1968

Diffusion coefficients of D-Glucose in aqueous Carboxymethylcellulose and Carboxypolymethylene solutions

Audrey Liu-Mei Huang

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DIFFUSION COEFFICIENTS OF D-GLUCOSE IN AQUEOUS CARBOXYMETHYLCBLLEULOSE AND CARBOXYPOLYMETHYLENE SOLUTIONS

BY

AUDREY LIU-MEI HUANG, 1942

A

THESIS

submitted to the faculty of the UNIVERSITY OF MISSOURI AT ROLLA in partial fulfillment of the requirements for the Degree of

MASTER OF SCIENCE IN CHEMICAL ENGINEERING

Rolla, Missouri 1968

Approved by

Frank H. Conrad

H. O. McDonald
ABSTRACT

A microinterferometric method was used to determine the concentration profiles in the infinite field unsteady state diffusion of D-Glucose in aqueous polymer solutions. Pseudo binary diffusion coefficients were determined as a function of reduced concentration both with and without the effect of liquid volume change during diffusion being considered. The systems studied were D-Glucose in aqueous Carboxymethylcellulose and D-Glucose in aqueous Carboxypolymethylene solutions. Solute concentration ranged from nearly zero to about 9% by weight D-Glucose in the aqueous polymer solutions.
ACKNOWLEDGEMENT

The author is greatly indebted to Dr. R. M. Wellek, Associate Professor of Chemical Engineering, who suggested this study and served as a research advisor. His help, guidance, kindness, and encouragement are sincerely appreciated.

The author wishes to dedicate this work to her loving parents, Dr. and Mrs. Chau-Lin Huang.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>ii</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENT</td>
<td>iii</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>viii</td>
</tr>
<tr>
<td>PROLOGUE TO THESIS</td>
<td>x</td>
</tr>
<tr>
<td>DIFFUSION COEFFICIENTS OF D-GLUCOSE IN AQUEOUS CARBOXYMETHYLCELLULOSE AND CARBOXYPOLYMETHYLINE SOLUTIONS</td>
<td>1</td>
</tr>
<tr>
<td>1. Introduction</td>
<td>1</td>
</tr>
<tr>
<td>2. Apparatus</td>
<td>3</td>
</tr>
<tr>
<td>3. Analysis of Data</td>
<td>3</td>
</tr>
<tr>
<td>4. Procedure and Results</td>
<td>7</td>
</tr>
<tr>
<td>5. Discussion of Results</td>
<td>8</td>
</tr>
<tr>
<td>6. Nomenclature</td>
<td>16</td>
</tr>
<tr>
<td>7. Bibliography</td>
<td>18</td>
</tr>
<tr>
<td>APPENDICES</td>
<td></td>
</tr>
<tr>
<td>A. Computer Programs</td>
<td>19</td>
</tr>
<tr>
<td>B. Data and Results</td>
<td>51</td>
</tr>
<tr>
<td>C. Theoretical Equation of Diffusion</td>
<td>64</td>
</tr>
<tr>
<td>D. Diffusivity Computation Techniques</td>
<td>66</td>
</tr>
<tr>
<td>E. Figures of Diffusivity (cm²/sec) Versus Reduced Concentration</td>
<td>80</td>
</tr>
<tr>
<td>F. Comparison for Five Different Methods of Calculating the Diffusivity</td>
<td>91</td>
</tr>
<tr>
<td>G. Measurement of the Density</td>
<td>102</td>
</tr>
<tr>
<td>H. Calculation of Differential Diffusion Coefficient of D-Glucose Using Wilke-Chang Correlation and Clough et al Correlation</td>
<td>103</td>
</tr>
</tbody>
</table>
I. Nomenclature.......................... 106
J. Bibliography.......................... 109
VITA........................................ 111
## LIST OF FIGURES

<table>
<thead>
<tr>
<th>FIGURE</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Differential Diffusivity vs. Solute Reduced Concentration for CMC-Water System</td>
<td>9</td>
</tr>
<tr>
<td>2.</td>
<td>Differential Diffusivity vs. Solute Reduced Concentration for Carbopol-Water System</td>
<td>10</td>
</tr>
<tr>
<td>D.1.</td>
<td>Experimental Reduced Concentration Profile for 0.25 wt.% Carbopol System</td>
<td>67</td>
</tr>
<tr>
<td>D.2.</td>
<td>Evaluation of ( \int_0^1 y^* x^* dy^* ) for ( \int_0^1 x^* dy^* = 0 )</td>
<td>77</td>
</tr>
<tr>
<td>D.3.</td>
<td>Evaluation of ( \int_0^1 y^* x^* dy^* ) and ( \int_0^1 y^* x^* d^* y^* ) for ( \int_0^1 x^* dy^* + 2A^* M^* A_1 ) ( \int_0^1 y^* x^* dy^* = 0 )</td>
<td>78</td>
</tr>
<tr>
<td>E.1.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 2.2 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with ( t = 12 ) seconds.</td>
<td>81</td>
</tr>
<tr>
<td>E.2.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 2.0 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with ( t = 50 ) seconds.</td>
<td>82</td>
</tr>
<tr>
<td>E.3.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 1.7 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with ( t = 20 ) seconds.</td>
<td>83</td>
</tr>
<tr>
<td>E.4.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 1.35 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with ( t = 18 ) seconds.</td>
<td>84</td>
</tr>
<tr>
<td>E.5.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 1.20 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with ( t = 20 ) seconds.</td>
<td>85</td>
</tr>
<tr>
<td>E.6.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 0.28 wt.% Carbopol in Water with D-Glucose as Solute, at 23°C, with ( t = 30 ) seconds.</td>
<td>86</td>
</tr>
<tr>
<td>E.7.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 0.25 wt.% Carbopol in Water with D-Glucose as Solute, at 21°C, with ( t = 24 ) seconds.</td>
<td>87</td>
</tr>
<tr>
<td>FIGURE</td>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>----------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>E.8.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 0.22 wt.% Carbopol in Water with D-Glucose as Solute, at 21°C, with t = 6 seconds</td>
<td>88</td>
</tr>
<tr>
<td>E.9.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 0.20 wt.% Carbopol in Water with D-Glucose as Solute, at 23°C, with t = 20 seconds</td>
<td>89</td>
</tr>
<tr>
<td>E.10.</td>
<td>Differential Diffusivity vs. Reduced Concentration for 0.18 wt.% Carbopol in Water with D-Glucose as Solute, at 23°C, with t = 20 seconds</td>
<td>90</td>
</tr>
</tbody>
</table>
LIST OF TABLES

<table>
<thead>
<tr>
<th>TABLE</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
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<tr>
<td>B.1</td>
<td>52</td>
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<td>53</td>
</tr>
<tr>
<td>B.3</td>
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<td>B.5</td>
<td>56</td>
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<td>B.6</td>
<td>57</td>
</tr>
<tr>
<td>B.7</td>
<td>58</td>
</tr>
<tr>
<td>B.8</td>
<td>59</td>
</tr>
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</tr>
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<td>61</td>
</tr>
<tr>
<td>B.11</td>
<td>62</td>
</tr>
<tr>
<td>B.12</td>
<td>63</td>
</tr>
<tr>
<td>D.1</td>
<td>72</td>
</tr>
<tr>
<td>F.1</td>
<td>92</td>
</tr>
<tr>
<td>F.2</td>
<td>93</td>
</tr>
<tr>
<td>F.3</td>
<td>94</td>
</tr>
<tr>
<td>F.4</td>
<td>95</td>
</tr>
<tr>
<td>Table</td>
<td>Description</td>
</tr>
<tr>
<td>-------</td>
<td>-------------</td>
</tr>
<tr>
<td>F.5</td>
<td>List of Five Values of Diffusivity for System 5</td>
</tr>
<tr>
<td>F.6</td>
<td>List of Five Values of Diffusivity for System 6</td>
</tr>
<tr>
<td>F.7</td>
<td>List of Five Values of Diffusivity for System 7</td>
</tr>
<tr>
<td>F.8</td>
<td>List of Five Values of Diffusivity for System 8</td>
</tr>
<tr>
<td>F.9</td>
<td>List of Five Values of Diffusivity for System 9</td>
</tr>
<tr>
<td>F.10</td>
<td>List of Five Values of Diffusivity for System 10</td>
</tr>
<tr>
<td>H.1</td>
<td>The Percentage Deviation of Wilke-Chang Value from the Experimental Values</td>
</tr>
</tbody>
</table>
The object of this investigation is to study the effect of solute concentration on the molecular diffusion coefficient in aqueous polymer solutions and also to determine the effect of polymer concentration on the diffusion coefficient. Besides these objectives, the importance of considering the effect of volume changes during the diffusion process is also investigated.

Information concerning molecular diffusion of solute-polymer pairs in concentrated solutions should be useful when considering many important polymer processing steps such as mixing, extraction, dissolution, and fiber formation by solution spinning.

The non-ionic, water-soluble polymers Carboxymethylcellulose (CMC) and Carboxypolymethylene (Carbopol) were used with D-Glucose as the solute. These particular polymer solutions were studied to aid in the prediction of molecular diffusivities for liquid extraction studies.

A microinterferometric technique was used to experimentally determine the diffusivities. Before 1967 the effect of volume changes during diffusion using the interferometric method was not considered. Previous measurements of the diffusivities by Desai(9) of the systems studied in this work were conducted before 1967. Therefore, Desai did not consider the effect of volume change on the diffusivity. In this study, the data of Desai were
reanalyzed considering the effect of volume changes.

The microinterferometric method analyzes the concentration profiles in a free diffusion experiment. Free diffusion will occur when two phases having different concentrations are brought in direct contact with each other. The diffusion process occurs in a cell of effectively infinite length in which there are no concentration changes at the ends of the cell during the period of observation. The most general method of determining binary diffusion coefficients from free diffusion data is that developed by Boltzmann in 1894 (3). However, all of the numerical methods had been derived for the case in which no volume change occurs during the mixing of the diffusion species. As a result of this limitation, many experimenters have chosen to examine diffusion between two solutions of very nearly the same concentration in an attempt to minimize the effect of the volume change during diffusion. From the equation of change and equation of motion, Duda and Vrentas (10) derived an equation from which diffusion coefficients can be obtained from free diffusion experiments. Paul (18) modified the relation to a form which was easier to use. The equations considering both volume with and without change on mixing were used in this study.

Free diffusion by microinterferometric means is currently one of the most accurate methods of measuring molecular diffusion coefficients. Its major advantages
in comparison with the normal interferometric method are, 1) the former equipment is less expensive; 2) the time required to obtain the data is much less; 3) only microgram amounts of solution are required in this method; and 4) since the microinterferometric diffusion cell is very thin, convection currents can be minimized; and hence temperature control is not as difficult to attain with the microinterferometry as it is with the macrointerferometry.
Diffusion Coefficients of D-Glucose in Aqueous Carboxymethylcellulose and Carboxypolymethylene Solutions

A. L. Huang, S. V. Desai, and R. M. Wellek
University of Missouri-Rolla, Rolla, Missouri

1. Introduction

Molecular diffusion coefficients of D-Glucose in aqueous Carboxymethylcellulose (CMC) and Carboxypolymethylene (Carbopol) solutions were measured in this work by a microinterferometric technique. Optical interference methods have been used previously by Kegeles and Gosting (9), Longsworth (10), Ambrose (1), Berg (2), Crank and Robinson (4), Robinson (15), Searle (16), Nishijima and Oster (11,12), and Secor (17). These workers assumed that there was no volume change on mixing during the diffusion process. However, Duda and Vrentas (6,7) derived a relation for calculating the molecular diffusivity which properly considers this effect. Paul (13) applied the relation of Duda and Vrentas for systems with linear density-concentration relations in a manner so that the calculations for diffusion coefficients using the interferometric technique is convenient.

In this investigation, one unsteady state solute concentration profile (observed at a certain time) was analyzed to study the effect of considering volume changes during mixing for the D-Glucose-CMC and D-Glucose-Carbopol systems. The ten systems studied are given in Table 1.
Table 1

Polymeric Systems Used

<table>
<thead>
<tr>
<th>System</th>
<th>Polymer</th>
<th>Solvent</th>
<th>Polymer conc. wt. %</th>
<th>Solute</th>
<th>Initial solute conc. gm/100 cm³ solution</th>
<th>Temperature Degrees C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CMC</td>
<td>Water</td>
<td>2.20</td>
<td>D-Glucose</td>
<td>10</td>
<td>23</td>
</tr>
<tr>
<td>2</td>
<td>CMC</td>
<td>Water</td>
<td>2.00</td>
<td>D-Glucose</td>
<td>10</td>
<td>23</td>
</tr>
<tr>
<td>3</td>
<td>CMC</td>
<td>Water</td>
<td>1.70</td>
<td>D-Glucose</td>
<td>10</td>
<td>23</td>
</tr>
<tr>
<td>4</td>
<td>CMC</td>
<td>Water</td>
<td>1.35</td>
<td>D-Glucose</td>
<td>10</td>
<td>23</td>
</tr>
<tr>
<td>5</td>
<td>CMC</td>
<td>Water</td>
<td>1.20</td>
<td>D-Glucose</td>
<td>10</td>
<td>23</td>
</tr>
<tr>
<td>6</td>
<td>Carbopol</td>
<td>Water</td>
<td>0.28</td>
<td>D-Glucose</td>
<td>10</td>
<td>23</td>
</tr>
<tr>
<td>7</td>
<td>Carbopol</td>
<td>Water</td>
<td>0.25</td>
<td>D-Glucose</td>
<td>10</td>
<td>21</td>
</tr>
<tr>
<td>8</td>
<td>Carbopol</td>
<td>Water</td>
<td>0.22</td>
<td>D-Glucose</td>
<td>10</td>
<td>21</td>
</tr>
<tr>
<td>9</td>
<td>Carbopol</td>
<td>Water</td>
<td>0.20</td>
<td>D-Glucose</td>
<td>10</td>
<td>23</td>
</tr>
<tr>
<td>10</td>
<td>Carbopol</td>
<td>Water</td>
<td>0.18</td>
<td>D-Glucose</td>
<td>10</td>
<td>23</td>
</tr>
</tbody>
</table>
2. Apparatus

The apparatus used in this work was basically the same as that used by Secor (16), except for the Carbopol systems for which platinum coated slides were used instead of aluminum coated slides to eliminate corrosion problems. In this study the range of the apparent viscosity of the polymer solutions used in the CMC system was from 635 centipoise to 9840 centipoise, and the range of viscosity used in the Carbopol system was from 819 centipoise to 17980 centipoise. For systems with viscosities significantly outside these ranges, the microinterferometric method could not be used; this effectively limited the range of polymer concentrations which could be studied.

3. Analysis of Data

Secor (16) used one concentration profile observed at a certain time and assumed no volume change on mixing during the diffusion process. The diffusion coefficient was calculated as a function of concentration using the following relation:

$$D_{AB}^{(3)} = - \int_0^Y \frac{x dy}{2t \frac{dy}{dx}}$$

Paul (13) observed that when the total fringe deflection was small and only a few fringes (10 or less) cross a line drawn parallel to the x axis, the errors involved in measuring the fringe deflection from a photograph as a
function of \( x \) would considerably affect the evaluation of the integrals and make graphical differentiation of these data very unreliable. In view of this problem, Paul used several concentration profiles which were observed at various times in order to help reduce the random error of transposing the fringe contour on a photograph into digital data. The profiles were combined into a master plot by using the Boltzmann transformation. The diffusion coefficient which considers volume changes during diffusion was then calculated as a function of reduced concentration from the following relation:

\[
D_{AB}^{(2)} = -\frac{2 \int_{0}^{y^*} (1-AW_A y^*) \eta dy^* + 2AW_A \int_{0}^{y^*} \eta y^* dy^*}{(1+AW_A y^*)(dy^*/d\eta)} \tag{2}
\]

where

\[ y^* = W_A/W_A = \text{reduced concentrations} \]
\[ W_A = \text{weight fraction of the solute} \]
\[ \rho = \rho_s (1+AW_A) = \text{solution density} \]
\[ \eta = x/2t^{1/2} \]

The effect of volume changes during diffusion is considered through the variable solution density, \( \rho \), for the different solute concentrations.

In this work, only one profile for each system was used -- both with and without the effects of volume changes during diffusion being considered in the calculations. The total fringe deflection in this work was not as small as Paul's; hence, the use of only one concentration profile probably does not contribute significantly to the possible errors mentioned by Paul. The time, \( t \), which was a
finite known value was separated from $\eta$ in this work for calculational convenience. Thus, in the case of diffusion with volume change, the pseudo binary diffusivity was calculated from the following relation:

$$D_{AB}^{(1)} = -\frac{(1-AW_{AL}y^*) \int_0^{y_*} xdy^* + 2AW_{AL} \int_0^{y_*} xy^* dy^*}{2t (1 + AW_{AL}y^*) \frac{dy^*}{dx}}$$  \hspace{1cm} (3)$$

When the volume change was not considered, the above relation was simplified as follows:

$$D_{AB}^{(2)} = -\frac{\int_0^{y_*} xdy^*}{2t (dy^*/dx)}$$  \hspace{1cm} (4)$$

which is, except for the concentration variable, essentially equivalent to equation (1).

In order to find the position of the original interface ($x=p$) when it is assumed that no volume change during diffusion occurs, the original interface was located so that the amount of substance leaving one half-plane is equal to the amount of substance arriving at the second half-plane (4,8,17). That is

$$-\int_0^{yp} xdy^* = \int_{yp}^{1} xdy^*$$  \hspace{1cm} (5)$$

where $yp$ is the value of $y^*$ corresponding to $p$. The relation for finding the original interface for volume changes during diffusion was presented by Paul (13) as follows:
The iterative procedure used to locate p is described in Appendix D.

In order to perform the integrations indicated in equations (1), (3), and (4), it is very useful to have an analytic relation between $y^*$ and $x$. The functional relation of the data is approximately represented by the following sigmoidal equation

$$y^* = ab^c G(x)$$

where

$$G(x) = \frac{x}{r} - 1$$

In this work, the scaling factor $r$ was taken to be 0.005.

