MASS TRANSFER PROCESS FOR PROLATE SPHEROIDAL DROPS IN ROTATING DISC CONTACTOR COLUMN

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DEDICATION

This thesis is dedicated to my mother, Bedah bt Hj Reduan who supported me through all the hardship and gives me the mentally support that I really need. I really appreciate her sacrifice all this time.

This thesis is also dedicated to my best friend, Dr Mastura Ab Wahid who gave me all the support that I needed during my study.

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ABSTRACT

A rotating disc contactor (RDC) column is one of the equipments that is commonly used in the chemical industry. This column is used for the liquid-liquid extraction process where it is a method to separate compounds based on their insolubility differences. The mass transfer process in the RDC column occurs due to the counter-current motion of the drop and continuous phases. The mass transfer process that occurs in the RDC column is also can be modelled mathematically. Previously, this process is modelled by assuming that the drops were spherical. After considering the research done on the distribution of drops and column properties, the drops have shapes closer to spheroidal rather than spherical. Therefore, a new model of the mass transfer process in the RDC column is proposed. This new model is developed by assuming that the drops are taking prolate spheroidal shape instead of oblate due to the properties of the column. The mass transfer process of the prolate spheroidal drops is determined by using Fick's second law in Cartesian coordinates to predict the diffusion for rectangular shape body. By using a suitable transformation equation, a three-dimensional partial differential equation is obtained. However, instead of solving Fick's second law analytically, the numerical approach is used. In this study, the finite difference method (FDM) is chosen. Since FDM is one of the methods that engineers usually use to solve modelling problems, the algorithm for this three-dimensional partial differential equation would help engineers increase the capability of the RDC column only by simulation, thus reducing the experimental cost. The algorithm developed in this study can be adjusted depending on the initial value and the boundary value of the system. This new model shows that the results obtained are satisfying the profile of concentration in the RDC column. After comparing the numerical results with the experimental results, this model's relative error was between 0.1% until 9%, which varied due to some stages. In conclusion, the results from the new model are closer to the experimental results compared to the older model. The algorithm obtained in this study can be used for references in solving the three-dimensional partial differential equation and this model would help engineers in improving the RDC column performance.

ABSTRAK

Turus pengekstrakan cakera berputar (RDC) adalah salah satu peralatan yang biasanya digunakan di dalam industri kimia. Turus ini digunakan untuk proses pengekstrakan cecair-cecair di mana ia adalah satu kaedah untuk mengasingkan sebatian bergantung kepada perbezaan keterlarutan masing-masing. Proses pemindahan jisim dalam turus RDC wujud disebabkan oleh pergerakan arus bertentangan di antara titisan dan fasa selanjar. Proses pemindahan jisim dalam turus RDC ini juga boleh dimodelkan secara matematik. Sebelum ini, proses tersebut dimodelkan dengan beranggapan bahawa titisan adalah berbentuk sfera. Setelah mengambil kira kajian yang telah dilakukan terhadap taburan titisan dan ciri-ciri turus, titisan lebih berbentuk kepada sferoid berbanding sfera. Oleh itu, model pemindahan jisim baharu dalam turus RDC telah dicadangkan. Model baharu ini dihasilkan dengan menganggap bahawa titisan adalah berbentuk sferoid bujur menegak daripada bujur melintang berdasarkan kepada ciri-ciri turus. Proses pemindahan jisim untuk sferoid bujur ini ditentukan menggunakan hukum kedua Fick pada koordinat Cartes untuk meramalkan resapan bagi bentuk segi empat tepat. Dengan menggunakan persamaan penjelmaan yang sesuai, satu persamaan pembezaan separa tiga dimensi diperoleh. Namun, daripada menyelesaikan hukum kedua Fick secara analitis, pendekatan berangka telah digunakan. Dalam kajian ini, kaedah perbezaan terhingga (FDM) telah dipilih. Oleh kerana FDM merupakan salah satu kaedah yang selalu digunakan oleh jurutera dalam menyelesaikan masalah permodelan, algoritma bagi persamaan pembezaan separa tiga dimensi ini akan membantu jurutera untuk meningkatkan kebolehan turus RDC melalui simulasi sahaja sekaligus mengurangkan kos eksperimen. Algoritma yang dihasilkan dalam kajian ini boleh dilaraskan bergantung kepada nilai awal dan nilai sempadan sistem tersebut. Model baharu ini menunjukkan bahawa keputusan yang diperoleh memenuhi profil kepekatan titisan di dalam turus RDC. Selepas membandingkan keputusan berangka dengan keputusan eksperimen, ralat relatif model ini adalah di antara 0.1% hingga 9% bergantung kepada tahap tertentu. Kesimpulannya, keputusan dari model baharu ini lebih menghampiri keputusan eksperimen berbanding dengan model yang lama. Algoritma yang diperoleh dalam kajian ini boleh digunakan sebagai rujukan dalam menyelesaikan persamaan pembezaan separa tiga dimensi dan model ini akan membantu jurutera dalam menambahbaikkan prestasi turus RDC.

