CHAPTER VIII

CONCLUSIONS

The first Taylor dispersion apparatus capable of measuring liquid phase mutual diffusion coefficients in substances which are solids at ambient conditions was successfully constructed. The apparatus is compatible with solvents which melt at temperatures up to 400 K. Using this apparatus, diffusion coefficients at infinite dilution were measured over a range of temperatures for hydrogen, carbon monoxide, carbon dioxide and several n-alkane solutes in the solvents n-eicosane (C_{20}), n-octacosane (C_{28}) and a sample of Fischer-Tropsch reactor wax. Solvent density was also measured at each experimental condition.

During the course of the experiments, an improved method for calculating the diffusion coefficient from Taylor dispersion data was also developed. The method is based on a non-linear curve fit of the analytical solution to the Taylor dispersion problem. A comparison of results calculated with the new method indicated that diffusion coefficients calculated with other techniques such as the "graphical method" and the "moment method" may be in error by several percent.

The experimental technique for determining gaseous solute diffusion coefficients using a Taylor dispersion apparatus was also improved and simplified. The previous method required a saturator to saturate a sample of pure liquid prior to injection. It has been demonstrated that a small quantity of pure gas may be injected under pressure directly into the diffusion tube, thus eliminating the need for an external saturator.

The Rough Hard Sphere theory was used to develop a correlation which has been demonstrated to predict both gaseous and liquid solute diffusion in normal alkane solvents with carbon numbers ranging from 7 to 28 at temperatures to 570

K. The data used to develop the model covered the solute/solvent molecular mass ratio range (m_1/m_2) of 0.005 for the H_2/C_{28} system to 2.26 for the C_{16}/C_7 system. The molecular diameter ratio ranged from 0.3 to 1.3 for the same systems. The ratio V/V_o ranged from 1.4 to 2.0. Molecular dynamics calculations for mutual diffusion coefficients are not yet available over the entire range of these conditions. The correlation demonstrated that the RHS theory can even be applied successfully to large chain molecules such as n-octacosane. For 143 measured diffusion coefficients used to develop the correlation, the average absolute percent error was only 6.3%. When the correlation was used to predict literature values, the agreement was also excellent, except for diffusion coefficients of small alkane solutes such as methane and ethane. Even for these solutes, the predicted values rarely disagreed with measured values by more than 30%. For most engineering design estimates, this agreement would be considered satisfactory.

The correlation was also used to predict literature data for the diffusion of noble gases in normal alkane solvents. For the noble gas data, the model predictions were high by an average of 12%. However a portion of this error may have been due to the analysis technique used to calculate the diffusion coefficients reported in the literature.

Diffusion coefficients were measured for several Fischer-Tropsch reactants and products in an actual sample of Fischer-Tropsch wax at reactor conditions. These diffusion coefficients can be conservatively estimated using the RHS correlation by modelling the FT wax as a pure normal alkane with carbon number equal to the mean carbon number of the wax. For mean carbon numbers greater than about 25, the mean carbon number does not need to be known accurately because the infinite dilution mutual diffusion coefficient is not a strong function of solvent carbon number for large carbon numbers.

The measured diffusion coefficients in the FT wax indicated that currently used correlations for predicting diffusion in FT wax grossly underestimates the diffusion coefficient. The results of this study also cast doubt on existing mass transfer correlations which are a function of the diffusion coefficient, but which were developed with low temperature mass transfer data. Furthermore, previous conclusions as to whether or not a reaction is mass transfer limited may be eventually rendered invalid by the results of this research.

CHAPTER IX

RECOMMENDATIONS FOR FUTURE WORK

In order to advance the development of the RHS theory for diffusion in liquid alkane solvents, measurements of diffusion coefficients for gaseous alkane solutes (C_1 through C_4) are desperately needed. There is also a strong need for measurements of diffusion coefficients near the solvent melting point, where most theories fail. Experiments should also be conducted to measure mutual diffusion coefficients as a function of composition. This data could then be used to develop a concentration dependent model for the RHS diffusion coefficient.