The method suggested by Davis (5) and used by Secor (17) required first that the data ($y^*$ versus $x$) be curve-fitted by passing a smooth curve through the data by "eye". From this smooth curve, values of $y^*$ at equal increments of $x$ are obtained for use in the method of Davis to determine the constants $a$, $b$, and $c$. It was found in this work, however, that human bias in the smoothing of the data often resulted in significantly different final results of the curve-fit of equation (7).

Thus in this work, an iterative non-linear least squares method was used to determine the curve-fit of equation (7) (which is non-linear in the constants $a$, $b$, and $c) directly from the original data—which in
general were at unequal increments in $x$. The least squares procedure used in this work resulted in a closer fit of the data to equation (7) than the procedure of Davis (5). See Appendix D.

The integrals $\int_0^{y^*} x \, dy^*$ and $\int_0^{y^*} xy^* \, dy^*$ were evaluated by Simpson's numerical method using equation (7). However, it was found convenient to first transform $x$ to function of $y^*$, i.e. $x = f(y^*)$, and then evaluate the integrals $\int_0^{y^*} f(y^*) \, dy^*$ and $\int_0^{y^*} f(y^*)y^* \, dy^*$. The derivative $dy^*/dx$ was easily obtained by directly differentiating the Gompertz equation.

A detailed discussion of the analysis of the data is given in Appendix D.

4. Procedure and Results

The experimental procedure used here was basically the same as that used by Secor (17).

The refractive index-concentration relationships were obtained by making measurements of a series of polymer solutions with known solute concentration using an Abbe Spencer refractometer. The index of refraction using an Abbe Spencer refractometer could be determined to $\pm 0.0001$. The resulting refractive index-concentration relationships were represented by the relation

$$ n = R_0 + R_1 y $$

(8)

The constants $R_0$ and $R_1$ are given in Table B.12 of Appendix B.
The densities were measured using a pycnometer using standard techniques (see Appendix G). The density and the concentration dependence of density are given in Table 2.

The molecular diffusion results are given in Figures 1 and 2 as the differential diffusion coefficient versus reduced concentration of the solute. Diffusion coefficient $D_{AB}^{(1)}$, presented in these figures were calculated using equation (3), which considers the density effect on mixing during molecular diffusion.

5. **Discussion of Results**

The diffusion coefficients were calculated for two cases: $D_{AB}^{(1)}$ using equation (3) and $D_{AB}^{(2)}$ using equation (4). For each system, each value of diffusivity, $D_{AB}^{(2)}$, which does not consider the volume change is always slightly smaller than the diffusivity, $D_{AB}^{(1)}$ which does consider volume changes. The absolute percentage deviation of $D_{AB}^{(2)}$ from $D_{AB}^{(1)}$ decreases as the reduced concentration increases. For all ten systems, the maximum percentage deviations ranged from -4.49% to -0.62%, depending on the system. Though the deviation is not large, the small changes in volume on mixing have been properly considered. See Appendix F for further analysis of the various differential diffusivities.
Figure 1. Differential Diffusivity vs. Solute Reduced Concentration for CMC-Water System
Figure 2. Differential Diffusivity vs. Solute Reduced Concentration for Carbopol-Water System
Table 2
Density of Pure Solvent and the Concentration Dependence of the Solution Density

<table>
<thead>
<tr>
<th>System Number</th>
<th>$\rho_s$</th>
<th>A</th>
<th>°C</th>
<th>W_{Al}</th>
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<tbody>
<tr>
<td>1</td>
<td>1.0089</td>
<td>0.3387</td>
<td>23</td>
<td>0.0902</td>
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<tr>
<td>2</td>
<td>1.0070</td>
<td>0.3507</td>
<td>23</td>
<td>0.0903</td>
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<tr>
<td>3</td>
<td>1.0048</td>
<td>0.3328</td>
<td>23</td>
<td>0.0905</td>
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<tr>
<td>4</td>
<td>1.0041</td>
<td>0.3132</td>
<td>23</td>
<td>0.0906</td>
</tr>
<tr>
<td>5</td>
<td>1.0029</td>
<td>0.2630</td>
<td>23</td>
<td>0.0907</td>
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<tr>
<td>6</td>
<td>0.9987</td>
<td>0.3790</td>
<td>23</td>
<td>0.0910</td>
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<tr>
<td>7</td>
<td>0.9999</td>
<td>0.3552</td>
<td>21</td>
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<td>8</td>
<td>0.9991</td>
<td>0.3750</td>
<td>21</td>
<td>0.0910</td>
</tr>
<tr>
<td>9</td>
<td>0.9990</td>
<td>0.3573</td>
<td>23</td>
<td>0.0910</td>
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<tr>
<td>10</td>
<td>0.9989</td>
<td>0.3558</td>
<td>23</td>
<td>0.0910</td>
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<tr>
<td>System Number</td>
<td>Polymer</td>
<td>Solvent</td>
<td>10 gm/100 cm$^3$ Solution</td>
<td>$\overline{D}_{AB}^{(1)}$ cm$^2$/sec$^{10^5}$</td>
</tr>
<tr>
<td>---------------</td>
<td>------------</td>
<td>---------</td>
<td>---------------------------</td>
<td>---------------------------------</td>
</tr>
<tr>
<td>1</td>
<td>CMC 2.20%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>1.140</td>
</tr>
<tr>
<td>2</td>
<td>CMC 2.00%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>1.121</td>
</tr>
<tr>
<td>3</td>
<td>CMC 1.70%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>0.969</td>
</tr>
<tr>
<td>4</td>
<td>CMC 1.35%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>1.292</td>
</tr>
<tr>
<td>5</td>
<td>CMC 1.20%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>1.717</td>
</tr>
<tr>
<td>6</td>
<td>Carbopol 0.28%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>0.874</td>
</tr>
<tr>
<td>7</td>
<td>Carbopol 0.25%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>1.120</td>
</tr>
<tr>
<td>8</td>
<td>Carbopol 0.22%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>0.878</td>
</tr>
<tr>
<td>9</td>
<td>Carbopol 0.20%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>0.861</td>
</tr>
<tr>
<td>10</td>
<td>Carbopol 0.18%</td>
<td>Water</td>
<td>D-Glucose</td>
<td>1.415</td>
</tr>
</tbody>
</table>
The integral average diffusivities, \( \overline{D} \), for the two polymers were given in Table 3. Though the data are somewhat scattered, the integral diffusivities of both D-Glucose-CMC and D-Glucose-Carbopol appear to increase with decreases of polymer concentration.

The diffusion coefficient of D-Glucose in pure water at 23°C calculated using the Wilke-Chang (18) equation (for dilute Newtonian solutions) was found to be 0.71(10)-5 cm²/sec, while at 21°C it was 0.67(10)-5 cm²/sec. These predictions may be compared with the experimental values (at the lowest value solute concentration for each system). The percentage deviation of the Wilke-Chang prediction from the experimental value ranged from -39.2% to 52.2% (the respective experimental diffusivities were 1.18(10)-5 cm²/sec and 0.439(10)-5 cm²/sec). For very low solute concentrations and low polymer concentrations, the Wilke-Chang equation may be used for only approximate estimations of the diffusivity.

Clough et al. (3) have suggested a semi-theoretical equation for predicting the diffusivity of a solute in non-Newtonian solutions.

\[
\frac{D_{NN}}{D} = X_{cp} \left( \frac{\xi}{\xi_{cp}} \right) \left( \frac{\mu}{\mu_{cp}} \right) \tag{9}
\]

Ree and Eyring (14) show that the average of \( \xi \) is about 6.0 in non-polar, organic fluids, and the best available average value of \( \xi \) is 15.5 in aqueous systems. Therefore, \( \xi / \xi_{cp} \) equal to 15.5/6.0 was used in this
work for comparisons with experimental data. Though the ratio $\mu/\mu_{cp}$ in the work of Clough et al may be established by means of direct rheological measurements, the rheological measurements for these ten systems were not performed in this study. Clough et al studied $\beta$-napthol diffusing through a 1% aqueous solution of sodium carboxymethylcellulose. None of ten systems in this work was exactly the same as those studied by Clough. However, system 5 (D-Glucose diffusing through a 1.2% aqueous solution of CMC) is relatively similar to the 1% CMC system used by Clough et al. Therefore, as an approximation Clough's value of $\mu_{cp}=3.0$ centipoise for a 1.0% CMC system was used here. If one assumes solvation to triple the effective volume of a CMC molecule in solution (3), $X_{cp}$ would be equal to 0.97. The Wilke-Chang (18) value of the diffusivity (in pure water) was calculated to be $0.71(10)^{-5}$cm$^2$/sec and was used as the diffusivity of Newtonian fluid, D. Then $D_{NN}$ for system 5 using equation (9) is predicted to be $0.547(10)^{-5}$cm$^2$/sec.

The lowest experimental value of the diffusivity for this system (at the solute concentration of 0.84 gm/100 cc solution) is $1.18(10)^{-5}$cm$^2$/sec. The percentage deviation of the Clough et al predicted value from this experimental value is -53.7%. The percentage deviation of the Wilke-Chang predicted value from this experimental value is
-39.8%. Thus, for this one particular system, the Wilke-Chang relation seemed to be slightly more accurate than the relation of Clough et al (3).
6. **Nomenclature**

\[ A = \text{concentration dependence of the solution density} \]
\[ a,b,c = \text{constants in Gompertz equation} \]
\[ D = \text{molecular diffusion coefficient of a solute, cm}^2/\text{sec} \]
\[ G = \text{coordinate, corresponds to distance after the changing of the scale} \]
\[ p = \text{original interface at x axis, cm} \]
\[ t = \text{time measured from the beginning of the experiment, seconds} \]
\[ x = \text{coordinate, corresponds to distance cm} \]
\[ Y = \text{concentration of solute, gm/100 cm}^3 \]
\[ y = \text{concentration of solute, gm/cm}^3 \]
\[ y* = \text{reduced concentration } \frac{W_A}{W_{Al}} \]
\[ yp = \text{reduced concentration } y* \text{ corresponds to } p \]
\[ W = \text{weight fraction of solute, } \frac{Y}{(Y + \text{wt. of Polymer solution})} \]
\[ X = \text{the volume fraction of the continuous phase} \]
\[ n = \text{refractive index} \]
\[ \bar{D} = \text{integral (average) diffusion coefficient of a solute, cm}^2/\text{sec} \]

**Subscripts**

A = solute A
B = solvent B
Al = initial weight fraction of solute
AO = solute free weight fraction
NN = diffusivity of a non-Newtonian fluid

cp = properties or parameters of the continuous phase portion of the non-Newtonian fluid

Greek Letters

\( \mu = \) viscosity of the fluid

\( \zeta = \) number of neighbors of the diffusing molecule which are sheared during its advancing a distance equal to one lattice parameter

\( \eta = \) Boltzmann transformation, \( x/2t^{1/2} \), cm/sec^{1/2}

\( \rho = \) total mass density (solution density) gm/cm^3

\( \rho_s = \) solute-free density, gm/cm^3
7. **BIBLIOGRAPHY**


## Appendix A
### Computer Programs

<table>
<thead>
<tr>
<th>Page</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A-1.</td>
<td>Calculation of Reduced Concentration from Concentration of Solute</td>
</tr>
<tr>
<td>A-2.</td>
<td>Calculation of the Concentration Dependence of Density</td>
</tr>
<tr>
<td>A-3.</td>
<td>Least-Squares Curve Fit of Gompertz Equations, for Equal Intervals of the Independent Variable (Method of Davis)</td>
</tr>
<tr>
<td>A-4.</td>
<td>Non-Linear, Iterative Least Squares Curve Fit to the Data of Gompertz Equations</td>
</tr>
<tr>
<td>A-5.</td>
<td>Reduced Concentration Gradient as a Function of Distance</td>
</tr>
<tr>
<td>A-6a.</td>
<td>Locating the Original Interface Considering Volume Changes</td>
</tr>
<tr>
<td>A-6b.</td>
<td>Locating the Original Interface Neglecting Volume Changes</td>
</tr>
<tr>
<td>A-7a.</td>
<td>Evaluation of Integral: $\int f(y*)dy*$</td>
</tr>
<tr>
<td>A-7b.</td>
<td>Evaluation of Integral: $\int f(y*)y<em>dy</em>$</td>
</tr>
<tr>
<td>A-7c.</td>
<td>Evaluation of Integral: $\int ydy*$</td>
</tr>
<tr>
<td>A-8a.</td>
<td>Calculation of the Diffusivity as a Function of Reduced Concentration for Systems with Volume Change</td>
</tr>
<tr>
<td>A-8b.</td>
<td>Calculation of the Diffusivity as a Function of Reduced Concentration for Systems without Volume Change</td>
</tr>
</tbody>
</table>
Program No. 1

Calculation of Reduced Concentration from Concentration of Solute

C A = WT. OF D-GLUCOSE DURING DIFFUSION
C P = WT. OF POLYMER AS SOLVENT
C AP = WT. OF SOLUTION DURING DIFFUSION
C C = WT. OF D-GLUCOSE AT THE BEGINNING
C RC = WT. OF SOLUTION AT THE BEGINNING
C AAB = WT. FRACTION DURING DIFFUSION
C CCA = WT. FRACTION AT THE BEGINNING
C DHO = DENSITY OF WATER
C WHO = WT. OF WATER 25ML
C WPO = WT. OF POLYMER 25ML
DIMENSION A(30), AP(30), AAB(30), RC(30), X(30), Z(30)
READ(I,100)K
DO 10 I=1,K
WRITE(3,1001)
WRITE(3,1002)K
READ(I,200)C,K
READ(I,300)DHO,WHO,WPO
READ(I,400)(A(I),I=1,K)
READ(I,400)(X(I),I=1,K)
BC=DHO*WPO/WHO
A=100.0*DHO*WPO/WHO
BC=BC+5
CCR=C/BC
WRITE(3,3001)K
WRITE(3,3002)
WRITE(3,3003)CCR
DO 20 I=1,K
A(I)=A(I)+5
AAB(I)=A(I)/AB(I)
RC(I)=AAB(I)/CCR
WRITE(3,4000)AAB(I),RC(I),X(I)
20 CONTINUE
10 CONTINUE
STOP

Continued on next page
kk = number of total systems

k = number of total data points (input) for each system

x = distance from original data.
Program No. 2

Calculation of the Concentration Dependence of Density A

C VS=WT. OF PURE POLYMER
C WS=WT. OF WATER
C V =WT. OF POLYMER DURING MIXING

DIMENSION D(20), A(20), W(20), V(20)
READ(1,100) KK
DO 10 I=1, KK
READ(1,200)N, VS, WS
READ(1,300) (V(I), W(I), I=1, N)
WRITE(2,1000) KK
DS = VS/WS
WRITE(2,3000) DS
WRITE(3,3000) SUM=0.0
DO 20 I=1, N
D(I)=V(I)/WS
A(I)=(D(I)-DS)/(DS*W(I))
WRITE(2,4000) D(I), W(I), A(I)
SUM=SUM+A(I)
20 CONTINUE
AA=SUM/N
WRITE(3,5000) AA
SUM1=0.0
SUM2=0.0
DO 30 I=1, N
DE=(AA-A(I))*100.0
DV=DE/AA
SUM1=SUM1+(ABS(DE))
SUM2=SUM2+(ABS(DV))
WRITE(3,6000) DE, DV
30 CONTINUE
DIFF=SUM1/N
DIFF2=SUM2/N
WRITE(3,6000) DIFF, DIFF2
10 CONTINUE
STOP

Continued on next page
kk = number of total systems
A = the concentration dependence of density
W = weight fraction
Program No. 3

Least-Square Curve Fit of Compertz Equations, for Equal Intervals of the Independent Variable (Method of Davis)

DIMENSION Y(30), YC(30)
READ(1, 905) KK

DO 900 IJK = 1, KK
WRITE (3, 901)
WRITE (3, 902) IJK
WRITE (3, 903)
WRITE (3, 904)
READ(1, 101) N
READ(1, 102) (X(I), Y(I), I = 1, N)

S(1) = 0.0
S(2) = C, C
S(3) = 0.0
DO 1 I = 1, N
1 S(I) = X(I) / 0.005 - 1.0
SUM = 0.0
K = N / 3
L = 1
1 K = L

DO 10 J = 1, 3
DO 11 I = 1, K
11 S(J) = S(J) + ALOG(Y(I))
L = K + 1
10 K = L + K
P = N / 3
2 = 1.0 / P
CN = (S(2) - S(3)) / (S(1) - S(2))
C = CN ** P
AL = (S(1) - ((S(1) - S(2)) / (1.0 - CN))) * P
AL = EXP(AL)
BL = (S(1) - S(2)) * (1.0 - C) / ((1.0 - CN) ** 2)
BL = EXP(BL)
SR = 0.0
WRITE (2, 103) AL, BL, C
WRITE (3, 105)
WRITE (3, 104)
DO 12 I = 1, N

Continued on next page
Y(C(I))=AL*(RL**(C**G(I))))
D=Y(C(I))-Y(I)
DV=(D/Y(I))*100.0
SUM=SUM+(ABS(DV))
SR=SR+(D**2)
WRITE(3,107)X(I),Y(I),Y(C(I)),D,DV

12 CONTINUE
WRITE(3,105)
WRITE(3,104)SR
E=N
DEV=SUM/E
WRITE(3,105)
WRITE(3,108)DEV
900 CONTINUE
STOP
101 FORMAT(15)
102 FORMAT(4F18.8)
103 FORMAT(4X,2HA=',F18.8,4X?HA=',E18.8,4X2HC=',E18.8)
104 FORMAT(4X4HX(I),14X4HY(I),12X8HY(I)CALC,12X4HDIFF,12X8HPER DEVI)
105 FORMAT(77)
106 FORMAT(25H SUM OF RESIDUAL SQUARE =E18.8)
107 FORMAT(5F18.8)
108 FORMAT(25H APS. AVE. PERCENT DEVI. =E18.8)
109 FORMAT(2F18.8)
901 FORMAT(1H1)
902 FORMAT(1X10HSYSTEM NO..I3)
903 FORMAT(77)
904 FORMAT(/)
905 FORMAT(15)
END

/data

kk = number of total system
N = number of total data points for each system
X = distance in cm
Y = reduced concentration

AL = constant of Gompertz equation a
BL = constant of Gompertz equation b
CL = constant of Gompertz equation c
Program No. 4

Non-Linear, Iterative Least Squares Curve Fit to the Data of Gompertz Equations.

