

FUZZY MODELLING OF HYDRODYNAMICS AND MASS TRANSFER OF
DROPS IN A ROTATING DISC CONTACTOR COLUMN

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To my family and friends

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ABSTRACT

Rotating Disc Contactor (RDC) column is one of the important equipments for separation process, because it gives high performance and is more efficient among equipments for solvent extraction. Over the years, researchers and engineers are designing and building models of hydrodynamics of drops and mass transfer to interpret the performance and to increase the efficiency of the RDC column. In this research, the main aim is to develop and design models of hydrodynamics and mass transfer of drops that are capable of work with any design of RDC column based on the experimental data and fuzzy modelling. Firstly, the Sauter mean diameter is calculated based on the flow rate of dispersed phase and Mamdani fuzzy model. Secondly, the fuzzy model based on optimal interval technique (FMBOIT) is established to predict models of the hydrodynamics of drops such as, mean number of daughter drops, probability of drop breakage, Sauter mean diameter and hold-up of dispersed phase from experimental data. Then, these models and beta distribution are incorporated to develop the forward model of drop size distribution, which is used to obtain the drop size distribution along RDC column. Besides the forward model, the inverse model of drop size distribution is constructed based on the optimization technique that determined the number of drops at bottom stages using the number of drops at top stages. The last model is the mass transfer model, which depends on the forward model of drop size distribution for calculating the amount of mass transfer from the continuous phase to the dispersed phase. In addition, the mass transfer model allows the usage of either the terminal or the characteristic velocity of drops which determines the lifetime of drops between compartments. All the models are developed based on three phases. Phase one is the literature review and problem formulation. Phase two is the design and development of the proposed models. Phase three is implementation, verification and validation of proposed models from phase two. Most of these models give less error when compared with simulation data of previous researchers against experimental data. Furthermore, the new mass transfer model allows parameters such as the height of the compartment, the number of stages or the diameter of the column to be changed at the same time. Thus, this new model is a powerful model for predicting the performance and design of RDC column.

ABSTRAK

Turus Penyentuh Cakera Berputar (RDC) adalah salah satu peralatan yang penting bagi proses pemisahan kerana ia memberikan prestasi yang tinggi dan lebih berkesan berbanding peralatan lain bagi pengekstrakan pelarut. Sejak beberapa tahun kebelakangan ini, penyelidik dan jurutera mereka bentuk dan membina model hidrodinamik titisan dan pemindahan jisim bagi mentafsirkan prestasi turus RDC serta meningkatkan kecekapannya. Tujuan utama kajian ini ialah untuk membangunkan dan mereka bentuk model hidrodinamik dan pemindahan jisim titisan yang mampu berfungsi dengan sebarang reka bentuk turus RDC berdasarkan data eksperimen dan pemodelan kabur. Pertama, purata diameter Sauter dikira berdasarkan kadar aliran fasa terserak dan model kabur Mamdani. Kedua, Model kabur berdasarkan teknik selang optimum (FMBOIT) diwujudkan untuk meramal model hidrodinamik titisan seperti purata titisan anak, kebarangkalian pemecahan titisan, purata diameter Sauter dan isi tertahan bagi fasa terserak daripada data eksperimen. Kemudian, model ini bersama dengan taburan beta digabungkan untuk membentuk model ke depan bagi taburan saiz titisan yang digunakan untuk mendapatkan taburan saiz titisan di sepanjang turus RDC. Selain daripada model ke depan, model songsang bagi taburan saiz model dibina berdasarkan teknik pengoptimuman bagi menentukan bilangan titisan pada peringkat bawah turus dengan menggunakan bilangan titisan pada peringkat atas turus tersebut. Model terakhir ialah model pemindahan jisim yang bergantung kepada model ke depan untuk taburan saiz titisan bagi mengira jumlah pemindahan jisim daripada fasa berterusan ke fasa terserak, dan juga membolehkan penggunaan sama ada halaju terminal atau cirian bagi titisan untuk menentukan tempoh hayat titisan antara kompartmen. Semua model dibina berdasarkan tiga fasa. Fasa pertama ialah tinjauan kajian dan perumusan masalah. Fasa kedua ialah reka bentuk dan pembangunan model yang dicadangkan. Fasa ketiga ialah pelaksanaan, penentusahan dan pengesahan model daripada fasa kedua. Kebanyakan model ini memberikan ralat yang lebih sedikit apabila dibandingkan dengan data simulasi yang diperolehi penyelidik terdahulu terhadap data eksperimen. Tambahan pula, model pemindahan jisim baharu membolehkan parameter seperti ketinggian ruang, bilangan peringkat atau diameter turus ditukar serentak. Maka, model ini berkeupayaan tinggi untuk meramal prestasi dan reka bentuk turus RDC.

