REFERENCES

Achilias, D., Kiparissides, C.," Modeling of Diffusion-Controlled Free Radical Polymerization Reactions", J. Appl. Polym. Sci., 35, 1303(1988).

Asua, J.M., Adams, M.E., and Sudol, E.D.," A New Approach for the Estimation in Emulsion Polymerization Systems. I. Homopolymerization under Zero-One Condition",J. Appl. Polym. Sci., 39, 1183(1990).

Asua, J.M., Sudol, E.D., El_aasser, M.S.," Radical Desorption in Emulsion Polymerization ", J. Polym. Sci.: Polym. Chem. Ed., 27, 3903(1989).

Badde, W., Moritz, H.U., and Reichert, K.H.," Kinetics of High Conversion Polymerization of Vinyl Acetate. Effects of Mixing and Reactor Type on Polymer Properties", J. Appl. Polym. Sci., 27, 2249(1982).

Challa, R.R., Drew. J.H., Stahel, E.P., and Stannett, V.," Radiation-Induced Emusion Polymerization of Vinyl Acetate in a Pilot Plant Reactor II. Kinetecs",J. Appl. Polym. Sci. 31, 27(1986).

Chapra, S.C. and Chanel, R.P.,"Numerical Method for Engineering". 2nd ed., McGraw Hill Inc., Singapore. 1987, pp. 576-609.

Chen,S., Wu,K.,"Emulsion Polymerization : On the Characterization of the Particle Size Distribution",J. Polym. Sci.: Polym Chem. Ed., 26, 1143(1988).

Chern, C., Poehlein, G.W.," Polymerization in Nonuniform Latex Particle : Distribution of free radicals",J. Polym. Sci. : Polym. Chem. Ed., 25, 617(1987).

Chern, C., Poehlein, G.W.," Reaction Kinetics of Vinyl Acetate Emulsion Polymerization", J. Appl. Polym. Sci., 33, 2217 (1987).

Chiang, A.T., Thompson, R.W.," Modeling the Transient Behavior of Continuous Emulsion Polymer Reactors", AIChE. J., 25,552 (1979).

Chen, S., Chang, H.,"Kinetics and Mechanism of Emulsion Polymerization : Styrene/Surface Active Ionic Comonomer System". J. Polym. Sci.: Polym. Chem. Ed., 23, 2615(1985).

Dietrich, B.K.,"Chain Transfer Constants of Mercaptants in the Emulsion Polymerization of Styrene",J. Appl. Polym. Sci. 36, 1129(1988).

Eliseeva, V.I., Ivanchev, S.S., Kuchanov, S.I., Lebedev, A.V., Translated by Teague, S.J.," Emulsion Polymerization and its Applications in Industry ",Consultants Bureau, New York, 1981.

Ellis, F.M., Taylor, T.W., Gonzalez, V., Jensen, K.F.,"Estimation of the Molecular Weight Distribution in Batch Polymerization", AIChE. J., 34, 1341(1988).

Gardon, G.L.,"Emulsion polymerization", Chap 6 in "Polymerization Processes", Schildknecht, C.E. and Skeist, I. eds., Wiley Interscience, New York, 1977.

Hamielec, A. E., Friis, N., " Lecture note on Polymerization kinetics", Department of Chemical Engineering, McMaster University, 1975.

Harkins, W. D.," A General Theory of Reaction Loci in Emulsion Polymerization", J. Chem. Phys., 14, 47(1946).

Harkins, W. D.," A General Theory of Emulsion Polymerization", J. Am. Chem. Soc., 69, 1428(1947).

Hasan S.M.," Mechanism of Styrene Emulsion Polymerization During Interval II", J. Polym. Sci.: Polym. Chem. Ed., 20, 3031 (1982).

Hasan, S.M.,"The Effect of the Purity of Ingredients, Oxygen, and Inorganic Particulate Dispersion on the Course of Styrene Emulsion Polymerization", J. Polym. Sci. : Polym. Chem. Ed., 20, 2969(1982).

Kirillov, V., Ray, W.," The Mathematical Modelling of Continuous Emulsion Polymerization Reactors", Chem. Eng. Sci., 33, 1499(1978).

Kiparissides, C., MacGregor, J.F. and Hamielec, A.E., "Continuous Emulsion Polymerization of Vinyl Acetate Part I : Experimental Studies", CJChE., 58, 48(1980).

Kiparissides, C., MacGregor, J.F. and Hamielec, A.E., "Continuous Emulsion Polymerization of Vinyl Acetate Part II : Parameter Estimation and Simulation Studies", CJChE., 58, 56 (1980).

Kiparissides, C., MacGregor, J.F. and Hamielec, A.E., "Continuous Emulsion Polymerization of Vinyl Acetate Part III : Detection of Reactor Performance by Turidity - Spectra and Liquid Exclusion Chromatography", CJChE., 58, 65(1980).

Kreyszig, E.,"Advance Engineering Mathematics", 5ht ed., John Wielh & Son, Inc., New York, 1983, pp. 830 - 869.

Lee, C.H., Mallinson, R.G.," A Model for Molecular Weights in Vinyl Acetate Emulsion Polymerization ", AIChE. J., 34, 840(1988).

Lichti, G., Gilbert, R.G., Donald, H.N.," The Mechanism of Latex Particle Formation and Growth in the Emulsion Polymerization", J. Polym. Sci.: Polym. Chem. Ed., 21, 269(1983).

Nomura, M.," Rate Coefficient for Radical Desorption in Emulsion Polymerization", J. Appl. Polym. Sci., 26, 17(1981).

Odian, G.,"Emulsion polymerization". Chap. 4 in " Principles of polymerization ", 2 nd Ed. Wiley-Interscience, New York, 1981.

Penlides, A., MacGregor, J.F. and Hamielec, A.E.," Effect of Impurities on Emulsion Polymerization : Case I Kinetics", J. Appl. Polym. Sci., 35, 2021(1988).

Piirma, I., Chang, M., " Emulsion Polymerization of Styrene : Nucleation Stuides with Nonionic Emulsifier ", J. Polym. Sci. : Polym. Chem. Ed., 20, 489(1982).

Piirma, I., ed.," Emulsion Polymerization ". Academic Press Inc., New York, 1982.

Pramojaney, N.," A Mathematical Model for an emulsion Polymerization Reactor ", Ph.D. Thesis, Lehigh University, 1982.

Ralings, J.B., and Ray, W.H.," Emulsion Polymerization Reactor Stability : Simplified Model Analysis ", AIChE. J., 33, 1663(1987).

Smith, W.V., Ewart, R.H.," Kinetics of Emulsion Polymerization", J. Chem. Phys., 16, 592(1948).

Soh, S.K., Sundberg, D.C.," Diffusion - Controlled Viniyl Polymerization. I The Gel Effect ", J. Polym. Sci. : Polym. Chem. Ed., 20, 1299(1982).

Stephanopoulos, G.,"Chemical Process Control : An Introduction to Theory and Practice", Prentice-Hall International, New York, 1984.

Taylor, T.W. and Reichert, K.H., "The Influence of Reactor Type and Operating Conditions on the Molecular Weight Distribution in Vinyl Acetate Polymerization", J. Appl. Polym. Sci., 30,227(1986).

Tornell, B., Uustalu, J.,"Formation of Primary Particles in Vinyl Chloride Polymerization", J. Appl. Polym. Sci., 35, 63 (1988).

Trivedi, M.K., Rajagopal, K.R. and Joshi, S.N.,"Emulsion Polymerization of Vinyl Acetate", J. Polym. Sci. : Polym. Chem. Ed., 21, 2011(1983).

Turbo Pascal 4.0 Owner's Handbook, Borland International, 1987.

Turbo Pascal 5.0 User's Guide, Borland International, 1988.

Turbo Pascal 5.0 Reference Guide, Borland International, 1988.

APPENDIX A

MOMENT EXPRESSIONS

1 i th moment of dead polymer without terminal double bond.

$$[M_i] = \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty}(j^i * P_{j,b})\right]$$

2 i th moment of living polymer without terminal double bond.

$$[M^*_i] = \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty}(j^i * P^*_{j,b})\right]$$

3 i th moment of dead polymer with terminal double bond.

$$[\underline{M}_i] = \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty}(j^i * \underline{P}_{j,b})\right]$$

4 i th moment of living polymer with terminal double bond.

$$[\underline{M}^*_i] = \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty}(j^i * \underline{P}^*_{j,b})\right]$$

APPENDIX B

SERIES REDUCTIONS

$$1\quad \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} P^*_{j-1,b}\right] - \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} P^*_{j,b}\right] = [P^*_{1,o}]$$

$$2\quad \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} (j*P^*_{j-1,b})\right] - \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} (j*P^*_{j,b})\right] = [P^*_{1,o}] + [M^*_{o}]$$

$$3\quad \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} (j^2*P^*_{j-1,b})\right] - \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} (j^2*P^*_{j,b})\right] = [P^*_{1,o}] + 2[M^*_{1}] + [M^*_{o}]$$

$$4\quad \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} \underline{P}^*_{j-1,b}\right] - \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} \underline{P}^*_{j,b}\right] = [\underline{P}^*_{1,o}]$$

$$5\quad \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} (j*\underline{P}^*_{j-1,b})\right] - \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} (j*\underline{P}^*_{j,b})\right] = [\underline{P}^*_{1,o}] + [M^*_{o}]$$

$$6\quad \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} (j^2*\underline{P}^*_{j-1,b})\right] - \left[\sum_{j=1}^{\infty}\sum_{b=1}^{\infty} (j^2*\underline{P}^*_{j,b})\right] = [\underline{P}^*_{1,o}] + 2[M^*_{1}] + [M^*_{o}]$$

$$7\quad \left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} \left(\sum_{b=1}^{\infty} P^*_{j-i,b}\sum_{c=1}^{\infty}\underline{P}_{i,c}\right)\right] = [M^*_{o}][\underline{M}_{o}]$$

$$8\quad \left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} j\left(\sum_{b=1}^{\infty} P^*_{j-i,b}\sum_{c=1}^{\infty}\underline{P}_{i,c}\right)\right] = [M^*_{1}][\underline{M}_{o}] + [M^*_{o}][\underline{M}_{1}]$$

$$9\quad \left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} j^2\left(\sum_{b=1}^{\infty} P^*_{j-i,b}\sum_{c=1}^{\infty}\underline{P}_{i,c}\right)\right] = [M^*_{2}][\underline{M}_{o}] + 2[M^*_{1}][\underline{M}_{1}] + [M^*_{o}][\underline{M}_{2}]$$

$$10\quad \left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} \left(\sum_{b=1}^{\infty} \underline{P}^*_{j-i,b}\sum_{c=1}^{\infty}\underline{P}_{i,c}\right)\right] = [\underline{M}^*_{o}][\underline{M}_{o}]$$

$$11\quad \left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} j\left(\sum_{b=1}^{\infty} \underline{P}^*_{j-i,b}\sum_{c=1}^{\infty}\underline{P}_{i,c}\right)\right] = [\underline{M}^*_{1}][\underline{M}_{o}] + [\underline{M}^*_{o}][\underline{M}_{1}]$$

$$12\quad \left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} j^2\left(\sum_{b=1}^{\infty} \underline{P}^*_{j-i,b}\sum_{c=1}^{\infty}\underline{P}_{i,c}\right)\right] = [\underline{M}^*_{2}][\underline{M}_{o}] + 2[\underline{M}^*_{1}][\underline{M}_{1}] + [\underline{M}^*_{o}][\underline{M}_{2}]$$

The full details of series reductions are shown below. To reduce the complexity of writing, the terms of branch point are omited. This series reduction can be applied to both systems that consider the effect of branch points and system which not consiter this effect.

$$1 \quad \left[\sum_{j=1}^{-} P^*_{j-1}\right] - \left[\sum_{j=1}^{-} P^*_{j}\right] = [P^*_1]$$

$$\left[\sum_{j=1}^{-} P^*_{j-1}\right] - \left[\sum_{j=1}^{-} P^*_{j}\right] = [P^*_1] - [P^*_2] \quad ; j = 2$$

$$+ [P^*_2] - [P^*_3] \quad ; j = 3$$

$$+ [P^*_3] - [P^*_4] \quad ; j = 4$$

$$+ [P^*_4] - [P^*_5] \quad ; j = 5$$

$$+ [P^*_5] - [P^*_6] \quad ; j = 6$$

$$+ \cdot$$

$$\cdot$$

$$\cdot$$

$$+ [P^*_{j-1}] - [P^*_j] \quad ; j = \infty$$

$$= [P^*_1] - [P^*_j]$$

assume $[P^*_1] \gg [P^*_j]$, thus

$$\left[\sum_{j=1}^{-} P^*_{j-1}\right] - \left[\sum_{j=1}^{-} P^*_{j}\right] = [P^*_1]$$

$$2 \left[\sum_{j=1}^{\infty} (j*P^*_{j-1})\right] - \left[\sum_{j=1}^{\infty} (j*P^*_{j})\right] = [P^*_1] + [M^*_0]$$

$$\left[\sum_{j=1}^{\infty} (j*P^*_{j-1})\right] - \left[\sum_{j=1}^{\infty} (j*P^*_{j})\right] = 2*[P^*_1] - 2*[P^*_2] \quad ; j = 2$$

$$+ 3*[P^*_2] - 3*[P^*_3] \quad ; j = 3$$

$$+ 4*[P^*_3] - 4*[P^*_4] \quad ; j = 4$$

$$+ 5*[P^*_4] - 5*[P^*_5] \quad ; j = 5$$

$$+ \; . \; . \; .$$

$$+ j*[P^*_{j-1}] - j*[P^*_j] \quad ; j = \infty$$

$$= 2*[P^*_1] + [P^*_2] + [P^*_3] + \ldots + [P^*_j]$$

$$= [P^*_1] + \left[\sum_{j=1}^{\infty} P^*_j\right]$$

$$\left[\sum_{j=1}^{\infty} (j*P^*_{j-1})\right] - \left[\sum_{j=1}^{\infty} (j*P^*_{j})\right] = [P^*_1] + [M^*_0]$$

$$3 \quad \left[\sum_{j=1}^{\infty} (j^2 * P^*_{j-1})\right] - \left[\sum_{j=1}^{\infty} (j^2 * P^*_{j})\right] = [P^*_1] + 2[M^*_1] + [M^*_o]$$

$$\begin{aligned}
\left[\sum_{j=1}^{\infty} (j^2 * P^*_{j-1})\right] - \left[\sum_{j=1}^{\infty} (j^2 * P^*_{j})\right] = \; & 2^2 * [P^*_1] - 2^2 * [P^*_2] && ; j = 2 \\
& + 3^2 * [P^*_2] - 3^2 * [P^*_3] && ; j = 3 \\
& + 4^2 * [P^*_3] - 4^2 * [P^*_4] && ; j = 4 \\
& + 5^2 * [P^*_4] - 5^2 * [P^*_5] && ; j = 5 \\
& + . \\
& \;\; . \\
& \;\; . \\
& + (j)^2 * [P^*_{j-1}] - (j)^2 * [P^*_j] && ; j = \infty
\end{aligned}$$

$$\begin{aligned}
= \; & [P^*_1] + 3*[P^*_1] + 5*[P^*_2] + 7*[P^*_3] \\
& + 9*[P^*_4] + \ldots + (2j+1)*[P^*_j]
\end{aligned}$$

$$= [P_1^*] + \left[\sum_{j=1}^{\infty} ((2j + 1) * P^*_j)\right]$$

$$= [P_1^*] + \left[\sum_{j=1}^{\infty} ((2j) * P^*_j)\right] + \left[\sum_{j=1}^{\infty} P^*_j\right]$$

$$= [P_1^*] + 2 * \left[\sum_{j=1}^{\infty} (j * P^*_j)\right] + \left[\sum_{j=1}^{\infty} P^*_j\right]$$

$$\left[\sum_{j=1}^{\infty} (j^2 * P^*_{j-1})\right] - \left[\sum_{j=1}^{\infty} (j^2 * P^*_{j})\right] = [P_1^*] + 2[M^*_o] + [M^*_o]$$

$$4 \quad \left[\sum_{j=1}^{\infty} \underline{P}^*_{j-1}\right] - \left[\sum_{j=1}^{\infty} \underline{P}^*_{j}\right] = [\underline{P}^*_1]$$

$$\begin{aligned}
\left[\sum_{j=1}^{\infty} \underline{P}^*_{j-1}\right] - \left[\sum_{j=1}^{\infty} \underline{P}^*_{j}\right] &= [\underline{P}^*_1] - [\underline{P}^*_2] && ; j = 2 \\
&+ [\underline{P}^*_2] - [\underline{P}^*_3] && ; j = 3 \\
&+ [\underline{P}^*_3] - [\underline{P}^*_4] && ; j = 4 \\
&+ [\underline{P}^*_4] - [\underline{P}^*_5] && ; j = 5 \\
&+ [\underline{P}^*_5] - [\underline{P}^*_6] && ; j = 6 \\
&+ \,. \\
&\;\;\;\;. \\
&\;\;\;\;. \\
&+ [\underline{P}^*_{j-1}] - [\underline{P}^*_j] && ; j = \infty \\
&= [\underline{P}^*_1] - [\underline{P}^*_j]
\end{aligned}$$

assume $[\underline{P}^*_1] >> [\underline{P}^*_j]$, thus

$$\left[\sum_{j=1}^{\infty} \underline{P}^*_{j-1}\right] - \left[\sum_{j=1}^{\infty} \underline{P}^*_{j}\right] = [\underline{P}^*_1]$$

$$5 \quad \left[\sum_{j=1}^{\infty}(j*\underline{P}^{*}_{j-1})\right] - \left[\sum_{j=1}^{\infty}(j*\underline{P}^{*}_{j})\right] = [\underline{P}^{*}_{1}] + [\underline{M}^{*}_{0}]$$

$$\begin{aligned}
\left[\sum_{j=1}^{\infty}(j*\underline{P}^{*}_{j-1})\right] - \left[\sum_{j=1}^{\infty}(j*\underline{P}^{*}_{j})\right] = \; & 2*[\underline{P}^{*}_{1}] - 2*[\underline{P}^{*}_{2}] && ;\ j = 2 \\
& + 3*[\underline{P}^{*}_{2}] - 3*[\underline{P}^{*}_{3}] && ;\ j = 3 \\
& + 4*[\underline{P}^{*}_{3}] - 4*[\underline{P}^{*}_{4}] && ;\ j = 4 \\
& + 5*[\underline{P}^{*}_{4}] - 5*[\underline{P}^{*}_{5}] && ;\ j = 5 \\
& + \,. \\
& \;\;\, . \\
& \;\;\, . \\
& + j*[\underline{P}^{*}_{j-1}] - j*[\underline{P}^{*}_{j}] && ;\ j = \infty
\end{aligned}$$

$$= 2*[\underline{P}^{*}_{1}] + [\underline{P}^{*}_{2}] + [\underline{P}^{*}_{3}] + \ldots + [\underline{P}^{*}_{j}]$$

$$= [\underline{P}^{*}_{1}] + \left[\sum_{j=1}^{\infty}\underline{P}^{*}_{j}\right]$$

$$\left[\sum_{j=1}^{\infty}(j*\underline{P}^{*}_{j-1}) - \left[\sum_{j=1}^{\infty}(j*\underline{P}^{*}_{j})\right] = [\underline{P}^{*}_{1}] + [\underline{M}^{*}_{0}]\right.$$

$$6 \quad \left[\sum_{j=1}^{\infty}(j^2 * \underline{P}^*_{j-1})\right] - \left[\sum_{j=1}^{\infty}(j^2 * \underline{P}^*_{j})\right] = [\underline{P}^*_1] + 2[\underline{M}^*_1] + [\underline{M}^*_0]$$

$$\begin{aligned}
\left[\sum_{j=1}^{\infty}(j^2 * \underline{P}^*_{j-1})\right] - \left[\sum_{j=1}^{\infty}(j^2 * \underline{P}^*_{j})\right] = \; & 2^2 * [\underline{P}^*_1] - 2^2 * [\underline{P}^*_2] && ;\ j = 2 \\
& + 3^2 * [\underline{P}^*_2] - 3^2 * [\underline{P}^*_3] && ;\ j = 3 \\
& + 4^2 * [\underline{P}^*_3] - 4^2 * [\underline{P}^*_4] && ;\ j = 4 \\
& + 5^2 * [\underline{P}^*_4] - 5^2 * [\underline{P}^*_5] && ;\ j = 5 \\
& + \, . \\
& \quad . \\
& \quad . \\
& + (j)^2 * [\underline{P}^*_{j-1}] - (j)^2 * [\underline{P}^*_j] && ;\ j = \infty
\end{aligned}$$

$$\begin{aligned}
= \; & [\underline{P}^*_1] + 3 * [\underline{P}^*_1] + 5 * [\underline{P}^*_2] + 7 * [\underline{P}^*_3] \\
& + 9 * [\underline{P}^*_4] + \ldots + (2j+1) * [\underline{P}^*_j]
\end{aligned}$$

$$= [\underline{P}_1^*] + \left[\sum_{j=1}^{\infty}((2j + 1) * \underline{P}^*_j)\right]$$

$$= [\underline{P}_1^*] + \left[\sum_{j=1}^{\infty}((2j) * \underline{P}^*_j)\right] + \left[\sum_{j=1}^{\infty} \underline{P}^*_j\right]$$

$$= [\underline{P}_1^*] + 2 * \left[\sum_{j=1}^{\infty}(j * \underline{P}^*_j)\right] + \left[\sum_{j=1}^{\infty} \underline{P}^*_j\right]$$

$$\left[\sum_{j=1}^{\infty}(j^2 * \underline{P}^*_{j-1})\right] - \left[\sum_{j=1}^{\infty}(j^2 * \underline{P}^*_{j})\right] = [\underline{P}_1^*] + 2[\underline{M}^*_0] + [\underline{M}^*_0]$$

7 $$\left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} P^{*}_{j-i}\underline{P}_{i}\right] = \left[\sum_{j=1}^{\infty} P^{*}_{j}\right]\left[\sum_{j=1}^{\infty} \underline{P}_{j}\right]$$

$$= [M^{*}_{o}][\underline{M}_{o}]$$

$$\left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} P^{*}_{j-i}\underline{P}_{i}\right] = P^{*}_{1}\underline{P}_{1}$$
$$+ P^{*}_{2}\underline{P}_{1} + P^{*}_{1}\underline{P}_{2}$$
$$+ P^{*}_{3}\underline{P}_{1} + P^{*}_{2}\underline{P}_{2} + P^{*}_{1}\underline{P}_{3}$$
$$+ P^{*}_{4}\underline{P}_{1} + P^{*}_{3}\underline{P}_{2} + P^{*}_{2}\underline{P}_{3} + P^{*}_{1}\underline{P}_{4}$$
$$+ \;.$$
$$.$$
$$.$$
$$+ P^{*}_{j}\underline{P}_{1} + P^{*}_{j-1}\underline{P}_{2} + P^{*}_{j-2}\underline{P}_{3} + \ldots + P^{*}_{1}\underline{P}_{j}$$

$$= P^{*}_{1}\underline{P}_{1} + P^{*}_{1}\underline{P}_{2} + P^{*}_{1}\underline{P}_{2} + P^{*}_{1}\underline{P}_{4} + \ldots + P^{*}_{1}\underline{P}_{j}$$
$$+ P^{*}_{2}\underline{P}_{1} + P^{*}_{2}\underline{P}_{2} + P^{*}_{2}\underline{P}_{3} + P^{*}_{2}\underline{P}_{4} + \ldots + P^{*}_{2}\underline{P}_{j}$$
$$+ P^{*}_{3}\underline{P}_{1} + P^{*}_{3}\underline{P}_{2} + P^{*}_{3}\underline{P}_{3} + P^{*}_{3}\underline{P}_{4} + \ldots + P^{*}_{3}\underline{P}_{j}$$
$$+ \;.$$
$$.$$
$$.$$
$$+ P^{*}_{j}\underline{P}_{1} + P^{*}_{j}\underline{P}_{2} + P^{*}_{j}\underline{P}_{2} + P^{*}_{j}\underline{P}_{4} + \ldots + P^{*}_{j}\underline{P}_{j}$$

$$= (P^{*}_{1} + P^{*}_{2} + P^{*}_{3} + \ldots + P^{*}_{j})(\underline{P}_{1} + \underline{P}_{2} + \underline{P}_{3} + \ldots + \underline{P}_{j})$$

$$= \left[\sum_{j=1}^{\infty} P^{*}_{j}\right]\left[\sum_{j=1}^{\infty} \underline{P}_{j}\right]$$

$$= [M^{*}_{o}][\underline{M}_{o}]$$

8 $$\left[\sum_{j=1}^{\infty}(j* \sum_{i=1}^{j-1} P^*_{j-i}\underline{P}_i)\right] = [M^*_1][\underline{M}_0] + [M^*_0][\underline{M}_1]$$

$$\left[\sum_{j=1}^{\infty}(j* \sum_{i=1}^{j-1} P^*_{j-i}\underline{P}_i)\right] = 2*P^*_1\underline{P}_1$$

$$+ 3*P^*_2\underline{P}_1 + 3*P^*_1\underline{P}_2$$

$$+ 4*P^*_3\underline{P}_1 + 4*P^*_2\underline{P}_2 + 4*P^*_1\underline{P}_3$$

$$+ 5*P^*_4\underline{P}_1 + 5*P^*_3\underline{P}_2 + 5*P^*_2\underline{P}_3 + 5*P^*_1\underline{P}_4$$

$$+ .$$

$$.$$

$$+ (j+1)P^*_j\underline{P}_1 + (j+1)P^*_{j-1}\underline{P}_2 +\ldots+ (j+1)P^*_1\underline{P}_j$$

$$= 1*P^*_1\underline{P}_1$$

$$+ 2*P^*_2\underline{P}_1 + 1*P^*_1\underline{P}_2$$

$$+ 3*P^*_3\underline{P}_1 + 2*P^*_2\underline{P}_2 + 1*P^*_1\underline{P}_3$$

$$+ 4*P^*_4\underline{P}_1 + 3*P^*_3\underline{P}_2 + 2*P^*_2\underline{P}_3 + 1*P^*_1\underline{P}_4$$

$$+ .$$

$$.$$

$$+ (j)*P^*_j\underline{P}_1 + (j-1)*P^*_{j-1}\underline{P}_2 + (j-2)*P^*_{j-2}\underline{P}_3$$

$$+ (j-3)*P^*_{j-3}\underline{P}_4 +\ldots+ (1)*P^*_1\underline{P}_j$$

$$+ 1*P^*_1\underline{P}_1$$

$$+ 2*P^*_1\underline{P}_2 + 1*P^*_2\underline{P}_1$$

$$+ 3*P^*_1\underline{P}_3 + 2*P^*_2\underline{P}_2 + 1*P^*_3\underline{P}_1$$

$$+ 4*P^*_1\underline{P}_4 + 3*P^*_2\underline{P}_3 + 2*P^*_3\underline{P}_2 + 1*P^*_4\underline{P}_1$$

$$+ .$$

$$.$$

$$+ (j)*P^*_1\underline{P}_j + (j-1)*P^*_2\underline{P}_{j-1} + (j-2)*P^*_3\underline{P}_{j-2}$$

$$+ (j-3)*P^*_4\underline{P}_{j-3} +\ldots+ (1)*P^*_j\underline{P}_1$$

$$= (1*P^*_1 + 2*P^*_2 + 3*P^*_3 +\ldots+ j*P^*_j)(\underline{P}_1 + \underline{P}_2 + \underline{P}_3 +\ldots+ \underline{P}_j)$$