C N = 3
C N9 = NUMBER OF DATA POINTS
C N = NUMBER OF PARAMETERS

DIMENSION A(30,30), D(30,30), F(30), C(1,30), X(30), Y(30), P(30), P0(30), P0(30)
DIMENSION AA(30,30), G(30), P(30), P(30), P0(30), P0(30)
READ(1,102)KK
DO 30 N9=1,30
WRITE(3,200)
READ(1,1001)N9,N
M=N+1
WRITE(3,202)N9,N
READ(1,103)A1,A2,A3
READ(1,101)G(I),Y(I),I=1,N9
WRITE(3,201)A1,A2,A3
ABC=1
DO 31 I=1,N9
31 X(I)=G(I)/0.005-1.0
GO TO 226
99 DO 90 J=1,N
90 A(I,J)=0
DO 10 I=1,N9
10 DO J=1,N
X(I)=G(I)/0.005-1.0
P(I)=A1*A2**A3**X(I)
AA(I,I)=P(I)/A1
AA(2,I)=(A3**X(I(I))*P(I))/A2
AA(3,I)=(X(I(I)*A3**X(I(I))-1.0))*P(I)**ALOG(A2)
AA(4,I)=(Y(I(I)-P(I))
A(K,J)=A(K,J)+AA(J,I)**AA(K,I)
10 CONTINUE
WRITE(3,1000)((A(I,J),J=1,M),I=1,N)
DO 11 I=1,N
11 DO J=1,M

continued on next page
DO 60 I=1,N
   K1=1
52  IF(I-N)=52,39,39
   N2=0
   NK=N-K1+1
   TEST=0
DO 12 I=K1,N
   IF(D(I1,1))=13,14,13
   TEST=TEST-ABS(D(I1,1))
   IF(ABS(I1))=15,12,12
   TEST=ABS(D(I1,1))
   IPR=I1
   GO TO 12
14  N2=N2+1
   IF(N2-NK)=12,16,16
16  WRITE(3,200)
   GO TO 969
12  CONTINUE
   DO 51 K2=K1,M
   C(I1,K2)=D(IPR,K2)
51  D(IPR,K2)=D(I1,K2)
   DO 39 I1=I+1
39  D(I1,K2)=C(I1,K2)
   DO 40 K3=K1,M
40  D(I1,K3)=D(I1,K3)/D11
   DO 60 J1=1,N
   DJ1=N(J1,1)
   IF(J1-T)=30,60,30
   DO 62 K4=K1,M
62  D(J1,K4)=D(J1,K4)-DJ1*D(I1,K4)
60  CONTINUE
   DO 19 I=1,N
19  SUM=0
   DO 20 J=1,N
   SUM=SUM+A(I,J)*D(J,M)
20  F(I)=A(I,M)-SUM
   WRITE(3,207)
   WRITE(3,208)(F(I),I=1,N)
   A1=A1+D(I1,M)
   A2=A2+D(I2,M)
   A3=A3+D(I3,M)
   WRITE(3,201)(A1,A2,A3)
   ABC=2
   DFVI=DEV
continued on next page
kk = number of total systems
A1 = constant of Gompertz equation a
A2 = constant of Gompertz equation b
A3 = constant of Gompertz equation c
G = distance in cm (original data)
Y = reduced concentration
Program No. 5

Reduced Concentration Gradient as a Function of Distance

DIMENSION X(I,5),PV(15),Y(I,5),C(I,5)
C(I,5) = X(I,5)
DO 100 IJK = 1, KY
WRITE(3,001)
WRITE(3,003)
WRITE(3,004)
READ(1,102)
READ(1,101)TAT,CL,CL
READ(3,101)AL,CL
READ1(1,101)G(I),V(I),I=1,K
DO 10 J = 1, K
Y(I) = G(I)/0.005-1.0
V(I) = 1./0.005*(AL**AL**CL**X(I)**AL**CL**X(I)**AL**CL))
WRITE(3,006)G(I),V(I)
10 CONTINUE
STOP
101 FORMAT(3IF15.8)
102 FORMAT(110)
103 FORMAT(315.8)
111 FORMAT(110)
16 FORMAT(VICEMAIL SYSTEM ND.),I3)
213 FORMAT(///)
264 FORMAT(/)
265 FORMAT(115)
266 FORMAT(215P8)
END

DATA
kk = number of total systems
k = number of total data points for each system
AL = constant of Gompertz equation a
BL = constant of Gompertz equation b
CL = constant of Gompertz equation c
G = distance in cm
Y = reduced concentration
Program No. 6a
Locating the Original Interface Considering Volume Changes

```
DIMENSION XA(50), YB(50), XA(50), XB(50), CCA(50), CGR(50), CA(50), GR(50)

READ(1, 001)
DO 30 IJK=1, KK
WRITE(3, 001)
WRITE(3, 002)
READ(1, 003)
WRITE(3, 003)
READ(1, 004)
WRITE(3, 004)
READ(1, 005)
WRITE(3, 005)
READ(1, 006)
WRITE(3, 006)
WRITE(3, 007)
DO=0.005
Y=(1+(1)**((1)**(1/1))**((1)**(1/1))**((1)**(1/1)))
PV=PV+PV
F=F+1
M=M/2.0+1.0
DA=(DA-1)/F
DAY=(DAY-DA)/F
X=X
Y=Y
10 IF I=I
X=X+DA
Y=Y+DAY
Y=(1+(1)**((1)**(1))**((1)**(1))**((1)**(1))
XA(1)=(ALOG((1+X/1)))*ALOG(1))
CCA(1)=(1.055*(1+1.0))
CCA(1)=Y-CCA(1)*Y
10 CONTINUE
S1=S1+C
S2=S2+C
STY=STY+C
```

Continued on next page
S1: Y = 10Y (1 + cp(n)) + 4,0*SIY + 2,0*S2Y*OBY/3,0
A2 = S1Y + S1Y*2,0*AN*WN
A3 = (P-0)*VAM(n) + (OBY-2OV)*2,0*AN*1,0*VAM(n) - (A1-A2)
P = A2-A3
DV = (A2-A2) / A2
PP = DV*100.0
WRITE (3,102) A1, A2, A3, P, PP, P
IF (ABS(DV) > 0.05) A, 5, 7

7 IF (A2-A3) P, 6, 14

12 P = P + DD
WRITE (3,105) P
GO TO 19

14 P = P - PP
GO TO 15

6 WRITE (3,104)
WRITE (3,102)
WRITE (3,105) A1, A2, A3, P, PP, P
VP = A1*PH**2 * CL**2 - (0.005-1.0)
WRITE (3,107) VP

000 CONTINUE
STOP

100 FORMAT (2F10.3,15)
101 FORMAT (2F10.3,15)
102 FORMAT (11Y,2HA1,15Y,2HA2,15X,2HA3,13X,SHA2-43,Y,SHO.O,DFV,16Y,1HO)
103 FORMAT (AF17.2)
104 FORMAT (11Y)
105 FORMAT (F10.2)
106 FORMAT (F10.2)
107 FORMAT (11Y) VP = IF18.2)
001 FORMAT (11Y)
002 FORMAT (1Y) CHSYSTEM NO. 0, 13)
003 FORMAT (1Y)
004 FORMAT (1Y)
005 FORMAT (1F)
END

/ DATA
 kk = number of total systems
 A = lower bound of distance
 B = upper bound of distance
 P = estimated interface from distance-reduced concentration plot
 N = any odd number
 AL = constant of Gompertz equation a
 BL = constant of Gompertz equation b
 CL = constant of Gompertz equation c
 AO = concentration dependence or density
 W0 = initial weight fraction W_A1
Problem No. 6b

Locating the Original Interface Neglecting Volume Changes

DIMENSION VA(50), VB(50)
READ(1,'(A50)') KV
DO 100 J=1, 50
WRITE(2,6151) J
WRITE(2,6152) IJK
WRITE(2,6153)
READ(1,'(I5,1X,E18.10)') I, P, D, N
WRITE(2,6154) I, P, D, N
READ(1,'(I5,1X,E18.10)') I, A, B, C
WRITE(2,6155) I, A, B, C
DO 20 I=1, 50
VA(I)=A1*(A1**((31***(X/C1*0.05-1.0))))
X=YA
10 CONTINUE
S1=C
S2=C
A=A-1
DO 20 I=2,*A,2
S1=S1+VA(I)
20 CONTINUE
M=I-2
DO 21 I=2, M, 2
S2=S2+VA(I)
21 CONTINUE
S1=(1.0+VA(M)+4.0*S1+2.0*S2)*DA/3.0
A1=S1
15 DO N=(D-1)/(F/2.0)
X=A
DO 11 I=1,*A
VB(I)=A1*(A1**((31***(X/C1*0.05-1.0))))

Continued on next page
\[ y = x + dr \]

11 CONTINUE
\[ s1 \equiv 0 \cdot c \]
\[ s2 \equiv 0 \cdot c \]
\[ ma \equiv m - 1 \]
\[ DO \ 22 \ 1 \equiv 2, \forall a, \? \]
\[ c1 \equiv c2 + \forall \theta (l) \]

22 CONTINUE
\[ m \equiv m - 2 \]
\[ DO \ 23 \ 1 \equiv 2, \forall a, \? \]
\[ c2 \equiv c2 + \forall \theta (l) \]

23 CONTINUE
\[ s1y \equiv s1y (l) + \forall \theta (n) + 4 \cdot s1 + 2 \cdot s21 * \forall v / 3 \cdot n \]
\[ a2 \equiv s1y \]
\[ a3 \equiv n - d \cdot \forall \theta (n) - (y) \cdot d - (y) \]
\[ p \equiv a2 - a2 \]
\[ dv \equiv (a2 - a2) / a2 \]
\[ p \equiv dv * 100.0 \]
\[ WRITE (2, 102) \(A1, A2, A3, \theta, p \)
\[ IF (A1 - A2) > 0.00006 \& 5.7 \]
\[ 7 \]
\[ p \equiv p + cp \]
\[ WRITE (2, 104) p \]
\[ GO TO 15 \]
\[ 12 \]
\[ p \equiv p - cp \]
\[ WRITE (2, 105) p \]
\[ GO TO 15 \]
\[ 14 \]
\[ WRITE (2, 106) \]
\[ WRITE (2, 107) \]
\[ WRITE (2, 108) \]
\[ WRITE (2, 109) \]
\[ \theta \equiv \theta / 0.00006 - 1.0 \]
\[ \forall \theta \equiv \forall \theta \star \star (0 / 0.00006 - 1.0) \]
\[ WRITE (2, 102) \forall \theta \]
\[ CONTINUE \]

100 FORMAT (2E10.5, 1P)
101 FORMAT (2E10.5)
103 FORMAT (AF17.9)
104 FORMAT (/ / I)
105 FORMAT (EY, 2ND., E18.2)
106 FORMAT (/4X *DP = E18.91

Continued on next page
kk = number of total systems
A = lower bound of distance
B = upper bound of distance
P = estimated interface from distance-reduced concentration plot
N = any odd number
AL = constant of Gompertz equation a
BL = constant of Gompertz equation b
CL = constant of Gompertz equation c
Problem No. 7a

Evaluation of Integral: \( \int f(y^*)dy^* \)

```
DIMENSION X(700), Y(700), GD(700), YD(700), G(700), GG(700)
READ(1, 005) YK
DO 20 IJ=1, YK
WRITE(2, 001)
WRITE(2, 002) IJ
WRITE(2, 003)
READ(1, 004) F
WRITE(1, 004) F
READ(1, 104) UD(I), YD(I), I=1, NT
J=1
YD=A1*12**A3*(P/0.008-1.4)
DO 10 J=1, N
G= (30, 31), JJ
30 M= JJ+1
J= JJ-1
G= (30, 31), JJ
31 M= (J+M)+1
J= JJ-1
G= (30, 31), JJ
32 G(1)= P-A
YA=M-1
MP=M-2
AM=M-A
V(1)= YD(I)
V(1)=P
DV=(Y(I)-V(1))/(AM)
S1=C+C
S2=C+C
DO 11 J=1, M
V(J+1)= V(J)+DV
Y(J+1)= (ALOG((ALOG((Y(J+1)))-1)/ALOG(A2)))/ALOG(A3)
SC(J+1)= C*C*C*(X(J+1)+1, C)
CG(J+1)= P-C*C*C*(X(J+1)+1, C)
11 CONTINUE
DO 12 J=2, M,
```

Continued on next page
\[ S1 = S1 + S(j) \]

\[ 12 \text{ CONTINUE} \]

\[ 13 \text{ J} = 2, M_\beta, ? \]

\[ S2 = S2 + S(j) \]

\[ 13 \text{ CONTINUE} \]

\[ S1 = (C(1) + C(1) + 4.0 * S1 + 2.0 * S2) * \Delta Y / 3.0 \]

\[ \text{WRITE}(3, 102) C(M), M(Y), S1, T \]

\[ JJ = JJ + 1 \]

\[ 20 \text{ I} = 1, L \]

\[ 23 \text{ TO } (40, 41), JJ \]

\[ 24 \text{ OF } 42 \]

\[ 25 \text{ J} = 1, M' \]

\[ M = (I * M) + 1 \]

\[ JJ = JJ + 1 \]

\[ 40 \text{ TO } 42 \]

\[ 41 \text{ M} = (I * M) + 1 \]

\[ JJ = JJ + 1 \]

\[ 42 \text{ C}(1) = \Delta Y - \Delta Y \]

\[ \text{IF}(KJ = NT) 24, 24, 990 \]

\[ 24 \text{ Y}(M) = Y(V(K, I)) \]

\[ 25 \text{ Y}(1) = \Delta Y \]

\[ \Delta Y = (Y(M) - Y(1)) / (AM) \]

\[ S1 = C \cdot C \]

\[ S2 = C \cdot C \]

\[ 26 \text{ DO } 21 \text{ J} = 1, M' \]

\[ Y(J+1) = \Delta Y + \Delta Y \]

\[ Y(J+1) = (\text{ALOG} \cdot \text{ALOG}(Y(J+1)) - \text{ALOG}(A1)) / \text{ALOG}(A2) / \text{ALOG}(A3) \]

\[ C(J+1) = 0.005 \times (X(J+1) + 1.0) - \Delta Y \]

\[ C(J+1) = 0.005 \times (X(J+1) + 1.0) - \Delta Y \]

\[ 21 \text{ CONTINUE} \]

\[ 22 \text{ DO } 21 \text{ J} = 1, M' \]

\[ S1 = S1 + C(J) \]

\[ 21 \text{ CONTINUE} \]

\[ 22 \text{ DO } 22 \text{ J} = 1, M' \]

\[ S2 = S2 + C(J) \]

\[ 23 \text{ CONTINUE} \]

\[ S1 = (C(1) + C(M) + 4.0 * S1 + 2.0 * S2) * \Delta Y / 3.0 \]

Continued on next page
kk = number of total systems
A1 = constant of Gompertz equation a
A2 = constant of Gompertz equation b
A3 = constant of Gompertz equation c
A = lower bound of distance
B = lower bound of reduced concentration
P = original interface
N = any odd number
K = number of data points before P add 1
L = number of data points after P
NT = K + L
GD = distance in cm
YD = reduced concentration
Program No. 7b

Evaluation of Integral: \( \int f(y*)y*dy* \)

```
DIMENSION X(700), Y(700), GD(70), YD(70), G(700), GY(700)
READ(1, CC1) KK
WRITE(3, CC1)
WRITE(3, CC2) IJK
WRITE(3, CC3)
READ(1, IT) A1, A2, A3
READ(1, IT) A, R, P
READ(1, IT) N, K, I, NT

E=M
READ(1, I04) (GD(I), YD(I), I=1, NT)
JJ=1
YP=A1*A2**A3**((P/C-0.005-1.0)
DO 20 I=1, K
20 GO TO (30, 31), JJ
30 GO TO 32
31 M=(I*N)+1
JJ=J-2
GO TO 32
32 G(1)=A
Y(1)=P*YP-G(1)*Y(1)
MA=M-1
MP=Y-2
AM=MA
YM=YD(I)
MY=(Y(M)-Y(1))/(AM)
S1=G.*C.
S2=G.*C.
DO 11 J=1, MA
11 Y(J+1)=Y(J)+MY
X(J+1)=ALOG((ALOG(Y(J+1)-ALOG(A1))/ALOG(A2))/ALOG(A3)
G(J+1)=C.*X(J+1)**(Y(J+1)+1.*Y)
GY(J+1)=P*YP-G(J+1)*Y(J+1)
```

Continued on next page
11 CONTINUE
DO 12 J=2,MA,2
S1=S1+GY(J)
12 CONTINUE
DO 13 J=3,MA,2
S2=S2+GY(J)
13 CONTINUE
SIM=(GY(1)+GY(M)+4.0*S1+2.0*S2)*DY1/3.0
WRITE(3,102)GY(M),Y(M),SIM,1
JJ=JJ+1
10 CONTINUE
MA=SIM
JJ=1
GO TO 20,1,1
GO TO 40
M=(I*M)+1
JJ=JJ-2
40 M=1
GO TO 42
41 M=(M+1)+1
42 G(1)=G
Y(1)=YP
GY(1)=G(1)*Y(1)-P*YP
MA=M+1
M=M+1
KJ=K+1
IF(KJ=NT)24,24,999
24 Y(M)=YD(KJ)
DY=(Y(M)-Y(1))/(AM)
S1=G*G
S2=C*G
DO 21 J=1,MA
Y(J+1)=Y(J)+DY
X(J+1)=ALOG((ALOG(Y(J+1))-ALOG(A1))/ALOG(A2))/ALOG(A3)
G(J+1)=0.095*(X(J+1)+1.0)
GY(J+1)=G(J+1)*Y(J+1)-P*YP
21 CONTINUE
DO 22 J=2,MA,2
S1=S1+GY(J)
22 CONTINUE

Continued on next page
kk = number of total systems
A1 = constant of Gompertza equation a
A2 = constant of Gompertz equation b
A3 = constant of Gompertz equation c
A = lower bound of distance
B = lower bound of reduced concentration
P = original interface
N = any odd number
K = number of data points before P add 1
L = number of data points after P
NT = K + L
GD = distance in cm
YD = reduced concentration
Program No. 7c