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LIST OF ABBREVIATIONS

RDC	–	Rotating Disc Contactor
FMMNDD	–	Fuzzy Model of Mean Number of Daughter Drops
FMBOIT	–	Fuzzy Model Based on Optimal Interval Technique
MISO	–	Multi Input Single Output
MIMO	–	Multi Input Multi Output
FMDS	–	Forward Model of Drop Size Distribution
SMDKH	–	Sauter Mean Diameter Based on Kumar and Hartland Equations
SMDFM	–	Sauter Mean Diameter Based on Fuzzy Model
IMDS	–	Inverse Model of Drop Size Distribution
MTDS	–	Mass Transfer Based on Drop Size Distribution

LIST OF SYMBOLS

a	–	radius of a sphere
A	–	Column cross sectional area (m^2)
C	–	Concentration (kg/m^3)
C_ψ	–	Dimensionless parameter allowing for the effect of mass transfer on the drop size
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_0	–	Initial drop diameter (m)
d_{dau}	–	Daughter drop diameter (m)
d_{mth}	–	Mother 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_{oe}	–	Overall effective diffusivity (m^2/s)
D_r	–	Rotor diameter (m)
D_s	–	Stator diameter (m)
E_o	–	Eotvos Number.
E_{O_n}	–	Nozzle Eotvos Number.
fl_d	–	Flow rate of dispersed phase (L/min)
fl_c	–	Flow rate of continuous phase (L/min)
g	–	Acceleration due to gravity (m^2/s)
h	–	Height of column (m)
h_c	–	Height of an element of compartment (m)
J_x, J_y	–	Mass flux
k_d	–	Drop film mass transfer coefficient (m/s)

m	–	Exponent in the equation of slip velocity
M	–	Morton number in terminal velocity
N_d	–	Number of drops
N_{br}	–	Number of broken drops
N_r	–	Rotor speed (s^{-1})
N_{cr}	–	Critical rotor speed for drop breakage
N_{cl}	–	Number of classes
n_{zd}	–	Nozzle diameter
P	–	Probability of breakage
P_r	–	Power consumption per disc (w/m^2)
Re	–	Drop Reynolds number
Re_k	–	Drop Reynolds number using v_k
$Re_{D,w}$	–	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}	–	Drop volume (m^3)
v_c	–	Continuous phase superficial velocity (m/s)
v_d	–	Dispersed phase superficial velocity (m/s)
v_n	–	nozzle velocity
v_k	–	Drop characteristic velocity (m/s)
v_S	–	Slip velocity (m/s)
v_{tw}	–	Drop terminal velocity (m/s)
V_{total}	–	Total drop volume (m^3)
We	–	Weber number for drop
We_m	–	Modified weber number for drop
We_n	–	Nozzle weber number
$We_{D,w}$	–	Disc angular Weber number
X_m	–	Mean number of daughter drops

Greek symbols

ε	–	Mechanical power dissipation per unit mass
γ	–	Interfacial tension (N/m)

μ_c, μ_d	–	Continuous and dispersed phase viscosities ($mPas$)
ρ_c, ρ_d	–	Continuous and dispersed phase densities (kg/m^3)
$\Delta\rho$	–	densities differences (kg/m^3)
κ	–	Viscosity ratio
ω	–	Angular velocity
ω_{cr}	–	Critical angular velocity

Subcripts

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 Introduction

Liquid-liquid extraction is one of the most important types of separation process for chemical systems, which is based on the different distribution of the separable components of two liquid phases (Molavi *et al.*, 2011a). Most types of liquid-liquid extraction equipment use two phases in the separation process, which are the dispersed phase and the continuous phase. The dispersed phase can be described as the phase that contains drops to provide the largest area of contact with the continuous phase (Talib, 1994). The process of liquid-liquid extraction is commonly used in chemical, biochemical and biotechnology industries (Maan, 2005; Molavi *et al.*, 2010b, 2011a).