Our study has been limited to diffusion in alkane solvents. Future studies could determine diffusion coefficients for various solute/solvent combinations of polar, non-polar, electrolytic, and non-electrolytic molecules. Eventually as more data becomes available, the RHS diffusion coefficient model could be refined.

Molecular dynamics studies are also required for both the mutual and the self diffusion coefficient. Future studies in this area should concentrate on accurately calculating the molecular dynamics ratios (used to correct the simple Chapman-Enskog theory) over a wide range of values for σ_1/σ_2, m_1/m_2, and V/V_o. Only molecular dynamics ratios for self-diffusion and infinitely dilute mutual diffusion have been published in the literature. Future studies should also calculate concentration dependent molecular dynamics ratios.

For this study, it was necessary to measure diffusion coefficients in an actual sample of Fischer-Tropsch wax so that the feasibility of using model compounds such as n-octacosane could be validated. For future work, it is recommended that diffusion coefficients be measured in different model compounds or in synthetic wax mixtures containing known fractions of alkanes, olefins, and or oxygenates. Such studies could quantitatively ascertain the effect of different types of compounds on the diffusion coefficient.

There is a desperate need for high temperature mass transfer coefficient data and a mass transfer coefficient correlation which is valid at the elevated temperatures typical of most industrial chemical processes. The diffusion coefficient measurements provided by this work should aid in the development of such a correlation once enough experimental mass transfer coefficients have been determined at elevated temperatures. Accurate measurements of diffusion coefficients and mass transfer coefficients at elevated temperatures will eventually lead to improved reactor models. Future studies could evaluate the overall effect of these coefficients on Fischer-Tropsch reactor design.

LITERATURE CITED

Akgerman, A., and J. L. Gainer, "Predicting Gas-Liquid Diffusivities," *J. Chem. Eng. Data*, **17**, 372 (1972).

Alder, B. J., W. E. Alley, and J. H. Dymond, "Studies in molecular dynamics. XIV. Mass and size dependence of the binary diffusion coefficient," *J. Chem. Phys.*, **61**, 1415 (1974).

Alder, B. J., D. M. Gass, and T. E. Wainwright, "Studies in Molecular Dynamics. VIII. The Transport Coefficients for a Hard Sphere Fluid," *J. Chem. Phys.*, **53**, 3813 (1970).

Alizadeh, A. A., C. A. Nieto de Castro, and W. A. Wakeham, "The Theory of the Taylor Dispersion Technique for Liquid Diffusivity Measurements," *Int. J. Thermophys.*, **1**, 243 (1980).

Alizadeh, A. A., and W. A. Wakeham, "Mutual Diffusion Coefficients for Binary Mixtures of Normal Alkanes," *Int. J. Thermophys.*, **3**, 307 (1982).

Anderson, R. B., *The Fischer-Tropsch Synthesis*, Academic Press, Orlando, Florida, 1984.

Anderson, R. P., G. P. Sturm, R. D. Grigsby, and J. W. Vogh, *Characterization of Waxes Derived From Fischer–Tropsch Reactors*, Department of Energy Contract DE-AC22-86PC90010, Proceedings of Indirect Liquefaction Contractors' Review Meeting, Pittsburgh, December, 1987.

Aris, R., "On the dispersion of a solute in a fluid flowing through a tube," *Proc. Roy. Soc.*, **A235**, 67 (1956).

Atwood, J. G., and J. Goldstein, "Measurements of Diffusion Coefficients in Liquids at Atmospheric and Elevated Pressure by the Chromatographic Broadening Technique," *J. Phys. Chem.*, **88**, 1875 (1984).

Baird, M. J., R. C. Schehl, and W. P. Haynes, "Fischer-Tropsch Processes Investigated at the Pittsburgh Energy Technology Center since 1944," *Ind. Eng. Chem. Prod. Res. Dev.*, **19**, 175 (1980).

Baldauf W., and H. Knapp, "Measurements of Diffusivities in Liquids by the Dispersion Method," *Chem. Eng. Sci.*, **38**, 1031 (1983).