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

Liquid-liquid extraction has become an important subject of discussion among engineers and mathematicians. Liquid-liquid extraction is a method to separate compounds based on their differences in insolubility. This extraction process is commonly used in the food industry, for example, the extraction of coffee with water in the production of instant coffee, and the process of perfume manufacturing; even biodiesel production (Assmann et al., 2013; Mustafa & Turner, 2011; Rezaee et al., 2010; Todd, 2014). Mathematical modelling commonly employed in this type of separation process is mass transfer model, which is important in determining the optimum concentration that has been absorbed by the substance. This mathematical model helps in determining the mass transfer process simply by using simulation only, thus concentration of a substance can be determined without needing manual measurement.

This mathematical modelling on mass transfer is usually applied with the use of an extraction machine. In order to determine the efficiency of the machine, a simulation is done, which can be used to improve the machine. Accurate design of the extraction column is important; sometimes, it requires experiment at a pilot-plant scale, which is expensive. By introducing accurate model of the mass transfer process, total cost can be reduced due to no requirement of the pilot-plant scale. In this study, the machine taken into consideration is a rotating disc contactor (RDC) column with a chemical system of cumene/isobutyric acid/water. This is one of the extraction equipment commonly used on a huge scale liquid-liquid extraction process in the industry (Aiffah et al., 2014; Attarakih et al., 2013; Ismail et al., 2015). Firstly, the whole column is filled with continuous phase. Then, the drops are dispersed by the disperser located at the bottom of the column. Due to difference in density, the drops float up to the end of the column, while the continuous phase flows down to the bottom of the column. This movement is known as countercurrent motion (Fakhrhoseini et al., 2013; Shehata et al., 2011).

Previous researchers such as Ford Versypt & Braatz (2014), Ismail et al. (2014), Kadam et al. (2009), Maan (2005), Mohamed Nor (2000), Shehata et al. (2011), and Talib (1994) modelled the mass transfer process inside the column based on the diffusion of a sphere, where the drops were assumed to be spherical. The diffusion equation of the sphere was as given by Crank (1999). The analytical solution for the diffusion equation was then published, and a lot of modifications have been developed ever since.

These days, most researchers have turned their focus from heat and mass transfer from a sphere to flowing continuous phase, due to its wide range of scientific and industrial applications. However, according to Juncu (2010), in many applications, the particle have shapes that are closer to spheroidal rather than spherical. Despite this fact, less attention is given to the transport phenomena around spheroids.

For example, in this study, due to the RDC column properties, the continuous phase, which has a higher density, enters the column from the top of the column, and then flows downwards before it exits through the bottom of the column. Meanwhile, the disperse phase, which has a lower density, is dispersed through a disperser at the bottom of the column, and then floats upward in the continuous phase due to different density. This movement in the RDC column is called counter current motion.

Due to this motion, drag force, which acts oppositely to the direction of the oncoming flow velocity, occurs, as stated by Liu et al (2019). The drag force drags the surface of the drops and elongates it into the shape of spheroidal instead. The drops size distribution is influenced by several factors, such as the liquid density, viscosity, and surface tension. Peng et al (2019) cited that liquid viscosity and surface tension are two parameters that affect the fluid dynamics in a column. Jildeh et al (2013) proposed a study on drops coalescence model in the RDC column. Instead of drops breaking, they suggested that the drops should collide and remain in contact for sufficient time, so that the process of film drainage, film rupture, and coalescence, can occur. Here, the possibility of the drops to be dragged into a prolate spheroidal shape is higher. Thus, this study is proposed, with assumption that the drops are to be in prolate spheroidal shape instead.

