

CO₂ Absorption and Mass Transfer in Film Flow on a Rotating Disc

MD S. Miah, Mohammad S. Hossain, Abid A. Khan, Muhammad A. Ashraf, and Zoubir Zouaoui

Abstract—The phenomenon of mass transfer is of vital importance in numerous industrial applications where gas and liquid phases interact. These mainly comprise chemical, semiconductor production, material industries etc. Separation of CO₂ and other gasses from different materials, generating impurities and compromising material's electrical and mechanical properties are of prime importance. CO₂ absorption of a film flow of poly-ethylene terephthalate (PET) on a rotating disc is taken as a sample case for investigation through advanced computational fluid dynamics (CFD) modelling. A survey was conducted for different degrees of polymerization and angular velocities. The Volume of Fluid model (VOF) was used to measure the layer thickness of the molten PET, which can affect the mass transfer phenomenon. The profile of the concentration of CO₂ was also investigated through user defined scalar (UDS) transport equations. This work is based on observation and investigation of the concentration profiles at different positions over the disc which emphasised the effects of the convective forces in the mass transfer phenomenon particularly at higher radial position. The results revealed that mass transfer of CO₂ depends on the thickness of PET layer and fluid viscosity. It was also observed that convection transport strongly influences the rate of absorption over different disc positions.

Index Terms—Absorption, Computational Fluid Dynamics (CFD), film flow, mass transfer, rotating disc, thickness.

I. INTRODUCTION

The phenomenon of mass transfer between a gas and a liquid is commonly encountered in many industrial applications. The chemical industries have perhaps the strongest mass transfer emphasis, notably through phenomena like extraction, separation, gas absorption or even adsorption [1]. An interesting application for the future is undoubtedly the capture and sequestration of greenhouse gas. In the light of increasing concerns about global warming caused by the effects of CO₂, companies have been urged to develop technologies to capture and sequester CO₂ from their emissions.

Different systems have been studied to remove carbon dioxide from gases employing liquid. Some of these comprise different physical techniques like absorption,

adsorption or membrane technique. The most famous and mature technology is the absorption process, using amine solutions such as mono-ethanolamine (MEA). It has been used in industry for 60 years, the CO₂ recovery rate with this technology is reported as 98%. However, regarding the energy consumption and the stability of the amines, many improvements need to be considered [2]. One of the main devices used here are the packed columns [3], which are commonly used to remove particular species from a gas stream by using a liquid. The liquid streams along the column and the wet surface in contact with the gas will be the place of the mass transfer of the species (absorption).

More recently, there has been increased interest on the mass transfer of film flow over rotating disc in order to improve the efficiency of classical systems. It is considered as a high performance device compared to conventional systems, many industrial applications which use mass transfer phenomenon employ this technology into their process. PET is the most common type of polyester and its properties make it suitable for a wide range of product applications including product packaging [4]. According to transparency market research (2012), 'the global PET market was estimated to be worth USD 23.3 billion in 2010 and is expected to reach USD 48.4 billion in 2016' [5]. During the synthesis of the PET, two monomers and a by-product component (Ethylene Glycol) are created [6]. In the last stage of poly-condensation process, the reactor must include the removal process for this by-product in order to get a high quality polymer. To separate this component from the melt polymer, the last stage reactor is made up with a large horizontal cylindrical vessel, which contains several vertical discs mounted along a rotating shaft. Each disc facilitates the removal of volatile product from the polymer by creating a film fluid over its surface where the diffusion of by-product takes place [6]. This emphasises the necessity of studying mass transfer phenomenon of film fluid created on a rotating disc in order to improve PET quality and the efficiency of PET polymerization technology. The work presented in this paper is aimed to be step ahead in this direction.

II. THEORETICAL ANALYSIS

Diffusion of CO₂ inside the film layer of PET is theoretically discussed. It was assumed that the mass transfer occurred by diffusion and not by convection. Earlier literature review focused on general mass transfer based on the Higbie's model to approximate the solution [7]. This section aims at applying this knowledge and study the diffusion term and the accumulation term of the equation for a rotating disc without using Higbie's model. Diffusion Equation can be approximated by equation 1 [8]:

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$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (1)$$

where,

C = Concentration of CO_2 (mol/kg)

D = Diffusivity of CO_2 in melt polymer

x = Axis perpendicular to the disc.

