of this study is to determine the concentration of dispersed and continuous phases in the RDC column. From the concentrations obtained, the efficiency of the column can be observed. The efficiency of the RDC column will increase if the extraction process that occurs in the column increases. In order to increase the extraction process, improvements can be made to the RDC column such as reducing the speed of the rotor discs in the column so that the drops will break into smaller. This will increase the surface area that was brought into contact with the continuous phase.

These concentrations also help in designing the RDC column by varying the geometric properties of the column. For example, by increase or decrease the radius of the column, the height of the column and etc depends on the extraction process happen, an efficient RDC column will be produce.

1.6 Thesis Organization

This thesis starts with Chapter 2, literature review on the liquid-liquid extraction. It is then followed by the introduction to the Rotating Disc Contactor (RDC) column and the hydrodynamics of mass transfer process that occurs in the RDC column. Discussion on the hydrodynamic, drop breakage, drop distribution and mass transfer process are also included. The existing models developed by previous researchers are presented.

Chapter 3 reviews on the existing mass transfer models. It discussed on the formulation of the varied boundary function. The details of the exact solution of the Initial Boundary Value Problem (IBVP) with the time depending function boundary condition will be shown and followed by the derivation of a new diffusion equation for sphere.

Chapter 4 discusses the formulation of the mass transfer process in the RDC column by using molarity. The new mass transfer process using molarity is presented. Molarity is a method that will be used to determine the concentration of both drops and continuous phase in the mass transfer process that occurs in the RDC column. Molarity will be embedded in the existing mass transfer model and this process will be explained further in this chapter.

Chapter 5 provided the explanation on the computer program that was build and the simulation data that were obtained from this simulation. The computer program was developed by using C programming. This simulation is then being run until 10000 iterations and the data obtained from this simulation will be compared with the SSPS data as cited in Talib [4]. The concentration error obtained from this comparison is then being compared with the concentration error obtained from the comparison S-DMT model and SSPS data.

The summarization and conclusion on the final findings and suggest areas for further research are given in Chapter 6.

1.7 Summary

In this introduction chapter, general information on the liquid-liquid extraction and the equipment is presented. The weakness of the existing model motivates this research to be done is given in the problem statement. Next, the research objectives and scope, and the contribution of this research are described in this chapter. Finally, the thesis organization is given.