Experiments on mean drop size and drop size distribution in a liquid-liquid extractor had been done by Jildeh et al. (2013), Hemmati et al. (2015), Schmidt et al. (2006) and Hosseinzadeh et al. (2018). However, they assumed the drops were spherical, despite some pictures taken showing that the drops were spheroidal. Therefore, by considering spheroidal shape being more legit, a new model of mass transfer process in the RDC column was then proposed (Favelukis & Ly, 2005; V. A. B. Oliveira & Lima, 2002).

In the previous study of the mass transfer process in the RDC column, the drops were assumed to be spherical. It means that the drops have the same radius from the center to the surface of the drops. Thus, the rate of diffusion for the drops are constant at all surface leads to the constant concentration on the whole drops. However, even from the previous study, there are proofs that the drops are in spheroidal shape instead. In RDC column, the drops are taking the prolate spheroidal shape where the distance from the center to the surface of the drops varies. Thus, the rate of diffusion is different and the concentration at each surface also different. This is the major difference between the spherical and the spheroidal drops.

A number of researchers had presented the analytical solution of mass transfer process in prolate spheroidal drops. On the contrary, for this study, a numerical approach had been used. A method known as the finite difference method (FDM) was implemented into the improved mass transfer model (Abadie & Chamorro, 2013; Duffy, 2013; Mish, 2016). An algorithm for this simulation had been presented. From engineering point of view, this method is more accessible and more practical since, researchers can manipulate the information quickly. Afterward, the stability of this numerical approach was tested. A constraint equation was presented after multiple tests of stability for different sizes of drops.

In order to determine the reliability of this FDM, this method had been implemented on the existing model, where the drops were assumed to be spherical. Another algorithm was evaluated as well, whose results obtained from simulation had been used in the comparison of data with those of prolate spheroidal.

1.2. Statement of Problem

A lot of modifications have been done to improve the performance of the RDC column, whether by the physical properties of the system, or the geometrical properties of the column itself. The most popular study is the mass transfer process that occurs inside the column. This is because the mass transfer process affects the performance of the column directly. Therefore, a model to help the engineers in adjusting the column's input whenever they need to has been developed, covering the transfer rate, the dispersed phase rate, the size of the disperser, etc.

Even with alterations by several researchers in this field, there is always room for improvement for the designated mathematical model. According to a previous research, the drops dispersed into this column are assumed to be spherical; therefore, the approach of diffusion equation for sphere is used in this mass transfer model.

However, the continuous phase in the RDC column moves downward through the inlet at the top of the column, and the drops are dispersed by disperser at the bottom of the column. The two liquids are brought into contact with each other, in which the frictional drag of the continuous phase will make it impossible for the drops to maintain their spherical shape. Therefore, a new assumption for the shape of the drop had been taken into consideration in order to develop mass transfer model in the RDC column.

In order to solve this problem, the drop is assumed to be a prolate spherical shape instead, and Fick's second law will be used. Instead of solving this problem analytically, numerical approach will be used. Then, finite difference method (FDM) is implemented into the initial boundary value problem (IBVP). Next, the stability of this numerical approach is determined to find the effect of step size on the process. Therefore, these are the research questions that need to be answered :

1. How to develop an improved mass transfer model for a single drop based on the concept of diffusion in prolate spheroidal drops and molarity?
2. How to develop an improved mass transfer model of multiple drops in the RDC column?
3. How to solve the two models?
4. How to validate the modified model?

1.3 Objectives of Study

1. To develop an improved mass transfer model for single drop based on the concept of diffusion in prolate spheroidal drops.
2. To develop an improved mass transfer model of multiple drops in the RDC column based on the developed model (from objective No 1) with consideration of the molarity of both phases.
3. To solve the two models by using finite difference method.
4. To validate the improved model by applying numerical approach to the existing mass transfer model.