The equation was solved neglecting the convective and the source terms. The boundary conditions of the system can be described by:

$$\begin{aligned} t = 0, \quad 0 < x < l \quad C &= C_i \\ t > 0, \quad x = l \quad C &= C^* \\ t > 0, \quad x = 0 \quad \partial C / \partial x &= 0 \end{aligned}$$

The solution of this equation associated with the boundary condition is as given in equation 2 [9]:

$$\sum_{n=0}^{\infty} (-1)^n \operatorname{erfc} \frac{(2n+1)l-x}{2\sqrt{Dt}} + \sum_{n=0}^{\infty} (-1)^n \operatorname{erfc} \frac{\frac{C-C_i}{C^*-C_i} \frac{(2n+1)l+x}{2\sqrt{Dt}}}{2\sqrt{Dt}} \quad (2)$$

where,

l = Thickness of the PET layer

C^* = Equilibrium concentration value of CO_2

C_i = Initial concentration value

erfc = Complementary error function defined by equation (3):

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy \quad (3)$$

The time dependent flux of CO_2 is worked out by differentiating the solution equation 4 using output from equation 5[10],

$$N_t = -(C^* - C_i) \sqrt{\frac{1}{\pi t}} \left[1 + 2 \sum_{n=1}^{\infty} (-1)^n \exp \left(-\frac{1}{Dt} \right) \right] \quad (4)$$

$$N_t = -D \left(\frac{\partial C}{\partial x} \right)_{x=l} \quad (5)$$

The average flux of CO_2 during the time interval t is defined by equation 6,

$$\begin{aligned} \bar{N}_t &= -2(C^* - C_i) \sqrt{\frac{1}{\pi t} - 4(C^* - C_i)} \\ &\quad \sqrt{\frac{1}{t} \sum_{n=1}^{\infty} (-1)^n \times \operatorname{ierfc} \left(\frac{1}{\sqrt{Dt}} \right)} \\ \bar{N}_t &= \frac{1}{t} \int_0^t N_t dt \quad (6) \end{aligned}$$

where ierfc is the integral complementary error function defined by equation 7,

$$\operatorname{ierfc}(x) = \int_x^{\infty} \operatorname{erfc}(y) dy$$

Since, $\bar{K}_L = \frac{|\bar{N}_t|}{C^* - C_i}$

$$\bar{K}_L = 2 \sqrt{\frac{D}{\pi t}} \left[1 + 2\sqrt{\pi} \sum_{n=1}^{\infty} (-1)^n \times \operatorname{ierfc} \left(\frac{nl}{\sqrt{Dt}} \right) \right] \quad (7)$$

The time dependent CO_2 mass flux relative to the time is plotted in Fig. 1, using $D_{X_n} = 82$ and $l = 3.4 \text{ mm}$. It was observed that N_t decreased with time. This is due to the fact that the more the liquid is in contact with the gas, the more it

will be filled by CO_2 . Consequently, the value of the mass flux decreases with the decrease of $C^* - C_i$.

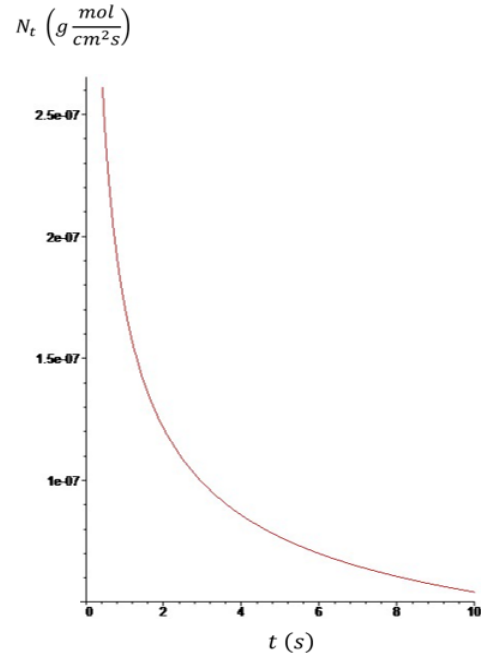


Fig. 1. Time dependent flux of CO_2 .