Batchinski, A. J., "Investigations on the Internal Friction of Liquids," *Z. Physik. Chem.*, **68**, 206 (1913).

Bidlack, D. L., and D. K. Anderson, "Mutual Diffusion in Nonideal, Nonassociating Liquid Systems," *J. Phys. Chem.*, **68**, 3790 (1964a).

Bidlack, D. L., and D. K. Anderson, "Mutual Diffusion in the Liquid System Hexane–Hexadecane," *J. Phys. Chem.*, **68**, 206 (1964b).

Bidlack, D.L., T. K. Kett, C. M. Kelly, and D. K. Anderson, "Diffusion in the Solvents Hexane and Carbon Tetrachloride," *J. Chem. Eng. Data*, **14**, 342 (1969).

Bondi, A., "van der Waals Volumes and Radii," *J. Phys. Chem*, **68**, 441 (1964)

Brush, S., *Kinetic Theory*, Pergamon Press, New York, 1972.

Calderbank P. H., and M. B. Moo-Young, "The continuous phase heat and mass-transfer properties of dispersions," *Chem. Eng. Sci.*, **16**, 39 (1961).

Chandler, D., "Rough hard sphere theory of the self–diffusion constant for molecular liquids," *J. Chem. Phys.*, **62**, 1358 (1975).

Chapman, S., and T. G. Cowling, *The Mathematical Theory of Non–Uniform Gases*, Third Edition, Cambridge University Press, London, 1970.

Chen, S.–H., H. T. Davis, and D. F. Evans, "Tracer Diffusion in Polyatomic Liquids. III," *J. Chem. Phys.*, **77**, 2540 (1982).

Cloeta, C. E., T. W. Smuts, and K. deClerk, "The Gas Chromatographic Determination of Binary Diffusion Coefficients I. A Theoretical Design Study," *J. Chromatography*, **120**, 1 (1976).

Davies, G. A., A. B. Ponter, and K. Craine, "The Diffusion of Carbon Dioxide in Organic Liquids," *Can. J. Chem. Eng.*, **45**, 372 (1967).

Doolittle A. K., and R. H. Peterson, "Preparation and Physical Properties of a Series of n-Alkanes," *J. Amer. Chem. Soc.*, **73**, 2145, (1951).

Douglass, D. C. and D. W. McCall, "Diffusion in Paraffin Hydrocarbons," *J. Phys. Chem.*, **62**, 1102 (1958).

Dymond, J. H., "Corrected Enskog theory and the transport coefficients of liquids," *J. Chem. Phys.*, **60**, 969 (1974).

Dymond, J. H., and L. A. Woolf, "Tracer Diffusion of Organic Solutes in n-Hexane at Pressures up to 400 MPa," *J. Chem. Soc. Farad. Trans. I*, **78**, 991 (1982).

Ertl, H., and F. A. Dullien, "Self-Diffusion and Viscosity of Some Liquids as a Function of Temperature," *A. I. Ch. E. J.*, **19**, 1215 (1973).

Esteal, A. J., L. A. Woolf, and D. L. Jolly, "Self-Diffusion in a Dense Hard Sphere Fluid: A Molecular Dynamics Simulation," *Physica*, **121A**, 286 (1983).

Evans, D. F., T. Tominaga, and C. Chan, "Diffusion of Symmetrical and Spherical Solutes in Protic, Aprotic, and Hydrocarbon Solvents," *J. Sol. Chem.*, **8**, 461 (1979).

Evans, E. V., and C. N. Kenney, "Gaseous dispersion in laminar flow through a circular tube," *Proc. Roy. Soc.*, **A284**, 540 (1965).

Fishman, E., "Self-Diffusion in Liquid n-Pentane and n-Heptane," *J. Phys. Chem.*, **59**, 469 (1955).

Gerrard, W., *Gas Solubilities: Widespread Applications*, Pergamon Press Ltd., Oxford (1980).

Giddings, J. C. and S. L. Seager, "Method for Rapid Determination of Diffusion Coefficients," *I. & E. C. Fund.*, 1, 277 (1962).