Evaluation of Integral: \( \int x \, dy \)

```
DIMENSION X(700), C(700), YO(70), YD(70)
READ(1, 205) X
WRITE(2, 201) X
WRITE(3, 202) I, J
WRITE(3, 203)
READ(1, 101) A1, P1, CL
READ(1, 101) A, P, D
READ(1, 103) N, K, L, NT

LEN
READ(1, 104) (X0(I), YD(I), I=1, NT)
JJ=1
DO 10 I=1, K
GO TO 20, JJ
10 JJ=JJ+1
GO TO 20
20 JJ=JJ-2
GO TO 30
30 X(1)=A
C(1)=AL*(RL**(CL**(X(1)/0.005-1.0)))
MA=M-1
MB=M-2
AM=MA
YM=YD(J)
DY=(X(N)-X(1))/AM
S=0.0
S2=0.0
10 M=1, MA
X(J+1)=X(J)+DY
C(J+1)=AL*(RL**(CL**(X(J+1)/0.005-1.0)))
11 CONTINUE
GO 12 J=2, MA
```

Continued on next page
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<td>FORMAT(4F18.9)</td>
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<td>FORMAT(2F18.9)</td>
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<td>105</td>
<td>FORMAT(1H1)</td>
</tr>
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<td>106</td>
<td>FORMAT(1X13,SYSTEM NO.,13)</td>
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<td>107</td>
<td>FORMAT(///)</td>
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<td>108</td>
<td>FORMAT(/)</td>
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<td>109</td>
<td>FORMAT(///)</td>
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</table>

DATA

kk = number of total systems
AL = constant of Gompertz equation a
BL = constant of Gompertz equation b
CL = constant of Gompertz equation c
A = lower bound of distance
B = upper bound of distance
P = original interface
N = any odd number
K = number of data points before P add 1
L = number of data points after P
NT = K + L
XD = distance in cm
YD = reduced concentration (or concentration)
AL = constant of Gompertz equation a
BL = constant of Gompertz equation b
CL = constant of Gompertz equation c
Program No. 8a

Calculation of the Diffusivity as a Function of Reduced Concentration for Systems with Volume Change

A = CONCENTRATION DEPENDENCE OF DENSITY
W = WEIGHT FRACTION
C = REDUCED CONCENTRATION
T = TIME IN SEC.
F1 = INTEGRAL OF XDC
Tf = INTEGRAL OF XDC
DF = WEIGHT FRACTION

Y = CONCENTRATION %/100CC SOLUTION

DIMENSION FI(20), TI(20), DT(20), C(20), X(20), CT2(20), RA(20), RB(20)
DIMENSION RC(200), D(20), WF(20), Y(20)
READ(1,100) KK
DO 10 IJK=1, KK
WRITE(3,1000) IJK
READ(1,200) NN
READ(1,300) A, W, T
READ(1,400) (X(K), C(K), K=1, NN)
READ(1,400) (FI(K), TI(K), K=1, NN)
READ(1,500) (DT(K), K=1, NN)
READ(1,600) (WF(K), K=1, NN)
READ(1,700) (Y(K), K=1, NN)
WRITE(3,3000) T
CT1 = A*W
DO 20 K=1, NN
CT2(K) = CT1*C(K)
RA(K) = (1-CT2(K))*FI(K)
RB(K) = 2*CT1*TI(K)
RC(K) = 2*T*(1+CT2(K))*DT(K)
D(K) = (RA(K)+RB(K))/RC(K)
D(K) = D(K)*10.**5
WRITE(3,2000) X(K), Y(K), WF(K), C(K), FI(K), TI(K), DT(K), D(K)
20 CONTINUE
TO CONTINUE
STOP
100 FORMAT(I5)
200 FORMAT(110)
300 FORMAT(3F18.8)
400 FORMAT(2F18.8)
500 FORMAT(F18.8)
600 FORMAT(4F18.8)
1000 FORMAT(1H1,4X,'SYSTEM NO.',15)
2000 FORMAT(/4X,'TIME',T='F5.1')
3000 FORMAT(/4X,'TIME',T='F5.1')
END

kk = number of total systems
NN = number of total data points for each system
X = distance in cm
C = reduced concentration
W = initial weight fraction WAl
WF = weight fraction during diffusion
D = diffusivity
Program No. 8b

Calculation of the Diffusivity as a Function of Reduced Concentration for Systems without Volume Change

```fortran
DIMENSION X(30), C(30), EN(30), ED(30), DC(30), R(30)

READ(1,905) KK
DO 900 IJK=1, KK
WRITE(3,901) IJK
WRITE(3,902) IJK
WRITE(3,903) IJK
READ(1,100) N, T
WRITE(3,200) T
WRITE(3,200) T
WRITE(3,200) T
READ(1,101) (X(I), C(I), I=1, N)
READ(1,102) (EN(I), I=1, N)
READ(1,102) (ED(I), I=1, N)
DO 10 I=1, N
DC(I)= (EN(I)/(2.*T*ED(I)))
ED(I)= ED(I)/100.*C
DC(I)= DC(I)*(100.*C**5)
WRITE(3,203) X(I), C(I), EN(I), ED(I), DC(I)
WRITE(3,904) I
10 CONTINUE
900 CONTINUE
STOP
100 FORMAT(110,F10.1)
101 FORMAT(2F18.8)
102 FORMAT(F18.8)
200 FORMAT(5X,8HTIME T = ,F5.1)
203 FORMAT(5X,F10.3,F11.3,F9.3,2F10.3)
901 FORMAT(1H1)
902 FORMAT(1X10HSYSTEM NO.,13)
903 FORMAT(/)
904 FORMAT(/)
905 FORMAT(15)
END
```

/*DATA*/
kk = number of total systems
T = time in seconds
N = number of total data points for each system
X = distance in cm
C = reduced concentration (or concentration)
EN = integral of ∫x dy* or ∫f(y*)dy* (or ∫xdy)
ED = derivative dy*/dx (or dy/dx)
DC = diffusivity
Appendix B

Data and Results

<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
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<tbody>
<tr>
<td>B.1</td>
<td>Polymeric Systems Used for the Study</td>
<td>52</td>
</tr>
<tr>
<td>B.2</td>
<td>Data and Results for System 1</td>
<td>53</td>
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<td>B.3</td>
<td>Data and Results for System 2</td>
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<td>Data and Results for System 3</td>
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<td>Data and Results for System 10</td>
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<td>B.12</td>
<td>Values of $R_0$ and $R_1$ in Equation (8)</td>
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### Table B.1

**Polymeric Systems Used for the Study**

<table>
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<tr>
<th>System Number</th>
<th>Polymer</th>
<th>Solvent</th>
<th>Polymer Concent. Wt.%</th>
<th>Solute</th>
<th>Initial Solute Conc. gm/100 cc Soln.</th>
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<td>1</td>
<td>CMC</td>
<td>Water</td>
<td>2.20%</td>
<td>D-Glucose</td>
<td>10.0</td>
</tr>
<tr>
<td>2</td>
<td>CMC</td>
<td>Water</td>
<td>2.00%</td>
<td>D-Glucose</td>
<td>10.0</td>
</tr>
<tr>
<td>3</td>
<td>CMC</td>
<td>Water</td>
<td>1.70%</td>
<td>D-Glucose</td>
<td>10.0</td>
</tr>
<tr>
<td>4</td>
<td>CMC</td>
<td>Water</td>
<td>1.35%</td>
<td>D-Glucose</td>
<td>10.0</td>
</tr>
<tr>
<td>5</td>
<td>CMC</td>
<td>Water</td>
<td>1.20%</td>
<td>D-Glucose</td>
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<tr>
<td>6</td>
<td>Carbopol</td>
<td>Water</td>
<td>0.28%</td>
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<tr>
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<td>Water</td>
<td>0.25%</td>
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<td>9</td>
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<td>D-Glucose</td>
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<tr>
<td>10</td>
<td>Carbopol</td>
<td>Water</td>
<td>0.18%</td>
<td>D-Glucose</td>
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Table B.2

Data and Results for System 1

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<th>X (cm)</th>
<th>gm solute/100cm³ sol.</th>
<th>Wₐ</th>
<th>y*</th>
<th>( \int_0^y y' dy' )</th>
<th>( \int_0^y y'^2 dy' )</th>
<th>dy*/dx</th>
<th>D(1) x 10⁵</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.008</td>
<td>0.047</td>
<td>0.099</td>
<td>0.099</td>
<td>0.0020</td>
<td>0.0012</td>
<td>17.070</td>
<td>0.512</td>
</tr>
<tr>
<td>0.14</td>
<td>2.667</td>
<td>0.226</td>
<td>0.236</td>
<td>0.0038</td>
<td>0.0027</td>
<td>25.716</td>
<td>0.627</td>
</tr>
<tr>
<td>0.19</td>
<td>3.432</td>
<td>0.033</td>
<td>0.368</td>
<td>0.0049</td>
<td>0.0037</td>
<td>28.803</td>
<td>0.719</td>
</tr>
<tr>
<td>0.23</td>
<td>4.664</td>
<td>0.044</td>
<td>0.482</td>
<td>0.0052</td>
<td>0.0042</td>
<td>28.422</td>
<td>0.784</td>
</tr>
<tr>
<td>0.288</td>
<td>5.861</td>
<td>0.055</td>
<td>0.612</td>
<td>0.0054</td>
<td>0.0044</td>
<td>25.466</td>
<td>0.902</td>
</tr>
<tr>
<td>0.35</td>
<td>7.674</td>
<td>0.071</td>
<td>0.776</td>
<td>0.0065</td>
<td>0.0059</td>
<td>19.374</td>
<td>1.415</td>
</tr>
<tr>
<td>0.41</td>
<td>8.606</td>
<td>0.079</td>
<td>0.877</td>
<td>0.0079</td>
<td>0.0077</td>
<td>14.255</td>
<td>2.317</td>
</tr>
<tr>
<td>0.482</td>
<td>9.923</td>
<td>0.086</td>
<td>0.992</td>
<td>0.0104</td>
<td>0.0112</td>
<td>7.353</td>
<td>5.902</td>
</tr>
</tbody>
</table>

Time t=12.0 seconds; T=23°C; Wₐ=0.0902
Concentration dependence of density A=0.3387
### Table B.3

Data and Results for System 2

<table>
<thead>
<tr>
<th>X (cm)</th>
<th>gm solute (100 cm³ sol.)</th>
<th>Y</th>
<th>( \frac{\int_y y^x dy}{\int_y y^x dy} )</th>
<th>( \frac{\int_y y^x dy}{\int_y y^x dy} ) dy*/dx</th>
<th>( D_{AB}^{(1)} \times 10^5 ) cm⁻¹ cm²/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.026</td>
<td>0.775</td>
<td>0.008</td>
<td>0.084</td>
<td>0.0045</td>
<td>0.0025</td>
</tr>
<tr>
<td>0.035</td>
<td>1.233</td>
<td>0.012</td>
<td>0.136</td>
<td>0.0065</td>
<td>0.0039</td>
</tr>
<tr>
<td>0.050</td>
<td>2.415</td>
<td>0.023</td>
<td>0.258</td>
<td>0.0095</td>
<td>0.0065</td>
</tr>
<tr>
<td>0.061</td>
<td>3.524</td>
<td>0.034</td>
<td>0.372</td>
<td>0.0108</td>
<td>0.0080</td>
</tr>
<tr>
<td>0.069</td>
<td>4.395</td>
<td>0.042</td>
<td>0.465</td>
<td>0.0111</td>
<td>0.0083</td>
</tr>
<tr>
<td>0.074</td>
<td>5.028</td>
<td>0.048</td>
<td>0.526</td>
<td>0.0113</td>
<td>0.0086</td>
</tr>
<tr>
<td>0.080</td>
<td>5.760</td>
<td>0.054</td>
<td>0.600</td>
<td>0.0120</td>
<td>0.0096</td>
</tr>
<tr>
<td>0.087</td>
<td>6.667</td>
<td>0.062</td>
<td>0.689</td>
<td>0.0134</td>
<td>0.0117</td>
</tr>
<tr>
<td>0.094</td>
<td>7.638</td>
<td>0.071</td>
<td>0.776</td>
<td>0.0154</td>
<td>0.0148</td>
</tr>
<tr>
<td>0.109</td>
<td>9.522</td>
<td>0.086</td>
<td>0.957</td>
<td>0.0215</td>
<td>0.0252</td>
</tr>
</tbody>
</table>

Time t=50.0 seconds; T=23°C; \( W_{Al} = 0.0903 \)

Concentration dependence of density \( A = 0.3507 \)
Table B.4

Data and Results for System 3

| X (g m solute/100 cm³ sol.) | WA |  |  |  |  |  |  |  |
|----------------------------|----|---|---|---|---|---|---|
|  |  |  |  |  |  |  |  |  |
| 0.017 | 1.018 | 0.010 | 0.112 | 0.0029 | 0.0018 | 12.834 | 0.572 |
| 0.022 | 1.726 | 0.017 | 0.187 | 0.0041 | 0.0029 | 16.800 | 0.628 |
| 0.026 | 2.423 | 0.024 | 0.259 | 0.0050 | 0.0037 | 19.169 | 0.667 |
| 0.030 | 3.207 | 0.031 | 0.339 | 0.0056 | 0.0044 | 20.644 | 0.698 |
| 0.036 | 4.378 | 0.047 | 0.465 | 0.0060 | 0.0048 | 21.150 | 0.725 |
| 0.040 | 5.271 | 0.050 | 0.549 | 0.0062 | 0.0050 | 20.544 | 0.763 |
| 0.046 | 6.428 | 0.060 | 0.667 | 0.0070 | 0.0061 | 18.636 | 0.947 |
| 0.051 | 7.410 | 0.069 | 0.755 | 0.0081 | 0.0077 | 16.538 | 1.232 |
| 0.055 | 8.026 | 0.074 | 0.818 | 0.0091 | 0.0092 | 14.739 | 1.563 |
| 0.064 | 9.255 | 0.084 | 0.932 | 0.0118 | 0.0122 | 10.344 | 2.742 |

Time t=20.0 seconds; T=23°C; WA = 0.0905

Concentration dependence of density A=0.3328
Table B.5
Data and Results for System 4

<table>
<thead>
<tr>
<th>X (cm)</th>
<th>Y</th>
<th>( \int_0^y y^2 dy )</th>
<th>( \int_0^y y^2 dy / dx )</th>
<th>( D^{(1)} \times 10^5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.208</td>
<td>0.825</td>
<td>0.008 0.085</td>
<td>0.0023 0.0013 11.838</td>
<td>0.558</td>
</tr>
<tr>
<td>0.217</td>
<td>2.035</td>
<td>0.020 0.229</td>
<td>0.0048 0.0032 19.467</td>
<td>0.704</td>
</tr>
<tr>
<td>0.222</td>
<td>3.107</td>
<td>0.030 0.332</td>
<td>0.0059 0.0043 21.501</td>
<td>0.782</td>
</tr>
<tr>
<td>0.228</td>
<td>4.381</td>
<td>0.042 0.462</td>
<td>0.0066 0.0050 21.595</td>
<td>0.865</td>
</tr>
<tr>
<td>0.232</td>
<td>5.263</td>
<td>0.050 0.547</td>
<td>0.0067 0.0051 20.520</td>
<td>0.919</td>
</tr>
<tr>
<td>0.238</td>
<td>6.396</td>
<td>0.060 0.663</td>
<td>0.0072 0.0057 17.921</td>
<td>1.131</td>
</tr>
<tr>
<td>0.245</td>
<td>7.599</td>
<td>0.070 0.776</td>
<td>0.0085 0.0073 14.316</td>
<td>1.656</td>
</tr>
<tr>
<td>0.252</td>
<td>8.528</td>
<td>0.078 0.864</td>
<td>0.0101 0.0095 10.878</td>
<td>2.585</td>
</tr>
<tr>
<td>0.265</td>
<td>9.667</td>
<td>0.083 0.971</td>
<td>0.0130 0.0135 6.317</td>
<td>6.043</td>
</tr>
</tbody>
</table>

Time \( t=18.0 \) seconds; \( T=23^\circ C; W_{Al}=0.0906 \)
Concentration dependence of density \( A=0.3132 \)
Table B.6
Data and Results for System 2

<table>
<thead>
<tr>
<th>X</th>
<th>gm solute</th>
<th>W_A</th>
<th>y* \int y<em>dy</em></th>
<th>y* \int y<em>dy</em></th>
<th>D_{AB}^{(1)} \times 10^5</th>
</tr>
</thead>
<tbody>
<tr>
<td>cm</td>
<td>100 cm^3 sol.</td>
<td></td>
<td>cm^{-1}</td>
<td>cm^{-1}</td>
<td>cm^2/sec</td>
</tr>
<tr>
<td>-------</td>
<td>------------</td>
<td>-----</td>
<td>---------------</td>
<td>---------------</td>
<td>--------------------------</td>
</tr>
<tr>
<td>0.016</td>
<td>0.840</td>
<td>0.008</td>
<td>0.091</td>
<td>0.0735</td>
<td>0.0019</td>
</tr>
<tr>
<td>0.026</td>
<td>1.730</td>
<td>0.017</td>
<td>0.196</td>
<td>0.0059</td>
<td>0.0037</td>
</tr>
<tr>
<td>0.032</td>
<td>2.438</td>
<td>0.024</td>
<td>0.261</td>
<td>0.0071</td>
<td>0.0048</td>
</tr>
<tr>
<td>0.039</td>
<td>3.340</td>
<td>0.037</td>
<td>0.361</td>
<td>0.0082</td>
<td>0.0059</td>
</tr>
<tr>
<td>0.045</td>
<td>4.363</td>
<td>0.042</td>
<td>0.453</td>
<td>0.0096</td>
<td>0.0063</td>
</tr>
<tr>
<td>0.052</td>
<td>5.339</td>
<td>0.051</td>
<td>0.564</td>
<td>0.0089</td>
<td>0.0067</td>
</tr>
<tr>
<td>0.058</td>
<td>6.352</td>
<td>0.060</td>
<td>0.658</td>
<td>0.0097</td>
<td>0.0078</td>
</tr>
<tr>
<td>0.063</td>
<td>7.187</td>
<td>0.067</td>
<td>0.734</td>
<td>0.0108</td>
<td>0.0093</td>
</tr>
<tr>
<td>0.068</td>
<td>7.931</td>
<td>0.073</td>
<td>0.806</td>
<td>0.0122</td>
<td>0.0114</td>
</tr>
<tr>
<td>0.073</td>
<td>8.636</td>
<td>0.079</td>
<td>0.873</td>
<td>0.0138</td>
<td>0.0139</td>
</tr>
<tr>
<td>0.081</td>
<td>9.647</td>
<td>0.088</td>
<td>0.971</td>
<td>0.0168</td>
<td>0.0137</td>
</tr>
</tbody>
</table>