$$+ (1*\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 +\ldots+ j*\underline{P}_j)(P^*_1 + P^*_2 + P^*_3 +\ldots+ P^*_j)$$

$$= \left[\sum_{j=1}^{\infty}(j*P^*_j)\right]\left[\sum_{j=1}^{\infty}\underline{P}_j\right] + \left[\sum_{j=1}^{\infty}(j*\underline{P}_j)\right]\left[\sum_{j=1}^{\infty}P^*_j\right]$$

$$= [M^*_1][\underline{M}_0] + [M^*_0][\underline{M}_1]$$

$$9 \quad \left[\sum_{j=1}^{\infty} \left(j^2 * \sum_{i=1}^{j-1} P^*_{j-i}\underline{P}_i\right)\right] = [M^*_2][\underline{M}_0] + 2[M^*_1][\underline{M}_1] + [M^*_0][\underline{M}_2]$$

$$\begin{aligned}
\left[\sum_{j=1}^{\infty} \left(j^2 * \sum_{i=1}^{j-1} P^*_{j-i}\underline{P}_i\right)\right] = \; & 4*P^*_1\underline{P}_1 \\
& + 9*P^*_2\underline{P}_1 + 9*P^*_1\underline{P}_2 \\
& + 16*P^*_3\underline{P}_1 + 16*P^*_2\underline{P}_2 + 16*P^*_1\underline{P}_3 \\
& + \;. \\
& \quad . \\
& + (j+1)^2 P^*_j\underline{P}_1 + (j+1)^2 P^*_{j-1}\underline{P}_2 + \ldots + (j+1)^2 P^*_1\underline{P}_j
\end{aligned}$$

$$\begin{aligned}
= \; & 1*P^*_1\underline{P}_1 \\
& + 4*P^*_2\underline{P}_1 + 1*P^*_1\underline{P}_2 \\
& + 9*P^*_3\underline{P}_1 + 4*P^*_2\underline{P}_2 + 1*P^*_1\underline{P}_3 \\
& + \;. \\
& \quad . \\
& + (j)^2*P^*_j\underline{P}_1 + (j-1)^2*P^*_{j-1}\underline{P}_2 + (j-2)^2*P^*_{j-2}\underline{P}_3 \\
& \qquad + (j-3)^2*P^*_{j-3}\underline{P}_4 + \ldots + (1)^2*P^*_1\underline{P}_j
\end{aligned}$$

$$\begin{aligned}
& + 2*P^*_1\underline{P}_1 \\
& + 4*P^*_2\underline{P}_1 + 4*P^*_1\underline{P}_2 \\
& + 6*P^*_3\underline{P}_1 + 8*P^*_2\underline{P}_2 + 6*P^*_1\underline{P}_3 \\
& + \;. \\
& \quad . \\
& + 2*j*1*P^*_j\underline{P}_1 + 2*(j-1)*2*P^*_{j-1}\underline{P}_2 \\
& \qquad + 2*(j-2)*3*P^*_{j-2}\underline{P}_3 + \ldots + 2*1*j*P^*_1\underline{P}_j
\end{aligned}$$

$$\begin{aligned}
& + 1*P^*_1\underline{P}_1 \\
& + 4*P^*_1\underline{P}_2 + 1*P^*_2\underline{P}_1 \\
& + 9*P^*_1\underline{P}_3 + 2*P^*_2\underline{P}_2 + 1*P^*_3\underline{P}_1 \\
& + \;. \\
& \quad . \\
& + (j)^2*P^*_1\underline{P}_j + (j-1)^2*P^*_2\underline{P}_{j-1} + (j-2)^2*P^*_3\underline{P}_{j-2} \\
& \qquad + (j-3)^2*P^*_4\underline{P}_{j-3} + \ldots + (1)^2*P^*_j\underline{P}_1
\end{aligned}$$

$$= \quad 1*P^*{}_1\underline{P}_1 + 1*P^*{}_1\underline{P}_2 + 1*P^*{}_1\underline{P}_3 + \ldots + 1*P_1{}^*\underline{P}_j$$
$$+\ 4*P^*{}_2\underline{P}_1 + 4*P^*{}_2\underline{P}_2 + 4*P^*{}_2\underline{P}_3 + \ldots + 4*P^*{}_2\underline{P}_j$$
$$+\ 9*P^*{}_3\underline{P}_1 + 9*P^*{}_3\underline{P}_2 + 9*P^*{}_3\underline{P}_3 + \ldots + 9*P^*{}_3\underline{P}_j$$
$$+\ .$$
$$.$$
$$+\ j^2*P^*{}_j\underline{P}_1 + j^2*P^*{}_j\underline{P}_2 + j^2*P^*{}_j\underline{P}_3 + \ldots + j^2*P^*{}_j\underline{P}_j$$

$$+\ 2*(1*P^*{}_1\underline{P}_1 + 2*P^*{}_1\underline{P}_2 + 3*P^*{}_1\underline{P}_3 + \ldots + 1*j*P^*{}_1\underline{P}_j)$$
$$+\ 2*(2*P^*{}_1\underline{P}_1 + 4*P^*{}_1\underline{P}_2 + 6*P^*{}_1\underline{P}_3 + \ldots + 2*j*P^*{}_1\underline{P}_j)$$
$$+\ 2*(3*P^*{}_1\underline{P}_1 + 6*P^*{}_1\underline{P}_2 + 9*P^*{}_1\underline{P}_3 + \ldots + 3*j*P^*{}_1\underline{P}_j)$$
$$+\ .$$
$$.$$
$$+\ 2*(j*1*P^*{}_1\underline{P}_1 + j*2*P^*{}_1\underline{P}_2 + j*3*P^*{}_1\underline{P}_3 + \ldots + j*j*P^*{}_1\underline{P}_j)$$

$$+\ 1*P^*{}_1\underline{P}_1 + 1*P^*{}_2\underline{P}_1 + 1*P^*{}_3\underline{P}_1 + \ldots + 1*P^*{}_j\underline{P}_1$$
$$+\ 4*P^*{}_1\underline{P}_2 + 4*P^*{}_2\underline{P}_2 + 4*P^*{}_3\underline{P}_2 + \ldots + 4*P^*{}_j\underline{P}_2$$
$$+\ 9*P^*{}_1\underline{P}_3 + 9*P^*{}_2\underline{P}_3 + 9*P^*{}_3\underline{P}_3 + \ldots + 9*P^*{}_j\underline{P}_3$$
$$+\ .$$
$$.$$
$$+\ j^2*P^*{}_1\underline{P}_j + j^2*P^*{}_2\underline{P}_j + j^2*P^*{}_3\underline{P}_j + \ldots + j^2*P^*{}_j\underline{P}_j$$

$$= \quad (1*P^*{}_1 + 2*P^*{}_2 + 3*P^*{}_3 + \ldots + j*P^*{}_j)(\underline{P}_1 + \underline{P}_2 + \underline{P}_3 + \ldots + \underline{P}_j)$$

$$+\ 2*(1*P^*{}_1(\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + 4*\underline{P}_4 + \ldots + j*\underline{P}_j))$$
$$+\ 2*(2*P^*{}_2(\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + 4*\underline{P}_4 + \ldots + j*\underline{P}_j))$$
$$+\ 2*(3*P^*{}_3(\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + 4*\underline{P}_4 + \ldots + j*\underline{P}_j))$$
$$+\ .$$
$$.$$
$$+\ 2*(j*P^*{}_j(\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + 4*\underline{P}_4 + \ldots + j*\underline{P}_j))$$

$$+\ (1*\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + \ldots + j*\underline{P}_j)(P^*{}_1 + P^*{}_2 + P^*{}_3 + \ldots + P^*{}_j)$$

$$= \left[\sum_{j=1}^{\infty} (j^2 * P^*_j)\right]\left[\sum_{j=1}^{\infty} \underline{P}_j\right]$$

$$+ 2(1*(P^*_1 * \left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right]) + 2*(P^*_2 * \left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right])$$

$$+ 3*(P^*_3 * \left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right]) + \ldots + j*(P^*_j * \left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right]))$$

$$+ \left[\sum_{j=1}^{\infty} (j^2 * \underline{P}_j)\right]\left[\sum_{j=1}^{\infty} P_j{}^*\right]$$

$$= \left[\sum_{j=1}^{\infty} (j^2 * P^*_j)\right]\left[\sum_{j=1}^{\infty} \underline{P}_j\right] + 2*\left[\sum_{j=1}^{\infty} (j*P^*_j)\right]\left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right]$$

$$+ \left[\sum_{j=1}^{\infty} (j^2 * \underline{P}_j)\right]\left[\sum_{j=1}^{\infty} P_j{}^*\right]$$

$$= [M^*_2][\underline{M}_0] + 2[M^*_1][\underline{M}_1] + [M^*_0][\underline{M}_2]$$

$$10 \qquad \left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} \underline{P}^*{}_{j-i}\underline{P}_i\right] = \left[\sum_{j=1}^{\infty} \underline{P}^*{}_j\right]\left[\sum_{j=1}^{\infty} \underline{P}_j\right]$$

$$= [\underline{M}^*{}_o][\underline{M}_o]$$

$$\begin{aligned}
\left[\sum_{j=1}^{\infty}\sum_{i=1}^{j-1} \underline{P}^*{}_{j-i}\underline{P}_i\right] = \; & \underline{P}^*{}_1\underline{P}_1 \\
& + \underline{P}^*{}_2\underline{P}_1 + \underline{P}^*{}_1\underline{P}_2 \\
& + \underline{P}^*{}_3\underline{P}_1 + \underline{P}^*{}_2\underline{P}_2 + \underline{P}^*{}_1\underline{P}_3 \\
& + \underline{P}^*{}_4\underline{P}_1 + \underline{P}^*{}_3\underline{P}_2 + \underline{P}^*{}_2\underline{P}_3 + \underline{P}^*{}_1\underline{P}_4 \\
& + \, . \\
& \quad . \\
& \quad . \\
& + \underline{P}^*{}_j\underline{P}_1 + \underline{P}^*{}_{j-1}\underline{P}_2 + \underline{P}^*{}_{j-2}\underline{P}_3 + \ldots + \underline{P}^*{}_1\underline{P}_j
\end{aligned}$$

$$\begin{aligned}
= \; & \underline{P}^*{}_1\underline{P}_1 + \underline{P}^*{}_1\underline{P}_2 + \underline{P}^*{}_1\underline{P}_2 + \underline{P}^*{}_1\underline{P}_4 + \ldots + \underline{P}^*{}_1\underline{P}_j \\
& + \underline{P}^*{}_2\underline{P}_1 + \underline{P}^*{}_2\underline{P}_2 + \underline{P}^*{}_2\underline{P}_3 + \underline{P}^*{}_2\underline{P}_4 + \ldots + \underline{P}^*{}_2\underline{P}_j \\
& + \underline{P}^*{}_3\underline{P}_1 + \underline{P}^*{}_3\underline{P}_2 + \underline{P}^*{}_3\underline{P}_3 + \underline{P}^*{}_3\underline{P}_4 + \ldots + \underline{P}^*{}_3\underline{P}_j \\
& + \, . \\
& \quad . \\
& \quad . \\
& + \underline{P}^*{}_j\underline{P}_1 + \underline{P}^*{}_j\underline{P}_2 + \underline{P}^*{}_j\underline{P}_2 + \underline{P}^*{}_j\underline{P}_4 + \ldots + \underline{P}^*{}_j\underline{P}_j
\end{aligned}$$

$$= (\underline{P}^*{}_1 + \underline{P}^*{}_2 + \underline{P}^*{}_3 + \ldots + \underline{P}^*{}_j)(\underline{P}_1 + \underline{P}_2 + \underline{P}_3 + \ldots + \underline{P}_j)$$

$$= \left[\sum_{j=1}^{\infty} \underline{P}^*{}_j\right]\left[\sum_{j=1}^{\infty} \underline{P}_j\right]$$

$$= [\underline{M}^*{}_o][\underline{M}_o]$$

$$11 \qquad \left[\sum_{j=1}^{\infty} \left(j * \sum_{i=1}^{j-1} \underline{P}^{*}_{j-i}\underline{P}_{i}\right)\right] = [\underline{M}^{*}_{1}][\underline{M}_{o}] + [\underline{M}^{*}_{o}][\underline{M}_{1}]$$

$$\begin{aligned}
\left[\sum_{j=1}^{\infty} \left(j * \sum_{i=1}^{j-1} \underline{P}^{*}_{j-i}\underline{P}_{i}\right)\right] = \; & 2*\underline{P}^{*}_{1}\underline{P}_{1} \\
& + 3*\underline{P}^{*}_{2}\underline{P}_{1} + 3*\underline{P}^{*}_{1}\underline{P}_{2} \\
& + 4*\underline{P}^{*}_{3}\underline{P}_{1} + 4*\underline{P}^{*}_{2}\underline{P}_{2} + 4*\underline{P}^{*}_{1}\underline{P}_{3} \\
& + 5*\underline{P}^{*}_{4}\underline{P}_{1} + 5*\underline{P}^{*}_{3}\underline{P}_{2} + 5*\underline{P}^{*}_{2}\underline{P}_{3} + 5*\underline{P}^{*}_{1}\underline{P}_{4} \\
& + \,. \\
& \;\;\; . \\
& + (j+1)\underline{P}^{*}_{j}\underline{P}_{1} + (j+1)\underline{P}^{*}_{j-1}\underline{P}_{2} + \ldots + (j+1)\underline{P}^{*}_{1}\underline{P}_{j}
\end{aligned}$$

$$\begin{aligned}
= \; & 1*\underline{P}^{*}_{1}\underline{P}_{1} \\
& + 2*\underline{P}^{*}_{2}\underline{P}_{1} + 1*\underline{P}^{*}_{1}\underline{P}_{2} \\
& + 3*\underline{P}^{*}_{3}\underline{P}_{1} + 2*\underline{P}^{*}_{2}\underline{P}_{2} + 1*\underline{P}^{*}_{1}\underline{P}_{3} \\
& + 4*\underline{P}^{*}_{4}\underline{P}_{1} + 3*\underline{P}^{*}_{3}\underline{P}_{2} + 2*\underline{P}^{*}_{2}\underline{P}_{3} + 1*\underline{P}^{*}_{1}\underline{P}_{4} \\
& + \,. \\
& \;\;\; . \\
& + (j)*\underline{P}^{*}_{j}\underline{P}_{1} + (j-1)*\underline{P}^{*}_{j-1}\underline{P}_{2} + (j-2)*\underline{P}^{*}_{j-2}\underline{P}_{3} \\
& \qquad + (j-3)*\underline{P}^{*}_{j-3}\underline{P}_{4} + \ldots + (1)*\underline{P}^{*}_{1}\underline{P}_{j} \\
& + \; 1*\underline{P}^{*}_{1}\underline{P}_{1} \\
& + \; 2*\underline{P}^{*}_{1}\underline{P}_{2} + 1*\underline{P}^{*}_{2}\underline{P}_{1} \\
& + \; 3*\underline{P}^{*}_{1}\underline{P}_{3} + 2*\underline{P}^{*}_{2}\underline{P}_{2} + 1*\underline{P}^{*}_{3}\underline{P}_{1} \\
& + \; 4*\underline{P}^{*}_{1}\underline{P}_{4} + 3*\underline{P}^{*}_{2}\underline{P}_{3} + 2*\underline{P}^{*}_{3}\underline{P}_{2} + 1*\underline{P}^{*}_{4}\underline{P}_{1} \\
& + \,. \\
& \;\;\; . \\
& + (j)*\underline{P}^{*}_{1}\underline{P}_{j} + (j-1)*\underline{P}^{*}_{2}\underline{P}_{j-1} + (j-2)*\underline{P}^{*}_{3}\underline{P}_{j-2} \\
& \qquad + (j-3)*\underline{P}^{*}_{4}\underline{P}_{j-3} + \ldots + (1)*\underline{P}^{*}_{j}\underline{P}_{1}
\end{aligned}$$

$$\begin{aligned}
= \; & (1*\underline{P}^{*}_{1} + 2*\underline{P}^{*}_{2} + 3*\underline{P}^{*}_{3} + \ldots + j*\underline{P}^{*}_{j})(\underline{P}_{1} + \underline{P}_{2} + \underline{P}_{3} + \ldots + \underline{P}_{j}) \\
& + (1*\underline{P}_{1} + 2*\underline{P}_{2} + 3*\underline{P}_{3} + \ldots + j*\underline{P}_{j})(\underline{P}^{*}_{1} + \underline{P}^{*}_{2} + \underline{P}^{*}_{3} + \ldots + \underline{P}^{*}_{j})
\end{aligned}$$

$$= \left[\sum_{j=1}^{\infty} (j*\underline{P}^{*}_{j})\right]\left[\sum_{j=1}^{\infty} \underline{P}_{j}\right] + \left[\sum_{j=1}^{\infty} (j*\underline{P}_{j})\right]\left[\sum_{j=1}^{\infty} \underline{P}^{*}_{j}\right]$$

$$= [\underline{M}^{*}_{1}][\underline{M}_{o}] + [\underline{M}^{*}_{o}][\underline{M}_{1}]$$

$$12 \quad \left[\sum_{j=1}^{-} (j^2 * \sum_{i=1}^{j-1} \underline{P}^*_{j-i}\underline{P}_i)\right] = [\underline{M}^*_2][\underline{M}_0] + 2[\underline{M}^*_1][\underline{M}_1] + [\underline{M}^*_0][\underline{M}_2]$$

$$\left[\sum_{j=1}^{-} (j^2 * \sum_{i=1}^{j-1} \underline{P}^*_{j-i}\underline{P}_i)\right] = 4*\underline{P}^*_1\underline{P}_1$$

$$+ 9*\underline{P}^*_2\underline{P}_1 + 9*\underline{P}^*_1\underline{P}_2$$

$$+ 16*\underline{P}^*_3\underline{P}_1 + 16*\underline{P}^*_2\underline{P}_2 + 16*\underline{P}^*_1\underline{P}_3$$

$$+ .$$

$$.$$

$$+ (j+1)^2\underline{P}^*_j\underline{P}_1 + (j+1)^2\underline{P}^*_{j-1}\underline{P}_2 + \ldots + (j+1)^2\underline{P}^*_1\underline{P}_j$$

$$= 1*\underline{P}^*_1\underline{P}_1$$

$$+ 4*\underline{P}^*_2\underline{P}_1 + 1*\underline{P}^*_1\underline{P}_2$$

$$+ 9*\underline{P}^*_3\underline{P}_1 + 4*\underline{P}^*_2\underline{P}_2 + 1*\underline{P}^*_1\underline{P}_3$$

$$+ .$$

$$.$$

$$+ (j)^2*\underline{P}^*_j\underline{P}_1 + (j-1)^2*\underline{P}^*_{j-1}\underline{P}_2 + (j-2)^2*\underline{P}^*_{j-2}\underline{P}_3$$

$$+ (j-3)^2*\underline{P}^*_{j-3}\underline{P}_4 + \ldots + (1)^2*\underline{P}^*_1\underline{P}_j$$

$$+ 2*\underline{P}^*_1\underline{P}_1$$

$$+ 4*\underline{P}^*_2\underline{P}_1 + 4*\underline{P}_1{}^*\underline{P}_2$$

$$+ 6*\underline{P}^*_3\underline{P}_1 + 8*\underline{P}^*_2\underline{P}_2 + 6*\underline{P}^*_1\underline{P}_3$$

$$+ .$$

$$.$$

$$+ 2*j*1*\underline{P}^*_j\underline{P}_1 + 2*(j-1)*2*\underline{P}^*_{j-1}\underline{P}_2$$

$$+ 2*(j-2)*3*\underline{P}^*_{j-2}\underline{P}_3 + \ldots + 2*1*j*\underline{P}^*_1\underline{P}_j$$

$$+ 1*\underline{P}^*_1\underline{P}_1$$

$$+ 4*\underline{P}^*_1\underline{P}_2 + 1*\underline{P}^*_2\underline{P}_1$$

$$+ 9*\underline{P}^*_1\underline{P}_3 + 2*\underline{P}^*_2\underline{P}_2 + 1*\underline{P}^*_3\underline{P}_1$$

$$+ .$$

$$.$$

$$+ (j)^2*\underline{P}^*_1\underline{P}_j + (j-1)^2*\underline{P}^*_2\underline{P}_{j-1} + (j-2)^2*\underline{P}^*_3\underline{P}_{j-2}$$

$$+ (j-3)^2*\underline{P}^*_4\underline{P}_{j-3} + \ldots + (1)^2*\underline{P}^*_j\underline{P}_1$$

$$= 1*\underline{P}^*{}_1\underline{P}_1 + 1*\underline{P}^*{}_1\underline{P}_2 + 1*\underline{P}^*{}_1\underline{P}_3 +\ldots+ 1*\underline{P}_1{}^*\underline{P}_j$$

$$+ 4*\underline{P}^*{}_2\underline{P}_1 + 4*\underline{P}^*{}_2\underline{P}_2 + 4*\underline{P}^*{}_2\underline{P}_3 +\ldots+ 4*\underline{P}^*{}_2\underline{P}_j$$

$$+ 9*\underline{P}^*{}_3\underline{P}_1 + 9*\underline{P}^*{}_3\underline{P}_2 + 9*\underline{P}^*{}_3\underline{P}_3 +\ldots+ 9*\underline{P}^*{}_3\underline{P}_j$$

$$+ \;.$$

$$.$$

$$+ j^2*\underline{P}^*{}_j\underline{P}_1 + j^2*\underline{P}^*{}_j\underline{P}_2 + j^2*\underline{P}^*{}_j\underline{P}_3 +\ldots+ j^2*P^*{}_j\underline{P}_j$$

$$+ 2*(1*\underline{P}^*{}_1\underline{P}_1 + 2*\underline{P}^*{}_1\underline{P}_2 + 3*\underline{P}^*{}_1\underline{P}_3 +\ldots+ 1*j*\underline{P}^*{}_1\underline{P}_j)$$

$$+ 2*(2*\underline{P}^*{}_1\underline{P}_1 + 4*\underline{P}^*{}_1\underline{P}_2 + 6*\underline{P}^*{}_1\underline{P}_3 +\ldots+ 2*j*\underline{P}^*{}_1\underline{P}_j)$$

$$+ 2*(3*\underline{P}^*{}_1\underline{P}_1 + 6*\underline{P}^*{}_1\underline{P}_2 + 9*\underline{P}^*{}_1\underline{P}_3 +\ldots+ 3*j*\underline{P}^*{}_1\underline{P}_j)$$

$$+ \;.$$

$$.$$

$$+ 2*(j*1*\underline{P}^*{}_1\underline{P}_1 + j*2*\underline{P}^*{}_1\underline{P}_2 + j*3*\underline{P}^*{}_1\underline{P}_3 +\ldots+ j*j*\underline{P}^*{}_1\underline{P}_j)$$

$$+ 1*\underline{P}^*{}_1\underline{P}_1 + 1*\underline{P}^*{}_2\underline{P}_1 + 1*\underline{P}^*{}_3\underline{P}_1 +\ldots+ 1*\underline{P}^*{}_j\underline{P}_1$$

$$+ 4*\underline{P}^*{}_1\underline{P}_2 + 4*\underline{P}^*{}_2\underline{P}_2 + 4*\underline{P}^*{}_3\underline{P}_2 +\ldots+ 4*\underline{P}^*{}_j\underline{P}_2$$

$$+ 9*\underline{P}^*{}_1\underline{P}_3 + 9*\underline{P}^*{}_2\underline{P}_3 + 9*\underline{P}^*{}_3\underline{P}_3 +\ldots+ 9*\underline{P}^*{}_j\underline{P}_3$$

$$+ \;.$$

$$.$$

$$+ j^2*\underline{P}^*{}_1\underline{P}_j + j^2*\underline{P}^*{}_2\underline{P}_j + j^2*\underline{P}^*{}_3\underline{P}_j +\ldots+ j^2*P^*{}_j\underline{P}_j$$

$$= (1*\underline{P}^*{}_1 + 2*\underline{P}^*{}_2 + 3*\underline{P}^*{}_3 +\ldots+ j*P^*{}_j)(\underline{P}_1 + \underline{P}_2 + \underline{P}_3 +\ldots+ \underline{P}_j)$$

$$+ 2*(1*\underline{P}^*{}_1(\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + 4*\underline{P}_4 +\ldots+ j*\underline{P}_j))$$

$$+ 2*(2*\underline{P}^*{}_2(\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + 4*\underline{P}_4 +\ldots+ j*\underline{P}_j))$$

$$+ 2*(3*\underline{P}^*{}_3(\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + 4*\underline{P}_4 +\ldots+ j*\underline{P}_j))$$

$$+ \;.$$

$$.$$

$$+ 2*(j*\underline{P}^*{}_j(\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 + 4*\underline{P}_4 +\ldots+ j*\underline{P}_j))$$

$$+ (1*\underline{P}_1 + 2*\underline{P}_2 + 3*\underline{P}_3 +\ldots+ j*\underline{P}_j)(P^*{}_1 + P^*{}_2 + P^*{}_3 +\ldots+ \underline{P}^*{}_j)$$

$$= \left[\sum_{j=1}^{\infty} (j^2 * \underline{P}^*_j)\right]\left[\sum_{j=1}^{\infty} \underline{P}_j\right]$$

$$+ 2(1*(\underline{P}^*_1 * \left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right]) + 2*(\underline{P}^*_2 * \left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right])$$

$$+ 3*(\underline{P}^*_3 * \left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right]) + \ldots + j*(\underline{P}^*_j * \left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right]))$$

$$+ \left[\sum_{j=1}^{\infty} (j^2 * \underline{P}_j)\right]\left[\sum_{j=1}^{\infty} \underline{P}_j^*\right]$$

$$= \left[\sum_{j=1}^{\infty} (j^2 * \underline{P}^*_j)\right]\left[\sum_{j=1}^{\infty} \underline{P}_j\right] + 2*\left[\sum_{j=1}^{\infty} (j*\underline{P}^*_j)\right]\left[\sum_{j=1}^{\infty} (j*\underline{P}_j)\right]$$

$$+ \left[\sum_{j=1}^{\infty} (j^2 * \underline{P}_j)\right]\left[\sum_{j=1}^{\infty} \underline{P}_j^*\right]$$

$$= [\underline{M}^*_2][\underline{M}_0] + 2[\underline{M}^*_1][\underline{M}_1] + [\underline{M}^*_0][\underline{M}_2]$$

APPENDIX C

SIMPLIFIED NOTATIONS

$$A_1 = k_p[M_p]$$

$$A_2 = k_{fm}[M_p] + k_{fp}[M_o] + k_{fp}[\underline{M}_o] + k_t[R_w]$$

$$A_3 = k_{fp}[M^*_o] + k_{fp}[\underline{M}^*_o]$$

$$A_4 = k_{pdb}[M^*_o] + k_{pdb}[\underline{M}^*_o]$$

$$A_5 = k_{td}[M^*_o] + k_{td}[\underline{M}^*_o]$$

$$A_6 = k_{td}[M^*_o] + (1/2)k_{td}[\underline{M}^*_o]$$

$$A_7 = k_{pdb}[M^*_o]$$

$$A_8 = k_t[R_w] + k_{fp}[M_o] + k_{fp}[\underline{M}_o] + k_{pdb}[\underline{M}_o]$$

$$A_9 = k_1[M_s]([R^*] + [M^*_1]) + k_2[N_o]([R^*] + [M^*_1])$$

$$A_{10} = (k_1[M_s] + k_2[N_o])[\underline{M}^*_1] + k_{fm}[M_p]([M^*_1] + [\underline{M}^*_1])$$

APPENDIX E

DESCRIPTIONS OF THE COMPUTER PROGRAM

The TUROBO PASCAL Version 5.0 Language is used in the developed computer program for the model calculation because of its flexibility, ease and available scientific parameters. The program is devided into four parts. Firstly, THE MAIN PROGRAM, all initial conditions are stated. Secondly, UNIT EQUATION, all model equations are calculated in this part. Thirdly, UNIT SHORGRP, this part shows the graphic results from model calculation on monitor. The results are shown with respect to the reaction time ranged form 0 to 12 residence time. Finally, UNIT PRINTGRP, this part provides the graphic print out.