The convection problem is converted to a diffusional one in which the adjustable parameter l is introduced. This method permits to deal with the steady-state mass transfer problem.

III. NUMERICAL ANALYSIS

A three dimensional model was developed for the modelling of the mass transfer of the PET film flow over one rotating disc, taking into account the mass transfer of the carbon dioxide. The model was generated in GAMBIT 2.4.6 and further simulated in FLUENT 6.4. Two different degrees of polymerization were set up in FLUENT to analyse the effect of the molecular weight on the rate of absorption. The simulations were run for different angular velocity. This section aims at providing the description of the 3D design and the numerical method developed for the task in hand.

A. Methodology

The current study was based on the work carried out in [6]. This permitted to design the system as well as check the validity of the simulation. The reference included an experimental study on the measurement of polymer melt film thickness in a rotating disc poly-condensation reactor. The layer thickness of molten PET was measured at 280°C , at two different angular velocities (10 and 20 rpm) and for three molecular weights (degree of polymerization). The film thickness was evaluated at different radial and angular positions by using an electrical conductivity probe.

The present simulation was run for two molecular weights [$X_n = 69$] and [$X_n = 82$]. For each molecular weight, two different disc speeds 20 rpm and 10 rpm were tested.

B. Model Design

A rotating disc was designed inside the reactor of 14cm diameter. The length of the reactor is also 14cm. The

diameter and the thickness of the disc were 12.7cm and 4mm respectively. The disc was immersed around 34% of the radius in the PET. The design of the system is illustrated in Fig. 2. The quality of the mesh was an important consideration for accurate prediction of the film thickness. The use of bias mesh permitted a very fine mesh near the disc and large cells at the border of the tank [11].

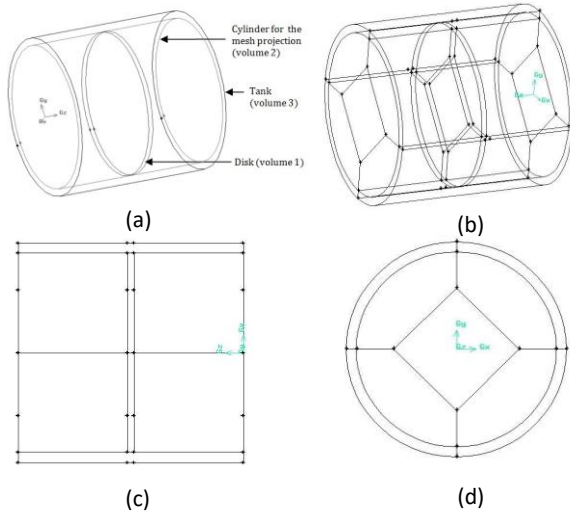


Fig. 2. Design of rotating disc reactor.

The predicted thickness of the film fluid near the disc surface was of main interest. Thickness near the tank borders was of no interest and therefore a rough mesh could suffice at tank borders. A minimal film thickness of 1mm was assumed [11], which was deemed an adequate thickness size. Thus, the minimal mesh size was 0.25mm (i.e. a quarter of the minimum thickness) to obtain a reasonable mesh quality and to ensure the reliability of the results.

C. Boundary Conditions

Table I lists the boundary conditions used in the model. Wall boundary conditions were used to bound fluid and solid regions. The fluid area was defined by interior boundary conditions. Symmetric boundary conditions are used for the vertical surfaces of the tank as seen in Fig. 3. This kind of boundary conditions was appropriate for the system as physical geometry and the expected flow pattern of the solution had mirror symmetry. It was considered that the fluid at the ends of the tank has no velocity [11].

TABLE I: DISC REACTOR BOUNDARY CONDITIONS

Subjective	Description	Boundary condition
[A]	Boarder of Reactor	Symmetry
[B]	Reactor	Wall
[C]	Boarder of Reactor	Symmetry
[D]	Disc	Wall
[E]	Fluid Area	Interior

Concerning the continuum types, one type of fluid was specified inside the reactor: 'PET plus air'. This fluid section is further divided into two fluids in FLUENT. A pressure based solver was used for the low speed incompressible flow. The two phase problem was solved using volume of fluid (VOF) model which permitted modelling of two immiscible fluids. It solves a single set of momentum equations and

marks the volume fraction of each fluid throughout the domain.