1.4 Scope of the Study

In this study, the rotating disc contactor (RDC) column with height of 1.75m had been used. Previously, RDC column was usually modelled into 23 stages, while in this study, the column is divided into partitions, where the number of partitions are the same as the time step size, nt. The time steps vary, depending on the simulation being done. The partitions are set equal to the number of stages. For example, if the number of time steps, nt chosen is 100, then the partitions are divided by 25. It is because, stage 0 is between the bottom of the column and the first stator ring, while stage 24 is between the 24^{th} stator ring and the top of the column. Thus, there are 25 stages overall. The partitions are divided into 25 to ease selecting which concentration of drops to be compared with the experimental data.

The chemical system used for the RDC column is a cumene/isobutyric acid/water. The physical properties of the column are given in Appendix A. This study focuses on developing a numerical scheme and algorithm in finding the total concentration of a prolate spheroidal drop. This algorithm is then used to develop a complete model for the mass transfer process in the RDC column, which involves multiple drops with various sizes, and a new algorithm will be developed.

In the RDC column, the whole column is assumed to be divided into 23 same size stages. Stage 1 is located in between the first and the second stator ring while stage 2 located in between the second and the third stator ring. The sequence continues till the stage 23 which is located between 23rd and 24th stator ring.

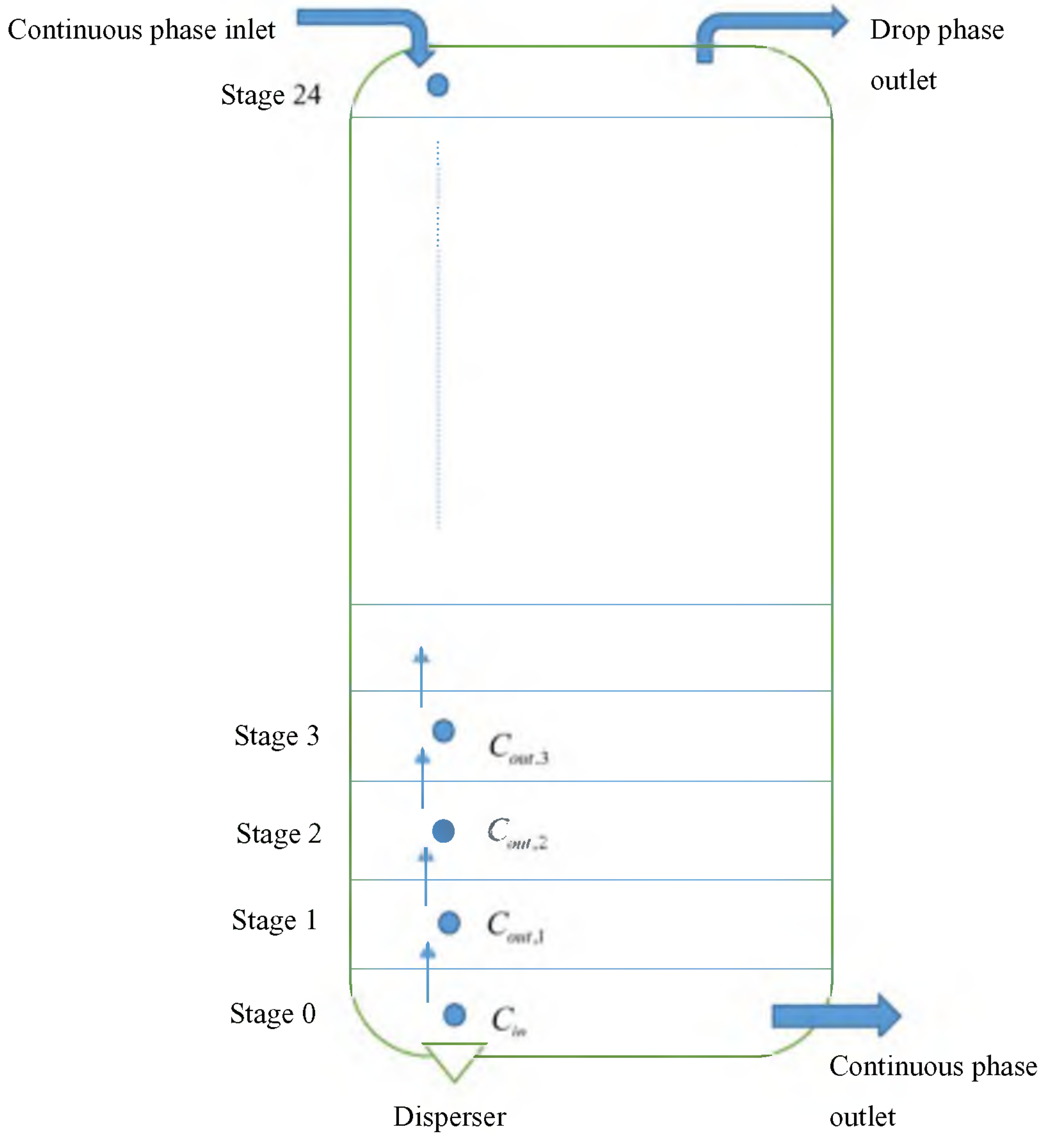

Figure 1.1 : Mapping of the process in the RDC column

The drops are dispersed into stage 0, located before the stage 1 which starts from the bottom of the column till the first stator ring. Here, the concentration of drops are assumed as C_{in} and the drops moves up to stage 1. With the initial concentration C_{in}, the new concentration for drops in stage 1, $C_{out,1}$ is obtained after diffusing from the concentration of dispersed phase which already filled the whole column and exited through the outlet at the bottom of the column. This new concentration becomes the new initial concentration for drop in stage 2. This process continues for all the drops and finally, the drops coalescence at the end (top) of the column, stage 24, located between 24th stator ring and the top of the column. It finally exited through the heavy phase outlet located at the top of the column. This process is shown in Figure 1.1 given below. Further explanation is given in Chapter 4.

1.5 Methodology