All kinetic parameters are the parameters at 60 $^{\circ}$C, if one wants to run the model at another temperature he or she should change the parameters stated in the model into those of the new temperature. The kinetic parameters of various sources are available in Appendix C.

The developde program must be run on IBM PC microcomputer with 80287/80387 math coprocessor. Half an hour is used for the calculation of the range form 0 to 12 residence time with 0.1 second increment.

There are some differences between the program parameters and the model parameters, the alphabetical comparison of both parameters is shown below.

Table D The variations in kinetics parameters of vinyl acetate at 60 °C.

Parameters	Friis et al. (1974)	Chiang & Thompson (1979 : 40 °C)	Baade et al. (1982)	Hamer (1983)
k_p	3910	4068	9500	5150
k_{pdb}	**	-	6270	3399
k_{fm}	1.19	0.75	2.26	1.23
k_{fp}	1.88	-	3.23	0.61
k_{td} ($*10^{-8}$)	-	-	3.55	3.93
k_t ($*10^{-8}$)	-	-	-	-

Table D (continued)

Parameters *	Villermaux (1983)	Taylor & Reichert (1985)	Lee & Mallinson (1988)	This work (1991)
k_p	11900	9500	9500	9500
k_{pdb}	2689	6270	**	**
k_{fm}	2.56	2.34	1.20	1.91
k_{fp}	3.61	0.46	1.88	3.23
k_{td} ($*10^{-8}$)	0.73	3.55	-	3.55
k_t ($*10^{-8}$)	-	-	0.73	0.73

* All units are dm^3/mol.s

** Parameters varies with conversion

$X < 0.21 \quad k_{pdb} = 2213.4$

$X > 0.21 \quad k_{pdb} = 2213.4 - 169.6*X - 479*X^2 - 1014*X^3$

APPENDIX E

DESCRIPTIONS OF THE COMPUTER PROGRAM

The TUROBO PASCAL Version 5.0 Language is used in the developed computer program for the model calculation because of its flexibility, ease and available scientific parameters. The program is devided into four parts. Firstly, THE MAIN PROGRAM, all initial conditions are stated. Secondly, UNIT EQUATION, all model equations are calculated in this part. Thirdly, UNIT SHORGRP, this part shows the graphic results from model calculation on monitor. The results are shown with respect to the reaction time ranged form 0 to 12 residence time. Finally, UNIT PRINTGRP, this part provides the graphic print out.

All kinetic parameters are the parameters at 60 $^{\circ}$C, if one wants to run the model at another temperature he or she should change the parameters stated in the model into those of the new temperature. The kinetic parameters of various sources are available in Appendix C.

The developde program must be run on IBM PC microcomputer with 80287/80387 math coprocessor. Half an hour is used for the calculation of the range form 0 to 12 residence time with 0.1 second increment.

There are some differences between the program parameters and the model parameters, the alphabetical comparison of both parameters is shown below.

1 The computer program.

```
PROGRAM Molecular_Weight_Development_Model_Unsteady_State_Hypothesis;
uses graph,printer,Crt,equation,showgrp,printgrp;
{$m $4000,$0,$a0000}
BEGIN {MAIN PROGRAM and initial conditions declaration}
ClrScr;
WRITE('ENTER INITIAL TIME (HOURS)                    '); READLN(InTime);
WRITE('ENTER FINAL   TIME (HOURS)                    '); READLN(FiTime);
WRITE('INITIATOR CONCENTRATION  IN FEED (mol/l)  '); READLN(Ifeed);
WRITE('EMULSIFIER CONCENTRATION IN FEED (mol/l)  '); READLN(Sfeed);
IntStep  :=   216000;
h        :=   3600*(FiTime - InTime)/IntStep;
t        :=   1e-5;
i        :=   0;

ClrScr;
writeln('The Proposed Model for Vinyl Acetate Molecular Weight at 60 C');
writeln;
writeln('                         INTEGRATION PARAMETERS');
writeln('Initiator  Concentration in Feed (mol/L)   =  ',Ifeed  :12:2);
writeln('Emulsifier Concentration in Feed (mol/L)   =  ',Sfeed  :12:2);
writeln('Initial Time (hrs)                         =  ',InTime :9:0);
writeln('Final   Time (hrs)                         =  ',FiTime :9:0);
writeln('Number of Integration Steps                =  ',IntStep:9);
writeln('Increment (sec)                            =  ',h      :12:2);
writeln;
writeln('                           KINETIC  PARAMETERS');
writeln('kp   (L/mol.s)                             =  ',kp  :12:2);
writeln('kfm  (L/mol.s)                             =  ',kfm :12:2);
writeln('kpdb (L/mol.s)                             =  ',kpp :12:2);
writeln('kfp  (L/mol.s)                             =  ',ktrp:12:2);
writeln('kt   (L/mol.s)                             =  ',kt  :12:2);
writeln('ktd  (L/mol.s)                             =  ',ktd :12:2);
writeln;
Y[Nt]   := 1;  Y[Dp]   := 0;  Y[Ap]   := 1;  Y[Vp]   := 0;  Y[Xt]   := 0;
Y[M0i]  := 0;  Y[M1i]  := 0;  Y[M2i]  := 0;  Y[M0a]  := 0;  Y[M1a]  := 0;  Y[M2a]  := 0;
Y[N0i]  := 0;  Y[N1i]  := 0;  Y[N2i]  := 0;  Y[N0a]  := 0;  Y[N1a]  := 0;  Y[N2a]  := 0;
psit    := 0;  P1wodb  := 0;  P1wdb   := 0;

writeln('INTEGRATION PLEASE WAIT !'); writeln(lst);
RUNGE_KUTTA; {calculation of the model equations}
WRITELN('Integration is completed press ENTER to begin the graphic result illustration'); READLN;
GRAPH1; {show the graphic results}
END. {MAIN PROGRAM}
```

The computer program(continued).

```
UNIT EQUATION;
interface
uses printer,Crt;
procedure adjust;
procedure model_equations;
procedure runge_kutta;

CONST  MAX     =   600;
       Difw    =   1.0E-7;
       Difp    =   1.40E-9;
       denm    =   930;
       denp    =   1150;
       dptt    =   5.4E-8;
       aptt    =   9.16E-15;
       vptt    =   8.24E-23;
       fkd     =   2.5E-7;
       kp      =   9500.0;
       kfm     =   1.91;
       ktrp    =   3.23;
       kt      =   7.3e+7;
       ktd     =   3.55E+8;
       kk1     =   2.736E-19;
       kh0     =   4.78E-5;
       L       =   1.29E-4;
       Mf      =   3.42;
       Mo      =   28;
       Scmc    =   4.0E-3;
       Salp    =   6.1E-17;
       delta   =   0.55;
       epsi    =   5;
       mu      =   1.6;
       psi     =   0.823;
       lamco   =   1.915E-12;
       kdeco   =   1.056E+5;
       hikdeco =   6.30E+4;
       Mw      =   86;
       theta   =   1800;
       Na      =   6.02E+23;
       clog    =   2.302585093;
TYPE   EQQ     =   (Nt,Dp,Ap,Vp,Xt,M0i,M1i,M2i,N0i,N1i,N2i,N0a,N1a,N2a,M0a,M1a,M2a);
       EQ      =   Nt..M2a;
       K       =   ARRAY[EQ] OF DOUBLE;
       EQQ1    =   (Ntt,Davt,Apt,Xtt,qav,FreM,Rvt,PriRadt,deRad,P1at,Mpt,Ratet,Mwc,Mnc,PDI);
       ANS     =   Ntt..PDI;
       AY1     =   ARRAY[1..MAX,ANS] OF REAL;
```

The computer program(continued).

```
VAR    AY    : AY1;
       K1,K2,K3,K4,DIFF,Y,Y1       : K;
       TEST,EQ1,EQ2,EQ3,EQ4,EQ5  : EQ;
       EQ6  : EQQ1;
       I,J  : INTEGER;                 {integrating parameters}
       n,IntStep  : LONGINT;           {integrating parameters}
       InTime,FiTime,h,t,t1 : DOUBLE; {integrating parameters}
       zetat,lamda,pseukde,ft,lot,kvt,Amt,Rate,psit,red,K1t,LYAPt : DOUBLE;
       Ifeed,Sfeed,Rw,P1wdb,P1wodb,Ms,Mp,M1wdb,M1wodb,PriRad       : DOUBLE;
       NO,Nact,kpp,kh,kk2,denominat,kde,dav,ctd,q,qpara            : DOUBLE;
       A1,A2,A3,A4,A5,A6,A7,A8,A9,A10                              : DOUBLE;
       a11,a12                                                     : DOUBLE;

implementation

PROCEDURE ADJUST;
   BEGIN
     FOR TEST  :=  MOi TO M2a DO
        BEGIN
            IF Y[TEST] < 1E-30  THEN  Y[TEST] :=  0;
        END;
   END;

PROCEDURE MODEL_EQUATIONS;
   BEGIN {model_equations}
      lamda      :=   lamco*kp*SQRT(kp*Ifeed/kfm);
if Y[Xt]  <=  0.21  then   kpp :=  2213.4   else
      kpp        :=   2213.4 - 169.6*Y[Xt] - 479*SQR(Y[Xt]) - 1014*Y[Xt]*SQR(Y[Xt]);
      red        :=   1-EXP(-t/theta);
      kvt        :=   Y[Vp]/(1-Y[Vp]);
      Amt        :=   (Sfeed*red-Scmc)*Salp*Na - Y[Ap];
if Amt        <  0   then Amt   :=   0;
if L*y[Ap]    >  4   then LYAPt :=   0  else
      LYAPt      :=   1 - L*Y[Ap]/4;
      K1t        :=   kvt*Amt + mu*LYAPt;
if Y[Xt]  >    0.35 then
      pseukde    :=   hikdeco*SQRT(kfm*Ifeed*red/kp)  else
      pseukde    :=   kdeco*SQRT(kfm*Ifeed/kp);
      lot        :=   2*fkd*Ifeed*red*Na + pseukde*Y[Nt]/SQRT(Y[Ap]);
      ft         :=   lot*K1t/(K1t + kvt*epsi*Y[Ap]);
      zetat      :=   red*psit/((1-psit)*SQRT(Y[Ap]));
      DIFF[Nt]   :=                            - Y[Nt]/theta + ft;
      DIFF[Dp]   :=   2*lamda*zetat*Y[Nt]      - Y[Dp]/theta + dptt*ft;
      DIFF[Ap]   :=   4*pi*lamda*zetat*Y[Dp] - Y[Ap]/theta + aptt*ft;
      DIFF[Vp]   :=   lamda*zetat*Y[Ap]        - Y[Vp]/theta + vptt*ft;
      Rate       :=   (1-psit)*denp*lamda*zetat*Y[Ap]/Mw;
      DIFF[Xt]   :=   (Rate/Mf - Y[Xt]/theta)/red;
if    Y[Xt] <  0.21  then  psit :=   psi  ELSE
      psit       :=   (1-Y[Xt])/(1-Y[Xt]*(1-denm/denp));
      Mp         :=   psit*denm/Mw;
      Ms         :=   Amt/Salp;
```

The computer program(continued).

```
    kh          :=   kh0*LYAPt;
    dav         :=   Y[Dp]/Y[Nt];
    kk2         :=   5*kk1*SQR(dav/dptt);
if  Y[Xt] )  0.4  then
    kde         :=   (6*Difp*kfm)/(SQR(dav)*kp)  else
    kde         :=   (12*Difw*delta*kfm)/(Mo*red*SQR(dav+1e-20)*kp);
    denominat :=   kk1*Ms + kk2*Y[Nt] + kh;
    PriRad      :=   2*fkd*Ifeed*red/denominat;
    M1wodb      :=   kde*P1wodb/denominat;
    M1wdb       :=   kde*P1wdb/denominat;
    Rw          :=   PriRad + M1wodb + M1wdb;
    qpara       :=   (2*fkd*Ifeed*red*Na)/(kde*Y[Nt]);
    q           :=   0.5*(SQRT(SQR(qpara) + 2*qpara) - qpara);
    Nact        :=   q*Y[Nt];
    N0          :=   Y[Nt] -  Nact; /
if  Y[Xt] )  0.35  then  ctd   :=  1  else   ctd   :=  0;
    A1    :=   kp*Mp;
    A2    :=   kt*Rw          + kfm*Mp    + ktrp*Y[M0i]    + ktrp*Y[N0i];
    A3    :=   ktrp*Y[M0a]    + ktrp*Y[N0a];
    A4    :=   kpp*Y[M0a]     + kpp*Y[N0a];
    A5    :=   ctd*ktd*Y[M0a] + ctd*ktd*Y[N0a];
    A6    :=   ctd*ktd*Y[M0a] + ctd*0.5*ktd*Y[N0a];
    A7    :=   kpp*Y[M0a];
    A8    :=   kt*Rw   + ktrp*Y[M0i]      + ktrp*Y[N0i]    + kpp*Y[N0i];
    A9    :=   (kk1*Ms + kk2*N0)*(PriRad  + M1wodb);
    A10   :=   (kk1*Ms + kk2*N0)*M1wdb    + kfm*Mp*(Y[M0a] + Y[N0a]);
P1wodb    :=  A9/( kde+A1 + A5 + A8 + 1/theta);
P1wdb     :=  A10/(kde+A1 + A5 + A8 + 1/theta);
DIFF[M0i] :=  (A2+A6)*Y[M0a]                - (A3+1/theta)*Y[M0i];
DIFF[M1i] :=  (A2+A6)*Y[M1a]                - (A3+1/theta)*Y[M1i];
DIFF[M2i] :=  (A2+A6)*Y[M2a]                - (A3+1/theta)*Y[M2i];
DIFF[N0i] :=  (A2+A5)*Y[N0a]                - (A3+A4+1/theta)*Y[N0i] + A6*Y[M0a];
DIFF[N1i] :=  (A2+A5)*Y[N1a]                - (A3+A4+1/theta)*Y[N1i] + A6*Y[M1a];
DIFF[N2i] :=  (A2+A5)*Y[N2a]                - (A3+A4+1/theta)*Y[N2i] + A6*Y[M2a];
DIFF[N0a] :=  A1*P1wdb                      - (A2+A5+1/theta)*Y[N0a] + A3*Y[N0i];
DIFF[N1a] :=  A1*(P1wdb+Y[N0a])             - (A2+A5+1/theta)*Y[N1a] + (A3+A7)*Y[N1i];
DIFF[N2a] :=  A1*(P1wdb+2*Y[N1a]+Y[N0a])   - (A2+A5+1/theta)*Y[N2a] + (A3+A7)*Y[N2i]
                                            + 2*kpp*Y[N1a]*Y[N1i];
DIFF[M0a] :=  A1*P1wodb                     - (A2+A5+1/theta)*Y[M0a] + A3*Y[M0i];
DIFF[M1a] :=  A1*(P1wodb+Y[M0a])            - (A2+A5+1/theta)*Y[M1a] + A3*Y[M1i]  + A7*Y[N1i];
DIFF[M2a] :=  A1*(P1wodb+2*Y[M1a]+Y[M0a]) - (A2+A5+1/theta)*Y[M2a] + A3*Y[M2i]  + A7*Y[N2i]
                                            + 2*kpp*Y[M1a]*Y[N1i];

   END; {model_equations}

PROCEDURE RUNGE_KUTTA;
   BEGIN {runge_kutta}
        FOR n := 1 TO IntStep  DO
        BEGIN {n}
              IF FRAC(n/100)  =  0 THEN
                   BEGIN
                        window(1,21,80,25);
                        ClrEol;
                        writeln('  n  =  ',n);
                   END;
```

The computer program(continued).

```
          FOR EQ1 := Nt  TO  M2a  DO
               BEGIN
                    Y1[EQ1]   :=   Y[EQ1];
               END; {EQ1}
               t1   :=   t;
          MODEL_EQUATIONS;
          FOR EQ2 := Nt  TO  M2a  DO
               BEGIN
                    K1[EQ2]   :=   DIFF[EQ2];
                    Y[EQ2]    :=   Y1[EQ2] + (h*K1[EQ2]/2);
               END; {EQ2}
               t    :=   t1 + h/2;
          ADJUST;
          MODEL_EQUATIONS;
          FOR EQ3 := Nt  TO  M2a  DO
               BEGIN
                    K2[EQ3]   :=   DIFF[EQ3];
                    Y[EQ3]    :=   Y1[EQ3] + (h*K2[EQ3]/2);
               END; {EQ3}
          ADJUST;
          MODEL_EQUATIONS;
          FOR EQ4 := Nt  TO  M2a  DO
               BEGIN
                    K3[EQ4]   :=   DIFF[EQ4];
                    Y[EQ4]    :=   Y1[EQ4] + (h*K3[EQ4]);
               END; {EQ4}
               t    :=   t1 + h;
          ADJUST;
          MODEL_EQUATIONS;
          FOR EQ5 := Nt  TO  M2a  DO
               BEGIN
                    K4[EQ5]   :=   DIFF[EQ5];
                    Y[EQ5]    :=   Y1[EQ5] + (h/6)*(K1[EQ5]+2*K2[EQ5]+2*K3[EQ5]+K4[EQ5]);
               END; {EQ5}
          ADJUST;
IF FRAC(n/360)  =  0  THEN
    BEGIN {collect the calcualted results}
     i := i + 1;
     AY[I,Ntt]      :=   Ln(Y[Nt])/clog - 15;
     AY[I,Davt]     :=   Y[Dp]/Y[Nt];
     AY[I,Apt]      :=   Y[Ap];
     AY[I,Xtt]      :=   Y[Xt];
     AY[I,qav]      :=   q;
     AY[I,FreM]     :=   Ms/Na;
     AY[I,Rwt]      :=   Rw;
     AY[I,PriRadt] :=   PriRad;
     AY[I,deRad]    :=   M1wdb + M1wdb;
     AY[I,P1at]     :=   P1wdb + P1wodb;
     AY[I,Mpt]      :=   Mp;
     AY[I,Ratet]    :=   Rate;
     AY[I,Mwc]      :=   Ln(Mw*((Y[M2i]+Y[M2a]+Y[N2i]+Y[N2a])/(Y[M1i]+Y[M1a]+Y[N1i]+Y[N1a])))/clog;
     AY[I,Mnc]      :=   Ln(Mw*((Y[M1i]+Y[M1a]+Y[N1i]+Y[N1a])/(Y[M0i]+Y[M0a]+Y[N0i]+Y[N0a])))/clog;
     AY[I,PDI]      :=   exp(clog*AY[I,Mwc])/exp(clog*AY[I,Mnc]);
    END; {collect the calculated results}
```

The computer program(continued).

```
        END; {n}
    END; {ruge_kutta}
BEGIN
END.

UNIT SHOWGRP;
interface
uses crt,dos,graph,printgrp,equation ;
procedure graph1;
implementation
procedure graph1;
VAR   gd,gm,k,select : integer;
      answer,head1,s : string;
      a3,a4,dd     : real;
      ch,ch1,ch2 : char;
      pixelcolor : word;
      c : longint;
PROCEDURE ntt1;
   begin
       a11  :=  250/4;
       a12  :=  4/250;
       eq6  :=  ntt;
   end;
PROCEDURE davt1;
   begin
       a11  :=  250/8E-6;
       a12  :=  8E-6/250;
       eq6  :=  davt;
   end;
PROCEDURE apt1;
   begin
       a11  :=  250/2.5E+6;
       a12  :=  2.5E+6/250;
       eq6  :=  apt;
   end;
PROCEDURE xtt1;
   begin
       a11  :=  250;
       a12  :=  1/250;
       eq6  :=  xtt;
   end;
PROCEDURE qav1;
   begin
       a11  :=  250/1;
       a12  :=  1/250;
       eq6  :=  qav;
   end;
PROCEDURE frem1;
   begin
       a11  :=  250/1E-2;
       a12  :=  1E-2/250;
       eq6  :=  frem;
   end;
```

The computer program(continued).

```
PROCEDURE Rw1;
  begin
     a11  :=  250/2E-10;
     a12  :=  2E-10/250;
     eq6  :=  Rwt;
  end;
PROCEDURE PriR1;
  begin
     a11  :=  250/2E-10;
     a12  :=  2E-10/250;
     eq6  :=  PriRadt;
  end;
PROCEDURE deRad1;
  begin
     a11  :=  250/2E-10;
     a12  :=  2E-10/250;
     eq6  :=  deRad;
  end;
PROCEDURE P1a1;
  begin
     a11  :=  250/2E-10;
     a12  :=  2E-10/250;
     eq6  :=  P1at;
  end;
PROCEDURE Mp1;
  begin
     a11  :=  250/10;
     a12  :=  10/250;
     eq6  :=  Mpt;
  end;
PROCEDURE Rate1;
  begin
     a11  :=  250/2E-3;
     a12  :=  2E-3/250;
     eq6  :=  Ratet;
  end;
PROCEDURE mwc1;
  begin
     a11  :=  250/7;
     a12  :=  7/250;
     eq6  :=  mwc;
  end;
PROCEDURE mnc1;
  begin
     a11  :=  250/7;
     a12  :=  7/250;
     eq6  :=  mnc;
  end;
PROCEDURE pdi1;
  begin
     a11  :=  250/5;
     a12  :=  5/250;
     eq6  :=  pdi;
  end;
```

The computer program(continued).

```
begin
  WINDOW(1,1,80,25);
  Clrscr;
  writeln(' 1. Total numbeer of polymer particle');
  writeln(' 2. Average particle diameter');
  writeln(' 3. Total particle surface area');
  writeln(' 4. Total conversion');
  writeln(' 5. Average number of free radical per particle');
  writeln(' 6. Free emulsifier concentration');
  writeln(' 7. Water phase radical concentration');
  writeln(' 8. Primary radical concentration');
  writeln(' 9. Desorbed radical concentration');
  writeln('10. Monomeric radical concentarition');
  writeln('11. Monomer concentration in particle');
  writeln('12. Rate of reaction');
  writeln('13. Weight average molecular weight');
  writeln('14. Number average molecular weight');
  writeln('15. Polydispersity index');
  writeln('16. exit');
  readln(select);
  WHILE select <> 16 DO
    BEGIN
      case select of
      1 : begin ntt1;  head1 := 'Total Number of Particle(particle/L)'; end;
      2 : begin davt1; head1 := 'Average Particle Diameter (dm/L)';     end;
      3 : begin apt1;  head1 := 'Total Particle Surface Area (dm2/L)';  end;
      4 : begin xtt1;  head1 := 'Conversion ';                          end;
      5 : begin qav1;  head1 := 'Average radical per particle';         end;
      6 : begin frem1; head1 := 'Free miclle concentration (1/L)';      end;
      7 : begin Rw1;   head1 := 'Water phase radical concentration';    end;
      8 : begin PriR1; head1 := 'Primary radical concentration';        end;
      9 : begin deRad1;head1 := 'Desorbed radical concentration';       end;
     10 : begin P1a1;  head1 := 'Monomeric radical concentration';      end;
     11 : begin Mp1;   head1 := 'Monomer concentration in particle';    end;
     12 : begin Rate1; head1 := 'Rate of reaction';                     end;
     13 : begin mwc1;  head1 := 'Weight average molecular weight';      end;
     14 : begin mnc1;  head1 := 'Number average molecular weight';      end;
     15 : begin pdi1;  head1 := 'Polydispersity index';                 end;
      else
      select := 16;
    END;
       SetGraphMode(GetGraphMode);
       gd := detect;
       initgraph(gd,gm,'');
       if graphresult <> grok then
       halt(1);
      cleardevice;
      line(50,48,50,298);
      line(50,298,700,298);
      moveto(650,250);
```

The computer program(continued).

```
FOR i := 1 TO 25 DO
  BEGIN
    settextstyle(2,horizdir,3);
    circle(50,298-i*10,2);
    moveto(30,298-i*10);
    str((i*10):1,s);
    outtext(s);
  END;
    settextstyle(2,vertdir,4);
    moveto(5,48);
    str(a12:5,s);
    outtext(head1+'x'+s);

FOR j := 1 TO 600 DO
  BEGIN {show graph}
    c := round((ay[j,eq6])*a11);
     putpixel(50+j,(298-c),1);
     settextstyle(2,horizdir,3);
     IF frac(j/50) = 0 THEN
        BEGIN
          settextstyle(2,1,4);
          Str(j:1,s);
          circle(50+j,298,2);
          moveto(50+j,298);
          outtext(s);
        END;
END; {show graph}
  moveto(300 ,320);
  settextstyle(2,horizdir,4);
  outtext('Time(x60 sec)');
  bar(50,10,150,25);
  moveto(50,10);
  setcolor(0);
  settextstyle(2,horizdir,5);
  outtext(' PRINT?(Y/N) ');
  setcolor(1);
  ch := readkey;
  outtext(ch);
  if (ch = 'y') or (ch = 'Y') then
    BEGIN
       setviewport(1,10,160,25,clipon);
       clearviewport;
       printgraph;
    END;{viewport}
  bar(500,10,650,25);
  setcolor(0);
  moveto(500,10);
  closegraph;
```

The computer program(continued).

```
      writeln(' 1. Total numbeer of polymer particle');
      writeln(' 2. Average particle diameter');
      writeln(' 3. Total particle surface area');
      writeln(' 4. Total conversion');
      writeln(' 5. Average number of free radical per particle');
      writeln(' 6. Free emulsifier concentration');
      writeln(' 7. Water phase radical concentration');
      writeln(' 8. Primary radical concentration');
      writeln(' 9. Desorbed radical concentration');
      writeln('10. Monomeric radical concentration');
      writeln('11. Monomer concentration in particle');
      writeln('12. Rate of reaction');
      writeln('13. Weight average molecular weight');
      writeln('14. Number average molecular weight');
      writeln('15. Polydispersity index');
      writeln('16. exit');
      write('your select ');
      readln(select);
         END;
   END;
END.

UNIT PRINTGRP;
interface
uses crt,dos,graph;
procedure printgraph;
implementation
procedure printgraph;
CONST  aspect  = $24;
TYPE   stroket = string[7];
VAR    prmode,maxx,maxy,maxstrip,n1,n2,ine : integer;
       gd,gm : integer;  {oldwnd : wndname;}
       reg   : registers;

PROCEDURE out1byte(dat : byte);
VAR    reg   : registers;
   BEGIN
     reg.ah := 0; reg.al := dat;
     reg.dx := $0000; intr($17,reg);
   END;
PROCEDURE sentcontrole(stroke : stroket);
VAR    id    : byte;
   BEGIN
     FOR id  := 1 TO length(stroke)  DO
       out1byte(ord(stroke[id]));
   END;
```