Time 5=20.0 seconds; T=23^oC; W_{Al}=0.0907
Concentration dependence of density A=0.2631
### Table B.7

**Data and Results for System 6**

<table>
<thead>
<tr>
<th>X (cm)</th>
<th>gm solute (100 cm³ sol.)</th>
<th>W_A</th>
<th>y*</th>
<th>$\int_{0}^{x} y^x dx$</th>
<th>$\int_{0}^{x} y^x dy dx$</th>
<th>$D_{AB}(1) \times 10^5$ cm²/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.11</td>
<td>0.715</td>
<td>0.007</td>
<td>0.077</td>
<td>0.0025</td>
<td>0.0015</td>
<td>9.258</td>
</tr>
<tr>
<td>0.17</td>
<td>1.335</td>
<td>0.013</td>
<td>0.146</td>
<td>0.0041</td>
<td>0.0027</td>
<td>13.410</td>
</tr>
<tr>
<td>0.23</td>
<td>2.198</td>
<td>0.022</td>
<td>0.237</td>
<td>0.0057</td>
<td>0.0040</td>
<td>16.804</td>
</tr>
<tr>
<td>0.29</td>
<td>3.282</td>
<td>0.032</td>
<td>0.345</td>
<td>0.0069</td>
<td>0.0053</td>
<td>18.834</td>
</tr>
<tr>
<td>0.34</td>
<td>4.125</td>
<td>0.040</td>
<td>0.440</td>
<td>0.0075</td>
<td>0.0059</td>
<td>19.377</td>
</tr>
<tr>
<td>0.40</td>
<td>5.268</td>
<td>0.050</td>
<td>0.556</td>
<td>0.0077</td>
<td>0.0061</td>
<td>18.335</td>
</tr>
<tr>
<td>0.47</td>
<td>6.580</td>
<td>0.067</td>
<td>0.682</td>
<td>0.0094</td>
<td>0.0071</td>
<td>17.046</td>
</tr>
<tr>
<td>0.51</td>
<td>7.365</td>
<td>0.069</td>
<td>0.747</td>
<td>0.0092</td>
<td>0.0082</td>
<td>15.707</td>
</tr>
<tr>
<td>0.56</td>
<td>8.092</td>
<td>0.075</td>
<td>0.821</td>
<td>0.0104</td>
<td>0.0099</td>
<td>13.892</td>
</tr>
<tr>
<td>0.61</td>
<td>8.740</td>
<td>0.080</td>
<td>0.886</td>
<td>0.0117</td>
<td>0.0119</td>
<td>12.062</td>
</tr>
<tr>
<td>0.72</td>
<td>9.862</td>
<td>0.091</td>
<td>0.998</td>
<td>0.0149</td>
<td>0.0167</td>
<td>8.424</td>
</tr>
</tbody>
</table>

**Time** t=30.0 seconds; **T=23°C;** $W_{Al}=0.0910$

**Concentration dependence of density** $A=0.3790$
### Table B.8

**Data and Results for System 7**

<table>
<thead>
<tr>
<th>X (cm)</th>
<th>gm solute/100cm³ sol.</th>
<th>W_A</th>
<th>y*</th>
<th>( \frac{\int_0^y d\gamma^<em>}{\int_0^y \gamma^</em>} )</th>
<th>( \frac{\int_0^y d\gamma^<em>}{\int_0^y \gamma^</em>} )</th>
<th>D(_{AB}) x 10^5 cm(^{-1}) cm²/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>0.734</td>
<td>0.007</td>
<td>0.078</td>
<td>0.0023</td>
<td>0.0014</td>
<td>11.197</td>
</tr>
<tr>
<td>0.015</td>
<td>1.355</td>
<td>0.013</td>
<td>0.146</td>
<td>0.0039</td>
<td>0.0026</td>
<td>15.936</td>
</tr>
<tr>
<td>0.020</td>
<td>2.140</td>
<td>0.021</td>
<td>0.235</td>
<td>0.0052</td>
<td>0.0039</td>
<td>19.516</td>
</tr>
<tr>
<td>0.024</td>
<td>2.894</td>
<td>0.029</td>
<td>0.317</td>
<td>0.0063</td>
<td>0.0049</td>
<td>21.107</td>
</tr>
<tr>
<td>0.028</td>
<td>3.741</td>
<td>0.036</td>
<td>0.403</td>
<td>0.0070</td>
<td>0.0057</td>
<td>21.528</td>
</tr>
<tr>
<td>0.031</td>
<td>4.455</td>
<td>0.043</td>
<td>0.467</td>
<td>0.0073</td>
<td>0.0060</td>
<td>21.173</td>
</tr>
<tr>
<td>0.034</td>
<td>5.111</td>
<td>0.049</td>
<td>0.529</td>
<td>0.0074</td>
<td>0.0062</td>
<td>20.362</td>
</tr>
<tr>
<td>0.038</td>
<td>5.882</td>
<td>0.056</td>
<td>0.608</td>
<td>0.0075</td>
<td>0.0063</td>
<td>18.775</td>
</tr>
<tr>
<td>0.043</td>
<td>6.727</td>
<td>0.063</td>
<td>0.696</td>
<td>0.0081</td>
<td>0.0070</td>
<td>16.338</td>
</tr>
<tr>
<td>0.047</td>
<td>7.367</td>
<td>0.069</td>
<td>0.757</td>
<td>0.0087</td>
<td>0.0079</td>
<td>14.275</td>
</tr>
<tr>
<td>0.052</td>
<td>8.070</td>
<td>0.075</td>
<td>0.822</td>
<td>0.0097</td>
<td>0.0093</td>
<td>11.785</td>
</tr>
<tr>
<td>0.061</td>
<td>9.013</td>
<td>0.083</td>
<td>0.910</td>
<td>0.0116</td>
<td>0.0119</td>
<td>7.967</td>
</tr>
<tr>
<td>0.076</td>
<td>9.970</td>
<td>0.091</td>
<td>0.995</td>
<td>0.0145</td>
<td>0.0159</td>
<td>3.828</td>
</tr>
</tbody>
</table>

Time \( t = 24.0 \) seconds; \( T = 21^\circ C; \) \( W_{Al} = 0.0909 \)

Concentration dependence of density \( A = 0.3552 \)
### Table B.9

**Data and Results for System 8**

<table>
<thead>
<tr>
<th>X (cm)</th>
<th>gm solute</th>
<th>W_A</th>
<th>Y</th>
<th>( \int_0^y y^k dy )</th>
<th>( \int_0^y y^k dy^k )</th>
<th>( \frac{dy^k}{dx} )</th>
<th>( D(1) \times 10^5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.17</td>
<td>1.217</td>
<td>0.012</td>
<td>0.132</td>
<td>0.0017</td>
<td>0.0010</td>
<td>22.747</td>
<td>0.640</td>
</tr>
<tr>
<td>0.217</td>
<td>2.501</td>
<td>0.024</td>
<td>0.269</td>
<td>0.0025</td>
<td>0.0017</td>
<td>31.528</td>
<td>0.687</td>
</tr>
<tr>
<td>0.322</td>
<td>3.382</td>
<td>0.033</td>
<td>0.368</td>
<td>0.0027</td>
<td>0.0019</td>
<td>34.151</td>
<td>0.685</td>
</tr>
<tr>
<td>0.372</td>
<td>4.290</td>
<td>0.041</td>
<td>0.437</td>
<td>0.0028</td>
<td>0.0020</td>
<td>34.708</td>
<td>0.681</td>
</tr>
<tr>
<td>0.425</td>
<td>5.144</td>
<td>0.049</td>
<td>0.541</td>
<td>0.0031</td>
<td>0.0023</td>
<td>33.988</td>
<td>0.765</td>
</tr>
<tr>
<td>0.526</td>
<td>6.148</td>
<td>0.058</td>
<td>0.640</td>
<td>0.0036</td>
<td>0.0031</td>
<td>31.344</td>
<td>0.967</td>
</tr>
<tr>
<td>0.630</td>
<td>6.786</td>
<td>0.064</td>
<td>0.702</td>
<td>0.0042</td>
<td>0.0038</td>
<td>29.890</td>
<td>1.175</td>
</tr>
<tr>
<td>0.844</td>
<td>8.007</td>
<td>0.074</td>
<td>0.817</td>
<td>0.0054</td>
<td>0.0055</td>
<td>25.354</td>
<td>1.801</td>
</tr>
</tbody>
</table>

Time \( t=6.0 \text{ seconds} \); \( T=21^\circ C \); \( W_{\text{Al}}=0.0910 \)

Concentration dependence of density \( A=0.3749 \)
### Table B.10

**Data and Results for System 9**

<table>
<thead>
<tr>
<th>X (cm)</th>
<th>gm solute W_A (100cm³/sol)</th>
<th>Y</th>
<th>$\int y^* , dy^*$</th>
<th>$\int y^* , dy^* , dy^* , dx$</th>
<th>$D_{AB} \times 10^5$ cm⁻¹ cm²/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.14</td>
<td>0.870</td>
<td>0.000</td>
<td>0.092</td>
<td>0.0024</td>
<td>0.0013 11.194</td>
</tr>
<tr>
<td>0.22</td>
<td>1.855</td>
<td>0.018</td>
<td>0.207</td>
<td>0.0322</td>
<td>0.0027 17.331</td>
</tr>
<tr>
<td>0.27</td>
<td>2.800</td>
<td>0.027</td>
<td>0.301</td>
<td>0.0050</td>
<td>0.0036 19.000</td>
</tr>
<tr>
<td>0.31</td>
<td>3.717</td>
<td>0.036</td>
<td>0.383</td>
<td>0.0054</td>
<td>0.0040 21.013</td>
</tr>
<tr>
<td>0.36</td>
<td>4.622</td>
<td>0.044</td>
<td>0.489</td>
<td>0.0056</td>
<td>0.0041 21.232</td>
</tr>
<tr>
<td>0.41</td>
<td>5.627</td>
<td>0.053</td>
<td>0.593</td>
<td>0.0060</td>
<td>0.0047 20.384</td>
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<tr>
<td>0.44</td>
<td>6.273</td>
<td>0.050</td>
<td>0.653</td>
<td>0.0066</td>
<td>0.0054 19.498</td>
</tr>
<tr>
<td>0.47</td>
<td>6.982</td>
<td>0.055</td>
<td>0.710</td>
<td>0.0072</td>
<td>0.0063 18.417</td>
</tr>
<tr>
<td>0.52</td>
<td>7.840</td>
<td>0.073</td>
<td>0.797</td>
<td>0.0086</td>
<td>0.0083 16.356</td>
</tr>
<tr>
<td>0.55</td>
<td>8.005</td>
<td>0.082</td>
<td>0.001</td>
<td>0.0103</td>
<td>0.0116 13.318</td>
</tr>
</tbody>
</table>

Time $t=20.0$ seconds; $T=23^\circ C$; $W_{A1}=0.0910$

Concentration dependence of density $A=0.3573$
Table B.11

Data and Results for System 10

<table>
<thead>
<tr>
<th>X cm solute / 100 cm³ sol</th>
<th>W_A</th>
<th>y*</th>
<th>∫y* dy* / dx</th>
<th>D(1) x 10^5 cm⁻¹ cm²/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.013</td>
<td>0.970</td>
<td>0.016</td>
<td>0.108</td>
<td>0.030</td>
</tr>
<tr>
<td>0.019</td>
<td>1.940</td>
<td>0.019</td>
<td>0.203</td>
<td>0.038</td>
</tr>
<tr>
<td>0.024</td>
<td>2.727</td>
<td>0.027</td>
<td>0.309</td>
<td>0.058</td>
</tr>
<tr>
<td>0.029</td>
<td>3.883</td>
<td>0.037</td>
<td>0.404</td>
<td>0.078</td>
</tr>
<tr>
<td>0.034</td>
<td>4.812</td>
<td>0.046</td>
<td>0.500</td>
<td>0.079</td>
</tr>
<tr>
<td>0.039</td>
<td>5.816</td>
<td>0.055</td>
<td>0.605</td>
<td>0.086</td>
</tr>
<tr>
<td>0.045</td>
<td>6.863</td>
<td>0.064</td>
<td>0.707</td>
<td>0.083</td>
</tr>
<tr>
<td>0.052</td>
<td>7.892</td>
<td>0.072</td>
<td>0.803</td>
<td>0.090</td>
</tr>
<tr>
<td>0.062</td>
<td>8.948</td>
<td>0.082</td>
<td>0.904</td>
<td>0.096</td>
</tr>
<tr>
<td>0.078</td>
<td>9.931</td>
<td>0.090</td>
<td>0.994</td>
<td>0.104</td>
</tr>
</tbody>
</table>

Time \( t = 20.0 \) seconds; \( T = 23^\circ C; W_{A1} = 0.0910 \)

Concentration dependence of density \( A = 0.3558 \)
<table>
<thead>
<tr>
<th>System Number</th>
<th>$R_0$</th>
<th>$R_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.3385</td>
<td>0.00120</td>
</tr>
<tr>
<td>2</td>
<td>1.3380</td>
<td>0.00127</td>
</tr>
<tr>
<td>3</td>
<td>1.3380</td>
<td>0.00118</td>
</tr>
<tr>
<td>4</td>
<td>1.3378</td>
<td>0.00117</td>
</tr>
<tr>
<td>5</td>
<td>1.3370</td>
<td>0.00123</td>
</tr>
<tr>
<td>6</td>
<td>1.3360</td>
<td>0.00130</td>
</tr>
<tr>
<td>7</td>
<td>1.3360</td>
<td>0.00122</td>
</tr>
<tr>
<td>8</td>
<td>1.3360</td>
<td>0.00123</td>
</tr>
<tr>
<td>9</td>
<td>1.3360</td>
<td>0.00130</td>
</tr>
<tr>
<td>10</td>
<td>1.3362</td>
<td>0.00118</td>
</tr>
</tbody>
</table>
Appendix C

Theoretical Equation of Diffusion

Duda and Vrentas (10) based their work on the assumptions of 1) free diffusion, 2) in an isothermal system of N components which do not react with each other, 3) the components involved are neither viscoelastic materials nor the polar materials, 4) $W_I = \rho_I / \rho$, 5) liquid system, 6) one directional motion with all variables changing only in that direction and derived from the equation of continuity and equation of motion the following:

$$v_i^1 = \frac{1}{\rho^2} \sum_{I=1}^{N-1} \frac{\partial \rho}{\partial W_I} j_I^1, i$$  \hspace{1cm} (C.1)

where

- $v_i^1$ is the $i$th component of mass average velocity
- $j_I^1$ is the $i$th component of mass diffusion flux of component $I$ relative to mass average velocity
- $W_I$ is the mass fraction of component $I$.

For binary free diffusion relative to rectangular cartesian coordinate axis, it became

$$\frac{\partial v}{\partial x} = -\frac{1}{\rho^2} \frac{\partial \rho}{\partial W_A} \frac{\partial^2 W_A}{\partial x^2}$$  \hspace{1cm} (C.2)

Equation (C.1), with the boundary conditions for one-dimensional free diffusion,

$$W_A (0, x) = W_{A0} \quad x < 0 \hspace{1cm} (C.3)$$
$$W_A (0, x) = W_{A1} \quad x > 0 \hspace{1cm} (C.4)$$
$$W_A (t, -\infty) = W_{A0} \hspace{1cm} (C.5)$$
$$W_A (t, +\infty) = W_{A1} \hspace{1cm} (C.6)$$
By applying the famous Boltzmann transformation
\[ \tau = \frac{x}{2t^\frac{1}{2}} \]
and constraining one of the infinite boundaries to set the velocity there equal to zero, equation (C.2) can be simplified to the form:
\[ \rho D \frac{dW_A}{d\eta} = -\int_{W_{AO}}^{W_A} 2 \rho \eta dW_A + \int_{W_{AO}}^{\rho_0} 2 \eta d\rho dW_A \quad (C.7) \]
If \( W_A \) is determined as a function of \( x \) and \( t \), integration by parts of the double integral transforms equation (C.7) into
\[ D = -2 \frac{d\eta}{dW_A} \left[ \frac{1}{2} \int_{W_{AO}}^{W_A} \eta \rho dW_A + \frac{1}{2} \int_{\rho_0}^{\rho} \eta W_A d\rho \right. \\
- \left. \left( \frac{W_A}{\rho} \right) \int_{\rho_0}^{\rho} \eta d\rho \right] \quad (C.8) \]
In the case when there is no volume change during diffusion, equation (C.8) will reduce to the familiar result (10).
\[ D = -2 \left( \frac{d\eta}{dW_A} \right) \int_{W_{AO}}^{W_A} \eta dW_A \quad (C.9) \]
Paul (18) pointed out that when the solution density is linear in the weight fraction of the solute
\[ \rho = \rho_s (1 + AW_A) \quad (C.10) \]
\[ y^* = W_A/W_{AI} \quad (C.11) \]
Equation (C.8) will transform to
\[ D = -2 \left[ \left( 1 - AW_{AI}y^* \right) \int_0^{y^*} \eta dy^* + 2AW_{AI} \int_0^{y^*} \eta y^* dy^* \right] \\
\frac{1 + AW_{AI}y^*}{(1 + AW_{AI}y^*)} \left( \frac{dy^*}{d\eta} \right) \quad (C.12) \]
Appendix D

Diffusivity Computation Techniques

The reduced concentration, \( y^* \), was defined by Paul (18) as

\[
y^* = \frac{W_A}{W_{Al}} \tag{D.1}
\]

where

\[
W_A = \text{weight fraction during diffusion}
\]

\[
W_{Al} = \text{weight fraction of initial solution on the solute rich side}
\]

From data given by Desai (9) in the concentration units (gm solute/100 cm\(^3\) solution), the weight fraction can be obtained as

\[
W = \frac{\text{gm solute/100 cm}^3\text{ solution}}{\text{gm solute/100 cm}^3\text{ solution} + (100)(\text{density of polymer solution})}
\]

The concentration dependence of density \( A \) was calculated from equation (C.10)

\[
\rho = \rho_s (1 + AW_A)
\]

From each known polymer solution density and the corresponding weight fraction, the value \( A \) can be obtained. For each system three different pairs -- weight fraction and solution density -- were used to calculate the arithmetic average \( A \).