In the last century, many types of equipment were used in the separation process of chemical fields, such as the Rotating Disc Contactor (RDC) column, which was developed during the period 1948–1952 by the Royal Dutch/Shell group in Amsterdam (Talib, 1994). The RDC column is more commonly used because it gives high performance and is more efficient when compared with other equipment for solvent extraction (Moris *et al.*, 1997).

However, the improvement of the design of the RDC column in recent years has increased the importance of this column among the extraction columns (Moreira *et al.*, 2005). Therefore, in this research our concern is the RDC column, especially for the modelling of the extraction process involved in the equipment. The modelling of the RDC column is related to the modelling of the drop size distribution and the modelling of the mass transfer.

Many researchers (Bahmanyar, 1988; Ghalehchian, 1996; Maan, 2005; Talib,

1994) introduced models for drop size distribution and mass transfer to improve the performance and capability of the RDC column. These models can be grouped into two categories, which are the forward model and inverse model. The forward model can be defined as the model that takes the geometrical and physical properties of the RDC column as inputs in determining of the drop size distribution and mass transfer along the RDC column, while the inverse model is usually used to obtain the input parameters or to determine the causes for the desired output parameters (Maan *et al.*, 2003).

1.2 Problem Background

Modelling the process involved in the RDC column is divided into two types of process, which is drop size distribution and the mass transfer process. Many researchers have focused on both of these processes to interpret the performance of the RDC column. Talib (1994) introduced three models of drop size distribution and two models of mass transfer. Then, Ghalehchian (1996) developed a new steady-state model for the mass transfer of the RDC column. After that, Arshad (2000) developed a new steady-state model for the hydrodynamic process, and used fuzzy logic to predict the input parameter for the specific given output. To get closer to reality, Maan (2005) modified the mass transfer model with a time dependent function boundary condition. Furthermore, Maan (2005) established a new technique for solving the inverse problem of determining the value of the input parameters for the desired values of the output parameters using the fuzzy approach. These models are mathematical forward models except Maan (2005), which introduced an inverse model of mass transfer based on the fuzzy approach.

Most of the models mentioned above were designed based on the geometrical and physical properties of a specific RDC column. Furthermore, the parameters of these models, such as the mean number of daughter drops, probability of drop breakage and Sauter mean diameter are calculated through equations based on these properties. These equations are called the empirical equations or empirical correlation, which means they are unsuitable for all chemical systems and the design of all RDC columns (Mohanty, 2000). In fact, the process of building these equations takes more time and more experimental work to get the final equations or models. Furthermore, it is well known that the measuring of drop size distribution in the liquid-liquid extraction industries is challenging, expensive and very tedious (Ismail Al-Rahawi,

2007). However, the following points explain the limitations and weakness of the previous models in this field:

- The current equation of the mean number of daughter drops (Hancil and Rod, 1988) depends on the ratio between the drop diameter and the critical drop diameter. Although this equation is used for a wide range of systems, and for different extraction equipment (Talib, 1994), it needs to be improved for two reasons. The first reason is that this equation was built based on particular experimental data and specific geometrical properties. However, the liquid-liquid extraction equipment has improved in recent years for use in various fields, which means that this equation must be improved to be applicable to the experimental data and design of the RDC column. For example, Garthe (2006) modified this equation based on his experimental data, also Kalem *et al.* (2011) used the modified equation by Garthe (2006) in his work. The second reason is that this equation does not depend on the volume of fractions of the mother drops in the calculation of the mean number of daughter drops. However, these fractions are considered to be the core of the process of determining the drop size distribution.
- The current equations for the probability of drop breakage (Bahmanyar and Slater, 1991) need to be improved for two reasons. The first reason is the same as the first reason in the previous point, which means that these equations are unsuitable for all designs of RDC columns. For example, Molavi *et al.* (2011a) proposed a new correlation for the probability of drop breakage to be compatible with their experimental data and design of the RDC column. The second reason is that these equations are built to obtain the probability of breakage at stage one, but, in fact, this probability varies from one stage to another (Bahmanyar, 1988).
- Many researchers (Ismail Al-Rahawi, 2007; Kumar and Hartland, 1982; Moreira *et al.*, 2005; Soltanali and Ziaie-Shirkolaee, 2008) focused on the generation and improvement of the correlation of the Sauter mean diameter, which is used in the models of drop size distribution (Ismail Al-Rahawi, 2007; Soltanali and Ziaie-Shirkolaee, 2008). Thus, the design of these models of drop size distribution must be based on the developed correlation of the Sauter mean diameter based on the experimental data or based on the flow rate.
- The distribution mechanism of the current forward models of the drop size distribution begins from the bottom stages to the top stages. The Sauter mean diameter can be calculated from the bottom stage, which leads to determining the initial drop diameter and drop size distribution along the RDC column. Sometimes, the experimental data are incomplete or contain the distribution of

drops for some stages, which means the existing forward models of drop size distribution fail to calculate the Sauter mean diameter for the bottom stage or cannot be used directly in these cases.

- The current computer programs need to be developed to be able to combine the hydrodynamics of the drops and mass transfer in one program that is capable of presenting the results, and which is also compatible with different systems (Arshad, 2000). For example, Attarakih *et al.* (2006) built a simulation tool named LLECMOD for the liquid-liquid extraction column.

1.3 Problem Statement

Several models for the hydrodynamics of drops and mass transfer have been proposed to improve the behaviour and performance of the RDC column. Most of these models have been successful in simulating the process of the hydrodynamics of the drops and mass transfer, and have given results close to the real process inside the RDC column. But, these models were built based on the empirical correlation. This means that these models are only valid for a specific RDC column or a particular chemical system. Furthermore, the parameters of these models, such as the mean number of daughter drops and probability of drop breakage might not be valid for the different types of RDC column.

The problem is how to design and develop the hydrodynamic models of drops and mass transfer to enable it to work with any design of RDC column based on the experimental data and fuzzy models.

1.4 Objectives of the Research

The objectives of this study are as follows:

1. To develop models for the mean number of daughter drops and probability of drop breakage along the RDC column using fuzzy models and experimental data.
2. To establish a new technique that can be incorporated in the fuzzy models to predict models from the experimental data.

3. To develop the correlation of the Sauter mean diameter and use it to formulate an equation to determine the initial drop diameter.
4. To develop a forward model of drop size distribution that depends on the flow rate and develop models for objectives 1, 2 and 3.
5. To construct an inverse model of drop size distribution that depends on the forward model of the drop size distribution and fuzzy approach.
6. To develop a mass transfer model by incorporating the forward model of the drop size distribution.
7. To create flexible simulation programs for all the models in this study.

1.5 Scope of Study

The main goals of this research are to determine models for the hydrodynamics of the drops and mass transfer process based on the experimental data, several equations of hydrodynamics and mass transfer of drops in the RDC columns from previous researchers in this field (Bahmanyar, 1988; Kumar and Hartland, 1982; Maan, 2005; Talib, 1994), and fuzzy modelling. As there is no experimental work involved in this study, the experimental data from previous researchers in this field will be used for developing and comparing the models. Furthermore, the drops assumed that are spherical in shape and that there is no coalescence between drops.

In this research, the hydrodynamics of the drops are determined using models of the mean number of daughter drops, the probability of drop breakage and the models of drop size distribution, which are forward and inverse. The forward model of drop size distribution is incorporated in developing the mass transfer model. These models are verified by many steps, such as check the theoretical description of each model and statistical analysis. Furthermore, these models are validated by comparison with experimental data and simulation data from previous researchers in this field. The experimental data used in this study are taken from Talib (1994), Bahmanyar (1988), Ghalehchian (1996), Molavi *et al.* (2011) and the simulation data are taken from Bahmanyar (1988), Talib (1994), Maan (2005). The simulation programs of the models are designed based on the MATLAB 2011 software.