The computer program(continued).

```
PROCEDURE printstrip(ine : integer);
CONST  bits    : array[0..7] of byte = (128,64,32,16,8,4,2,1);
VAR    bit,dat : byte;
       xx,yy   :integer;
   BEGIN
     yy := ine *8;
     sentcontrole(#27 + '*' + chr(prmode) + chr(n1) + chr(n2) + #0);
     FOR  xx := 0 TO maxx DO
       BEGIN
          dat := 0;
          for bit := 0 to 7 do
          if getpixel(xx,yy+bit) () 0 then
          dat := dat or bits[bit];
          reg.ah :=0 ; reg.dx := $0000;
          reg.al := dat;   intr($17,reg);
       END;
         out1byte(10);
   END;

BEGIN {printgraph};
   reg.ah := 1; reg.dx :=0; intr($17,reg);
   IF (reg.ah () 16 ) AND (reg.ah () 8 ) THEN
      BEGIN
         write('  printer no ready try again');
         write(^g); exit end;
         sentcontrole(#27+'3'+aspect);
         sentcontrole(#27 + '1' + #10);
         maxx := getmaxx ; maxy := getmaxy;
         maxstrip := maxy div 8;
         detectgraph(gd,gm);
   IF (gd = cga ) AND (gm in [0..3]) THEN
         prmode := 0   ELSE
         prmode := 1;
         n1 := lo(succ(maxx));
         n2 := hi(succ(maxx));
   FOR ine := 0 TO maxstrip  DO
         printstrip(ine);
         sentcontrole (#27+'2');
         sentcontrole (#27 +'1'+#0);
         sentcontrole(#13);
      END;
END.
```

2 The alphabatical comparison between program parameters model parameters.

program	model	meaning
Amt	$A_m(t)$	total micelle surface area
dav	-	average particle diameter
aptt	$a_p(t,t)$	surface area of micelle
DIFF[A_p]	$dA_p(t)/dt$	change rate of total particle surface area
DIFF[Dp]	$dD(t)/dt$	change rate of total particle diameter
DIFF[M0i]	$d[M_o]/dt$	change rate of zero moment for dead polymer without terminal double bond
DIFF[M1i]	$d[M_1]/dt$	change rate of first moment for dead polymer without terminal double bond
DIFF[M2i]	$d[M_2]/dt$	change rate of second moment for dead polymer without terminal double bond
DIFF[M0a]	$d[M^*_o]/dt$	change rate of zero moment for living polymer without terminal double bond
DIFF[M1a]	$d[M^*_1]/dt$	change rate of first moment for living polymer without terminal double bond
DIFF[M2a]	$d[M^*_2]/dt$	change rate of second moment for living polymer without terminal double bond
DIFF[N0i]	$d[\underline{M}_o]/dt$	change rate of zero moment for dead polymer with terminal double bond
DIFF[N1i]	$d[\underline{M}_1]/dt$	change rate of first moment for dead polymer with terminal double bond
DIFF[N2i]	$d[\underline{M}_2]/dt$	change rate of second moment for dead polymer with terminal double bond
DIFF[N0a]	$d[\underline{M}^*_o]/dt$	change rate of zero moment for living polymer with terminal double bond
DIFF[N1a]	$d[\underline{M}^*_1]/dt$	change rate of first moment for living polymer with terminal double bond
DIFF[N2a]	$d[\underline{M}^*_2]/dt$	change rate of second moment for living polymer with terminal double bond

program	model	meaning
DIFF[Nt]	$dN(t)/dt$	change rate of total number of particle
DIFF[Vp]	$dV_p(t)/dt$	change rate of total particle volume
DIFF[Xt]	$dX(t)/dt$	change rate of total conversion
dptt	$D_p(t,t)$	micelle size, micelle diameter
Difw	D_w	diffusion coefficient of monomeric radical in water phase
Difp	D_p	diffusion coefficient of monomeric radical in polymer particle
denm	d_m	monomer density
denp	d_p	polymer density
f	f	initiator decomposition efficiency
kd	k_d	initiator decomposition rate constant
ft	$f(t)$	particle nucleation rate
Ifeed	$[I]_{feed}$	initiator concentration in feed
hikdeco	-	constant for k_{de} at high conversion = $\frac{6D_p}{m_o d_p^2}$
kdeco	-	constant for k_{de} at low conversion = $\frac{12D_w}{m_o d_p^2}$
kk1	k_1	radical absorption rate constant to micelles
kk2	k_2	radical absorption rate constant to particles
kfm	k_{fm}	rate coefficient of chain transfer to monomer
kfp	k_{fp}	rate coefficient of chain transfer to polymer
kh, kh0	k_h, k_{ho}	rate coefficient of homogeneous nucleation
kp	k_p	rate coefficient of polymer propagation
kpdb	k_{pdb}	rate coefficient for terminal double bond reaction
ktd	k_{td}	rate coefficient for termination by disproportionation
kt	k_t	termination rate constant with water phase radicals
kv	k_v	volume ratio of polymer to aqueous phase
L	L	critical diffusion length

program	model	meaning
LYAPt	-	time dependent function, $(1-LA_p(t)/4)$
lamda		constant $= \frac{d_m}{N_A d_p}\left[\frac{fk_d m_o}{12\pi D_w}\right]^{1/2}$
M1wodb	M^*_1	monomeric concentration without terminal double bond in water phase
M1wdb	$\underline{M}^*_1$	monomeric concentration without terminal double bond in water phase
Mf	M_f	monomer concentartion in feed
Mo	Mm, m(t)	partition coefficient of monomeric radicals between water and particle phase
Mp	$[M_p]$	monomer concentration in particles
Ms	-	free micelle concentration .
Mw	Mw	molecular weight of vinyl acetate monomer
Na	N_A	Avogadro's number
NO	$[N_O]$	dead partecle concentration
Nact	$[N^*]$	active partecle concentration
P1wodb	$[P^*_1]$	monomeric radical without terminal double bond in particles
P1wdb	$[\underline{P}^*_1]$	monomeric radical with terminal double bond in particles
PDI	PDI	polydispersity index
PriRad	$[R^*]$	primary radical concentration
Rate	R_p	total rate of polymerization
Rw	$[R_w]$	water phase radical concentration
red	$(1-e^{-t/\theta})$	time dependent function
Sfeed	S_F	emulsifier concentration in feed
Scmc	S_{cmc}	critical micelle concentration
Salp	S_α	area cover by one molecule of emulsifier
t	t	time
$Y[A_p]$	$A_p(t)$	total surface area of polymer particles
Y[Dp]	D(t)	total polymer particle diameter

program	model	meaning
Y[M0i]	$[M_0]$	zero moment for dead polymer without terminal double bond
Y[M1i]	$[M_1]$	first moment for dead polymer without terminal double bond
Y[M2i]	$[M_2]$	second moment for dead polymer without terminal double bond
Y[M0a]	$[M^*_0]$	zero moment for living polymer without terminal double bond
Y[M1a]	$[M^*_1]$	first moment for living polymer without terminal double bond
Y[M2a]	$[M^*_2]$	second moment for living polymer without terminal double bond
Y[N0i]	$[\underline{M}_0]$	zero moment for dead polymer with terminal double bond
Y[N1i]	$[\underline{M}_1]$	first moment for dead polymer with terminal double bond
Y[N2i]	$[\underline{M}_2]$	second moment for dead polymer with terminal double bond
Y[N0a]	$[\underline{M}^*_0]$	zero moment for living polymer with terminal double bond
Y[N1a]	$[\underline{M}^*_1]$	first moment for living polymer with terminal double bond
Y[N2a]	$[\underline{M}^*_2]$	second moment for living polymer with terminal double bond
Y[Mwc]	M_w	weight average molecular weight
Y[Mnc]	M_n	number average molecular weight
Y[Nt]	$N(t)$	total number of particle at time t
Y[Vp]	$V_p(t)$	total particle volume at time t
Y[Xt]	$X(t)$	total monomer conversion

Greek letters

program	model	meaning
mu	μ	constant equal to k_{ho}/k_m ratio
delta	δ	lumped monomeric radical diffusion coefficient
epsi	ε	ratio of radical desorption rate to micella nucleation rate
psi	ϕ_{sat}	saturated monomer volume fraction in particle
psit	$\phi(t)$	monomer volume fraction in particle
lamda	λ	constant $= \dfrac{k_p d_m}{N_A d_p}\left[\dfrac{k_p f k_d [I]_{feed} m_o}{12 \pi D_w \delta k_{fm}}\right]^{1/2}$
lot		free radical production rate
theta	θ	mean residence time
zetat	$\zeta(t)$	time dependent function $= \dfrac{(1-e^{-t/\theta})\phi(t)}{(1-\phi(t))A^{1/2}(t)}$

3 Examples of the calculated results.

The following are the examples of the calculated results of the proposed model.

Table E1 Calculated results of moments at $[I]_{feed}$ = 0.01 mole/dm^3, $[S]_{feed}$ = 0.01 mole/dm^3, θ = 30 min. VAc/Water = 4/10.

Time min.	M0i mol/L	M1i mol/L	M2i mol/L	N0i mol/L	N1i mol/L	N2i mol/s	Mv	Mn	PDI
12	5.5E-0007	2.8E-0003	3.0E+0001	6.4E-0004	3.2E+0000	3.3E+0004	8.9E+0005	4.3E+0005	2.1E+0000
24	1.7E-0006	1.1E-0002	1.6E+0002	3.5E-0003	1.7E+0001	2.3E+0005	1.1E+0006	4.3E+0005	2.6E+0000
36	3.0E-0006	2.1E-0002	3.8E+0002	3.7E-0003	1.8E+0001	2.7E+0005	1.3E+0006	4.3E+0005	2.9E+0000
48	4.1E-0006	2.8E-0002	5.1E+0002	2.5E-0003	1.2E+0001	1.8E+0005	1.3E+0006	4.3E+0005	2.9E+0000
60	5.0E-0006	3.2E-0002	5.5E+0002	1.7E-0003	8.3E+0000	1.2E+0005	1.3E+0006	4.3E+0005	2.9E+0000
72	5.7E-0006	3.5E-0002	5.5E+0002	1.1E-0003	5.7E+0000	8.2E+0004	1.3E+0006	4.3E+0005	2.9E+0000
84	6.3E-0006	3.6E-0002	5.2E+0002	7.8E-0004	3.9E+0000	5.6E+0004	1.2E+0006	4.3E+0005	2.9E+0000
96	6.6E-0006	3.6E-0002	4.9E+0002	5.5E-0004	2.7E+0000	3.8E+0004	1.2E+0006	4.2E+0005	2.9E+0000
108	6.8E-0006	3.5E-0002	4.5E+0002	3.9E-0004	1.9E+0000	2.7E+0004	1.2E+0006	4.2E+0005	2.9E+0000
120	6.8E-0006	3.5E-0002	4.1E+0002	2.8E-0004	1.4E+0000	1.9E+0004	1.2E+0006	4.2E+0005	2.8E+0000
132	6.7E-0006	3.3E-0002	3.7E+0002	2.1E-0004	1.0E+0000	1.4E+0004	1.1E+0006	4.2E+0005	2.7E+0000
144	6.5E-0006	3.2E-0002	3.4E+0002	1.6E-0004	7.9E-0001	1.0E+0004	1.1E+0006	4.1E+0005	2.6E+0000
156	6.2E-0006	3.0E-0002	3.1E+0002	1.3E-0004	6.3E-0001	7.7E+0003	1.0E+0006	4.1E+0005	2.5E+0000
168	5.9E-0006	2.8E-0002	2.9E+0002	1.1E-0004	5.2E-0001	6.1E+0003	1.0E+0006	4.1E+0005	2.4E+0000
180	5.6E-0006	2.6E-0002	2.6E+0002	9.6E-0005	4.5E-0001	5.0E+0003	9.5E+0005	4.1E+0005	2.3E+0000
192	5.4E-0006	2.5E-0002	2.5E+0002	8.7E-0005	4.1E-0001	4.3E+0003	9.1E+0005	4.0E+0005	2.3E+0000
204	5.2E-0006	2.4E-0002	2.4E+0002	8.1E-0005	3.8E-0001	3.9E+0003	8.8E+0005	4.0E+0005	2.2E+0000
216	5.0E-0006	2.4E-0002	2.3E+0002	7.7E-0005	3.6E-0001	3.6E+0003	8.6E+0005	4.0E+0005	2.1E+0000
228	4.9E-0006	2.4E-0002	2.4E+0002	1.0E-0003	5.2E+0000	5.6E+0004	9.3E+0005	4.3E+0005	2.2E+0000
240	5.7E-0006	3.2E-0002	4.1E+0002	3.1E-0003	1.5E+0001	2.0E+0005	1.1E+0006	4.3E+0005	2.6E+0000
252	6.6E-0006	4.1E-0002	6.4E+0002	3.1E-0003	1.6E+0001	2.1E+0005	1.2E+0006	4.3E+0005	2.7E+0000
264	7.0E-0006	4.6E-0002	7.8E+0002	3.6E-0003	1.8E+0001	2.6E+0005	1.2E+0006	4.3E+0005	2.9E+0000
276	6.9E-0006	4.6E-0002	8.1E+0002	2.8E-0003	1.4E+0001	2.0E+0005	1.3E+0006	4.3E+0005	2.9E+0000
288	6.6E-0006	4.3E-0002	7.4E+0002	1.9E-0003	9.3E+0000	1.4E+0005	1.2E+0006	4.3E+0005	2.9E+0000
300	6.3E-0006	3.9E-0002	6.4E+0002	1.3E-0003	6.4E+0000	9.2E+0004	1.2E+0006	4.3E+0005	2.9E+0000
312	5.9E-0006	3.5E-0002	5.4E+0002	8.8E-0004	4.4E+0000	6.3E+0004	1.2E+0006	4.3E+0005	2.9E+0000
324	5.5E-0006	3.2E-0002	4.6E+0002	6.1E-0004	3.0E+0000	4.3E+0004	1.2E+0006	4.3E+0005	2.9E+0000
336	5.2E-0006	2.9E-0002	3.9E+0002	5.2E-0004	2.6E+0000	3.4E+0004	1.2E+0006	4.3E+0005	2.7E+0000
348	5.0E-0006	2.8E-0002	3.9E+0002	1.9E-0003	9.2E+0000	1.1E+0005	1.0E+0006	4.3E+0005	2.4E+0000
360	6.0E-0006	3.7E-0002	5.7E+0002	3.5E-0003	1.7E+0001	2.3E+0005	1.2E+0006	4.3E+0005	2.7E+0000

Table E2 Calculated results of polymer properties at $[I]_{feed}$ = 0.01 mole/dm^3, $[S]_{feed}$ = 0.01 mole/dm^3, θ = 30 min. VAc/Water = 4/10.

Time min.	Nt 1/L	Dav dm	Ap dm2/L	Xt	q	freeMi mol/L	Mp mol/L	Rate mol/s	Mw	Mn	PDI
12	2.0E+0018	3.4E-0007	7.2E+0005	8.6E-0002	1.4E-0003	0.0E+0000	8.9E+0000	4.0E-0004	8.9E+0005	4.3E+0005	2.1E+0000
24	1.3E+0018	6.6E-0007	1.8E+0006	2.7E-0001	5.6E-0003	0.0E+0000	8.3E+0000	9.9E-0004	1.1E+0006	4.3E+0005	2.6E+0000
36	8.9E+0017	8.6E-0007	2.1E+0006	4.1E-0001	2.2E-0002	0.0E+0000	6.9E+0000	1.1E-0003	1.3E+0006	4.3E+0005	2.9E+0000
48	6.0E+0017	1.0E-0006	1.9E+0006	4.8E-0001	3.4E-0002	0.0E+0000	6.2E+0000	1.1E-0003	1.3E+0006	4.3E+0005	2.9E+0000
60	4.0E+0017	1.2E-0006	1.7E+0006	5.1E-0001	4.8E-0002	0.0E+0000	5.9E+0000	1.0E-0003	1.3E+0006	4.3E+0005	2.9E+0000
72	2.7E+0017	1.3E-0006	1.4E+0006	5.2E-0001	6.7E-0002	0.0E+0000	5.8E+0000	1.0E-0003	1.3E+0006	4.3E+0005	2.9E+0000
84	1.8E+0017	1.5E-0006	1.2E+0006	5.2E-0001	9.1E-0002	0.0E+0000	5.8E+0000	9.6E-0004	1.2E+0006	4.2E+0005	2.9E+0000
96	1.2E+0017	1.7E-0006	1.1E+0006	5.1E-0001	1.2E-0001	0.0E+0000	5.9E+0000	9.2E-0004	1.2E+0006	4.2E+0005	2.9E+0000
108	8.1E+0016	1.9E-0006	9.1E+0005	5.0E-0001	1.6E-0001	0.0E+0000	6.0E+0000	8.8E-0004	1.2E+0006	4.2E+0005	2.8E+0000
120	5.4E+0016	2.1E-0006	7.8E+0005	4.8E-0001	2.1E-0001	0.0E+0000	6.2E+0000	8.5E-0004	1.2E+0006	4.2E+0005	2.7E+0000
132	3.6E+0016	2.4E-0006	6.8E+0005	4.7E-0001	2.6E-0001	0.0E+0000	6.3E+0000	8.1E-0004	1.1E+0006	4.1E+0005	2.6E+0000
144	2.4E+0016	2.8E-0006	5.9E+0005	4.5E-0001	3.2E-0001	0.0E+0000	6.5E+0000	7.8E-0004	1.1E+0006	4.1E+0005	2.5E+0000
156	1.6E+0016	3.2E-0006	5.1E+0005	4.4E-0001	3.7E-0001	0.0E+0000	6.7E+0000	7.5E-0004	1.0E+0006	4.1E+0005	2.4E+0000
168	1.1E+0016	3.6E-0006	4.4E+0005	4.2E-0001	4.2E-0001	0.0E+0000	6.8E+0000	7.2E-0004	1.0E+0006	4.1E+0005	2.3E+0000
180	7.3E+0015	4.1E-0006	3.9E+0005	4.0E-0001	4.5E-0001	0.0E+0000	7.0E+0000	6.9E-0004	9.5E+0005	4.1E+0005	2.3E+0000
192	4.9E+0015	4.7E-0006	3.4E+0005	3.9E-0001	4.3E-0001	0.0E+0000	7.2E+0000	6.6E-0004	9.1E+0005	4.0E+0005	2.2E+0000
204	3.3E+0015	5.3E-0006	3.0E+0005	3.7E-0001	4.6E-0001	0.0E+0000	7.3E+0000	6.3E-0004	8.8E+0005	4.0E+0005	2.2E+0000
216	2.2E+0015	6.1E-0006	2.6E+0005	3.6E-0001	4.8E-0001	0.0E+0000	7.5E+0000	6.0E-0004	8.6E+0005	4.0E+0005	2.1E+0000
228	1.5E+0015	7.0E-0006	2.3E+0005	3.4E-0001	4.9E-0001	0.0E+0000	7.6E+0000	5.8E-0004	9.3E+0005	4.3E+0005	2.2E+0000
240	3.6E+0016	4.8E-0007	2.1E+0005	3.3E-0001	4.3E-0002	3.1E-0004	7.8E+0000	5.6E-0004	1.1E+0006	4.3E+0005	2.6E+0000
252	3.5E+0016	1.3E-0006	3.1E+0005	3.3E-0001	1.1E-0001	0.0E+0000	7.8E+0000	6.8E-0004	1.2E+0006	4.3E+0005	2.7E+0000
264	2.3E+0016	2.0E-0006	3.9E+0005	3.5E-0001	1.9E-0001	0.0E+0000	7.6E+0000	7.5E-0004	1.2E+0006	4.3E+0005	2.9E+0000
276	1.6E+0016	2.7E-0006	4.1E+0005	3.6E-0001	2.6E-0001	0.0E+0000	7.4E+0000	7.6E-0004	1.3E+0006	4.3E+0005	2.9E+0000
288	1.0E+0016	3.3E-0006	4.0E+0005	3.7E-0001	3.3E-0001	0.0E+0000	7.3E+0000	7.3E-0004	1.2E+0006	4.3E+0005	2.9E+0000
300	7.0E+0015	3.9E-0006	3.7E+0005	3.7E-0001	3.9E-0001	0.0E+0000	7.3E+0000	7.0E-0004	1.2E+0006	4.3E+0005	2.9E+0000
312	4.7E+0015	4.6E-0006	3.3E+0005	3.7E-0001	4.3E-0001	0.0E+0000	7.3E+0000	6.7E-0004	1.2E+0006	4.3E+0005	2.9E+0000
324	3.2E+0015	5.3E-0006	2.9E+0005	3.6E-0001	4.6E-0001	0.0E+0000	7.4E+0000	6.3E-0004	1.2E+0006	4.3E+0005	2.9E+0000
336	2.1E+0015	6.1E-0006	2.5E+0005	3.5E-0001	4.8E-0001	0.0E+0000	7.5E+0000	6.0E-0004	1.2E+0006	4.3E+0005	2.7E+0000
[illegible]	[illegible]	7.0E-0006	2.2E+0005	3.4E-0001	4.9E-0001	0.0E+0000	7.7E+0000	5.8E-0004	1.0E+0006	4.3E+0005	2.4E+0000
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	3.0E-0002	1.7E-0004	7.8E+0000	5.7E-0004	1.2E+0006	4.3E+0005	2.7E+0000

Table E3 Calculated results of moments at $[I]_{feed}$ = 0.01 mole/dm^3, $[S]_{feed}$ = 0.03 mole/dm^3, 0 = 30 min. VAc/Water = 4/10.

Time min.	M0i mol/L	M1i mol/L	M2i mol/L	N0i mol/L	N1i mol/L	N2i mol/s	Mv	Mn	PDI
12	5.5E-0007	2.8E-0003	3.0E+0001	6.4E-0004	3.2E+0000	3.3E+0004	8.9E+0005	4.3E+0005	2.1E+0000
24	1.7E-0006	1.1E-0002	1.6E+0002	3.5E-0003	1.7E+0001	2.3E+0005	1.1E+0006	4.3E+0005	2.6E+0000
36	3.0E-0006	2.1E-0002	3.8E+0002	3.7E-0003	1.8E+0001	2.7E+0005	1.3E+0006	4.3E+0005	2.9E+0000
48	4.1E-0006	2.8E-0002	5.1E+0002	2.5E-0003	1.2E+0001	1.8E+0005	1.3E+0006	4.3E+0005	2.9E+0000
60	5.0E-0006	3.2E-0002	5.5E+0002	1.7E-0003	8.3E+0000	1.2E+0005	1.3E+0006	4.3E+0005	2.9E+0000
72	5.7E-0006	3.5E-0002	5.5E+0002	1.1E-0003	5.7E+0000	8.2E+0004	1.3E+0006	4.3E+0005	2.9E+0000
84	6.3E-0006	3.6E-0002	5.2E+0002	7.8E-0004	3.9E+0000	5.6E+0004	1.2E+0006	4.3E+0005	2.9E+0000
96	6.6E-0006	3.6E-0002	4.9E+0002	5.5E-0004	2.7E+0000	3.8E+0004	1.2E+0006	4.2E+0005	2.9E+0000
108	6.8E-0006	3.6E-0002	4.5E+0002	3.9E-0004	1.9E+0000	2.7E+0004	1.2E+0006	4.2E+0005	2.9E+0000
120	7.3E-0006	3.7E-0002	4.3E+0002	2.8E-0004	1.4E+0000	1.9E+0004	1.2E+0006	4.2E+0005	2.8E+0000
132	7.7E-0006	3.7E-0002	4.1E+0002	2.2E-0004	1.0E+0000	1.4E+0004	1.1E+0006	4.2E+0005	2.7E+0000
144	7.9E-0006	3.8E-0002	4.0E+0002	1.7E-0004	8.1E-0001	1.0E+0004	1.1E+0006	4.1E+0005	2.6E+0000
156	8.1E-0006	3.8E-0002	3.9E+0002	1.4E-0004	6.5E-0001	7.8E+0003	1.0E+0006	4.1E+0005	2.5E+0000
168	8.1E-0006	3.8E-0002	3.7E+0002	1.2E-0004	5.4E-0001	6.2E+0003	9.8E+0005	4.0E+0005	2.4E+0000
180	8.2E-0006	3.8E-0002	3.6E+0002	1.0E-0004	4.7E-0001	5.1E+0003	9.3E+0005	4.0E+0005	2.3E+0000
192	8.1E-0006	3.7E-0002	3.5E+0002	9.1E-0005	4.1E-0001	4.3E+0003	8.9E+0005	3.9E+0005	2.3E+0000
204	8.0E-0006	3.7E-0002	3.4E+0002	8.4E-0005	3.8E-0001	3.8E+0003	8.6E+0005	3.9E+0005	2.2E+0000
216	8.0E-0006	3.6E-0002	3.4E+0002	8.0E-0005	3.6E-0001	3.5E+0003	8.4E+0005	3.9E+0005	2.1E+0000
228	8.1E-0006	3.7E-0002	3.4E+0002	7.9E-0005	3.5E-0001	3.4E+0003	8.2E+0005	3.9E+0005	2.1E+0000
240	8.3E-0006	3.7E-0002	3.5E+0002	7.8E-0005	3.5E-0001	3.3E+0003	8.0E+0005	3.9E+0005	2.1E+0000
252	8.3E-0006	3.8E-0002	3.5E+0002	7.8E-0005	3.5E-0001	3.2E+0003	8.0E+0005	3.9E+0005	2.1E+0000
264	8.4E-0006	3.8E-0002	3.5E+0002	7.7E-0005	3.4E-0001	3.2E+0003	7.9E+0005	3.9E+0005	2.0E+0000
276	8.3E-0006	3.8E-0002	3.4E+0002	7.6E-0005	3.4E-0001	3.1E+0003	7.9E+0005	3.8E+0005	2.0E+0000
288	8.3E-0006	3.7E-0002	3.4E+0002	7.4E-0005	3.3E-0001	3.0E+0003	7.8E+0005	3.8E+0005	2.0E+0000
300	8.2E-0006	3.7E-0002	3.4E+0002	7.3E-0005	3.3E-0001	3.0E+0003	7.8E+0005	3.8E+0005	2.0E+0000
312	8.0E-0006	3.6E-0002	3.3E+0002	7.3E-0005	3.2E-0001	2.9E+0003	7.8E+0005	3.8E+0005	2.0E+0000
324	8.1E-0006	3.7E-0002	3.3E+0002	7.3E-0005	3.3E-0001	3.0E+0003	7.8E+0005	3.8E+0005	2.0E+0000
336	8.3E-0006	3.7E-0002	3.4E+0002	7.5E-0005	3.3E-0001	3.0E+0003	7.8E+0005	3.8E+0005	2.0E+0000
348	8.4E-0006	3.8E-0002	3.4E+0002	7.6E-0005	3.4E-0001	3.1E+0003	7.8E+0005	3.8E+0005	2.0E+0000
360	8.4E-0006	3.8E-0002	3.4E+0002	7.6E-0005	3.4E-0001	3.1E+0003	7.8E+0005	3.8E+0005	2.0E+0000

Table E4 Calculated results of polymer properties at $[I]_{feed}$ = 0.01 mole/dm^3, $[S]_{feed}$ = 0.03 mole/dm^3, 0 = 30 min. VAc/Water = 4/10.