In order to determine the concentration of a prolate spheroidal drop, the Fick's second law in Cartesian coordinates is used. This equation is said to be the most appropriate equation to predict the mass transfer in bodies with a rectangular shape. With suitable transformation, which in this case is the prolate spheroidal coordinate system, the mass transfer process for the prolate spheroid dal drop can be determined.

After completing the transformation of the equation, a three-dimensional partial differential equation is obtained. It involves time, radius of the drops, and angle of rotation that generates the body of the prolate spheroidal. This equation is used to determine the concentration of prolate spheroidal drops with the most suitable initial and boundary value. However, instead of solving this equation analytically, a numerical approach is used.

The numerical approach taken into consideration in this study is finite difference method (FDM). This method discretises the cross-section of the drops into a mesh grid. Thus, each layer of the drops, from the center to the surface concentration of the drops, can be calculated. However, in this case, only the surface concentration of drops is considered. This method is frequently used to solve differential equations by replacing the derivatives in the equation with differential quotients. The domain is partitioned in space and in time, and approximations of the solution are computed at the space and time points.

Numerical method is a method to solve mathematical modelling which involves partial differential equation. One of the commonly used methods is finite difference method, usually to obtain numerical solution for a PDE. Zhang & Guo (2018) applied finite difference method into fractional diffusion equation. Gelu et al. (2017) applied a sixth order compact finite difference method into a 1D reaction diffusion problem. Prieto et al. (2011) described how generalized finite difference method is used to solve the advection-diffusion equation. Martín-Vaquero & Sajavičius (2019) explained a two-level finite difference scheme for heat equation with nonlocal initial conditions. Malek & Momeni-Masuleh (2008) solved a novel microscopic heat evacuation by using mixed-collocation finite difference method in and on the boundaries of a particle when the thickness was much smaller than both the length and width. Recktenwald (2014) applied a finite difference approximation into a heat equation.

The application of finite difference method into partial differential equation of diffusion/heat equations by all the above mentioned researchers has inspired this research to use the same method in solving the diffusion equation of prolate spheroidal drops in RDC column.