The curve of reduced concentration vs. distance (i.e., \( y^* \) vs. \( x \)) is sigmoid (see Figure D.1). The curve is characterized by a very small initial slope followed
Figure D.1. Experimental Reduced Concentration Profile for 0.25 wt.% Carbopol System.
by a period of rapidly increasing slope which gives way to an interval of nearly constant slope succeeded by a period when the rapidly decreasing slope approaches zero. The Gompertz equation

\[ y^* = ab^c \]

where

G is a linear function of x used in order to scale the x variables, has been found to satisfactorily represent such data (8). Davis' method of determining the constants, a, b, and c, in the Gompertz equation requires that the independent variable be in equal intervals. (The independent variable may be time or distance for instance, and the data may appear as the dates 1890, 1900, 1910, and 1920, or the distance 0.005, 0.010, 0.015, and 0.020 to which are assigned values of G of 0, 1, 2, and 3. See Davis (8).)

In this work, the data were not in equal intervals. From the y* vs. x plot, the equal interval 0.005 cm of x were picked up through the use of a curve which was fitted by "eye". Therefore, following linear relationship between G and x was used:

\[ G = \left( \frac{x}{0.005} \right) - 1 \]

Whenever y* is calculated, the x scale must be changed to the G scale, i.e.

\[ y^* = ab^c \] or \[ y^* = ab^c \left( \frac{x}{0.005} - 1 \right) \]
The data are divided into three parts of \( n \) entries each. \( S_1, S_2, \) and \( S_3 \) represent the sums of the three groups of values of \( \log y \), starting with the lowest values. The constants \( a, b, \) and \( c \) can then be evaluated from the equations

\[
c = \left( \frac{S_2 - S_3}{S_1 - S_2} \right)^{1/n} \quad (D.3)
\]

\[
\log a = \frac{1}{n} \left( S_1 - \frac{S_1 - S_2}{1 - c^n} \right)
\]

and

\[
\log b = \left( S_1 - S_2 \right)(1-c)/(1-c^n)^2 \quad (D.5)
\]

where \( n \) equals one-third of the total data points used.

It was found that using the same data, when curves were passed through the data points by "eye," several slightly different curves would be obtained.

In order to eliminate human bias when passing a curve through the \( y^* \) vs. \( x \) data (as is possible in the previous method of Davis), a non-linear least squares method was used. The Gompertz equation is non-linear in the constants \( a, b, \) and \( c \). Therefore the Gompertz equation was linearized in terms of the constants, \( a, b, \) and \( c \), before the least squares technique was applied.

The resulting least square "normal" equations were:

\[
\Delta a \sum_{i=1}^{N} \left( \frac{P_i}{a_0} \right)^2 + \Delta b \sum_{i=1}^{N} \left( c_o p_i^{G_1}/a_o b_o \right) + \Delta c \sum_{i=1}^{N} \left( G_1 c_o p_i^{(G_1-1)}/a_o \right) \ln \left( b_o \right)/a_o = \sum_{i=1}^{N} \left[ \left( \frac{P_i}{a_o} \right) y^*_i - \left( \frac{P_i^2}{a_o} \right) \right]
\]
\[ \Delta a \sum_{i=1}^{N} \left( p_i^2 c_i^0 / a_o b_o \right) + \Delta b \sum_{i=1}^{N} \left( p_i c_i^0 / b_o \right)^2 \]

\[ + \Delta c \sum_{i=1}^{N} \left( p_i^2 c_i^0 / c_o \right) \ln(b_o) / b_o \]

\[ = \sum_{i=1}^{N} \left( p_i c_i^0 y_i^x / b_o \right) - p_i c_i^0 / b_o \] (D.7)

\[ \Delta a \sum_{i=1}^{N} \left( p_i^2 c_i^0 / c_o \right) (G_i - 1) \ln(b_o) / a_o \]

\[ + \Delta b \sum_{i=1}^{N} \left( p_i^2 c_i^0 / c_o \right) (G_i - 1) \ln(b_o) / b_o \]

\[ + \Delta c \sum_{i=1}^{N} \left( p_i c_i^0 (G_i - 1) \right) \ln(b_o)^2 \]

\[ = \sum_{i=1}^{N} \left( p_i c_i^0 (G_i - 1) \ln(b_o) y_i^x - p_i c_i^0 (G_i - 1) \ln(b_o) \right) \] (D.8)

where \[ G_i \]

\[ p_i = a_o b_o \]

\[ \Delta a = a - a_o \]

\[ \Delta b = b - b_o \]

\[ \Delta c = c - c_o \]

\( a_o, b_o, \) and \( c_o \) (obtained from Davis' method) represent initial estimates of \( a, b, \) and \( c, \) for \( \Delta a, \Delta b, \) and \( \Delta c. \)

This 3 by 4 matrix was solved by an iterative process to obtain the best values of \( a, b, \) and \( c. \) The iterative process was terminated when \( \text{DDEV/DEV} \leq 5 \times 10^{-3}. \)
where

\[
DEV = \sum \left| \frac{\hat{y}_i - y_i}{y_i} \right| \times 100 / \text{number of data points}
\]

and

\[
DDEV = (DEV)_j - (DEV)_{j-1}
\]

and \( j \) is iteration index.

Dalal (7) and Desai (9) used a modified Gompertz equation \( y = \alpha + abcG \) instead of \( y^* = abc \), where \( \alpha \) is intercept of \( y^* \). In these systems, \( \alpha \) is nearly zero for all loces. In Desai's analysis, all \( \alpha \)'s were zero. When the modified Gompertz equation is used, there are four parameters \( \alpha, a, b, \) and \( c \) instead of three \( a, b, \) and \( c \). Some \( \alpha \)'s from the least squares method were negative; but the limits of \( y^* \) in this study were from 0 to 1. Therefore, the unmodified Gompertz equation was used here.

In Desai's program No. 2-A: "Experimental Concentration Gradient as a Function of Distance", Desai treated the derivative as

\[
dy/dx = (ab^c)(\ln b) c^G(\ln c).
\]

Actually, it is

\[
dy/dx = (dy/dG)(dG/dx) = (1/0.005)(ab^c)
\]

\[
(\ln b) c^G(\ln c)
\]

where \( x \) is the experimental scale, and \( G \) is the changing scale for \( y \) value. The unit for \( dy/dx \) in this program is gm/100 cm³/cm. Even using the \( a, b, \) and \( c \) which Desai obtained from Gompertz equation to calculate \( dy/dx \) by his program 2-A, the results are different from the
Table D-1

Constants of Gompertz Equation from Non-Linear Least Squares Method and the Initial Values $a_0$, $b_0$, $c_0$

<table>
<thead>
<tr>
<th>System Number</th>
<th>$a_0$</th>
<th>$b_0$</th>
<th>$c_0$</th>
<th>AAPD$_0$</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>AAPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.1305</td>
<td>0.0509</td>
<td>0.7106</td>
<td>1.4829</td>
<td>1.1006</td>
<td>0.0508</td>
<td>0.6996</td>
<td>1.4741</td>
</tr>
<tr>
<td>2</td>
<td>1.5335</td>
<td>0.0083</td>
<td>0.8966</td>
<td>2.5353</td>
<td>1.8039</td>
<td>0.0103</td>
<td>0.9094</td>
<td>0.4613</td>
</tr>
<tr>
<td>3</td>
<td>1.1788</td>
<td>0.0162</td>
<td>0.7958</td>
<td>1.1963</td>
<td>1.1840</td>
<td>0.0146</td>
<td>0.7839</td>
<td>0.4899</td>
</tr>
<tr>
<td>4</td>
<td>1.0983</td>
<td>0.0482</td>
<td>0.7641</td>
<td>1.6161</td>
<td>1.0878</td>
<td>0.0498</td>
<td>0.7612</td>
<td>0.9621</td>
</tr>
<tr>
<td>5</td>
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<td>0.0195</td>
<td>0.8515</td>
<td>1.7370</td>
<td>1.4295</td>
<td>0.0214</td>
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</tr>
<tr>
<td>6</td>
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<td>1.2122</td>
<td>0.0282</td>
<td>0.8047</td>
<td>0.6252</td>
</tr>
<tr>
<td>7</td>
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<td>0.0314</td>
<td>0.7590</td>
<td>1.1034</td>
<td>1.0677</td>
<td>0.0321</td>
<td>0.7602</td>
<td>0.8460</td>
</tr>
<tr>
<td>8</td>
<td>1.8502</td>
<td>0.0214</td>
<td>0.7563</td>
<td>3.5711</td>
<td>1.2137</td>
<td>0.0218</td>
<td>0.6779</td>
<td>1.0257</td>
</tr>
<tr>
<td>9</td>
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<td>0.7887</td>
<td>1.5168</td>
<td>1.2353</td>
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<td>0.7912</td>
<td>1.3758</td>
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<td>10</td>
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<td>0.7600</td>
<td>1.1031</td>
<td>1.0658</td>
<td>0.0298</td>
<td>0.7647</td>
<td>1.0266</td>
</tr>
</tbody>
</table>
values he presented in his thesis. The values of $\frac{dy}{dx}$ for comparison for system 9 are given below:

<table>
<thead>
<tr>
<th>From Desai's Thesis</th>
<th>Using Desai's Constants &amp; His prog. 2-A</th>
<th>After prog. 2-A Corrected</th>
</tr>
</thead>
<tbody>
<tr>
<td>gm/cm$^3$/cm</td>
<td>gm/100 cm$^3$/cm</td>
<td>gm/100 cm$^3$/cm</td>
</tr>
<tr>
<td>1.077</td>
<td>0.518</td>
<td>103.155</td>
</tr>
<tr>
<td>1.640</td>
<td>0.830</td>
<td>163.596</td>
</tr>
<tr>
<td>1.939</td>
<td>0.959</td>
<td>191.410</td>
</tr>
<tr>
<td>2.079</td>
<td>1.034</td>
<td>205.186</td>
</tr>
<tr>
<td>2.115</td>
<td>1.057</td>
<td>211.437</td>
</tr>
<tr>
<td>2.057</td>
<td>1.024</td>
<td>206.989</td>
</tr>
<tr>
<td>1.975</td>
<td>0.984</td>
<td>200.274</td>
</tr>
<tr>
<td>1.849</td>
<td>0.934</td>
<td>191.302</td>
</tr>
<tr>
<td>1.652</td>
<td>0.834</td>
<td>172.989</td>
</tr>
<tr>
<td>1.346</td>
<td>0.684</td>
<td>144.250</td>
</tr>
</tbody>
</table>

The results in columns one and three are quite close; but column two differs greatly from columns one and three. Thus it appears that the program 2-A in Desai's thesis is an incorrect earlier version from his work which he included in the thesis instead of the correct program which leads to the results indicated in column one.

Dalal (7) used Davis' method to calculate the derivative $\frac{dy}{dx}$. Desai (9) also presented this method for comparison (prog. no. 2-B in Desai's thesis).

$$\phi = \frac{(x-x_1)}{(a+bx)} \quad \text{(D.9)}$$

where $x_1$ corresponds to $y=-.1$

$$\phi = \log \left[ \frac{20y}{\log (100-y)} \right] \quad \text{(D.10)}$$

$$\frac{dy}{dx} = \frac{(a+bx_1)}{(a+bx)^2} S \quad \text{(D.11)}$$

where

$$S = 0.434 \left[ \frac{1}{y} + 0.434 \log(100-y) \right]$$

The constants, $a$ and $b$ are not the same as from Gompertz equation. For instance consider system 9.
The derivatives were also different.

Therefore Davis' method for evaluating the derivative was not considered here.

After the Gompertz equation was obtained from the least squares method, the location of the original interface, i.e., the locus of $x=0$, was obtained. Simpson's numerical method was used to evaluate the areas $A_1$ and $A_2$ at a distance $x=p$ as shown in Figure D.2 and Figure D.3. Area $A_3$ was then evaluated and compared with $A_2$. If these were unequal, then another value of $p$ was specified, $(p_j=p_{j-1}+Dp)$ depending on which area is large or small. This trial and error procedure was followed until the percentage deviation is defined as follows:

$$\text{percentage deviation} = \left(\frac{(A_2-A_3)}{A_2}\right)(100)$$

In other words, the absolute value of $(A_2-A_3)/A_2$ should be less than $8(10)^{-3}$ for all the systems at a final value of $p$. This very closely satisfied the requirement that
for neglecting volume change during diffusion; and

\[ - \int_0^{\infty} x \, dy^* = \int_{y^*}^{1} x \, dy^* \quad \text{(i.e. } \int_{y^*}^{1} x \, dy^* = 0) \]  \hspace{1cm} (D.12)

\[ (i.e. \int_{y^*}^{1} x \, dy^* + 2AW_1 \int_{y^*}^{1} xy^* \, dy^* = 0) \]  \hspace{1cm} (D.13)

for volume change during diffusion. Thus the location of the original interface was obtained.

Consider program number 6 for locating the original interface. In this program, \( N \) is any odd number, \( DP \) is the increment of the iteration. If these two numbers were not suitably used, the satisfactory value of \( (A_2 - A_3)/A_2 \), i.e. \( (A_2 - A_3)/A_2 \leq 8(10)^{-3} \), would not be obtained.

In Desai's analysis, \( DP = 0.0002 \) was small enough; but in this work, only \( DP = 0.00005 \) satisfied all the systems.

There are two ways to evaluate the integral of

\[ \int x \, dy^* : \]

1. \( I_1 = \int_{y^*_1}^{y^*_2} x \, dy^* = \int_{x_1}^{x_2} x \, dy^* \) } \hspace{1cm} \text{(P,YP)}

\[ \begin{align*}
I_1 &= \int_{y^*_1}^{y^*_2} x \, dy^* \\
&= \int_{x_1}^{x_2} x \, dy^* + (p - x_2)(y^*_2 - y^*_1)
\end{align*} \]

\[ \left( P, Y_P \right) \]
2. $x$ was first changed to a function of $y^*$. 

$$x = f(y^*) = 0.005 \left( \frac{\ln((\ln(y^*) - \ln(a))/\ln(b))}{\ln(c)} + 1.0 \right) \quad (D.12)$$

The results of system 9 by these two ways are given below:

<table>
<thead>
<tr>
<th>$I_1$</th>
<th>$I_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00235</td>
<td>0.00235</td>
</tr>
<tr>
<td>0.00412</td>
<td>0.00411</td>
</tr>
<tr>
<td>0.00496</td>
<td>0.00496</td>
</tr>
<tr>
<td>0.00533</td>
<td>0.00533</td>
</tr>
<tr>
<td>0.00547</td>
<td>0.00547</td>
</tr>
<tr>
<td>0.00598</td>
<td>0.00598</td>
</tr>
<tr>
<td>0.00651</td>
<td>0.00651</td>
</tr>
<tr>
<td>0.00719</td>
<td>0.00719</td>
</tr>
<tr>
<td>0.00857</td>
<td>0.00857</td>
</tr>
<tr>
<td>0.01083</td>
<td>0.01083</td>
</tr>
</tbody>
</table>

They are almost the same, as they should be. For evaluating $\int x^*y^*dy^*$, the $I_1$ method is not valid. Therefore, for consistency, $I_2$ method was used to calculate $\int xdy^*$ and $\int x^*dy^*$ for the final results present in this work.