Time min.	Nt 1/L	Dav dm	Ap dm2/L	Xt	q	freeMi mol/L	Mp mol/L	Rate mol/s	Mw	Mn	PDI
12	2.0E+0018	3.4E-0007	7.2E+0005	8.6E-0002	1.4E-0003	0.0E+0000	8.9E+0000	4.0E-0004	8.9E+0005	4.3E+0005	2.1E+0000
24	1.3E+0018	6.6E-0007	1.8E+0006	2.7E-0001	5.6E-0003	0.0E+0000	8.3E+0000	9.9E-0004	1.1E+0006	4.3E+0005	2.6E+0000
36	8.9E+0017	8.6E-0007	2.1E+0006	4.1E-0001	2.2E-0002	0.0E+0000	6.9E+0000	1.1E-0003	1.3E+0006	4.3E+0005	2.9E+0000
48	6.0E+0017	1.0E-0006	1.9E+0006	4.8E-0001	3.4E-0002	0.0E+0000	6.2E+0000	1.1E-0003	1.3E+0006	4.3E+0005	2.9E+0000
60	4.0E+0017	1.2E-0006	1.7E+0006	5.1E-0001	4.8E-0002	0.0E+0000	5.9E+0000	1.0E-0003	1.3E+0006	4.3E+0005	2.9E+0000
72	2.7E+0017	1.3E-0006	1.4E+0006	5.2E-0001	6.7E-0002	0.0E+0000	5.8E+0000	1.0E-0003	1.3E+0006	4.3E+0005	2.9E+0000
84	1.8E+0017	1.5E-0006	1.2E+0006	5.2E-0001	9.1E-0002	0.0E+0000	5.8E+0000	9.6E-0004	1.2E+0006	4.3E+0005	2.9E+0000
96	1.2E+0017	1.7E-0006	1.1E+0006	5.1E-0001	1.2E-0001	0.0E+0000	5.9E+0000	9.2E-0004	1.2E+0006	4.2E+0005	2.9E+0000
108	8.3E+0016	1.8E-0006	9.1E+0005	5.0E-0001	1.6E-0001	4.9E-0004	6.0E+0000	8.8E-0004	1.2E+0006	4.2E+0005	2.9E+0000
120	3.0E+0017	5.0E-0007	8.0E+0005	4.8E-0001	2.6E-0002	3.8E-0003	6.2E+0000	8.6E-0004	1.2E+0006	4.2E+0005	2.8E+0000
132	1.7E+0018	2.4E-0007	9.1E+0005	4.8E-0001	5.4E-0003	8.9E-0004	6.2E+0000	9.3E-0004	1.1E+0006	4.2E+0005	2.7E+0000
144	1.2E+0018	4.7E-0007	1.2E+0006	4.9E-0001	1.3E-0002	0.0E+0000	6.0E+0000	1.1E-0003	1.1E+0006	4.1E+0005	2.6E+0000
156	8.0E+0017	6.6E-0007	1.4E+0006	5.2E-0001	2.2E-0002	0.0E+0000	5.8E+0000	1.1E-0003	1.0E+0006	4.1E+0005	2.5E+0000
168	5.3E+0017	8.4E-0007	1.4E+0006	5.3E-0001	3.3E-0002	0.0E+0000	5.7E+0000	1.0E-0003	9.8E+0005	4.0E+0005	2.4E+0000
180	3.6E+0017	1.0E-0006	1.3E+0006	5.3E-0001	4.8E-0002	0.0E+0000	5.6E+0000	1.0E-0003	9.3E+0005	4.0E+0005	2.3E+0000
192	2.4E+0017	1.2E-0006	1.2E+0006	5.3E-0001	6.8E-0002	0.0E+0000	5.7E+0000	9.7E-0004	8.9E+0005	3.9E+0005	2.3E+0000
204	1.6E+0017	1.4E-0006	1.0E+0006	5.2E-0001	9.4E-0002	0.0E+0000	5.8E+0000	9.3E-0004	8.6E+0005	3.9E+0005	2.2E+0000
216	1.2E+0017	1.5E-0006	9.2E+0005	5.1E-0001	1.1E-0001	9.7E-0004	5.9E+0000	9.0E-0004	8.4E+0005	3.9E+0005	2.1E+0000
228	3.8E+0017	4.6E-0007	8.3E+0005	4.9E-0001	2.2E-0002	3.4E-0003	6.1E+0000	8.8E-0004	8.2E+0005	3.9E+0005	2.1E+0000
240	1.4E+0018	2.7E-0007	9.3E+0005	4.9E-0001	6.9E-0003	7.5E-0004	6.1E+0000	9.4E-0004	8.0E+0005	3.9E+0005	2.1E+0000
252	9.5E+0017	5.0E-0007	1.2E+0006	5.0E-0001	1.5E-0002	0.0E+0000	6.0E+0000	1.0E-0003	8.0E+0005	3.9E+0005	2.1E+0000
264	6.4E+0017	7.0E-0007	1.3E+0006	5.1E-0001	2.6E-0002	0.0E+0000	5.8E+0000	1.0E-0003	7.9E+0005	3.9E+0005	2.0E+0000
276	4.3E+0017	8.9E-0007	1.3E+0006	5.2E-0001	3.9E-0002	0.0E+0000	5.7E+0000	1.0E-0003	7.9E+0005	3.8E+0005	2.0E+0000
288	2.9E+0017	1.1E-0006	1.2E+0006	5.2E-0001	5.7E-0002	0.0E+0000	5.7E+0000	9.8E-0004	7.8E+0005	3.8E+0005	2.0E+0000
300	1.9E+0017	1.3E-0006	1.1E+0006	5.2E-0001	8.0E-0002	0.0E+0000	5.8E+0000	9.5E-0004	7.8E+0005	3.8E+0005	2.0E+0000
312	1.3E+0017	1.5E-0006	9.6E+0005	5.1E-0001	1.1E-0001	0.0E+0000	5.9E+0000	9.1E-0004	7.8E+0005	3.8E+0005	2.0E+0000
324	2.2E+0017	7.6E-0007	8.6E+0005	5.0E-0001	4.6E-0002	2.7E-0003	6.0E+0000	8.8E-0004	7.8E+0005	3.8E+0005	2.0E+0000
336	1.1E+0018	2.7E-0007	8.6E+0005	4.9E-0001	7.6E-0003	2.6E-0003	6.1E+0000	9.0E-0004	7.8E+0005	3.8E+0005	2.0E+0000
348	1.1E+0018	4.3E-0007	1.1E+0006	4.9E-0001	1.2E-0002	0.0E+0000	6.1E+0000	1.0E-0003	7.8E+0005	3.8E+0005	2.0E+0000
360	7.1E+0017	6.4E-0007	1.2E+0006	5.1E-0001	2.2E-0002	0.0E+0000	5.9E+0000	1.0E-0003	7.8E+0005	3.8E+0005	2.0E+0000

Table E5 Calculated results of moments at $[I]_{feed}$ = 0.01 mole/dm^3, $[S]_{feed}$ = 0.05 mole/dm^3, Θ = 30 min. VAc/Water = 4/10.

Time min.	M0i mol/L	M1i mol/L	M2i mol/L	N0i mol/L	N1i mol/L	N2i mol/s	Mw	Mn	PDI
12	5.5E-0007	2.8E-0003	3.0E+0001	6.4E-0004	3.2E+0000	3.3E+0004	8.9E+0005	4.3E+0005	2.1E+0000
24	1.7E-0006	1.1E-0002	1.6E+0002	3.5E-0003	1.7E+0001	2.3E+0005	1.1E+0006	4.3E+0005	2.6E+0000
36	3.0E-0006	2.1E-0002	3.8E+0002	3.7E-0003	1.8E+0001	2.7E+0005	1.3E+0006	4.3E+0005	2.9E+0000
48	4.1E-0006	2.8E-0002	5.1E+0002	2.5E-0003	1.2E+0001	1.8E+0005	1.3E+0006	4.3E+0005	2.9E+0000
60	5.0E-0006	3.2E-0002	5.5E+0002	1.7E-0003	8.3E+0000	1.2E+0005	1.3E+0006	4.3E+0005	2.9E+0000
72	5.8E-0006	3.5E-0002	5.5E+0002	1.1E-0003	5.7E+0000	8.2E+0004	1.3E+0006	4.3E+0005	2.9E+0000
84	6.5E-0006	3.7E-0002	5.4E+0002	7.8E-0004	3.9E+0000	5.6E+0004	1.2E+0006	4.3E+0005	2.9E+0000
96	7.0E-0006	3.8E-0002	5.1E+0002	5.5E-0004	2.7E+0000	3.8E+0004	1.2E+0006	4.2E+0005	2.9E+0000
108	7.4E-0006	3.8E-0002	4.8E+0002	3.9E-0004	1.9E+0000	2.7E+0004	1.2E+0006	4.2E+0005	2.9E+0000
120	7.7E-0006	3.8E-0002	4.5E+0002	2.8E-0004	1.4E+0000	1.9E+0004	1.2E+0006	4.2E+0005	2.8E+0000
132	7.9E-0006	3.8E-0002	4.2E+0002	2.1E-0004	1.0E+0000	1.3E+0004	1.1E+0006	4.1E+0005	2.7E+0000
144	8.0E-0006	3.8E-0002	4.0E+0002	1.6E-0004	7.6E-0001	9.8E+0003	1.1E+0006	4.1E+0005	2.7E+0000
156	8.1E-0006	3.8E-0002	3.8E+0002	1.3E-0004	6.0E-0001	7.3E+0003	1.0E+0006	4.0E+0005	2.6E+0000
168	8.2E-0006	3.8E-0002	3.7E+0002	1.1E-0004	5.0E-0001	5.8E+0003	9.8E+0005	4.0E+0005	2.5E+0000
180	8.3E-0006	3.8E-0002	3.6E+0002	9.4E-0005	4.3E-0001	4.7E+0003	9.3E+0005	3.9E+0005	2.4E+0000
192	8.4E-0006	3.8E-0002	3.6E+0002	8.5E-0005	3.9E-0001	4.1E+0003	8.9E+0005	3.9E+0005	2.3E+0000
204	8.4E-0006	3.8E-0002	3.5E+0002	8.0E-0005	3.6E-0001	3.6E+0003	8.6E+0005	3.9E+0005	2.2E+0000
216	8.4E-0006	3.8E-0002	3.5E+0002	7.6E-0005	3.4E-0001	3.3E+0003	8.3E+0005	3.8E+0005	2.2E+0000
228	8.4E-0006	3.8E-0002	3.4E+0002	7.2E-0005	3.2E-0001	3.0E+0003	8.1E+0005	3.8E+0005	2.1E+0000
240	8.4E-0006	3.7E-0002	3.4E+0002	7.0E-0005	3.1E-0001	2.9E+0003	8.0E+0005	3.8E+0005	2.1E+0000
252	8.4E-0006	3.7E-0002	3.4E+0002	6.8E-0005	3.0E-0001	2.8E+0003	7.9E+0005	3.8E+0005	2.1E+0000
264	8.4E-0006	3.7E-0002	3.4E+0002	6.8E-0005	3.0E-0001	2.7E+0003	7.8E+0005	3.8E+0005	2.1E+0000
276	8.5E-0006	3.8E-0002	3.4E+0002	6.8E-0005	3.0E-0001	2.7E+0003	7.7E+0005	3.8E+0005	2.0E+0000
288	8.5E-0006	3.8E-0002	3.4E+0002	6.8E-0005	3.0E-0001	2.7E+0003	7.7E+0005	3.8E+0005	2.0E+0000
300	8.5E-0006	3.8E-0002	3.4E+0002	6.8E-0005	3.0E-0001	2.7E+0003	7.7E+0005	3.8E+0005	2.0E+0000
312	8.5E-0006	3.8E-0002	3.4E+0002	6.7E-0005	3.0E-0001	2.6E+0003	7.7E+0005	3.8E+0005	2.0E+0000
324	8.5E-0006	3.7E-0002	3.4E+0002	6.7E-0005	2.9E-0001	2.6E+0003	7.7E+0005	3.8E+0005	2.0E+0000
336	8.4E-0006	3.7E-0002	3.3E+0002	6.6E-0005	2.9E-0001	2.6E+0003	7.7E+0005	3.8E+0005	2.0E+0000
348	8.4E-0006	3.7E-0002	3.4E+0002	6.6E-0005	2.9E-0001	2.6E+0003	7.7E+0005	3.8E+0005	2.0E+0000
360	8.5E-0006	3.8E-0002	3.4E+0002	6.7E-0005	2.9E-0001	2.6E+0003	7.7E+0005	3.8E+0005	2.0E+0000

Table E6 Calculated results of polymer properties at $[I]_{feed}$ = 0.01 mole/dm^3, $[S]_{feed}$ = 0.05 mole/dm^3, θ = 30 min. VAc/Water = 4/10.

Time min.	Nt 1/L	Dav dm	Ap dm2/L	Xt	q	freeMi mol/L	Mp mol/L	Rate mol/s	Mw	Mn	PDI
12	2.0E+0018	3.4E-0007	7.2E+0005	8.6E-0002	1.4E-0003	0.0E+0000	8.9E+0000	4.0E-0004	8.9E+0005	4.3E+0005	2.1E+0000
24	1.3E+0018	6.6E-0007	1.8E+0006	2.7E-0001	5.6E-0003	0.0E+0000	8.3E+0000	9.9E-0004	1.1E+0006	4.3E+0005	2.6E+0000
36	8.9E+0017	8.6E-0007	2.1E+0006	4.1E-0001	2.2E-0002	0.0E+0000	6.9E+0000	1.1E-0003	1.3E+0006	4.3E+0005	2.9E+0000
48	6.0E+0017	1.0E-0006	1.9E+0006	4.8E-0001	3.4E-0002	0.0E+0000	6.2E+0000	1.1E-0003	1.3E+0006	4.3E+0005	2.9E+0000
60	4.0E+0017	1.2E-0006	1.7E+0006	5.1E-0001	4.8E-0002	0.0E+0000	5.9E+0000	1.0E-0003	1.3E+0006	4.3E+0005	2.9E+0000
72	3.0E+0017	1.2E-0006	1.4E+0006	5.2E-0001	5.9E-0002	2.3E-0003	5.8E+0000	1.0E-0003	1.3E+0006	4.3E+0005	2.9E+0000
84	1.1E+0018	3.2E-0007	1.3E+0006	5.2E-0001	8.5E-0003	8.4E-0003	5.8E+0000	9.7E-0004	1.2E+0006	4.3E+0005	2.9E+0000
96	6.4E+0018	1.7E-0007	1.5E+0006	5.2E-0001	2.0E-0003	2.6E-0003	5.7E+0000	1.1E-0003	1.2E+0006	4.2E+0005	2.9E+0000
108	4.6E+0018	3.1E-0007	2.0E+0006	5.5E-0001	4.2E-0003	0.0E+0000	5.4E+0000	1.2E-0003	1.2E+0006	4.2E+0005	2.9E+0000
120	3.1E+0018	4.3E-0007	2.2E+0006	5.8E-0001	7.2E-0003	0.0E+0000	5.2E+0000	1.2E-0003	1.2E+0006	4.2E+0005	2.8E+0000
132	2.0E+0018	5.4E-0007	2.1E+0006	5.9E-0001	1.1E-0002	0.0E+0000	5.0E+0000	1.1E-0003	1.1E+0006	4.1E+0005	2.7E+0000
144	1.4E+0018	6.5E-0007	2.0E+0006	5.9E-0001	1.6E-0002	0.0E+0000	5.0E+0000	1.1E-0003	1.1E+0006	4.1E+0005	2.7E+0000
156	9.2E+0017	7.6E-0007	1.8E+0006	5.8E-0001	2.3E-0002	0.0E+0000	5.1E+0000	1.1E-0003	1.0E+0006	4.0E+0005	2.6E+0000
168	6.7E+0017	8.2E-0007	1.6E+0006	5.7E-0001	2.9E-0002	1.9E-0003	5.2E+0000	1.0E-0003	9.8E+0005	4.0E+0005	2.5E+0000
180	1.3E+0018	4.0E-0007	1.5E+0006	5.6E-0001	1.0E-0002	6.0E-0003	5.3E+0000	1.0E-0003	9.3E+0005	3.9E+0005	2.4E+0000
192	4.2E+0018	2.0E-0007	1.5E+0006	5.6E-0001	2.9E-0003	4.4E-0003	5.4E+0000	1.1E-0003	8.9E+0005	3.9E+0005	2.3E+0000
204	3.9E+0018	3.0E-0007	1.8E+0006	5.6E-0001	4.5E-0003	0.0E+0000	5.3E+0000	1.1E-0003	8.6E+0005	3.9E+0005	2.2E+0000
216	2.6E+0018	4.2E-0007	1.9E+0006	5.7E-0001	7.7E-0003	0.0E+0000	5.2E+0000	1.1E-0003	8.3E+0005	3.8E+0005	2.2E+0000
228	1.7E+0018	5.4E-0007	1.9E+0006	5.8E-0001	1.2E-0002	0.0E+0000	5.1E+0000	1.1E-0003	8.1E+0005	3.8E+0005	2.1E+0000
240	1.2E+0018	6.6E-0007	1.8E+0006	5.8E-0001	1.8E-0002	0.0E+0000	5.1E+0000	1.1E-0003	8.0E+0005	3.8E+0005	2.1E+0000
252	7.9E+0017	7.8E-0007	1.7E+0006	5.8E-0001	2.6E-0002	5.2E-0004	5.2E+0000	1.1E-0003	7.9E+0005	3.8E+0005	2.1E+0000
264	1.0E+0018	5.2E-0007	1.5E+0006	5.7E-0001	1.5E-0002	4.6E-0003	5.3E+0000	1.0E-0003	7.8E+0005	3.8E+0005	2.1E+0000
276	2.9E+0018	2.4E-0007	1.5E+0006	5.6E-0001	4.2E-0003	5.5E-0003	5.4E+0000	1.0E-0003	7.7E+0005	3.8E+0005	2.0E+0000
288	4.1E+0018	2.6E-0007	1.7E+0006	5.6E-0001	3.8E-0003	0.0E+0000	5.3E+0000	1.1E-0003	7.7E+0005	3.8E+0005	2.0E+0000
300	2.7E+0018	3.9E-0007	1.9E+0006	5.7E-0001	7.0E-0003	0.0E+0000	5.2E+0000	1.1E-0003	7.7E+0005	3.8E+0005	2.0E+0000
312	1.8E+0018	5.1E-0007	1.9E+0006	5.8E-0001	1.1E-0002	0.0E+0000	5.1E+0000	1.1E-0003	7.7E+0005	3.8E+0005	2.0E+0000
324	1.2E+0018	6.4E-0007	1.8E+0006	5.8E-0001	1.7E-0002	0.0E+0000	5.1E+0000	1.1E-0003	7.7E+0005	3.8E+0005	2.0E+0000
336	8.3E+0017	7.6E-0007	1.7E+0006	5.7E-0001	2.4E-0002	5.0E-0004	5.2E+0000	1.1E-0003	7.7E+0005	3.8E+0005	2.0E+0000
348	1.0E+0018	5.3E-0007	1.5E+0006	5.7E-0001	1.5E-0002	4.4E-0003	5.3E+0000	1.0E-0003	7.7E+0005	3.8E+0005	2.0E+0000
360	2.8E+0018	2.5E-0007	1.5E+0006	5.6E-0001	4.5E-0003	5.4E-0003	5.3E+0000	1.0E-0003	7.7E+0005	3.8E+0005	2.0E+0000

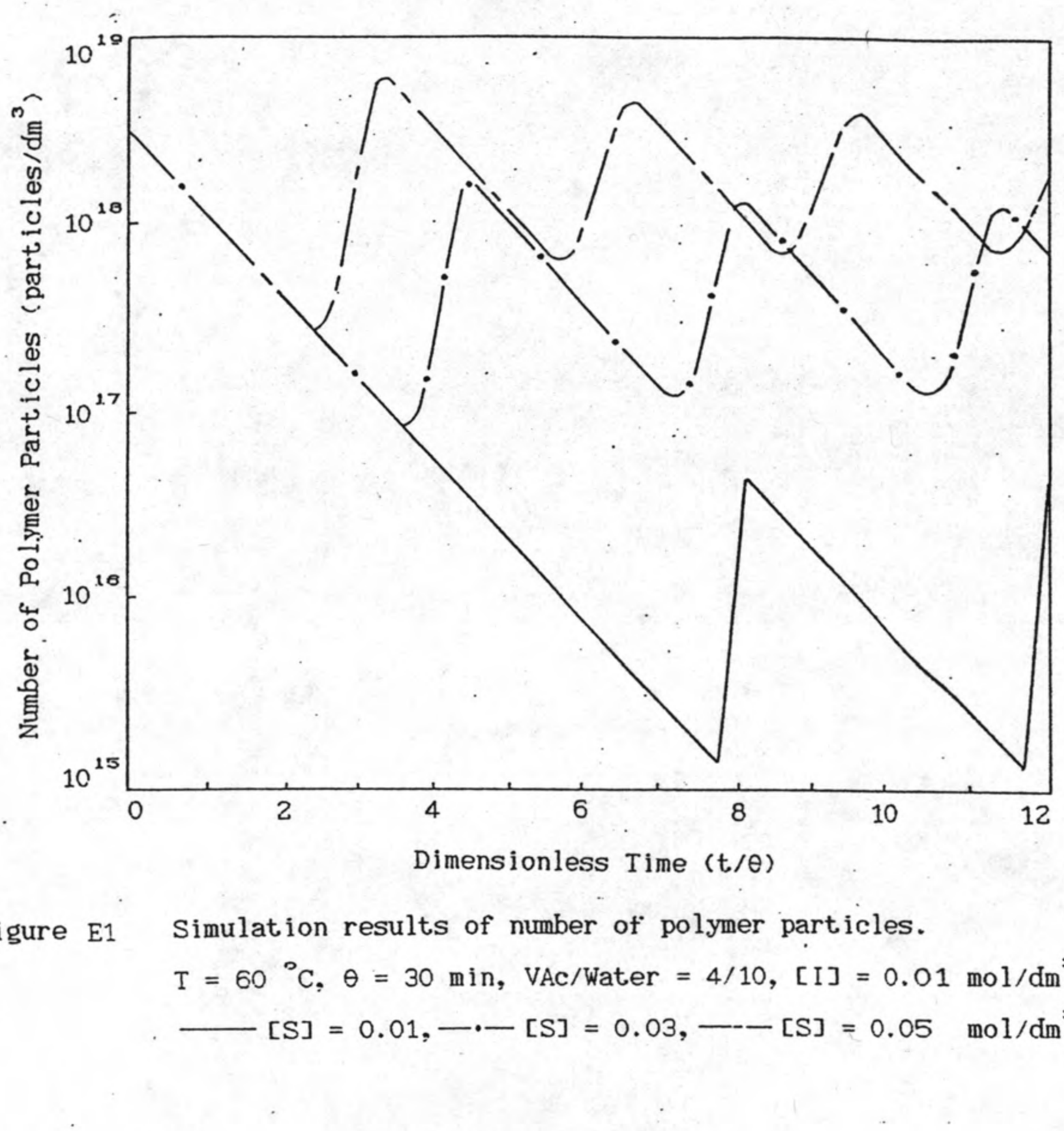

Figure E1 Simulation results of number of polymer particles.
T = 60 °C, θ = 30 min, VAc/Water = 4/10, [I] = 0.01 mol/dm^3
—— [S] = 0.01, —·— [S] = 0.03, ---- [S] = 0.05 mol/dm^3

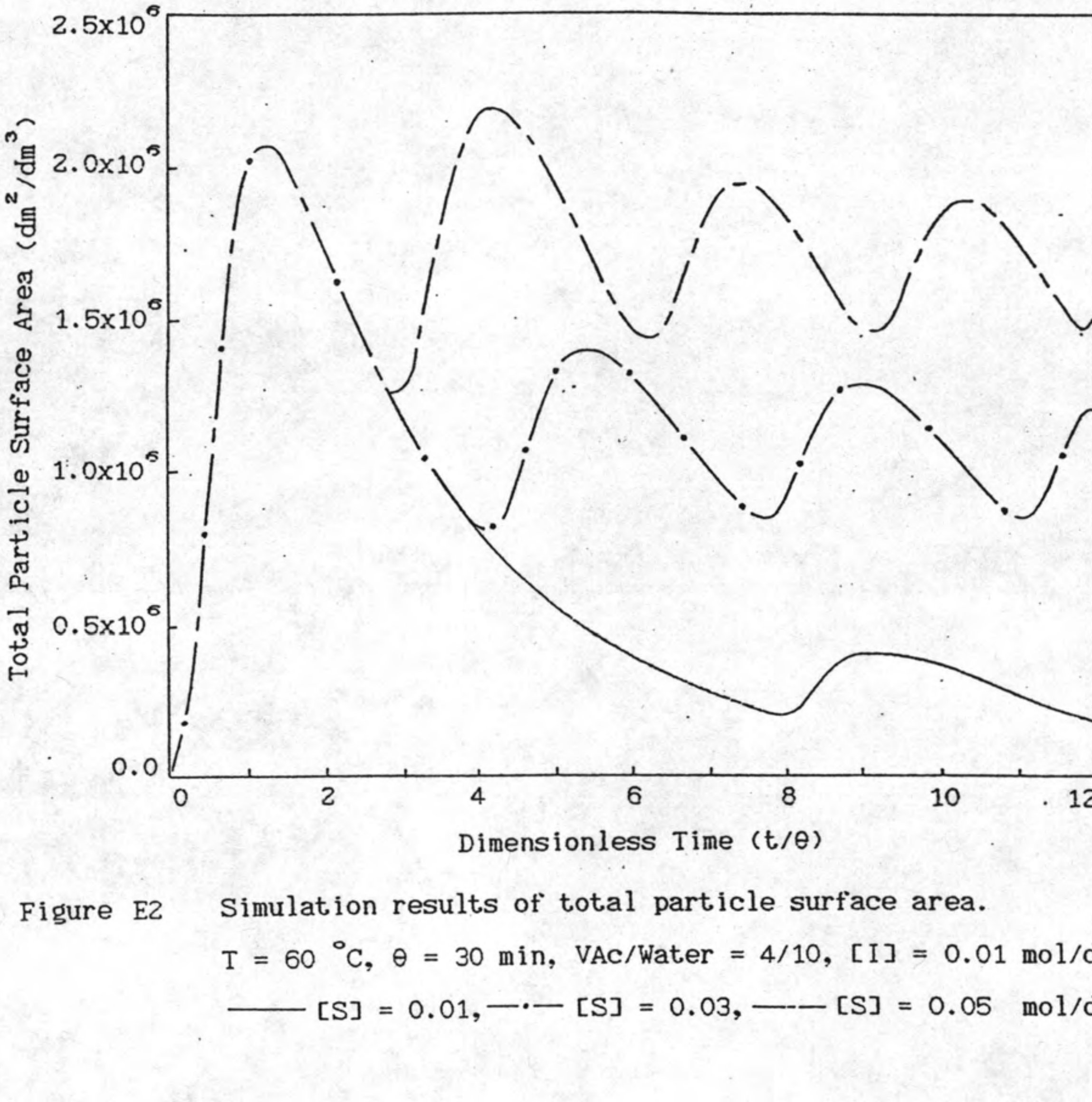

Figure E2 Simulation results of total particle surface area.