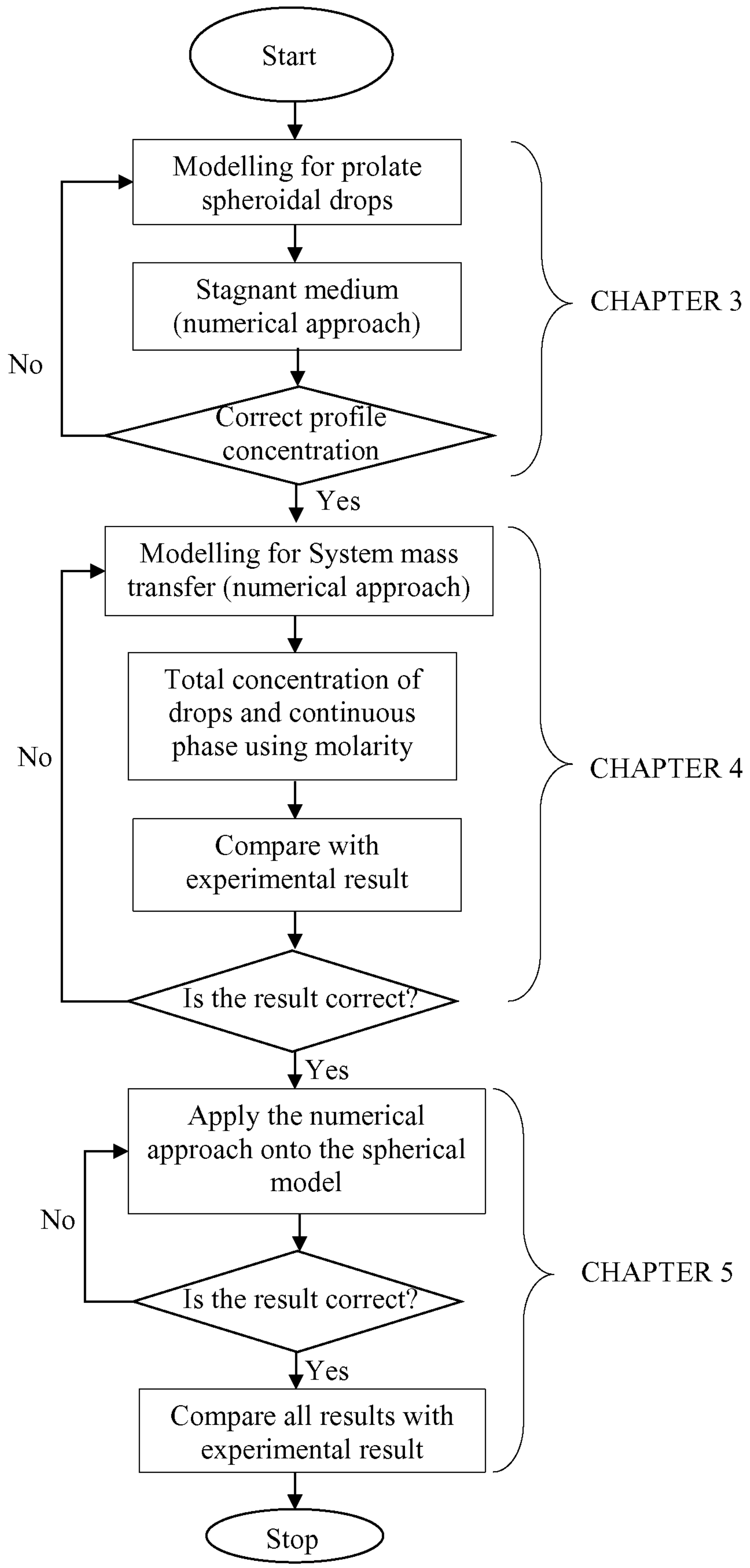

Figure 1.2 : The flow chart of the project.

The molarity of the concentration for both phases has also been taken into consideration. First, the total concentration of drops is calculated by using molarity. Once the total concentration is obtained, the balance concentration for the continuous phase is calculated. In order to determine the balance concentration of the continuous phase inside the column, molar concentration concept is used. The comparison between the numerical results and the experimental results is done since there is no numeric results obtained from the previous study. Most of the researchers presented their results using graph. The profile of this graph is used as well. The flow of this project is as expressed in Figure 1.2.

1.6 Significant of Study

RDC column is widely used in industry, as part of large scale extraction process. It is tedious for engineers to check each machine manually. This study is aimed to contribute significantly in the form of algorithms, which is hoped able to help engineers in increasing the capability of the machine only by simulation, thus reducing experimental cost. The results of this study indicate that these algorithms are able to calculate the mass transfer process for prolate spheroidal drops in the RDC column. This shall also be future reference for diffusion equation for prolate spheroidal drops and the application for the mass transfer process in RDC column.