This volume fraction was essential to measure the thickness of the film layer. To create the PET Fluid, the non-Newtonian power law was used to set the parameters of the viscosity.

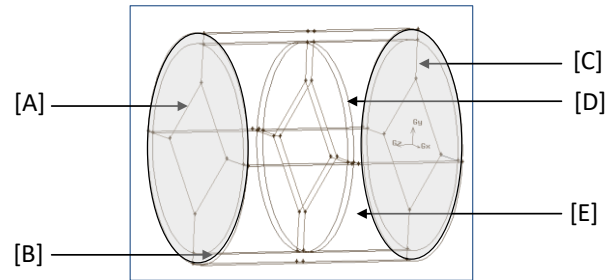


Fig. 3. Boundary conditions.

One of the main objectives of this work was to get the concentration profile in the PET layer. FLUENT needs to solve the UDS transport equations for the solution. CO₂ concentration was considered as a UDS and applied to the air fluid. The mass flow rate for the flux function and the default unsteady function were applied. After the creation of UDS, diffusivity of CO₂ inside the PET must be defined, however this value was hard to obtain in the literature as it depends on the molecular weight, temperature and fluid pressure [12]. Nevertheless, the value of the diffusion coefficient of CO₂ inside the water was easily found in the literature.

IV. NUMERICAL RESULTS AND DISCUSSION

The numerical results were obtained through ANSYS FLUENT 6.4 post processing software package. To confirm the stability of system, film thickness was computed at different number of rotations. The film thickness has been acquired for different molecular weights and rotating speeds of the disc as depicted in Fig. 4. It has been noticed that a higher film thickness can be obtained at a higher rotating speed and higher molecular weight which conforms to the published experimental results in literature [6].

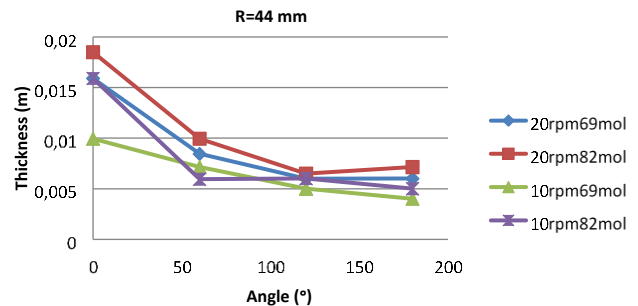


Fig. 4. Film thickness at different angular positions.

The concentration profiles inside the film layer are presented in Figs. 5 and 6. It is worth mentioning that concentration is measured in a flow that is constantly altering/updated due to disc motion. Therefore, for all the positions, the concentration values increase from 0 to 1 due to the boundary conditions set in the solver. It is known that the rate of absorption depends on concentration slope relative to

the distance. The time dependent flux of CO₂ is determined by differentiating the solution of diffusion equation (5).

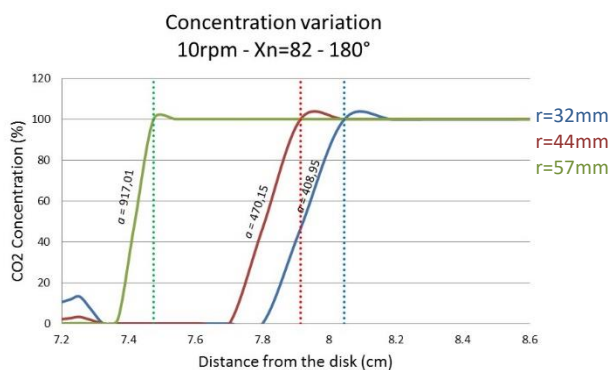


Fig. 5. Concentration slope, 10rpm.

The numerical results in Figs. 5 and 6 can provide the slope of the concentration by linear approximation. The graphs show that the concentration slope increases with radial position. This phenomenon can be explained by the cylindrical diffusion equation.