$T = 60\ ^{\circ}C$, $\theta = 30$ min, VAc/Water = 4/10, [I] = 0.01 mol/dm^3

—— [S] = 0.01, —·— [S] = 0.03, —-— [S] = 0.05 mol/dm^3

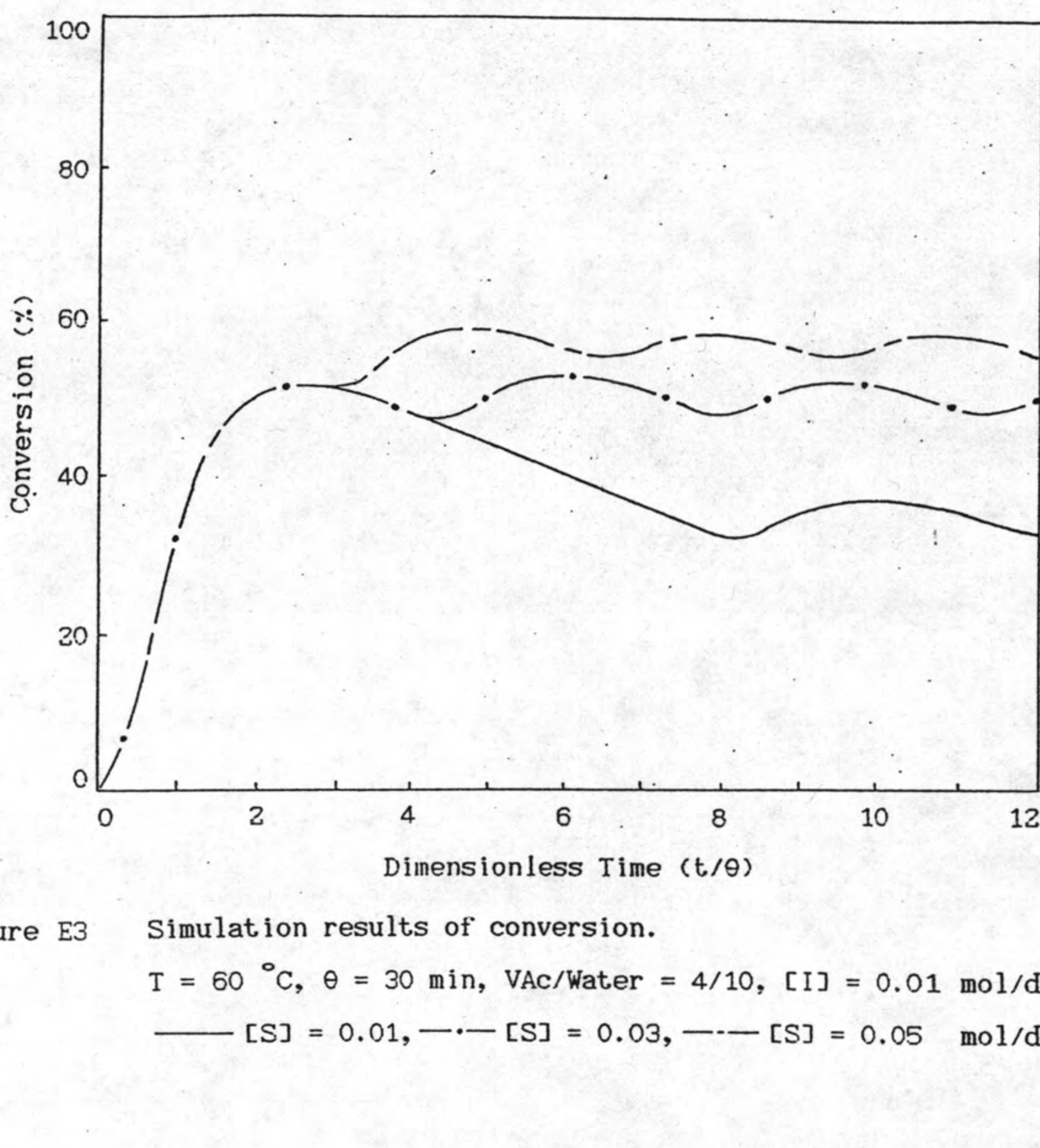

Figure E3 Simulation results of conversion.

T = 60 °C, θ = 30 min, VAc/Water = 4/10, [I] = 0.01 mol/dm^3

——— [S] = 0.01, —·— [S] = 0.03, —·-— [S] = 0.05 mol/dm^3

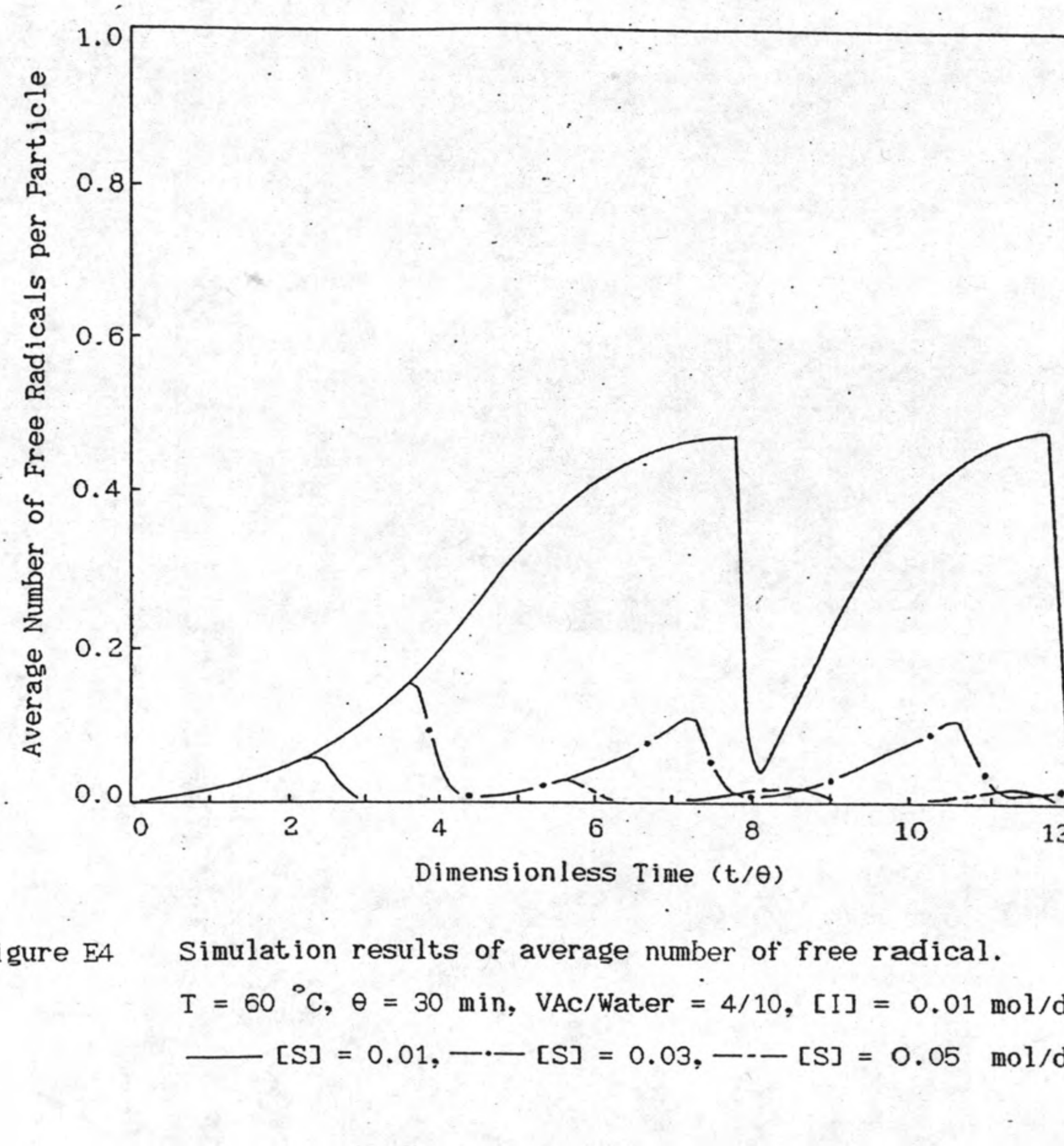

Figure E4 Simulation results of average number of free radical.
T = 60 °C, θ = 30 min, VAc/Water = 4/10, [I] = 0.01 mol/dm^3
—— [S] = 0.01, —·— [S] = 0.03, —-— [S] = 0.05 mol/dm^3

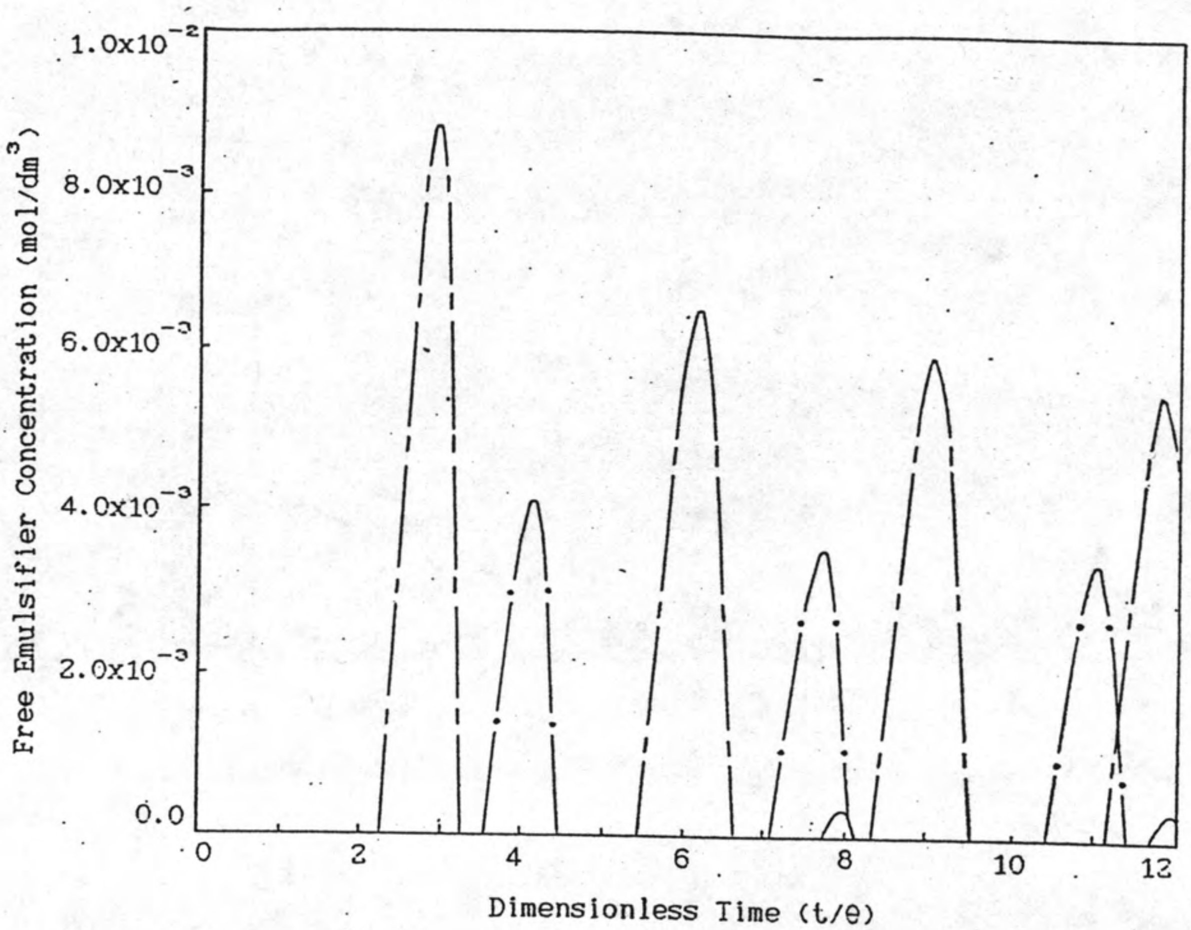

Figure E5 Simulation results of free emulsifier concentration.
T = 60 °C, θ = 30 min, VAc/Water = 4/10, [I] = 0.01 mol/dm^3
——— [S] = 0.01, —·— [S] = 0.03, —··— [S] = 0.05 mol/dm^3

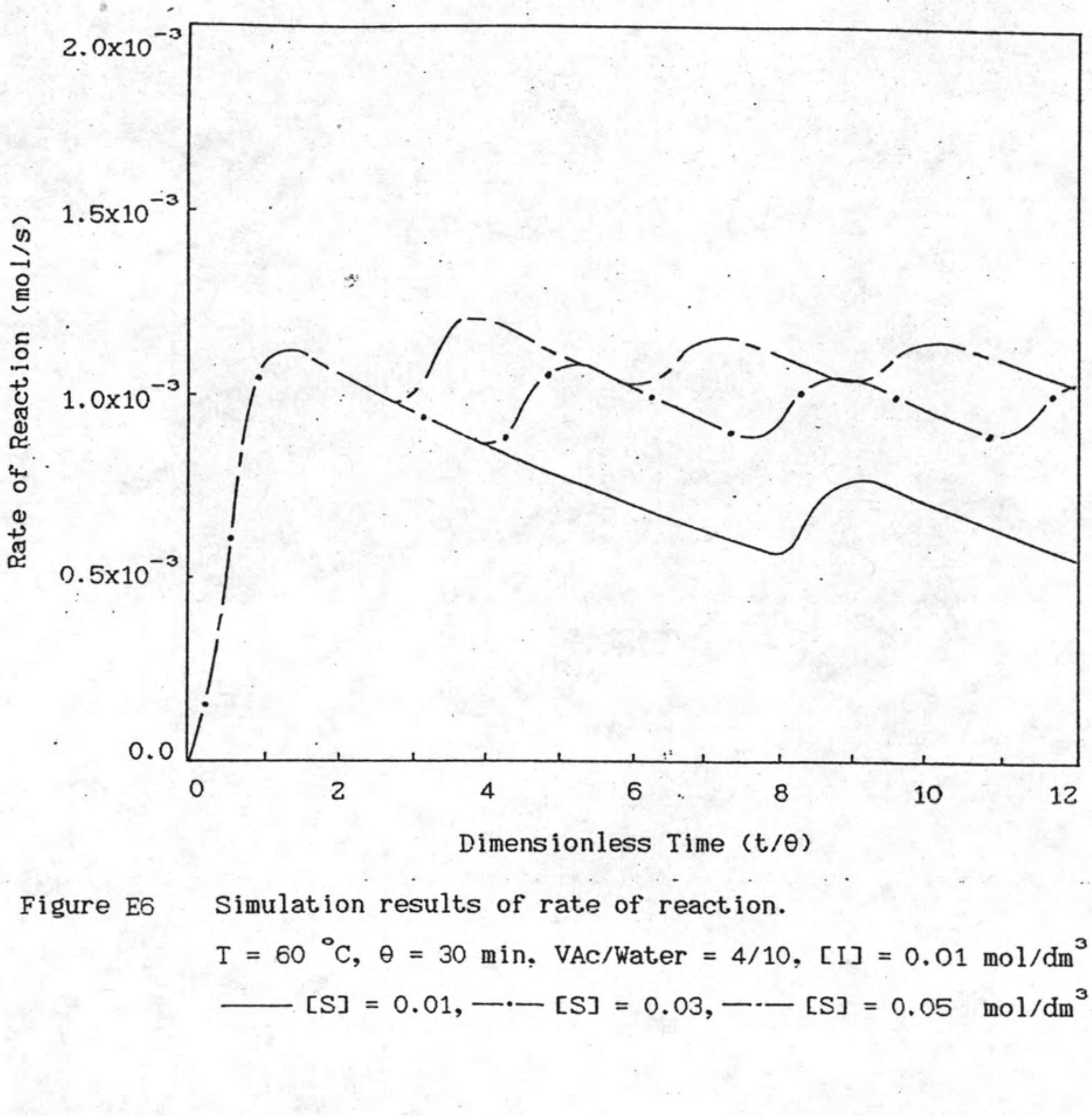

Figure E6 Simulation results of rate of reaction.

T = 60 °C, θ = 30 min, VAc/Water = 4/10, [I] = 0.01 mol/dm^3

—— [S] = 0.01, —·— [S] = 0.03, —··— [S] = 0.05 mol/dm^3

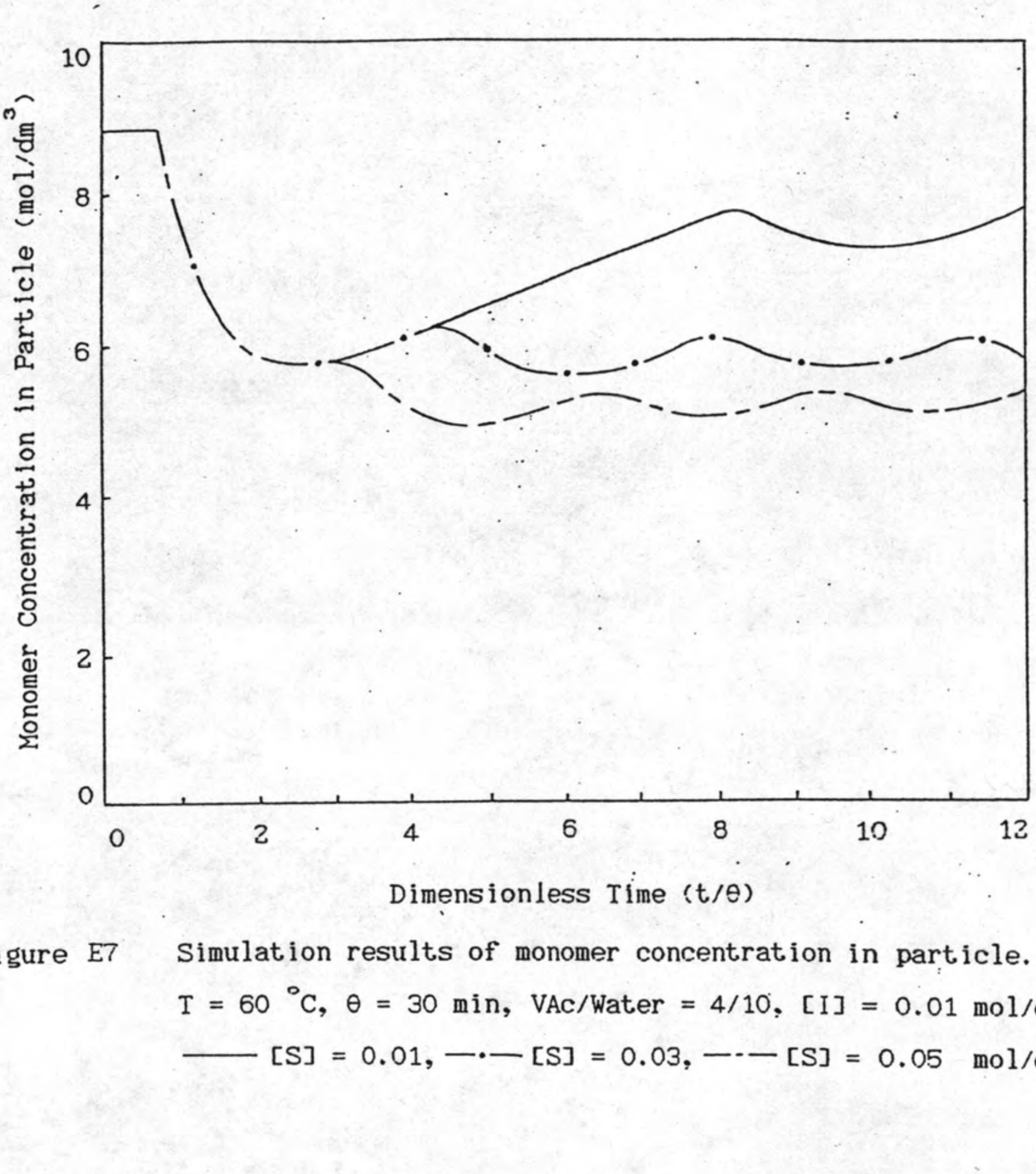

Figure E7 Simulation results of monomer concentration in particle.
T = 60 °C, θ = 30 min, VAc/Water = 4/10, [I] = 0.01 mol/dm^3
——— [S] = 0.01, —•— [S] = 0.03, —·— [S] = 0.05 mol/dm^3

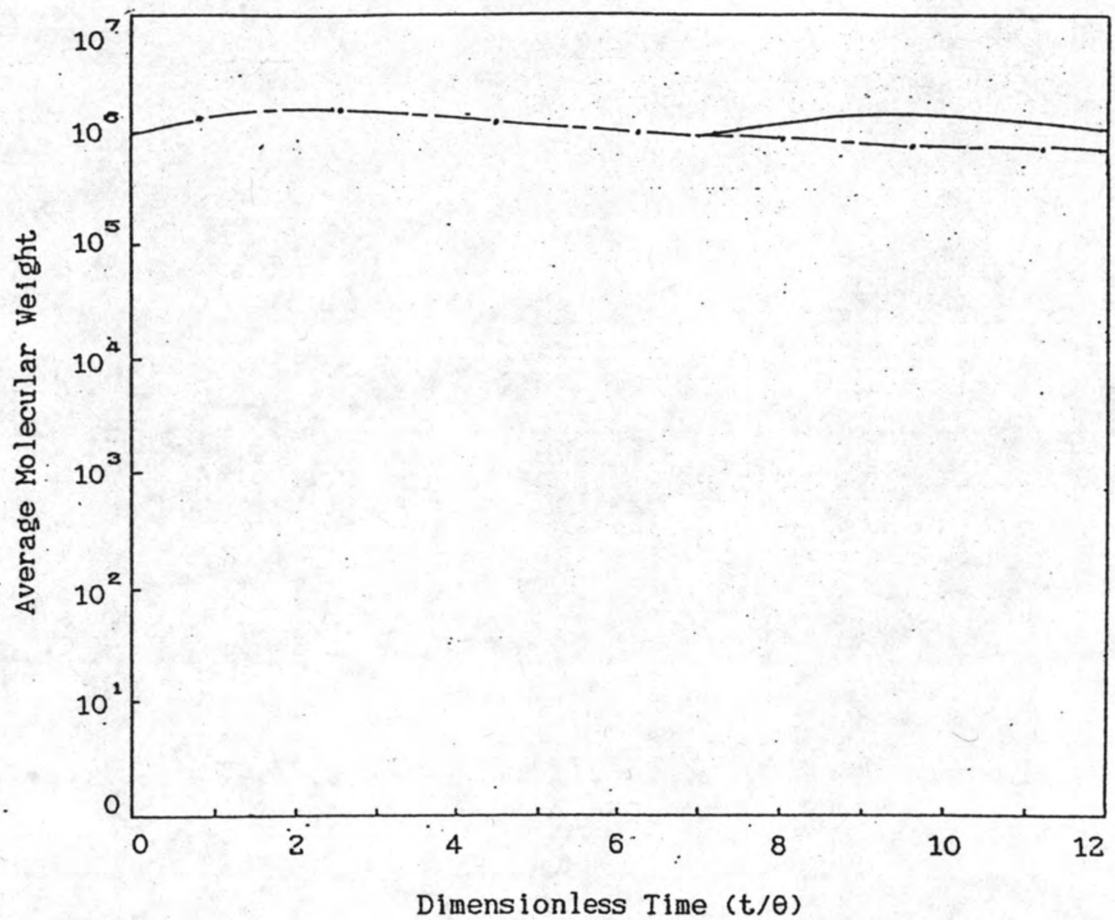

Figure E8 Simulation results of weight average molecular weights.
T = 60 °C, θ = 30 min, VAc/Water = 4/10, [I] = 0.01 mol/dm^3
—— [S] = 0.01, —·— [S] = 0.03, —··— [S] = 0.05 mol/dm^3

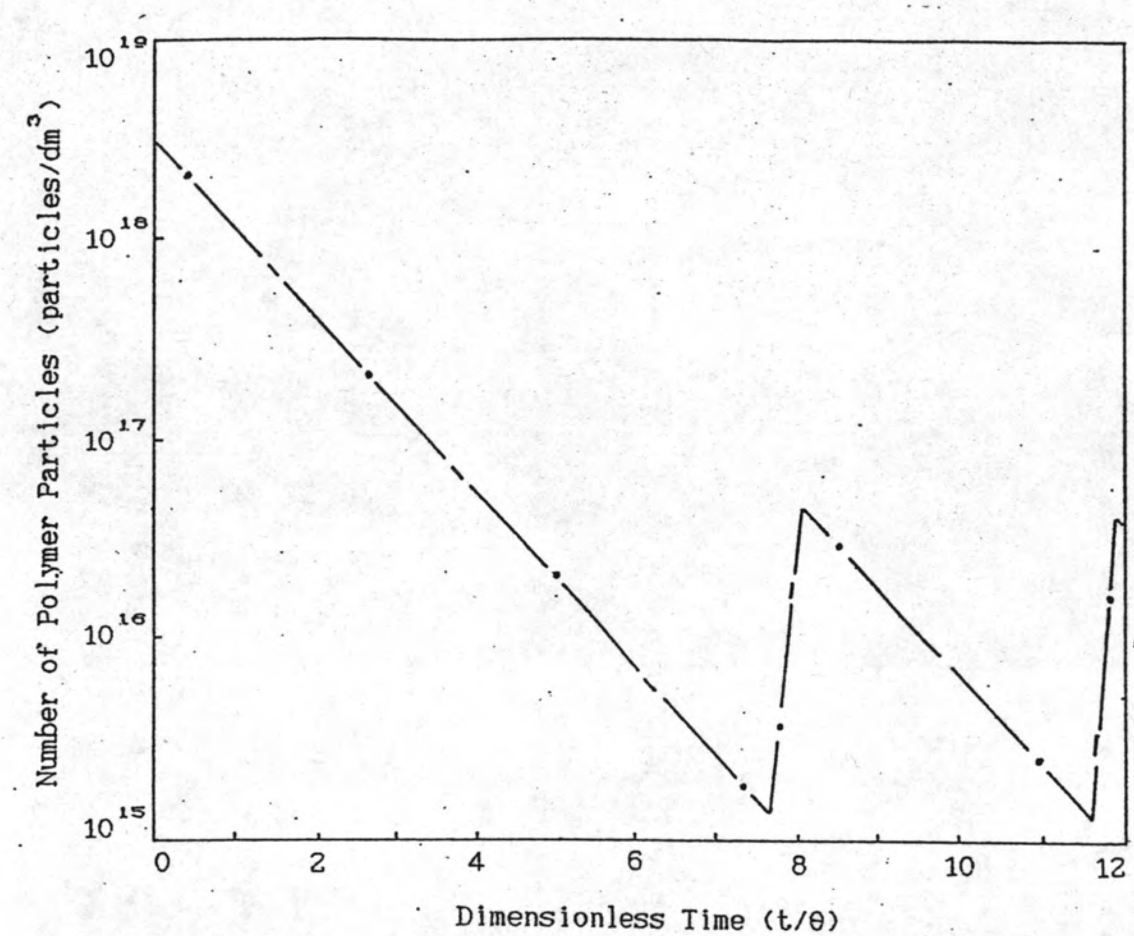

Figure E9 Simulation results of number of polymer particles.