1.6 Significance of the Findings

This study introduces a new concept for building models of the hydrodynamics of drops and the mass transfer of the RDC column based on the fuzzy models and experimental data. The fuzzy models of the mean number of daughter drops and the probability of drops gives results very close to the experimental data. Furthermore, these models can be easily modified based on the size of the experimental data. The Sauter mean diameter is developed based on the experimental data, and is used it to determine the initial drop diameter through a linear equation. The forward model of drop size distribution is designed based on the developed models of the mean number of daughter drops, the probability of drop breakage and initial drop diameter, which is calculated based on that linear equation. Furthermore, this model is able to work with the flow rate directly. Moreover, it gives results closer to the reality of the distribution of drops inside the RDC column.

The inverse model of drop size distribution has many advantages besides the distribution of drops, which can be used to control the drop distribution between stages. This research gives a flexible mass transfer model that is capable of working with different velocities of drops and allows for a change in the value of the geometrical and physical properties of the RDC column. This work provides a new technique, named the optimal interval technique, which merges with the fuzzy models to obtain models for the probability of drop breakage, the Sauter mean diameter and hold-up of the dispersed phase from the experimental data directly. Furthermore, this study provides computer programs of all the models, which can help engineers in designing the RDC column. Finally, these models will enhance our understanding of the performance and capability of the RDC column.

1.7 Organization of Thesis

This thesis consists of seven chapters. The present chapter gives a general background, problem background, problem statement, objective of the research, scope of study and significance of the findings. Chapter 2 consists of ten sections. The first and second section presents the literature review of the liquid-liquid extraction in general. The third and fourth sections present liquid-liquid equipment, especially the RDC column, and the hydrodynamics of drops, such as drop velocities, hold-up of the dispersed phase and the probability of drop breakage. The fifth and sixth sections

provide a review of the mass transfer and previous work of researchers in this field, such as the probability of drop breakage, forward model of drop size distribution and mass transfer. The seventh and eighth section provide a review of the inverse problem and fuzzy models. The ninth section shows the relationship between the literature and the objectives of this study. The last section provides the summary of this chapter.

The third chapter presents two models and a technique, which are the fuzzy models of the mean number of daughter drops and the probability of drop breakage, and the new technique called the optimal interval technique. The first model describes the process for obtaining the mean number of daughter drops by determining the volume fraction of mother drops using the fuzzy model. The second model describes the process of obtaining the probability of drop breakage along the RDC column using two steps. The first step is using the optimal interval technique with the fuzzy model to determine the probability of drop breakage at stage one, while the second step is calculating the variation in the value of probability in step one for the remaining stages.

In Chapter 4, the Sauter mean diameter will be determined by two methods. The first method develops the Kumar and Hartland (1982) equation based on the experimental data. The second method is calculating it direct from the experimental data using the fuzzy model. After that, the Sauter mean diameter is used for calculating the initial drop diameter through a linear equation. The main aim of this chapter is to determine the forward model of the drop size distribution. This model is developed using the fuzzy models in Chapter 3, in which the Sauter mean diameter, initial drop diameter and beta distribution with the random number of volume fraction are developed. Furthermore, it presents the distribution of drops along the RDC column and plotting the volume fraction for each stage.

The fifth chapter presents the inverse model of drop size distribution, which is used to determine the number of drops at the bottom stage by the number of drops at the top stage using the fuzzy approach. Furthermore, this model can be used for the control of the distribution of drops between stages. This chapter provides a new relationship for all the Sauter mean diameters along the RDC column.

In Chapter 6, the model of mass transfer is developed that can be incorporated in the forward model of drop size distribution to determine the concentrations of the continuous and dispersed phase. This model can be considered as the flexible model, which is able to work with different velocities of drops and allows for a change in the value of the geometrical and physical properties of the RDC column, such as

rotor speed, height of compartment and flow rate. Furthermore, it is considered as a predictive model that can be used to determine the relationship between the geometrical and physical properties of the RDC column, such as the relationship between the rotor speed and flow rate, concentration of phases and interfacial tension.