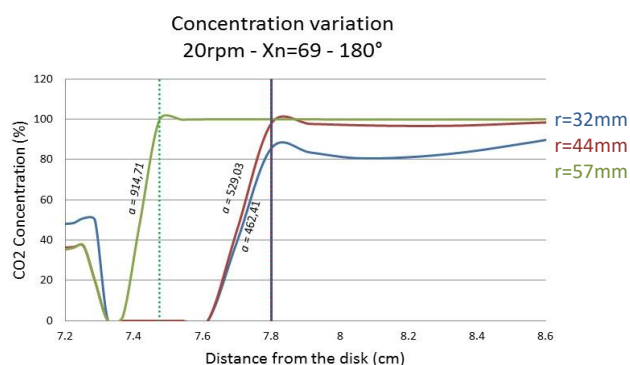


Fig. 6. Concentration slope, 20rpm.

Concerning the diffusive term, it seems that its effect on the rate of absorption is smaller than the convective term at high radial position. The diffusive term, contrary to the convection, represents the fact that the particles of CO₂ diffuses through the film layer, regardless of the motion of the fluid due to concentration gradient. The graphical representation of the liquid mass transfer coefficient K_L as plotted in Fig. 7 reveals that higher mass transfer coefficient is resulted due to higher thickness. Furthermore, in case of very thin film layer the mass transfer coefficient tends to become insufficient to permit a mass transfer by diffusion. It is pertinent to mention that no such case has been observed in the results. However, beyond a certain value, thickness has no influence over the rate of absorption. This statement is verified in the plots of concentration shown in Fig. 5 & 6, where it is evident that after a certain depth inside the layer, the concentration reaches a minimum value and after which rate of absorption is not effected due to film thickness.

We can notice from the diffusion equation (5) that the mass transfer by diffusion strongly depends on the diffusivity of the CO₂ inside the PET layer. The diffusivity equals to 2.31×10^{-14} m²/sec and 4.22×10^{-14} m²/sec for $X_n=82$ and $X_n=69$ respectively.

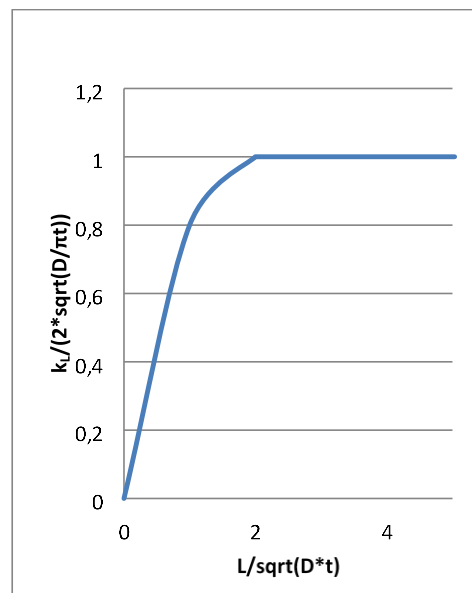


Fig. 7. Graphical representation of K_L .

The results reveal that diffusion is more efficient at low molecular weight which is $X_n=69$.

V. CONCLUSION

The mass transfer phenomenon is widely used in daily life and has many industrial applications, particularly for polymer synthesis. It was in this context that investigation of the CO₂ absorption of a film fluid of PET over a rotating disc was performed. Theoretical and numerical investigations were conducted to develop a full understanding of the effect of different parameters. In order to find the parameters that influence CO₂ absorption, two degrees of PET polymerization $X_n=69,82$ and two disc rotating speeds of 10 and 20 rpm were investigated through advanced CFD modelling. In each case, the layer thickness and the concentration profile were computed at different radial and angular positions.

The theoretical study focused on the mass transfer by diffusion. The diffusion term depends on the layer thickness and the contact time. The fluid viscosity affects the diffusivity and so the rate of absorption. The acquired numerical results for film thickness match well with empirical data [4]. The concentration profile inside the PET layer was determined through UDS transport equations. Analysis revealed that the rate of absorption increases with the radial position. The results also show that the mass transfer of CO₂ is dependent on the thickness of PET layer and fluid viscosity. It was further noticed that the position over the disc strongly influences the rate of absorption.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

Dr. MD Salim Miah headed the research on which Dr. Abid Ali Khan, Dr. Mohammad Sayeed Hossain and Dr. Muhammad Arif Ashraf became active contributors. The paper draft was prepared by the first author and all other four authors helped him in finalizing the draft. However, Dr

Zoubir Zouaoui was involved in vetting and finalizing of the manuscript's final version. All authors had approved the final version.

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