T = 60 °C, θ = 30 min, VAc/Water = 4/10, [S] = 0.01 mol/dm^3

—— [I] = 0.01, —·— [I] = 0.03, —··— [I] = 0.05 mol/dm^3

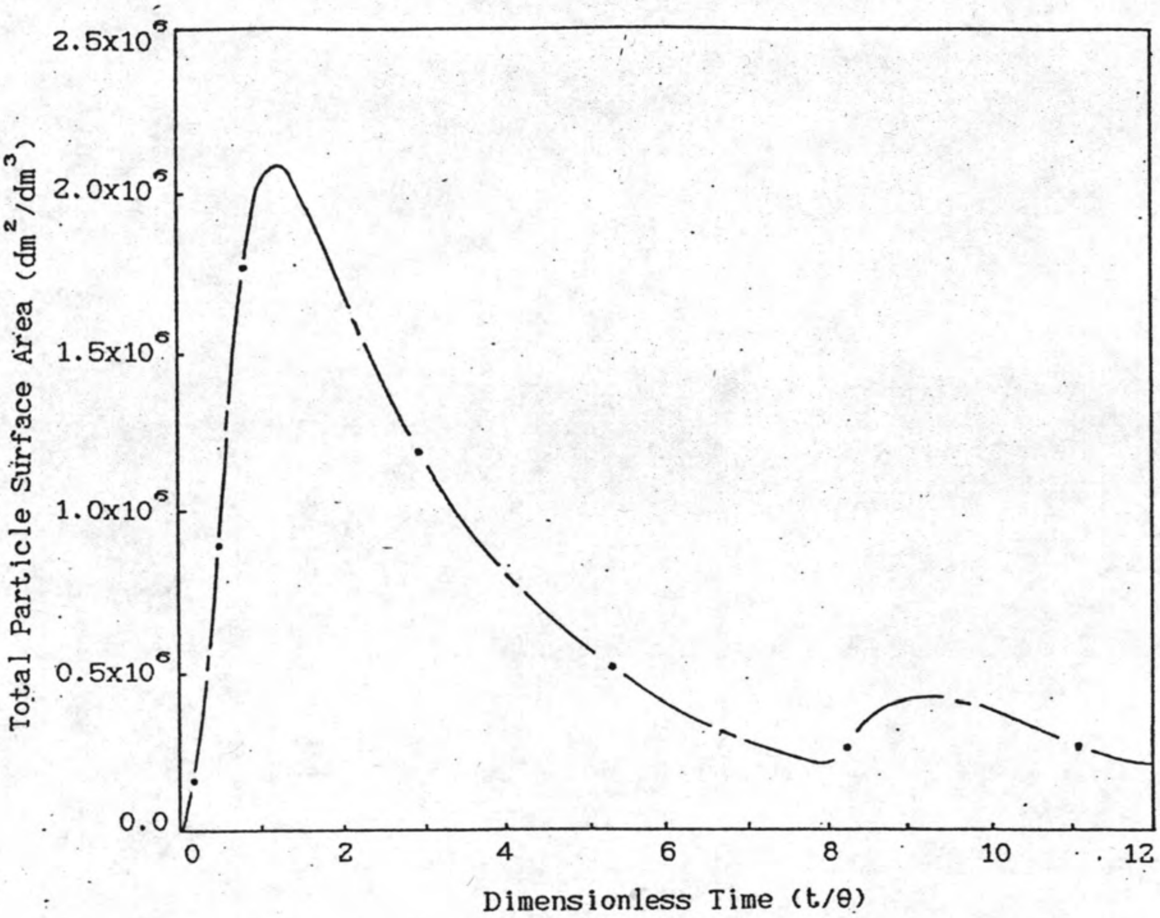

Figure E10 Simulation results of total particle surface area.

$T = 60\ ^{\circ}C$, $\theta = 30$ min, VAc/Water = 4/10, [S] = 0.01 mol/dm^3

—— [I] = 0.01, —·— [I] = 0.03, —-— [I] = 0.05 mol/dm^3

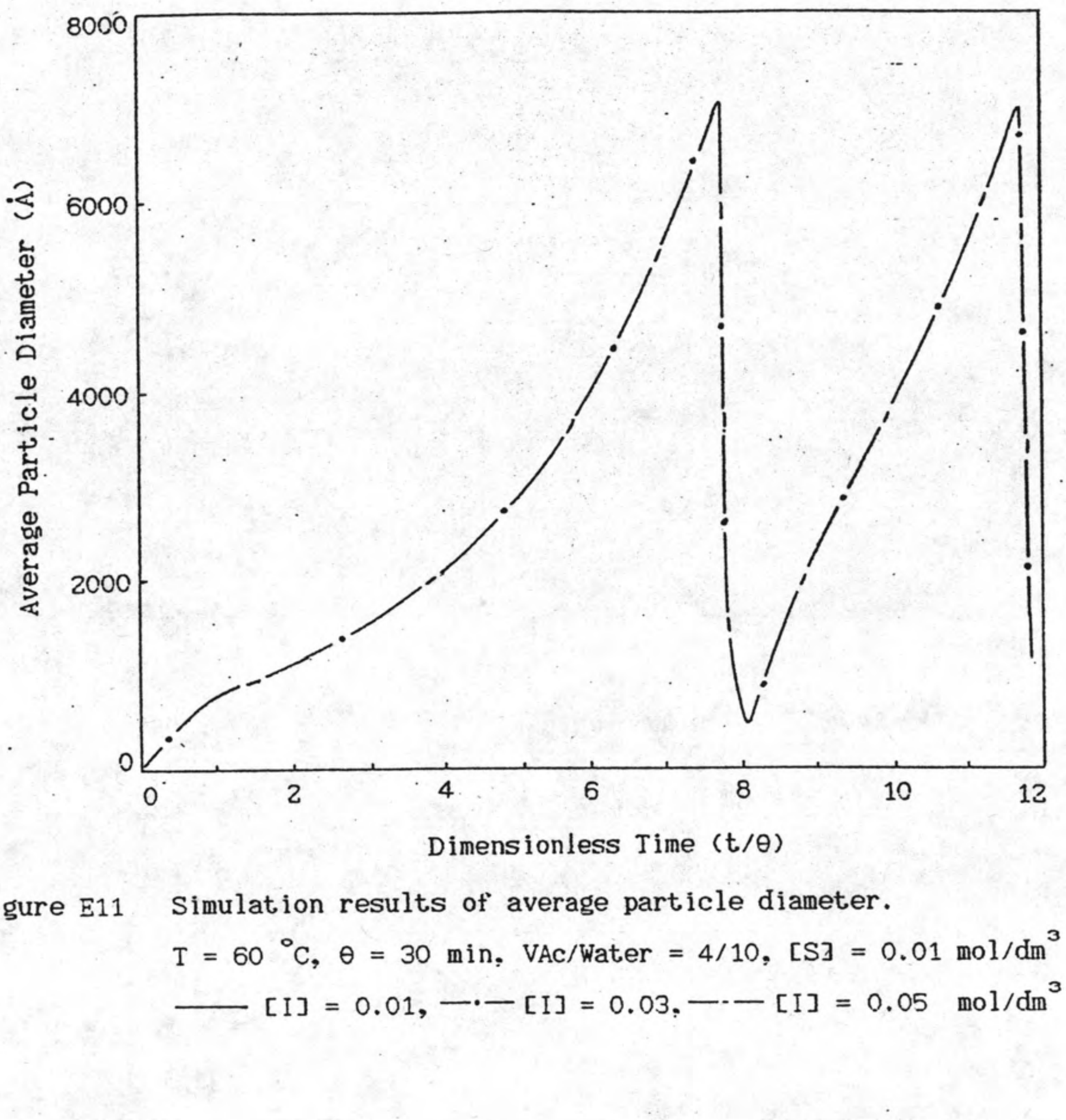

Figure E11 Simulation results of average particle diameter.

T = 60 °C, θ = 30 min, VAc/Water = 4/10, [S] = 0.01 mol/dm^3

—— [I] = 0.01, —·— [I] = 0.03, —·-— [I] = 0.05 mol/dm^3

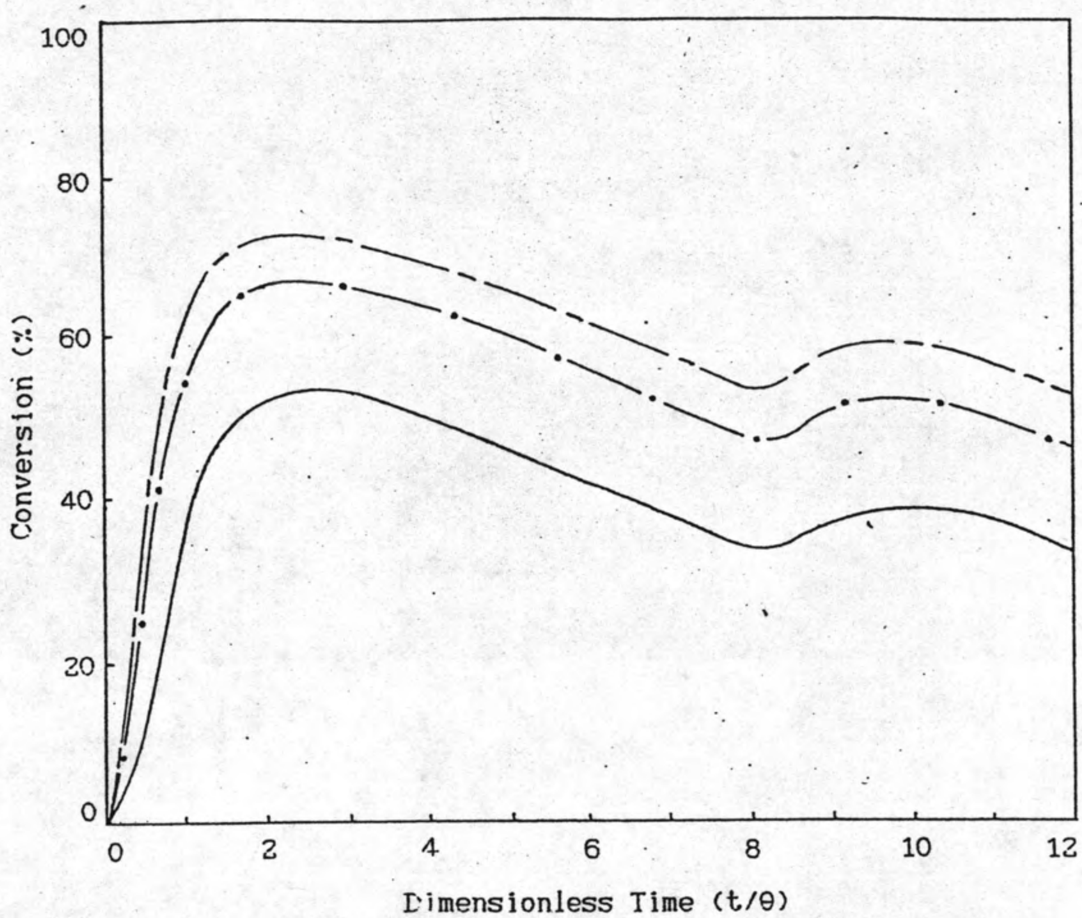

Figure E12 Simulation results of conversion.

T = 60 °C, θ = 30 min, VAc/Water = 4/10, [S] = 0.01 mol/dm^3

—— [I] = 0.01, —•— [I] = 0.03, —·— [I] = 0.05 mol/dm^3

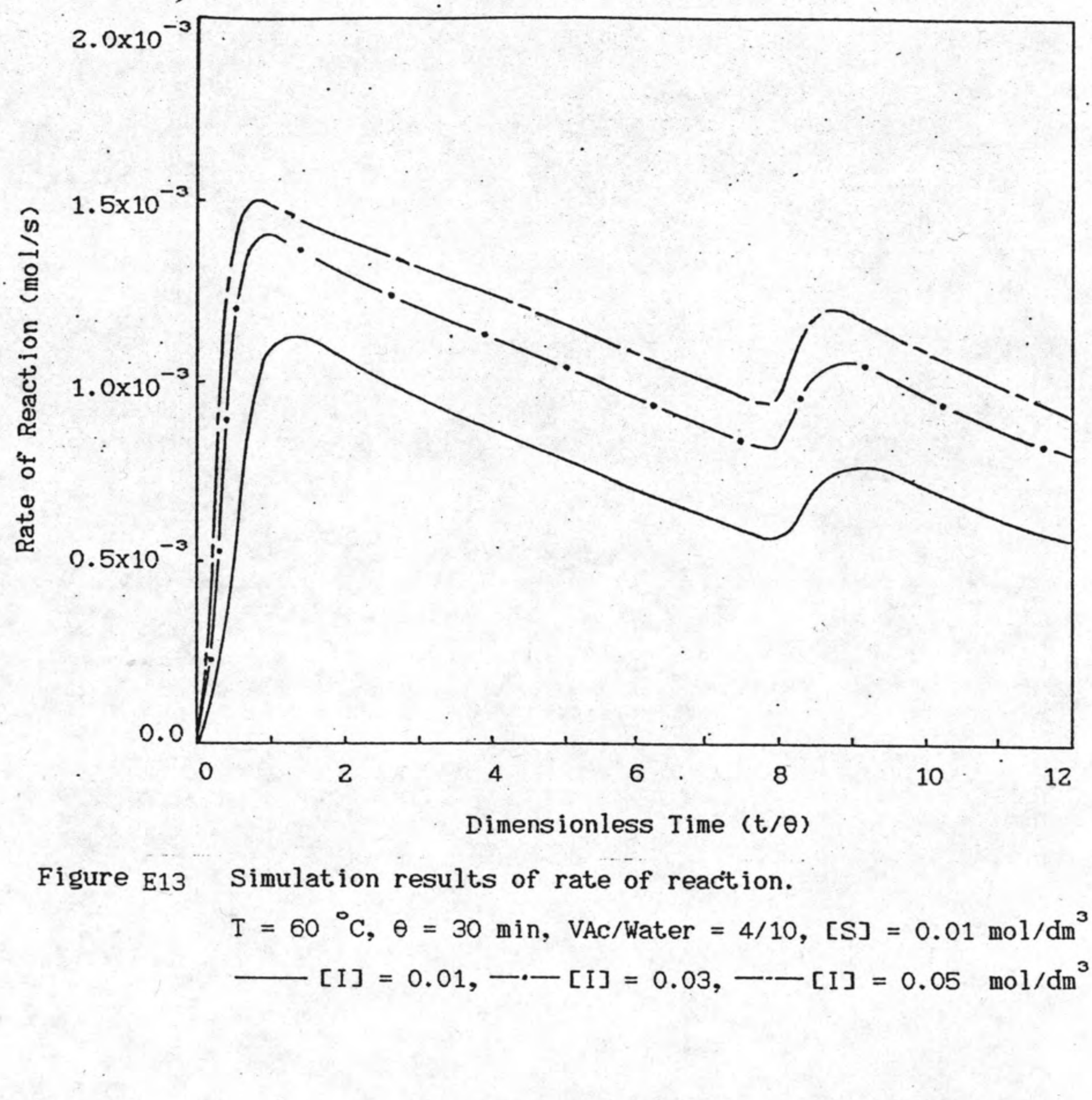

Figure E13 Simulation results of rate of reaction.

T = 60 °C, θ = 30 min, VAc/Water = 4/10, [S] = 0.01 mol/dm^3

—— [I] = 0.01, —·— [I] = 0.03, —··— [I] = 0.05 mol/dm^3

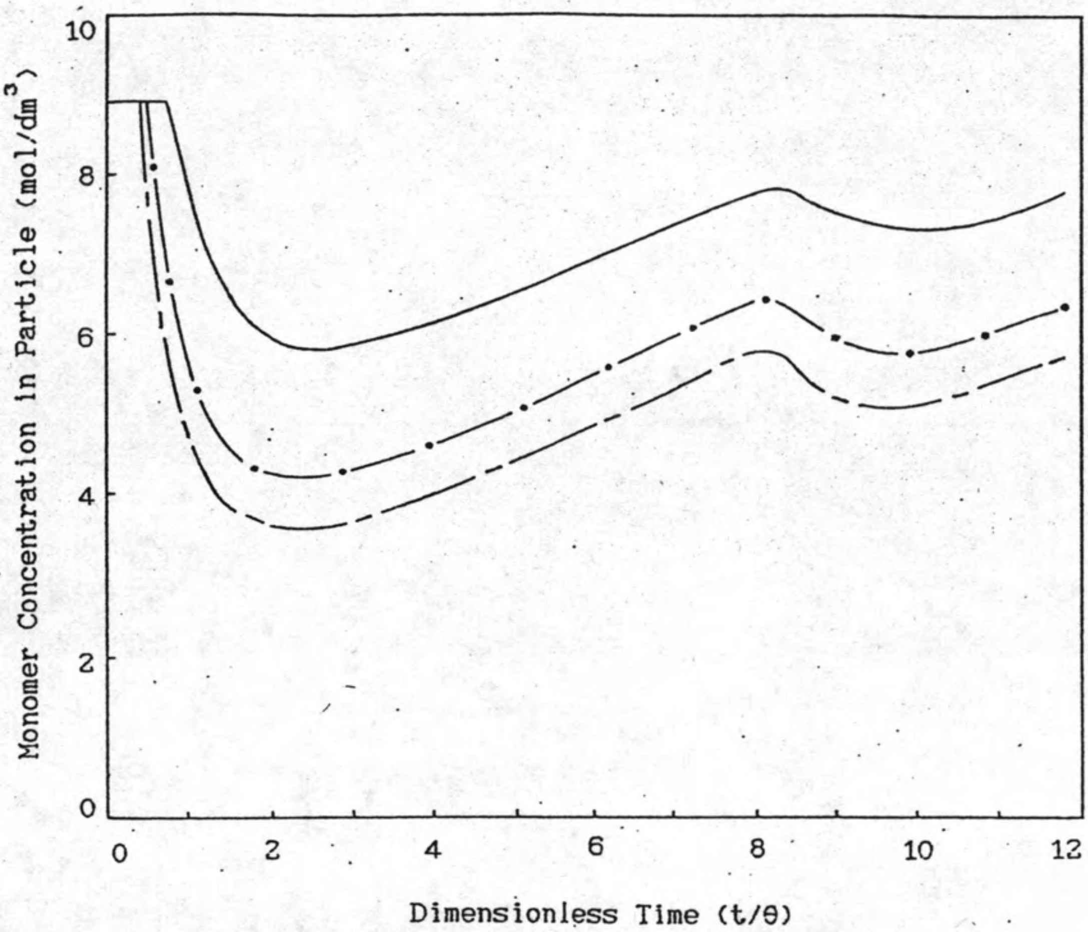

Figure E14 Simulation results of monomer concentration in particle.
T = 60 °C, θ = 30 min, VAc/Water = 4/10, [S] = 0.01 mol/dm^3
——— [I] = 0.01, —·— [I] = 0.03, —·-— [I] = 0.05 mol/dm^3

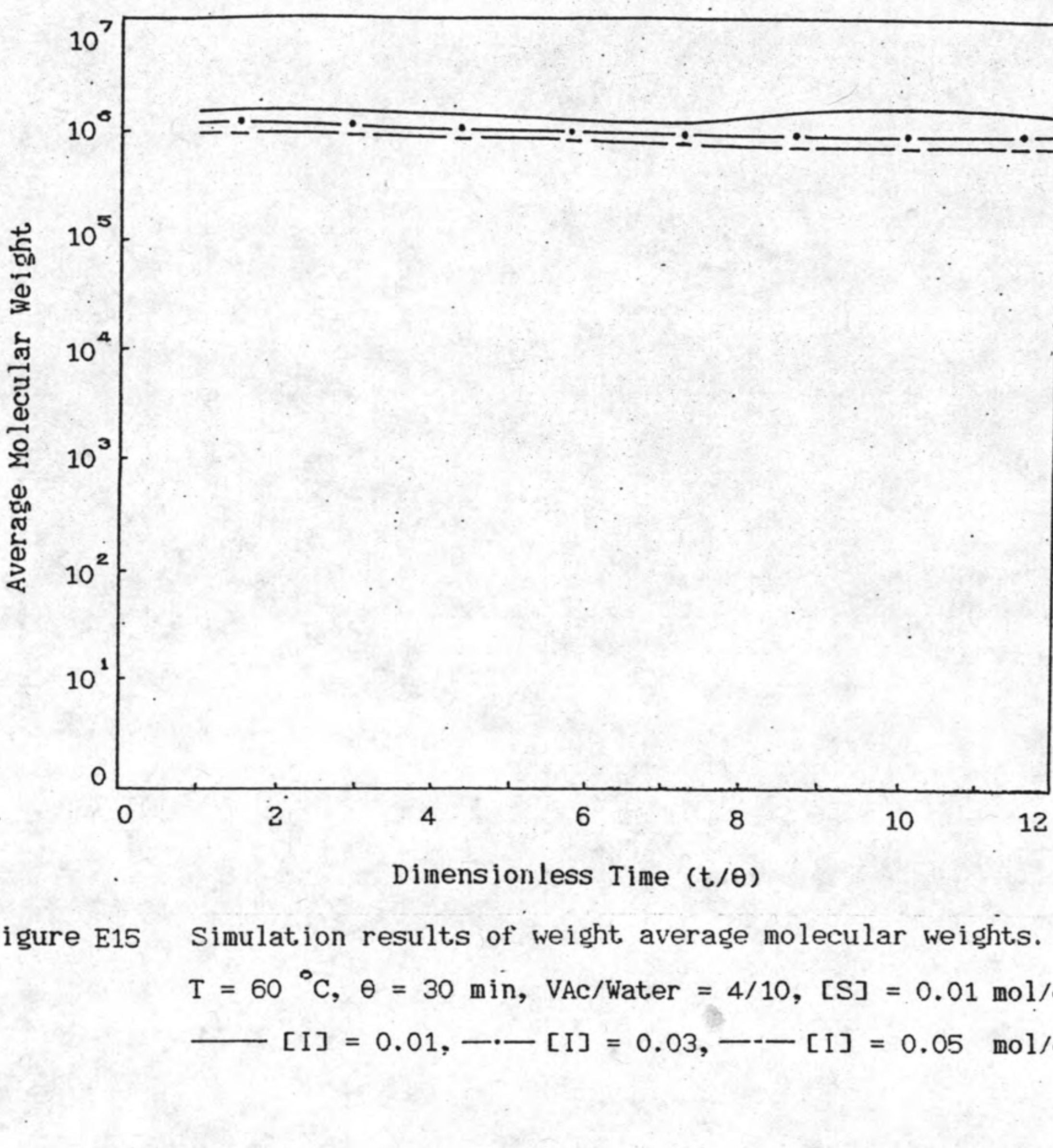

Figure E15 Simulation results of weight average molecular weights.
T = 60 °C, θ = 30 min, VAc/Water = 4/10, [S] = 0.01 mol/dm^3
—— [I] = 0.01, —·— [I] = 0.03, —--— [I] = 0.05 mol/dm^3

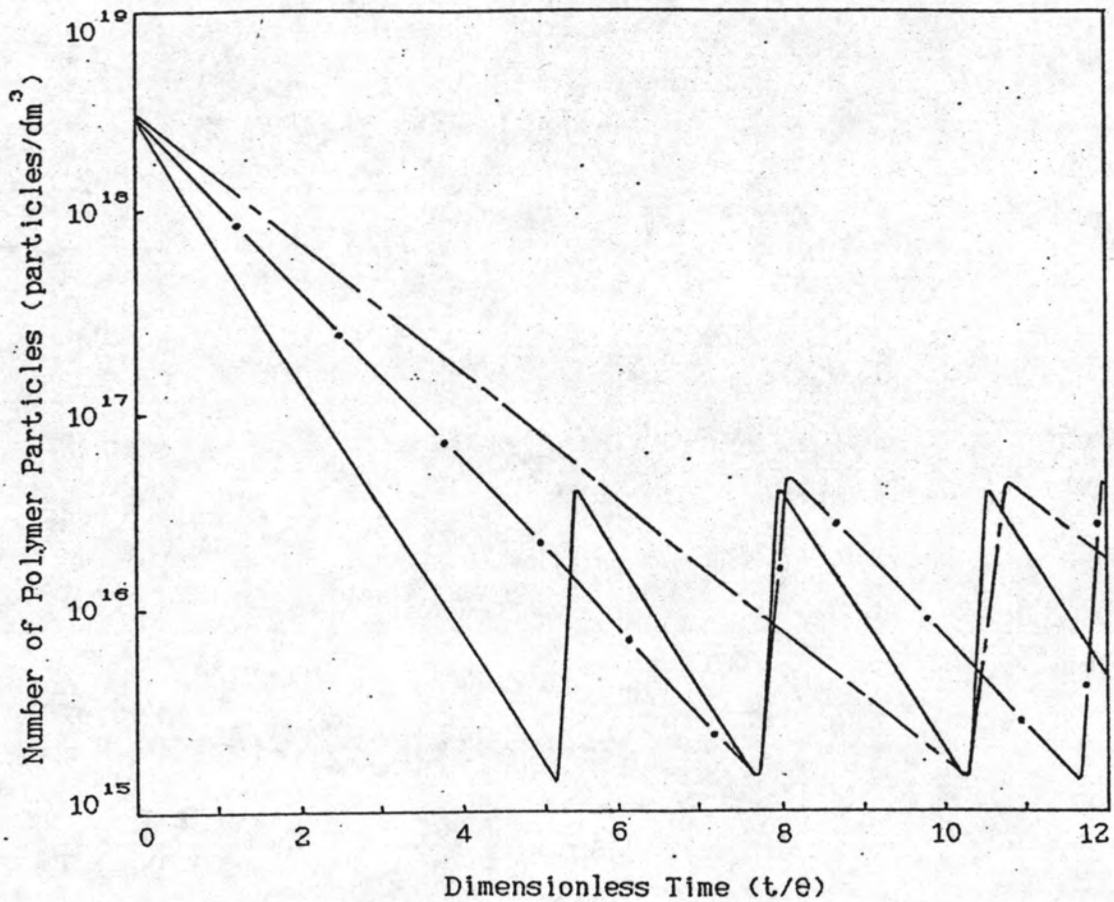

Figure E16 Simulation results of number of polymer particles.
T = 60 °C, [I] = 0.01 mol/dm^3, [S] = 0.01 mol/dm^3
VAc/Water = 4/10, —— θ = 20, —·— θ = 30, —·—— θ = 40 min.

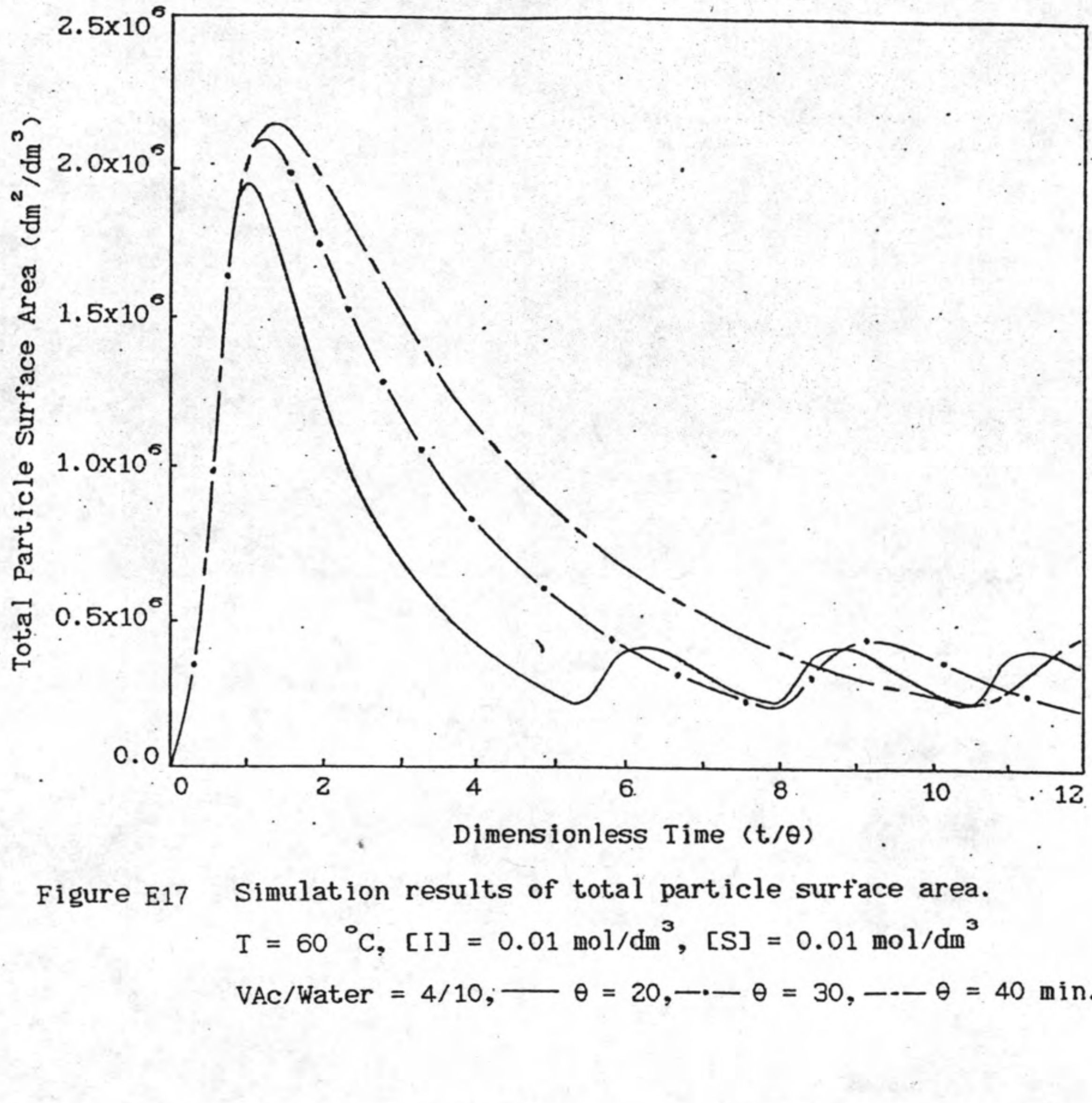

Figure E17 Simulation results of total particle surface area.
$T = 60\ ^{\circ}C$, $[I] = 0.01\ mol/dm^3$, $[S] = 0.01\ mol/dm^3$
VAc/Water = 4/10, —— θ = 20, —·— θ = 30, --- θ = 40 min.