In Appendix F, five different values of diffusion coefficient are presented. $D^{(1)}_{AB}$ is calculated considering volume change during diffusion with the integration technique of $I_2$. $D^{(2)}_{AB}$ is calculated for no volume change during diffusion with the integration technique of $I_2$. $D^{(3)}_{AB}$ is calculated in the same manner as Secor, i.e. the
Figure D-2. Evaluation of \( \int_{0}^{\infty} x \, dy^* \) for \( \int_{0}^{1} x \, dy^* = 0 \).
Figure D-3. Evaluation of $\int_0^y x \, dy^*$ and $\int_0^y xy^* \, dy^*$ for

$$\int_0^1 x \, dy^* + 2A_1\int_0^1 xy^* \, dy^*$$

$= 0$; $A_1 = A_1^{'''} + 2AW_{A_1}A_2^{'''}$, $A_2 = A_2^{'''} + 2AW_{A_1}A_2^{'''}$, $A_3 = A_3^{'''} + 2AW_{A_1}A_3^{'''}$. 

\[\text{For Figure A:} \quad A_1^{'''} \quad A_2^{'''} \quad A_3^{'''}\] 

\[\text{For Figure B:} \quad A_1^{''''} \quad A_2^{''''} \quad A_3^{''''}\]
diffusivity is function of the concentration without
volume change during diffusion. $D_{AB}^{(4)}$ is calculated for
no volume change during diffusion with the integration
technique of $I_1$. $D_{AB}^{(5)}$ considers volume changes during
diffusion with the integration technique $I_1$ for $\int x dy^*$
and $I_2$ for $\int x y^* dy^*$. The five different values are given
in Appendix F.
Appendix E

Figures of Diffusivity (cm^2/sec)  
Versus Reduced Concentration
Figure E.1. Differential Diffusivity vs. Reduced Concentration for 2.2 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with t=12 seconds.
Figure E.2. Differential Diffusivity vs. Reduced Concentration for 2.0 wt.% CMC in Water with D-Glucose as Solute at 23°C, with t=50 seconds.
Figure E.3. Differential Diffusivity vs. Reduced Concentration for 1.7 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with t=20 seconds
Figure E.4. Differential Diffusivity vs. Reduced Concentration for 1.35 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with t=18 seconds.
Figure E.5. Differential Diffusivity vs. Reduced Concentration for 1.20 wt.% CMC in Water with D-Glucose as Solute, at 23°C, with t=20 seconds.
Figure E.6. Differential Diffusivity vs. Reduced Concentration for 0.28 wt.% Carbopol in Water with D-Glucose as Solute, at 23°C, with t=30 seconds
Figure E.7. Differential Diffusivity vs. Reduced Concentration for 0.25 wt.% Carbopol in Water with D-Glucose as Solute, at 21°C, with t=24 seconds.
Figure E.8. Differential Diffusivity vs. Reduced Concentration for 0.22 wt.% Carbopol in Water with D-Glucose as Solute, at 21°C, with t=6 seconds.
Figure E.9. Differential Diffusivity vs. Reduced Concentration for 0.20 wt.% Carbopol in Water with D-Glucose as Solute, at 23°C, with t=20 seconds
Figure E.10. Differential Diffusivity vs. Reduced Concentration for 0.18 wt.% Carbopol in Water with D-Glucose as Solute, at 23°C, with t=20 seconds
Appendix F

Comparison for Five Different Methods of Calculating the Diffusivity

\[
D_{AB}^{(1)} = \frac{(1 - AW_{Al} y^*) \int_0^y f(y^*) dy^* + 2AW_{Al} \int_0^y f(y^*) y dy^*}{2t(1 + AW_{Al} y^*)(dy^*/dx)} \quad (F.1)
\]

\[
D_{AB}^{(2)} = \frac{\int_0^y f(y^*) dy^*}{2t(dy^*/dx)} \quad (F.2)
\]

\[
D_{AB}^{(3)} = \frac{\int_0^y x dy}{2t(dy^*/dx)} \quad (F.3)
\]

\[
D_{AB}^{(4)} = \frac{\int_0^y x dy^*}{2t(dy^*/dx)} \quad (F.4)
\]

\[
D_{AB}^{(5)} = \frac{(1 - AW_{Al} y^*) \int_0^y x dy^* + 2AW_{Al} \int_0^y f(y^*) y dy^*}{2t(1 + AW_{Al} y^*)(dy^*/dx)} \quad (F.5)
\]
Table F.1
List of Five Values of Diffusivity for System 1

<table>
<thead>
<tr>
<th>y*</th>
<th>(D_{AB}^{(1)}) cm²/sec(10^5)</th>
<th>(D_{AB}^{(2)}) cm²/sec(10^5)</th>
<th>(D_{AB}^{(3)}) cm²/sec(10^5)</th>
<th>(D_{AB}^{(4)}) cm²/sec(10^5)</th>
<th>(D_{AB}^{(5)}) cm²/sec(10^5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.099</td>
<td>0.512</td>
<td>0.491</td>
<td>0.501</td>
<td>0.490</td>
<td>0.510</td>
</tr>
<tr>
<td>0.230</td>
<td>0.627</td>
<td>0.602</td>
<td>0.610</td>
<td>0.601</td>
<td>0.626</td>
</tr>
<tr>
<td>0.368</td>
<td>0.719</td>
<td>0.691</td>
<td>0.697</td>
<td>0.690</td>
<td>0.718</td>
</tr>
<tr>
<td>0.483</td>
<td>0.784</td>
<td>0.755</td>
<td>0.758</td>
<td>0.755</td>
<td>0.783</td>
</tr>
<tr>
<td>0.619</td>
<td>0.902</td>
<td>0.878</td>
<td>0.855</td>
<td>0.876</td>
<td>0.916</td>
</tr>
<tr>
<td>0.776</td>
<td>1.415</td>
<td>1.394</td>
<td>1.304</td>
<td>1.392</td>
<td>1.413</td>
</tr>
<tr>
<td>0.877</td>
<td>2.317</td>
<td>2.294</td>
<td>2.107</td>
<td>2.291</td>
<td>2.315</td>
</tr>
<tr>
<td>0.992</td>
<td>5.902</td>
<td>5.865</td>
<td>5.285</td>
<td>5.860</td>
<td>5.897</td>
</tr>
</tbody>
</table>

Range of % DEV of \(D_{AB}^{(2)}\) from \(D_{AB}^{(1)}\): \(-4.10\) to \(-0.63\)

where \(\%\, DEV = \left(\frac{D_{AB}^{(2)} - D_{AB}^{(1)}}{D_{AB}^{(1)}}\right) \times 100\)
Table F.2
List of Five Values of Diffusivity for System 2

<table>
<thead>
<tr>
<th>y*</th>
<th>D(1)_{AB} cm^2/sec(10^5)</th>
<th>D(2)_{AB} cm^2/sec(10^5)</th>
<th>D(3)_{AB} cm^2/sec(10^5)</th>
<th>D(4)_{AB} cm^2/sec(10^5)</th>
<th>D(5)_{AB} cm^2/sec(10^5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.084</td>
<td>0.953</td>
<td>0.915</td>
<td>0.941</td>
<td>0.913</td>
<td>0.952</td>
</tr>
<tr>
<td>0.136</td>
<td>0.997</td>
<td>0.956</td>
<td>0.973</td>
<td>0.951</td>
<td>0.993</td>
</tr>
<tr>
<td>0.258</td>
<td>1.020</td>
<td>0.976</td>
<td>0.985</td>
<td>0.974</td>
<td>1.019</td>
</tr>
<tr>
<td>0.372</td>
<td>0.993</td>
<td>0.949</td>
<td>0.951</td>
<td>0.948</td>
<td>0.992</td>
</tr>
<tr>
<td>0.465</td>
<td>0.942</td>
<td>0.904</td>
<td>0.896</td>
<td>0.903</td>
<td>0.942</td>
</tr>
<tr>
<td>0.526</td>
<td>0.934</td>
<td>0.901</td>
<td>0.877</td>
<td>0.900</td>
<td>0.933</td>
</tr>
<tr>
<td>0.600</td>
<td>0.970</td>
<td>0.944</td>
<td>0.900</td>
<td>0.943</td>
<td>0.969</td>
</tr>
<tr>
<td>0.689</td>
<td>1.078</td>
<td>1.056</td>
<td>0.987</td>
<td>1.054</td>
<td>1.077</td>
</tr>
<tr>
<td>0.776</td>
<td>1.255</td>
<td>1.235</td>
<td>1.139</td>
<td>1.234</td>
<td>1.254</td>
</tr>
<tr>
<td>0.957</td>
<td>1.892</td>
<td>1.872</td>
<td>1.697</td>
<td>1.879</td>
<td>1.891</td>
</tr>
</tbody>
</table>

Range of % DEV of $D(2)_{AB}$ from $D(1)_{AB}$: -3.98 to -1.06
Table F.3

List of Five Values of Diffusivity for System 3

<table>
<thead>
<tr>
<th>y*</th>
<th>D_{AB}^{(1)}</th>
<th>D_{AB}^{(2)}</th>
<th>D_{AB}^{(3)}</th>
<th>D_{AB}^{(4)}</th>
<th>D_{AB}^{(5)}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>cm^2/sec(10^5)</td>
<td>cm^2/sec(10^5)</td>
<td>cm^2/sec(10^5)</td>
<td>cm^2/sec(10^5)</td>
<td>cm^2/sec(10^5)</td>
</tr>
<tr>
<td>0.112</td>
<td>0.572</td>
<td>0.549</td>
<td>0.561</td>
<td>0.551</td>
<td>0.574</td>
</tr>
<tr>
<td>0.187</td>
<td>0.628</td>
<td>0.602</td>
<td>0.611</td>
<td>0.603</td>
<td>0.629</td>
</tr>
<tr>
<td>0.259</td>
<td>0.667</td>
<td>0.640</td>
<td>0.646</td>
<td>0.640</td>
<td>0.668</td>
</tr>
<tr>
<td>0.339</td>
<td>0.698</td>
<td>0.670</td>
<td>0.673</td>
<td>0.671</td>
<td>0.699</td>
</tr>
<tr>
<td>0.465</td>
<td>0.725</td>
<td>0.697</td>
<td>0.696</td>
<td>0.698</td>
<td>0.726</td>
</tr>
<tr>
<td>0.549</td>
<td>0.763</td>
<td>0.739</td>
<td>0.721</td>
<td>0.740</td>
<td>0.763</td>
</tr>
<tr>
<td>0.667</td>
<td>0.947</td>
<td>0.926</td>
<td>0.876</td>
<td>0.927</td>
<td>0.948</td>
</tr>
<tr>
<td>0.755</td>
<td>1.232</td>
<td>1.211</td>
<td>1.127</td>
<td>1.212</td>
<td>1.233</td>
</tr>
<tr>
<td>0.818</td>
<td>1.563</td>
<td>1.540</td>
<td>1.420</td>
<td>1.541</td>
<td>1.563</td>
</tr>
<tr>
<td>0.932</td>
<td>2.742</td>
<td>2.711</td>
<td>2.469</td>
<td>2.713</td>
<td>2.743</td>
</tr>
</tbody>
</table>

Range of % DEV or D_{AB}^{(2)} from D_{AB}^{(1)}: -4.19 to -1.14
Table F.4

List of Five Values of Diffusivity for System 4

<table>
<thead>
<tr>
<th>y*</th>
<th>(D^{(1)}_{AB}) cm(^2)/sec(10(^5))</th>
<th>(D^{(2)}_{AB}) cm(^2)/sec(10(^5))</th>
<th>(D^{(3)}_{AB}) cm(^2)/sec(10(^5))</th>
<th>(D^{(4)}_{AB}) cm(^2)/sec(10(^5))</th>
<th>(D^{(5)}_{AB}) cm(^2)/sec(10(^5))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.085</td>
<td>0.558</td>
<td>0.539</td>
<td>0.541</td>
<td>0.531</td>
<td>0.551</td>
</tr>
<tr>
<td>0.229</td>
<td>0.704</td>
<td>0.679</td>
<td>0.682</td>
<td>0.675</td>
<td>0.701</td>
</tr>
<tr>
<td>0.332</td>
<td>0.782</td>
<td>0.755</td>
<td>0.756</td>
<td>0.752</td>
<td>0.779</td>
</tr>
<tr>
<td>0.462</td>
<td>0.865</td>
<td>0.837</td>
<td>0.834</td>
<td>0.833</td>
<td>0.862</td>
</tr>
<tr>
<td>0.547</td>
<td>0.919</td>
<td>0.892</td>
<td>0.879</td>
<td>0.888</td>
<td>0.915</td>
</tr>
<tr>
<td>0.663</td>
<td>1.131</td>
<td>1.109</td>
<td>1.058</td>
<td>1.105</td>
<td>1.126</td>
</tr>
<tr>
<td>0.776</td>
<td>1.656</td>
<td>1.637</td>
<td>1.523</td>
<td>1.631</td>
<td>1.651</td>
</tr>
<tr>
<td>0.864</td>
<td>2.585</td>
<td>2.564</td>
<td>2.354</td>
<td>2.557</td>
<td>2.578</td>
</tr>
<tr>
<td>0.971</td>
<td>6.043</td>
<td>6.016</td>
<td>5.442</td>
<td>6.002</td>
<td>6.030</td>
</tr>
</tbody>
</table>

Range of % DEV of \(D^{(2)}_{AB}\) from \(D^{(1)}_{AB}\): \(-3.41\) to \(-0.45\)
Table F.5

List of Five Values of Diffusivity for System $5$

<table>
<thead>
<tr>
<th>$y^*$</th>
<th>$D_{AB}^{(1)}$</th>
<th>$D_{AB}^{(2)}$</th>
<th>$D_{AB}^{(3)}$</th>
<th>$D_{AB}^{(4)}$</th>
<th>$D_{AB}^{(5)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{cm}^2/\text{sec}(10^5)$</td>
<td>$\text{cm}^2/\text{sec}(10^5)$</td>
<td>$\text{cm}^2/\text{sec}(10^5)$</td>
<td>$\text{cm}^2/\text{sec}(10^5)$</td>
<td>$\text{cm}^2/\text{sec}(10^5)$</td>
</tr>
<tr>
<td>0.091</td>
<td>1.181</td>
<td>1.149</td>
<td>1.164</td>
<td>1.141</td>
<td>1.174</td>
</tr>
<tr>
<td>0.186</td>
<td>1.306</td>
<td>1.268</td>
<td>1.275</td>
<td>1.262</td>
<td>1.299</td>
</tr>
<tr>
<td>0.261</td>
<td>1.357</td>
<td>1.319</td>
<td>1.319</td>
<td>1.313</td>
<td>1.351</td>
</tr>
<tr>
<td>0.361</td>
<td>1.387</td>
<td>1.349</td>
<td>1.341</td>
<td>1.344</td>
<td>1.382</td>
</tr>
<tr>
<td>0.453</td>
<td>1.380</td>
<td>1.343</td>
<td>1.327</td>
<td>1.338</td>
<td>1.375</td>
</tr>
<tr>
<td>0.564</td>
<td>1.410</td>
<td>1.383</td>
<td>1.329</td>
<td>1.377</td>
<td>1.404</td>
</tr>
<tr>
<td>0.658</td>
<td>1.582</td>
<td>1.560</td>
<td>1.466</td>
<td>1.554</td>
<td>1.576</td>
</tr>
<tr>
<td>0.734</td>
<td>1.835</td>
<td>1.615</td>
<td>1.682</td>
<td>1.808</td>
<td>1.828</td>
</tr>
<tr>
<td>0.806</td>
<td>2.194</td>
<td>2.175</td>
<td>1.997</td>
<td>2.168</td>
<td>2.188</td>
</tr>
<tr>
<td>0.873</td>
<td>2.673</td>
<td>2.653</td>
<td>2.420</td>
<td>2.646</td>
<td>2.666</td>
</tr>
<tr>
<td>0.971</td>
<td>3.729</td>
<td>3.706</td>
<td>3.356</td>
<td>3.697</td>
<td>3.721</td>
</tr>
</tbody>
</table>

Range of $\%$ DEV of $D_{AB}^{(2)}$ from $D_{AB}^{(1)}$: $-2.71$ to $-0.62$
Table F.6

List of Five Values of Diffusivity for System 6

<table>
<thead>
<tr>
<th>( y^* )</th>
<th>( D_{AB}^{(1)} ) cm(^2)/sec(10(^5))</th>
<th>( D_{AB}^{(2)} ) cm(^2)/sec(10(^5))</th>
<th>( D_{AB}^{(3)} ) cm(^2)/sec(10(^5))</th>
<th>( D_{AB}^{(4)} ) cm(^2)/sec(10(^5))</th>
<th>( D_{AB}^{(5)} ) cm(^2)/sec(10(^5))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.077</td>
<td>0.468</td>
<td>0.467</td>
<td>0.454</td>
<td>0.444</td>
<td>0.465</td>
</tr>
<tr>
<td>0.146</td>
<td>0.528</td>
<td>0.505</td>
<td>0.510</td>
<td>0.502</td>
<td>0.528</td>
</tr>
<tr>
<td>0.237</td>
<td>0.583</td>
<td>0.557</td>
<td>0.561</td>
<td>0.555</td>
<td>0.581</td>
</tr>
<tr>
<td>0.345</td>
<td>0.631</td>
<td>0.603</td>
<td>0.604</td>
<td>0.601</td>
<td>0.629</td>
</tr>
<tr>
<td>0.440</td>
<td>0.661</td>
<td>0.633</td>
<td>0.631</td>
<td>0.631</td>
<td>0.660</td>
</tr>
<tr>
<td>0.556</td>
<td>0.692</td>
<td>0.667</td>
<td>0.654</td>
<td>0.665</td>
<td>0.690</td>
</tr>
<tr>
<td>0.682</td>
<td>0.834</td>
<td>0.813</td>
<td>0.771</td>
<td>0.812</td>
<td>0.832</td>
</tr>
<tr>
<td>0.747</td>
<td>0.984</td>
<td>0.965</td>
<td>0.901</td>
<td>0.963</td>
<td>0.982</td>
</tr>
<tr>
<td>0.821</td>
<td>1.254</td>
<td>1.235</td>
<td>1.139</td>
<td>1.233</td>
<td>1.252</td>
</tr>
<tr>
<td>0.886</td>
<td>1.633</td>
<td>1.613</td>
<td>1.474</td>
<td>1.610</td>
<td>1.630</td>
</tr>
<tr>
<td>0.998</td>
<td>2.976</td>
<td>2.952</td>
<td>2.663</td>
<td>2.948</td>
<td>2.973</td>
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</table>

Range of % DEV of \( D_{AB}^{(2)} \) from \( D_{AB}^{(1)} \): -4.49 to -0.81
<table>
<thead>
<tr>
<th>y*</th>
<th>$D_{AB}^{(1)}$</th>
<th>$D_{AB}^{(2)}$</th>
<th>$D_{AB}^{(3)}$</th>
<th>$D_{AB}^{(4)}$</th>
<th>$D_{AB}^{(5)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>cm$^2$/sec(10$^5$)</td>
<td>cm$^2$/sec(10$^5$)</td>
<td>cm$^2$/sec(10$^5$)</td>
<td>cm$^2$/sec(10$^5$)</td>
<td>cm$^2$/sec(10$^5$)</td>
</tr>
<tr>
<td>0.078</td>
<td>0.439</td>
<td>0.421</td>
<td>0.431</td>
<td>0.420</td>
<td>0.438</td>
</tr>
<tr>
<td>0.146</td>
<td>0.508</td>
<td>0.487</td>
<td>0.496</td>
<td>0.485</td>
<td>0.507</td>
</tr>
<tr>
<td>0.235</td>
<td>0.579</td>
<td>0.554</td>
<td>0.562</td>
<td>0.553</td>
<td>0.578</td>
</tr>
<tr>
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<td>0.636</td>
<td>0.609</td>
<td>0.616</td>
<td>0.609</td>
<td>0.635</td>
</tr>
<tr>
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<td>0.691</td>
<td>0.664</td>
<td>0.670</td>
<td>0.663</td>
<td>0.691</td>
</tr>
<tr>
<td>0.467</td>
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<td>0.704</td>
<td>0.708</td>
<td>0.703</td>
<td>0.731</td>
</tr>
<tr>
<td>0.529</td>
<td>0.770</td>
<td>0.752</td>
<td>0.745</td>
<td>0.741</td>
<td>0.769</td>
</tr>
<tr>
<td>0.608</td>
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<td>0.822</td>
<td>0.807</td>
<td>0.821</td>
<td>0.846</td>
</tr>
<tr>
<td>0.696</td>
<td>1.039</td>
<td>1.016</td>
<td>0.973</td>
<td>1.015</td>
<td>1.038</td>
</tr>
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<td>0.757</td>
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<td>1.260</td>
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<td>1.259</td>
<td>1.282</td>
</tr>
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<td>0.822</td>
<td>1.728</td>
<td>1.703</td>
<td>1.582</td>
<td>1.701</td>
<td>1.727</td>
</tr>
<tr>
<td>0.910</td>
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<td>3.031</td>
<td>2.767</td>
<td>3.028</td>
<td>3.060</td>
</tr>
<tr>
<td>0.995</td>
<td>7.922</td>
<td>7.863</td>
<td>7.045</td>
<td>7.856</td>
<td>7.916</td>
</tr>
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</table>