Chapter 7, the final chapter concludes the thesis and includes suggestions for the further research of this field. Figure 1.1 shows the flow chart of the organization of the thesis.

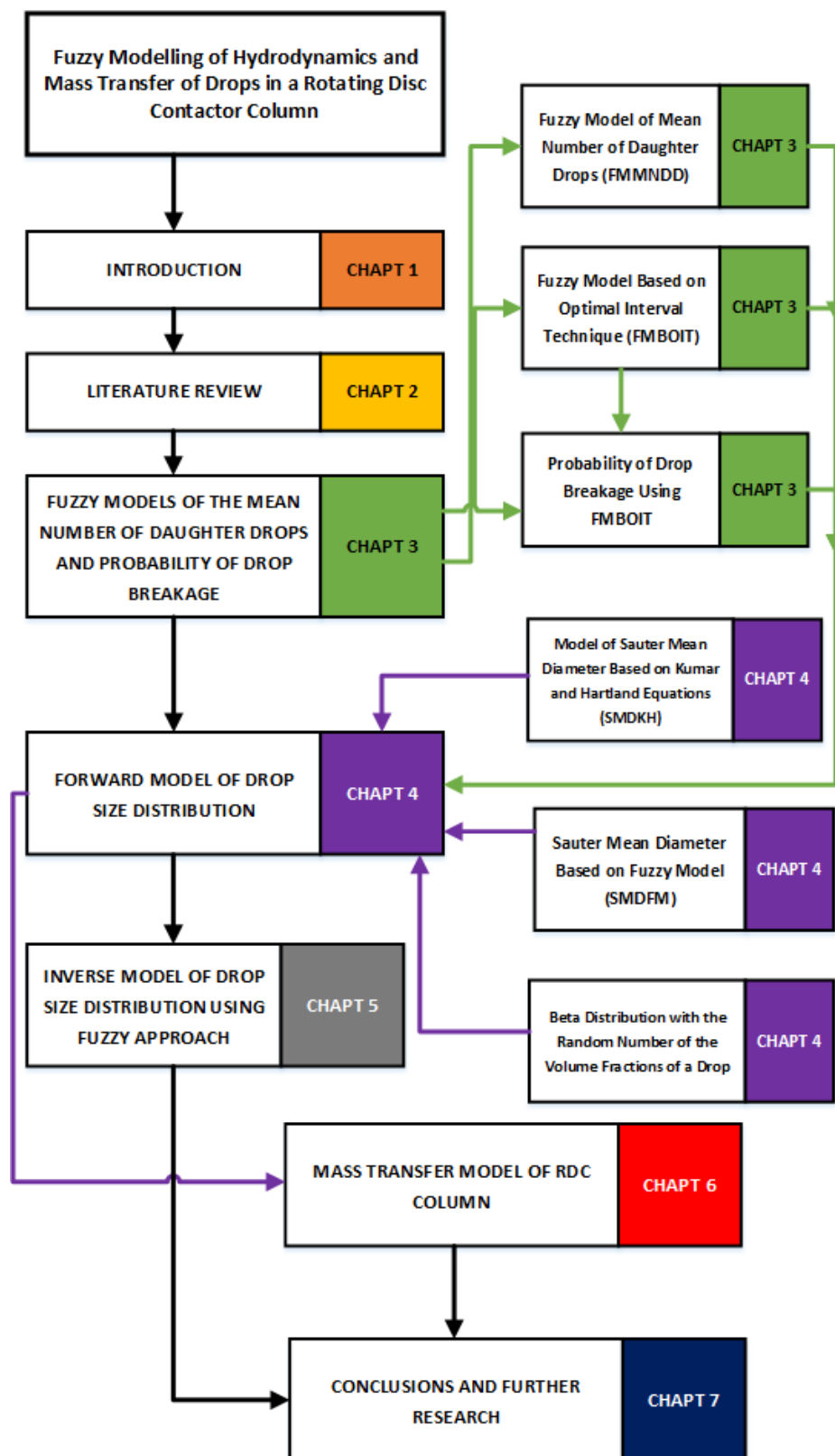


Figure 1.1: Organization of the Thesis

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