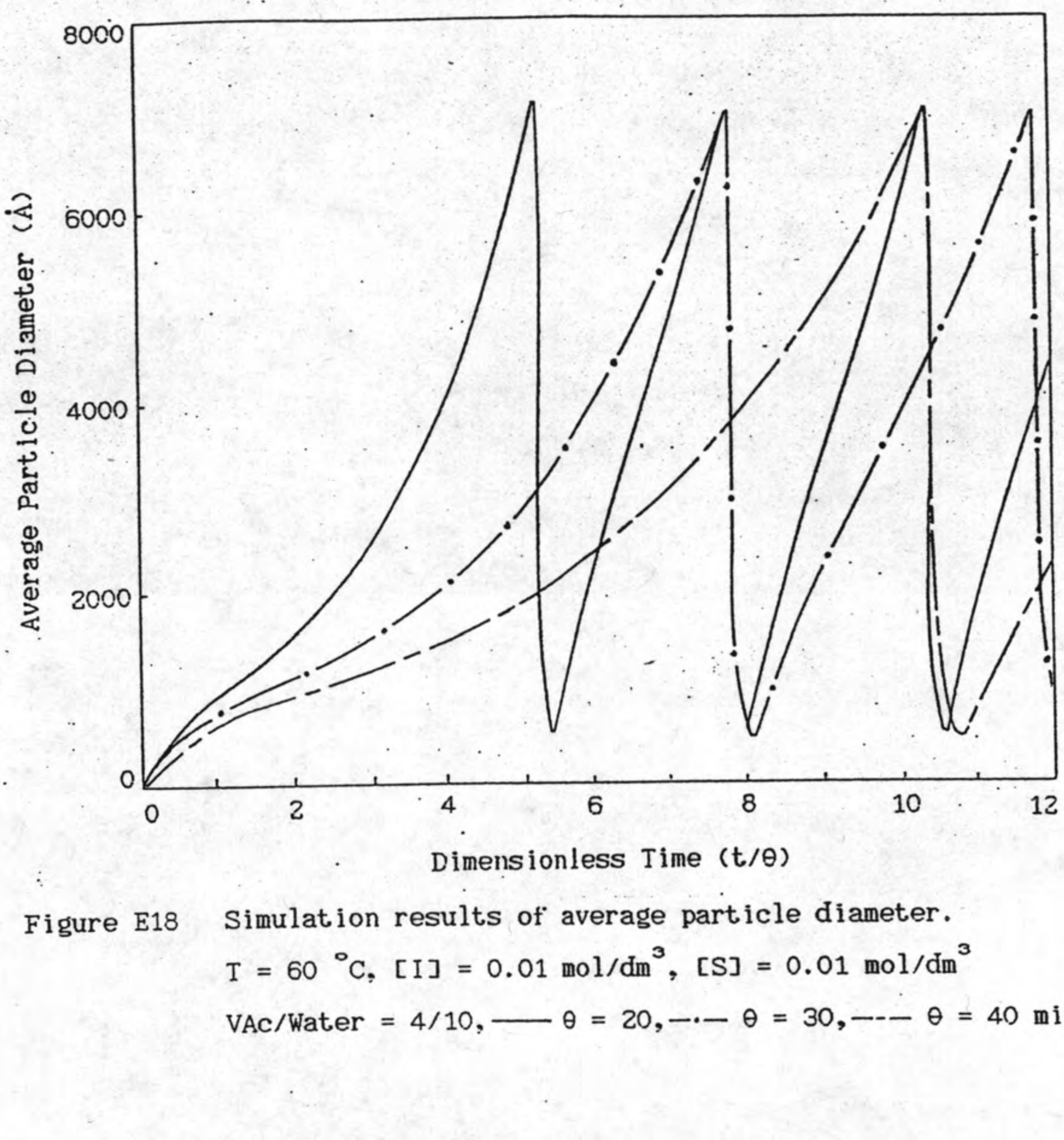

Figure E18 Simulation results of average particle diameter.
T = 60 °C, [I] = 0.01 mol/dm^3, [S] = 0.01 mol/dm^3
VAc/Water = 4/10, —— θ = 20, —·— θ = 30, --- θ = 40 min.

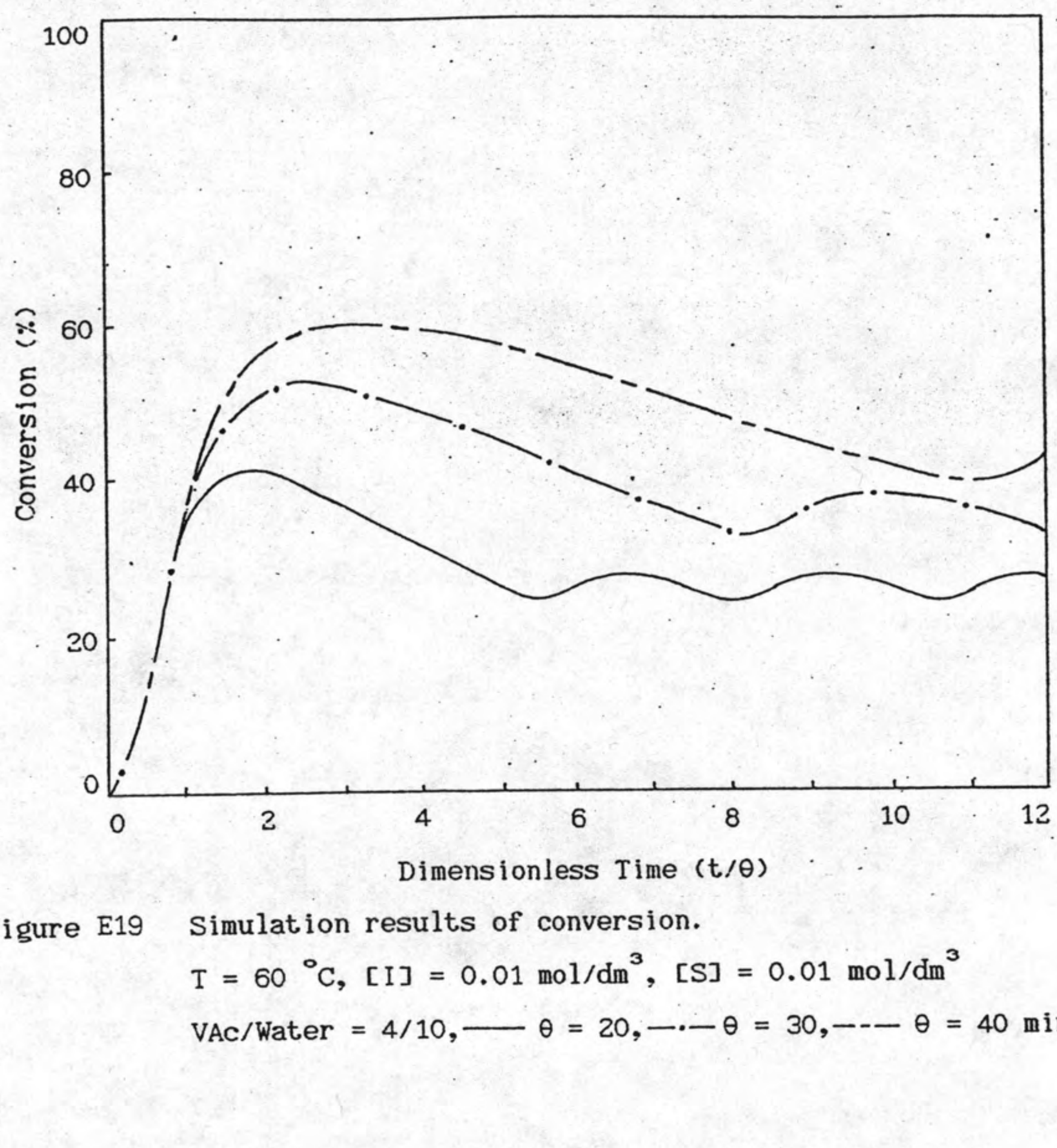

Figure E19 Simulation results of conversion.

$T = 60\ ^{\circ}C$, $[I] = 0.01\ mol/dm^3$, $[S] = 0.01\ mol/dm^3$

VAc/Water = 4/10, —— θ = 20, —·— θ = 30, - - - θ = 40 min.

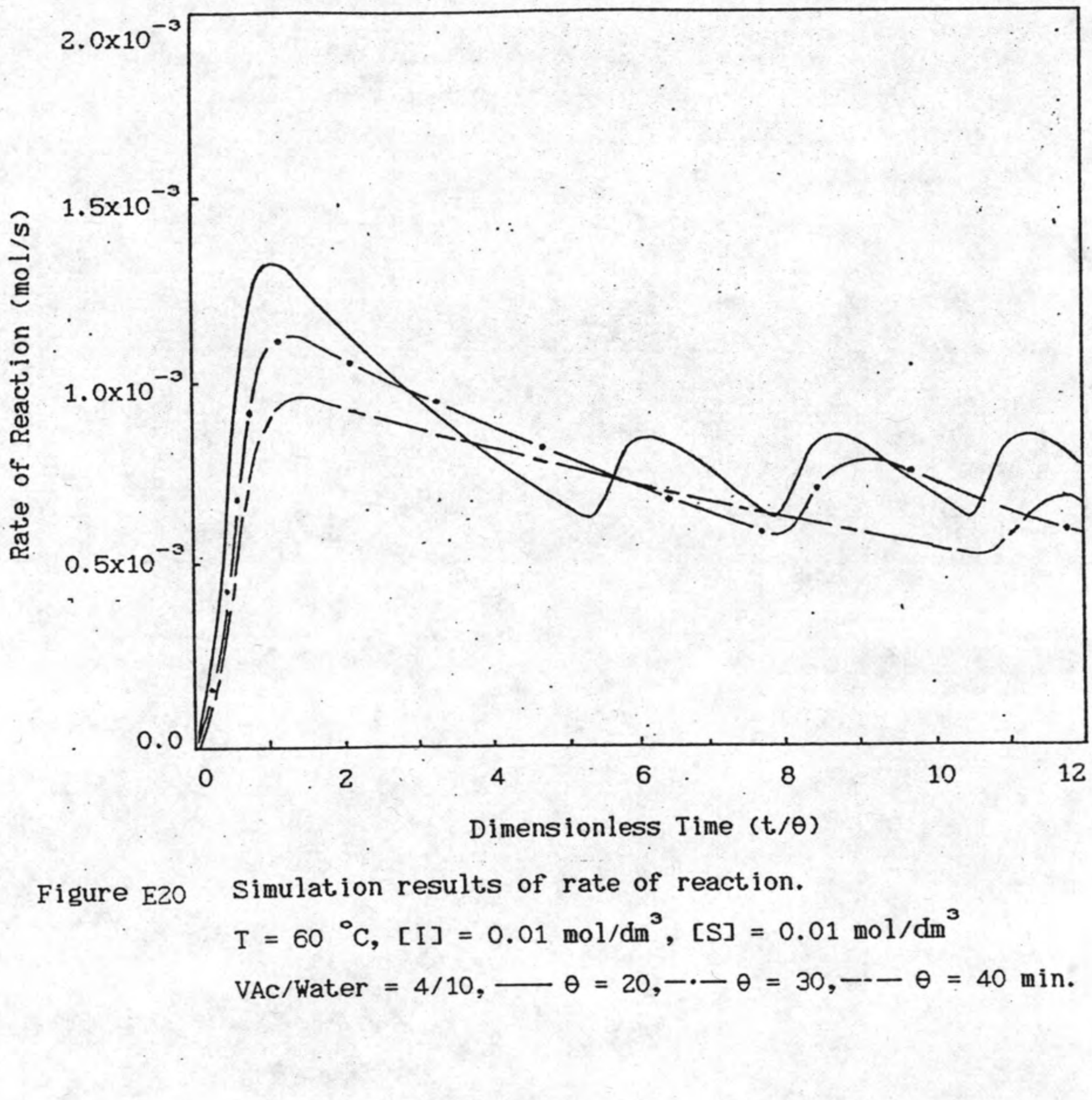

Figure E20 Simulation results of rate of reaction.

T = 60 °C, [I] = 0.01 mol/dm^3, [S] = 0.01 mol/dm^3

VAc/Water = 4/10, —— θ = 20, —·— θ = 30, —-— θ = 40 min.

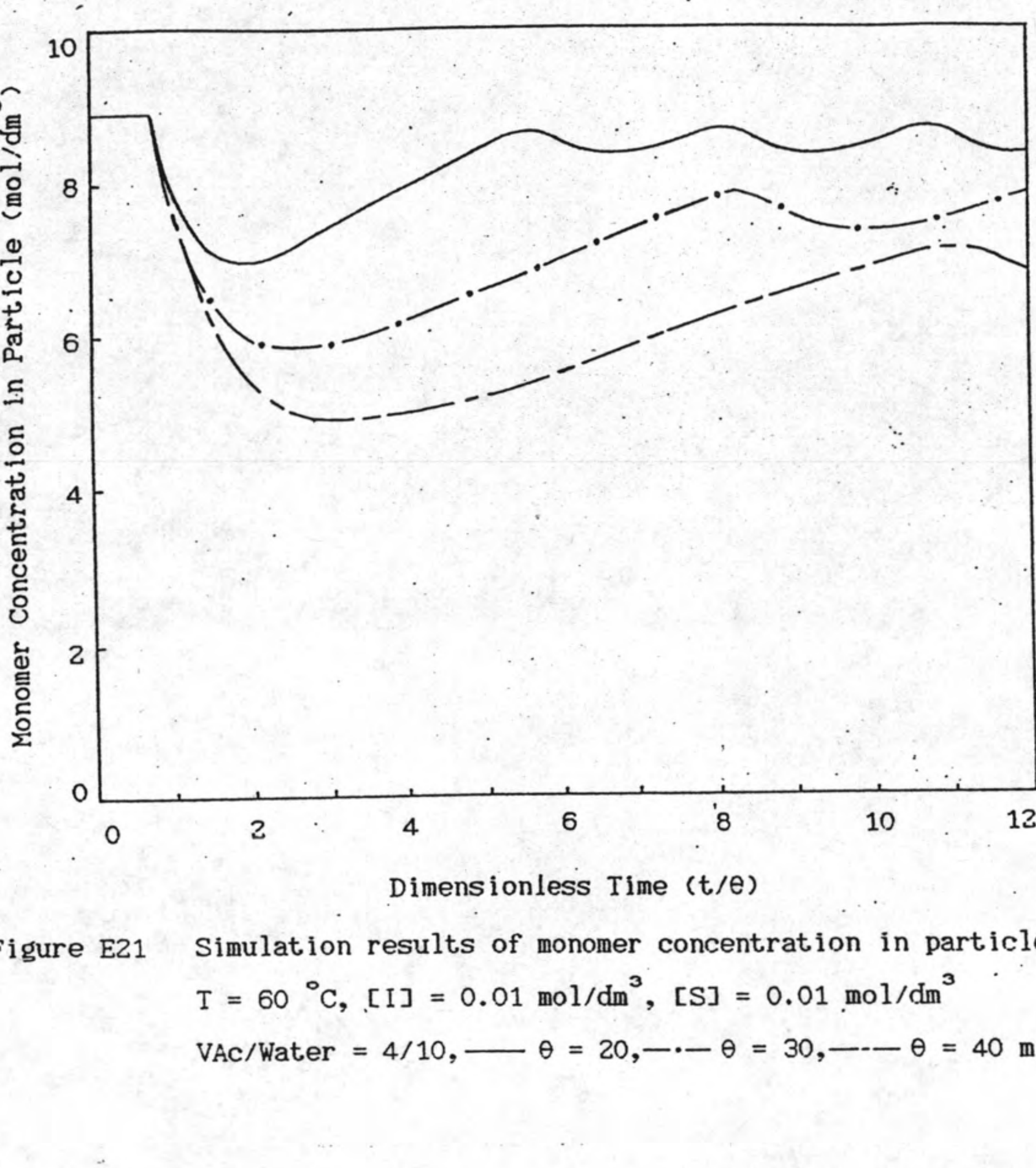

Figure E21 Simulation results of monomer concentration in particle.
T = 60 °C, [I] = 0.01 mol/dm^3, [S] = 0.01 mol/dm^3
VAc/Water = 4/10, —— θ = 20, —·— θ = 30, ---- θ = 40 min.

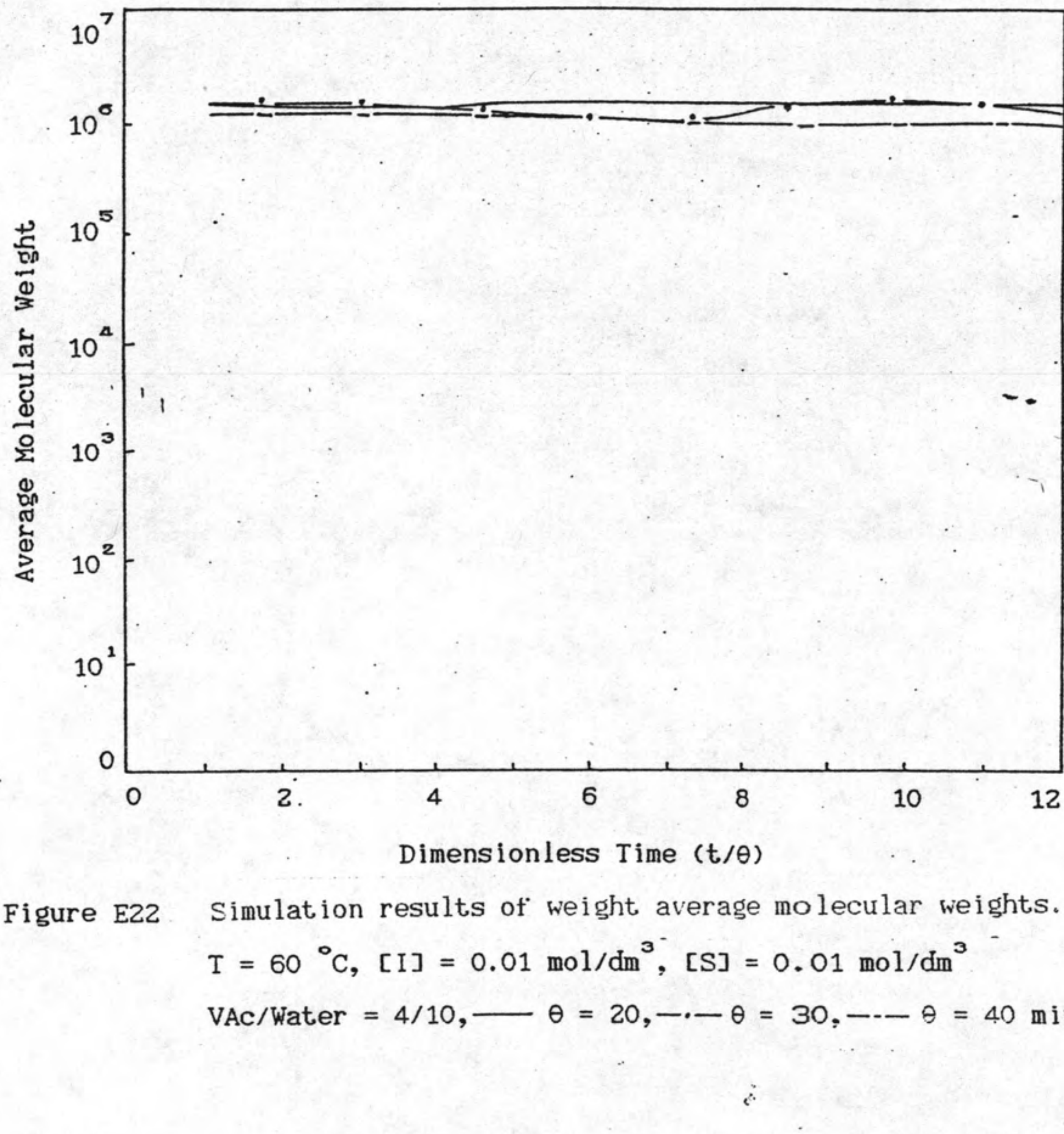

Figure E22 Simulation results of weight average molecular weights.

T = 60 °C, [I] = 0.01 mol/dm^3, [S] = 0.01 mol/dm^3

VAc/Water = 4/10, —— θ = 20, —·— θ = 30, –·– θ = 40 min.

APPENDIX F
NUMERICAL CALCULATION

This present section is devoted to solving the differential equation numerically. There are a very large number of available techniques for numerical integration of differential equations. Numerical integration implies an approximation of the continuous differential equations with discrete finite-difference equations. The various integration methods differ in the way they implement their approximation. Thus, the key questions for an intregation technique are the stability of the procedure and speed with it reaches the solution. The most popular integration method is the fourth-order Runge-Kutta, which provides satisfactory accuracy and stability of computations.

Linearization is the process by which we approximate nonlinear systems with linear ones. It is widely used in the numerical calculation because we can have closed-form, analytical solution for linear systems. Thus, we can have a complete and general picture of the behaviour of the equations. Consider the following nonliner differential equation

$$dy/dx = f(x,y) \tag{1}$$

x - independent variable

y - dependent variable

If the solution of the equation, function describing the behaviour of y, has continuous derivative, it can be represented by a Taylor series expansion about a starting value (x_i, y_i), then the nonlinear equation is changed into the related linear equation as

$$y_{i+1} = y_i + \frac{y'_i h}{1!} + \frac{y''_i h^2}{2!} + \frac{y'''_i h^3}{3!} + \ldots + \frac{y^n{}_i h^n}{n!} \tag{2}$$

Where $h = x_{i+1} - x_i$

An alternative form can be developed by substituting equation 1 into equation 2 then

$$y_{i+1} = y_i + \frac{f(x_i,y_i)h}{1!} + \frac{f'(x_i,y_i)h^2}{2!} + \frac{f''(x_i,y_i)h^3}{3!} + \ldots + \frac{f^{(n-1)}(x_i,y_i)h^n}{n!} \quad (3)$$

Runge-Kutta methods achive the accuracy of a Tayler series approch without requiring the calculation of higher derivative. Many variations exist but all can be cast in the general form as

$$y_{i+1} = y_i + \phi(x_i, y_i, h)h \quad (4)$$

Where $\phi(x_i,y_i,h)$ is an increment function which can be interpreted as a representative slope over the interval (x_i,x_{i+1}), the increment function can be written in the general form as

$$\phi = a_1k_1 + a_2k_2 + a_3k_3 + \ldots + a_nk_n \quad (5)$$

$$k_1 = f(x_i, y_i) \quad (6)$$

$$k_2 = f(x_i+p_1h, y_i + q_{11}k_1h) \quad (7)$$

$$k_3 = f(x_i+p_2h, y_i+q_{21}k_1h + q_{22}k_2h) \quad (8)$$

$$k_n = f(x_i+p_{n-1}h, y_i+q_{n-1,1}k_1h + q_{n-2,2}k_2h + q_{n-1,n-1}k_{n-1}h) \quad (9)$$

Where a's are constant

Notice that the k's are recurrence relationships. That is, k_1 appears in the equation for k_2. which arrears in the equation for k_3 and so forth. This recurrence relation makes Runge-Kutta methods efficient for computer calculations.

Various types of Runge-Kutta methods can be devided by employing different numbers of terms in the increment function as specified by n. For the fourth-order Runge-kutta method, the method that is used in this model calculation and is the most popualr Runge-Kutta methods, this method uses an increment function with 4 terms ($n = 4$) and y_{i+1} is expressed in the term of y_i and the increment function as

$$y_{i+1} = y_i + (k_1 + 2k_2 + 2k_3 + k_4)h/6 \quad (10)$$

$$k_1 = f(x_i, y_i) \quad (11)$$

$$k_2 = f(x_i + h/2, y_i + k_1h/2) \quad (12)$$

$$k_3 = f(x_i + h/2, y_i + k_2h/2) \quad (13)$$

$$k_4 = f(x_i + h, y_i + k_3h) \quad (14)$$

The developed model in this study comprises of many differential equations and the system equations of differential equation are formed, thus, the fourth-order Runge-Kutta are applied for numerical calculation of this system equations.

The system equation may be represented in the general form as

$$dy_1/dx = f_1(x, y_1, y_2, y_3, \ldots, y_n) \quad (15)$$

$$dy_2/dx = f_2(x, y_1, y_2, y_3, \ldots, y_n) \quad (16)$$

$$dy_3/dx = f_3(x, y_1, y_2, y_3, \ldots, y_n) \quad (17)$$

$$dy_n/dx = f_n(x, y_1, y_2, y_3, \ldots, y_n) \quad (18)$$

The solution of such a system requires n initial conditions and the starting value of x.

For example the system equation with m differential equations. The y_{i+1} value of the j th differential equation can be express as

$$y_{j,i+1} = y_{j,i} + (k_{j,1} + 2k_{j,2} + 2k_{j,3} + k_{j,4})h/6 \quad (19)$$

$$k_{j,1} = f_j(x_i, y_{1,i}, y_{2,i}, y_{3,i}, \ldots, y_{m,i}) \quad (20)$$

$$k_{j,2} = f_j(x_i+h/2, y_{1,i}+k_{1,1}h/2, y_{2,i}+k_{2,1}h/2, y_{3,i}+k_{3,1}h/2, \ldots, y_{m,i}+k_{m,1}h/2) \quad (21)$$

$$k_{j,3} = f_j(x_i+h/2, y_{1,i}+k_{1,2}h/2, y_{2,i}+k_{2,2}h/2, y_{3,i}+k_{3,2}h/2, \ldots, y_{m,i}+k_{m,2}h/2) \quad (23)$$

$$k_{j,4} = f_j(x_i+h, y_{1,i}+k_{1,3}h, y_{2,i}+k_{2,3}h, y_{3,i}+k_{3,3}h, \ldots, y_{m,i}+k_{m,3}h) \quad (24)$$

From the system solution express in equation 19 to 24 one can solve the system epuations which consist of any m equations in the consecutive manner if the initial value of all m equations and initial value of x are known. One must keep in mind that the small value of the increment, h, the more accuracy of the obtained solution.

APPENDIX G
BIOGRAPHY

Sanong Ekgasit, a son of Mrs. Tham and Mr. Charad Ekgasit, was born on March 5, 1966 in Nakhornrachasima province, Thailand. After finish high school from Wat Saket school, he entered Chulalonngkron university as a scholarship under the Development and Promotion of Science and Technology Talent Project(DPST) and received Bachelor of Science degree majoring in Chemistry on May 15, 1989. He continued his graduate study at The Petroleum and Petrochemical college,Chulalongkorn University, majoring in polymer technology, on his master degree study he continue his scholarship under the DPST Project as well.