1.7 Thesis Organization

Chapter 2 presents literature review of the RDC column and the liquid-liquid process in general. Mass transfer process that occurs in the column will also be discussed thoroughly. Previous researches on mass transfer and finite difference method are deliberated as well. These reviews have been used in developing the modified mass transfer model, which will be discussed in Chapter 3.

Chapter 3 gives the formulation of the diffusion equation for the prolate spheroidal drops, which is the main purpose of this study. In this method, FDM is applied to the partial differential published by using Fick's second law. This equation is used to determine the concentration of drops in the stagnant medium for some time. The solution for different sizes of drops is also presented, along with analysis on the stability of this model.

Chapter 4 entails the solution for multiple drops in the RDC column. Mass transfer by using molarity will be discussed thoroughly, followed by explanation on tests of different step sizes for all spaces and time steps, to choose which one is the most suitable choice for the RDC column.

Chapter 5 explains the application of FDM into the mass transfer process for the spherical drops. This is to validate the modified model developed before. This chapter presents comparison of results of this study with the results of the modified model. Verification of this method by assuming that a spherical drop is brought in contact with a stagnant medium. The concentration at some time is then determined before the model of mass transfer in the RDC column is developed by implementation of FDM in the diffusion equation.

Chapter 6 presents the results, conclusion, and suggestions for future researches; more into two-dimensional diffusion equation, which has not been widely explored. Perhaps the analytical solution for this particular differential equation can be developed, or another numerical approach that can give better solution can be used.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter explains the application of rotating disc contactor (RDC) column in general. The process involved in the RDC column in this study is liquid-liquid extraction. Discussion also covers the theoretical concept and mathematical equation involved in the RDC column such as hydrodynamics, drops distribution, and general form of the mass transfer process. Previous works with regards to mass transfer process in RDC column are also discussed. Finally, the application of numerical approach involved in this study is explained.

2.2 Rotating Disc Contactor Column

Rotating disc contactor (RDC) column is one of the process columns that is used in chemical industry to extract impurities from liquids. This equipment consists of a vertical cylindrical vessel, whose length is divided into a number of equally spaced compartments by a series of stator rings. In the center of each compartment, there is a rotor disc supported by a shaft. In the RDC column, the process involved in the column is called solvent extraction, where liquid is brought in contact with another liquid.

In the column, the drops (lower density liquid) are dispersed through the bottom of the column, while the continuous phase (higher density liquid) enters the column through the vessel at the top, which is called the counter current principle. Due to the difference in their density, the drops will move up inside the continuous phase along the column. The rotation of rotor discs may influence the process of extracting the two liquids. The column length, compartment height, column diameter, flow speed, and rotational speed also affect the droplet size.

One of the phase's flow rate can be controlled, while the other maximum rate will be limited, due to the rate of the first phase and physical properties of the system. However, there is still a maximum rate at which the phases can flow through the column; once this happens, the column is considered flooded, and the dispersed phase is rejected at its point of entry. This will influence the rate of extraction process that occurs in the column.

The separation efficiency of this type of extractors is very high compared to the mixer settler. There are several important factors that need to be considered when selecting extractor types, such as the stage requirements, fluid properties, and operational considerations. Table 2.1 summarizes the abilities and characteristics of different extractor-types.

The column contactors performance is more efficient and gives better operational flexibility compared to non-agitated column type.

The rotating disc contactor (RDC) column, schematically shown in Figure 2.1, was developed in Europe by Reman in 1951. They used the shearing action of a rapidly rotating disc to interdisperse the phases. Since then, RDC contactors have been widely used in large scale liquid-liquid extraction in industry, particularly in the petroleum and petrochemical industries because of their high throughput, low investment, as well

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LIST OF PUBLICATION

Indexed Conference Proceedings

1. Nurul Nadiya binti Abu Hassan, Jamalludin Talib (2015). Concentration Profile of Spherical Drops in Rotating Disc Contactor (RDC) Column Using Finite Difference Method (FDM). *3rd International Science Postgraduate Conference 2015 (ISPC 2015)* - 978-967-0194-51-6, 301-310