Range of % DEV of $D_{AB}^{(2)}$ from $D_{AB}^{(1)}$: -0.41 to -0.74
Table F.8

List of Five Values of Diffusivity for System 8

<table>
<thead>
<tr>
<th>$y^*$</th>
<th>$D_{AB}^{(1)}$ cm$^2$/sec(10$^5$)</th>
<th>$D_{AB}^{(2)}$ cm$^2$/sec(10$^5$)</th>
<th>$D_{AB}^{(3)}$ cm$^2$/sec(10$^5$)</th>
<th>$D_{AB}^{(4)}$ cm$^2$/sec(10$^5$)</th>
<th>$D_{AB}^{(5)}$ cm$^2$/sec(10$^5$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.132</td>
<td>0.640</td>
<td>0.614</td>
<td>0.632</td>
<td>0.616</td>
<td>0.643</td>
</tr>
<tr>
<td>0.269</td>
<td>0.687</td>
<td>0.658</td>
<td>0.668</td>
<td>0.660</td>
<td>0.689</td>
</tr>
<tr>
<td>0.368</td>
<td>0.685</td>
<td>0.657</td>
<td>0.662</td>
<td>0.658</td>
<td>0.687</td>
</tr>
<tr>
<td>0.437</td>
<td>0.681</td>
<td>0.657</td>
<td>0.651</td>
<td>0.658</td>
<td>0.682</td>
</tr>
<tr>
<td>0.541</td>
<td>0.765</td>
<td>0.745</td>
<td>0.716</td>
<td>0.746</td>
<td>0.766</td>
</tr>
<tr>
<td>0.640</td>
<td>0.967</td>
<td>0.949</td>
<td>0.892</td>
<td>0.950</td>
<td>0.968</td>
</tr>
<tr>
<td>0.702</td>
<td>1.175</td>
<td>1.157</td>
<td>1.076</td>
<td>1.158</td>
<td>1.177</td>
</tr>
<tr>
<td>0.812</td>
<td>1.801</td>
<td>1.778</td>
<td>1.633</td>
<td>1.780</td>
<td>1.803</td>
</tr>
</tbody>
</table>

Range of % DEV of $D_{AB}^{(2)}$ from $D_{AB}^{(1)}$: -4.06 to -1.28
Table F.9

List of Five Values of Diffusivity for System 9

<table>
<thead>
<tr>
<th>( y^* )</th>
<th>( D_{AB}^{(1)} ) cm(^2)/sec(10(^5))</th>
<th>( D_{AB}^{(2)} ) cm(^2)/sec(10(^5))</th>
<th>( D_{AB}^{(3)} ) cm(^2)/sec(10(^5))</th>
<th>( D_{AB}^{(4)} ) cm(^2)/sec(10(^5))</th>
<th>( D_{AB}^{(5)} ) cm(^2)/sec(10(^5))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.092</td>
<td>0.545</td>
<td>0.524</td>
<td>0.538</td>
<td>0.525</td>
<td>0.546</td>
</tr>
<tr>
<td>0.207</td>
<td>0.618</td>
<td>0.593</td>
<td>0.602</td>
<td>0.594</td>
<td>0.619</td>
</tr>
<tr>
<td>0.301</td>
<td>0.648</td>
<td>0.622</td>
<td>0.628</td>
<td>0.623</td>
<td>0.649</td>
</tr>
<tr>
<td>0.383</td>
<td>0.660</td>
<td>0.635</td>
<td>0.637</td>
<td>0.644</td>
<td>0.661</td>
</tr>
<tr>
<td>0.489</td>
<td>0.666</td>
<td>0.644</td>
<td>0.635</td>
<td>0.644</td>
<td>0.666</td>
</tr>
<tr>
<td>0.593</td>
<td>0.751</td>
<td>0.733</td>
<td>0.702</td>
<td>0.733</td>
<td>0.751</td>
</tr>
<tr>
<td>0.653</td>
<td>0.851</td>
<td>0.835</td>
<td>0.788</td>
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<td>0.852</td>
</tr>
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<td>0.710</td>
<td>0.992</td>
<td>0.976</td>
<td>0.911</td>
<td>0.976</td>
<td>0.992</td>
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<tr>
<td>0.797</td>
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<td>1.207</td>
<td>1.310</td>
<td>1.327</td>
</tr>
<tr>
<td>0.901</td>
<td>2.054</td>
<td>2.033</td>
<td>1.854</td>
<td>2.033</td>
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</tr>
</tbody>
</table>

Range of % DEV of \( D_{AB}^{(2)} \) from \( D_{AB}^{(1)} \): -3.85 to -1.02
Table F.10

List of Five Values of Diffusivity for System 10

<table>
<thead>
<tr>
<th>$y^*$</th>
<th>$D_{AB}^{(1)}$ cm$^2$/sec</th>
<th>$D_{AB}^{(2)}$ cm$^2$/sec</th>
<th>$D_{AB}^{(3)}$ cm$^2$/sec</th>
<th>$D_{AB}^{(4)}$ cm$^2$/sec</th>
<th>$D_{AB}^{(5)}$ cm$^2$/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.108</td>
<td>0.591</td>
<td>0.565</td>
<td>0.578</td>
<td>0.566</td>
<td>0.592</td>
</tr>
<tr>
<td>0.203</td>
<td>0.695</td>
<td>0.664</td>
<td>0.674</td>
<td>0.664</td>
<td>0.695</td>
</tr>
<tr>
<td>0.300</td>
<td>0.783</td>
<td>0.748</td>
<td>0.757</td>
<td>0.748</td>
<td>0.783</td>
</tr>
<tr>
<td>0.404</td>
<td>0.869</td>
<td>0.832</td>
<td>0.838</td>
<td>0.832</td>
<td>0.869</td>
</tr>
<tr>
<td>0.508</td>
<td>0.950</td>
<td>0.912</td>
<td>0.916</td>
<td>0.912</td>
<td>0.950</td>
</tr>
<tr>
<td>0.605</td>
<td>1.058</td>
<td>1.024</td>
<td>1.006</td>
<td>1.023</td>
<td>1.058</td>
</tr>
<tr>
<td>0.707</td>
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<td>1.321</td>
<td>1.261</td>
<td>1.320</td>
<td>1.353</td>
</tr>
<tr>
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<td>1.956</td>
<td>1.826</td>
<td>1.955</td>
<td>1.989</td>
</tr>
<tr>
<td>0.904</td>
<td>3.693</td>
<td>3.650</td>
<td>3.344</td>
<td>3.649</td>
<td>3.692</td>
</tr>
</tbody>
</table>

Range of % DEV of $D_{AB}^{(2)}$ from $D_{AB}^{(1)}$: -0.40 to -0.80
Appendix G

Measurement of the Density

Four different weight concentrations of D-Glucose in the solution were measured for each system. The corresponding weight percentages of D-Glucose in the solutions are 0, 3, 6, and 10%. The D-Glucose used here is anhydrous, but the D-Glucose used by Desai (9) was hydrous. It was, therefore, necessary to correct the equivalent weight from anhydrous to hydrous form. The true weights of anhydrous D-Glucose used are 2.7272 gm, 5.4444 gm, and 9.0907 gm corresponding to 3.0 gm, 6.0 gm, and 10 gm of hydrous D-Glucose.

The procedures for measuring the density are as follow:

1. Measure the weight of empty pycnometer.
2. Place the solution in the pycnometer; then let it be in the constant temperature water bath for about 15 minutes.
3. Dry and weigh.

The weight of pure water at the same temperature was also measured. From equation (G.1) the densities of the solutions can be determined.

\[
\text{Density of solution} = \frac{(\text{density of water/weight of water}) \times (\text{weight of solution})}{\text{(G.1)}}
\]

The density of water was obtained from Perry's Handbook (19) as 0.99757 gm/cm\(^3\) at 23°C and 0.99802 gm/cm\(^3\) at 21°C.
Appendix H

Calculation of Differential Diffusion Coefficient of D-Glucose Using Wilke-Chang Correlation and Clough et al Correlation

The form suggested by Wilke and Chang (24, 25) is

\[ D_{AB} = \left[ (7.4)(10)^{-8} \left( \psi_B^m B \right)^{1/3} T \right] / \mu V_A^{0.6} \]  \hspace{1cm} (H.1)

where

- \( D_{AB} \) = diffusivity of solute A in dilute solution in solvent B, cm²/sec
- \( M_B \) = mol. wt. of solvent
- \( T \) = temperature, °K
- \( \mu \) = viscosity of solution, centipoise
- \( V_A \) = solute molal volume of the normal boiling point, cm³/cm mole
- \( \psi_B \) = an association factor for the solvent, 2.6 for water as solvent.

The differential diffusion coefficient of D-Glucose in water at 21 °C is calculated as follows:

- \( M_B = 18 \)
- \( T = 294 \°K \)
- \( \mu = 0.9810 \text{ cp} \)
- \( \psi_B = 2.6 \)
- \( V_A = 177.6 \)

\[ D_{AB} = \left[ 7.4(10)^{-8} (2.6)(18)^0.5 (294) \right] / [(177.6)^0.6 (0.9810)] \]

\[ = 0.67(10)^{-5} \text{ cm}²/\text{sec} \]

In a similar way the differential diffusion coefficient of D-Glucose in water at 23 °C is calculated to be
The percentage deviation of Wilke-Chang value from the experimental value for each system is given in Table H.1.

The form suggested by Clough et al. for predicting the diffusivity of a solute in non-Newtonian solutions is

\[ \frac{D_{NN}}{D} = X_{cp} \left( \frac{\xi}{\xi_{cp}} \right) \left( \frac{\mu}{\mu_{cp}} \right) \]  

(H.2)

For 1.0% CMC system at 23°C

\[ D = \text{Wilke-Chang value for the diffusivity of a Newtonian (low viscosity) fluid,} \]
\[ 0.71(10)^{-5} \text{cm}^2/\text{sec} \]
\[ X_{cp} = \text{the volume fraction of the continuous phase,} \]
\[ 0.97 \]
\[ \frac{\xi}{\xi_{cp}} = \text{ratio of number of neighbors of the diffusing molecule which are sheared during its advancing a distance equal to one lattice parameter,} \]
\[ 15.5/6.0 \]
\[ \mu_{cp} = \text{viscosity of the continuous phase portion of the non-Newtonian fluid.} \]

\[ D_{NN} = (0.71)(10)^{-5}(0.97)(15.5/6.0)(0.92/3.0) \]
\[ = 0.547(10)^{-5} \text{cm}^2/\text{sec} \]

Comparing this predicted value to the lowest value (the solute concentration is 0.84 gm/cm³ solution) for the 1.20 wt.% CMC system in the experiments:

\[ \% \text{ deviation} = \left( \frac{0.547(10)^{-5} - 1.181(10)^{-5}}{1.181(10)^{-5}} \right) \]
\[ = -53.7\% \]
Table H.1

The Percentage Deviation of Wilke-Chang Value from the Experimental Values: Wilke-Chang Values:
$0.71(10)\times10^{-5} \text{cm}^2/\text{sec}$ at $23^\circ\text{C}$ and $0.67(10)\times10^{-5} \text{cm}^2/\text{sec}$ at $21^\circ\text{C}$

<table>
<thead>
<tr>
<th>System Number</th>
<th>Temperature $^\circ\text{C}$</th>
<th>Polymer</th>
<th>Polymer conc. wt.%</th>
<th>$D_{AB}^{(1)}$ $(10)\times10^{-5} \text{cm}^2/\text{sec}$</th>
<th>$Y_{\text{sol.}}$ gm/100cm$^3$</th>
<th>% Dev</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>23</td>
<td>CMC</td>
<td>2.20</td>
<td>0.512</td>
<td>0.947</td>
<td>-39</td>
</tr>
<tr>
<td>2</td>
<td>23</td>
<td>CMC</td>
<td>2.00</td>
<td>0.953</td>
<td>0.775</td>
<td>25</td>
</tr>
<tr>
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<td>23</td>
<td>CMC</td>
<td>1.70</td>
<td>0.572</td>
<td>1.018</td>
<td>-25</td>
</tr>
<tr>
<td>4</td>
<td>23</td>
<td>CMC</td>
<td>1.35</td>
<td>0.558</td>
<td>0.825</td>
<td>-27</td>
</tr>
<tr>
<td>5</td>
<td>23</td>
<td>CMC</td>
<td>1.20</td>
<td>1.181</td>
<td>0.840</td>
<td>40</td>
</tr>
<tr>
<td>6</td>
<td>23</td>
<td>Carbopol</td>
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<td>0.468</td>
<td>0.715</td>
<td>-51</td>
</tr>
<tr>
<td>7</td>
<td>21</td>
<td>Carbopol</td>
<td>0.25</td>
<td>0.439</td>
<td>0.734</td>
<td>-52</td>
</tr>
<tr>
<td>8</td>
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<td>Carbopol</td>
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</tr>
<tr>
<td>9</td>
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<td>Carbopol</td>
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<td>0.545</td>
<td>0.870</td>
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</tr>
<tr>
<td>10</td>
<td>23</td>
<td>Carbopol</td>
<td>0.18</td>
<td>0.591</td>
<td>0.970</td>
<td>-20</td>
</tr>
</tbody>
</table>
Appendix I

Nomenclature

$A =$ concentration dependence of the solution density

$A_1, A_2, A_3 =$ area under the curve of reduced concentration versus distance, cm

$a, b, c =$ constants in Gompertz equation

$D =$ molecular diffusion coefficient of a solute, cm$^2$/sec

$D_{AB}^{(1)} =$ diffusivity as function of reduced concentration. Calculated with integral $I_2$ considering volume change, cm$^2$/sec

$D_{AB}^{(2)} =$ diffusivity as function of reduced concentration. Calculated with integral $I_2$ neglecting volume change, cm$^2$/sec

$D_{AB}^{(3)} =$ diffusivity as function of concentration. Calculated with integral $I_1$ neglecting volume change, cm$^2$/sec

$D_{AB}^{(4)} =$ diffusivity as function of reduced concentration. Calculated with integral $I_1$ neglecting volume change, cm$^2$/sec

$D_{AB}^{(5)} =$ diffusivity as function of reduced concentration. Calculated with integral $I_1$ for $x dy$ and integral $I_2$ for $xy dy$ considering volume change, cm$^2$/sec

$G =$ coordinate, corresponds to distance after the changing of the scale ($G=(x/0.005)-1$)

$\bar{D} =$ integral (average) diffusion coefficient of a solute cm$^2$/sec
\[ I_1 = \int x \, dy^* \]
\[ I_2 = \int f(y^*) \, dy^* \]
\[ j_i^I = \text{ith component of mass diffusion flux of component I relative to mass average velocity, sec}^{-1} \]
\[ M = \text{mol. wt.} \]
\[ p = \text{original interface at x axis, cm.} \]
\[ t = \text{time, seconds} \]
\[ T = \text{temperature, } ^o \text{K} \]
\[ V = \text{volume, cm}^3 \]
\[ v = \text{x component of mass average velocity cm/sec} \]
\[ x = \text{coordinate, corresponds to distance cm} \]
\[ Y = \text{concentration of solute, gm/100cm}^3 \]
\[ y = \text{concentration of solute, gm/cm}^3 \]
\[ y^* = \text{reduced concentration } w_A/w_{A1} \]
\[ y_p = \text{reduced concentration } y^* \text{ corresponds to } p \]
\[ W = \text{weight fraction of solute, } Y/(Y + \text{wt. of Polymer solution}) \]
\[ X = \text{the volume fraction of the continuous phase} \]
\[ n = \text{refractive index} \]

**Subscripts:**

\[ A = \text{solute A} \]
\[ B = \text{solvent B} \]
\[ A_1 = \text{initial weight fraction of solute} \]
\[ A_0 = \text{solute free weight fraction} \]
NN = diffusivity of a non-Newtonian fluid

\( \rho = \) properties or parameters of the continuous phase portion of the non-Newtonian fluid.

Greek and Other Letters:

\( \rho = \) total mass density, \( \text{gm/cm}^3 \)

\( \rho_I = \) mass density of component I, \( \text{gm/cm}^3 \)

\( \rho_s = \) density of solute-free polymer solution, \( \text{gm/cm}^3 \)

\( \phi = \) symbol used for sigmoid function

\( \psi = \) an association factor for solvent

\( \mu = \) viscosity of the fluid, centipoise

\( \xi = \) number of neighbors of the diffusing molecule which are sheared during its advancing a distance equal to one lattice parameter

\( \eta = \) Boltzmann transformation, \( x/2t^{\frac{3}{2}}, \text{cm/sec}^{\frac{3}{2}} \)
Appendix J

Bibliography


VITA

The author was born on February 4, 1942, in San-Chung, Taipei, Taiwan, Republic of China. She received her Primary education in San-Chung Primary School and Pun-Lai Primary School; and her secondary education in Taipei First Girls' Middle and High School. She entered Tunghai University in Tai-Chung, Taiwan in September 1961 and graduated in June 1965 with a Bachelor of Science Degree in Chemical Engineering.

She has been enrolled in the Graduate School of the University of Missouri at Rolla since September, 1966.