Glasstone, S., K. Laidler, and H. Eyring, *The Theory of Rate Processes*, McGraw–Hill, New York, 1941.

Golay M. J., "The HETP of an Unretained Component of Fluid Flow in a Coiled Round Pipe," *J. Chromatography*, **186**, 341 (1979).

Grushka, E., and J. Kikta, "Extension of the Chromatographic Broadening Method of Measuring Diffusion Coefficients to Liquid Systems. I. Diffusion Coefficients of Some Alkylbenzenes in Chloroform," *J. Phys. Chem.*, **78**, 2297 (1974).

Hayduk, W., and W. D. Buckley, "Effect of molecular size and shape on diffusivity in dilute liquid solutions," *Chem. Eng. Sci.*, **27**, 1997 (1972).

Hayduk, W., R. Castaneda, H. Bromfield, and R. R. Perras, "Diffusivities of Propane in Normal Paraffin, Chlorobenzene, and Butanol Solvents," *A. I. Ch. E. J.*, **19**, 859 (1973).

Hayduk, W., and S. C. Cheng, "Review of relation between diffusivity and solvent viscosity in dilute liquid solution," *Chem. Eng. Sci*, **26**, 635 (1971).

Hayduk, W., and S. Iokimidis, "Liquid Diffusivities in Normal Paraffin Solutions," *J. Chem. Eng. Data*, **21**, 255 (1976).

Herman, P. T., and B. J. Alder, "Studies in Molecular Dynamics. XI. Correlation Functions of a Hard–Sphere Test Particle," *J. Chem. Phys.*, **56**, 987 (1972).

Hildebrand, J. H., "Motions of Molecules in Liquids: Viscosity and Diffusivity," *Science*, **174**, 490 (1971).

Hildebrand, J. H., *Viscosity and Diffusivity: A Predictive Treatment*, John Wiley & Sons, Inc., New York (1977).

Hirschfelder O., C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids*, John Wiley & Sons, Inc., New York (1954).

Hunt, B, "Diffusion in Laminar Pipe Flow," *Int. J. Heat Mass Trans.*, **20**, 393 (1976).

Kuo J. C. (ed.), *Slurry Fischer-Tropsch/Mobil Two Stage Process for Converting Syngas to High Octane Gasoline* , Final Contract Report, U. S. Department of Energy Contract No. DE-AC22-80PC30022, 1983.

Lebowitz, J. L., "Exact Solution of Generalized Percus–Yevick Equation for a Mixture of Hard Spheres," *Phys. Rev.*, **133**, A895 (1964).

Levenspiel, O., and W.K. Smith, "Notes on the diffusion–type model for the longitudinal mixing and flow," *Chem. Eng. Sci.*, **6**, 227 (1957).

Lo, H. Y., "Diffusion Coefficients in Binary Liquid n–Alkane Systems," *J. Chem. Eng. Data*, **19**, 236 (1974).

Longuet-Higgins, H. C., "Solutions of Chain Molecules - A New Statistical Theory," *Disc. Faraday Soc.*, **15**, 73 (1953).

Malik, V. K. and W. Hayduk, "A Steady-State Capillary Cell Method for Measuring Gas-Liquid Diffusion Coefficients," *Can. J. Chem. Eng.*, **46**, 462 (1968).

Matthews, M. A., *Diffusion Coefficients at Infinite Dilution in n-Alkane Solvents at Temperatures to 573 K and Pressures to 3.5 MPa*, Ph.D. dissertation, Texas A&M University (1986).

Matthews, M. A., and A. Akgerman, "Diffusion Coefficients for Binary Alkane Mixtures to 573 K and 3.5 MPa," *A. I. Ch. E. J.*, **33**, 881 (1987a).

Matthews, M. A., and A. Akgerman, "Hard-sphere theory for correlation of tracer diffusion of gases and liquids in alkanes," *J. Chem. Phys.*, **87**, 2285 (1987b).

Matthews, M. A., and A. Akgerman, "A New Method for Measuring Fluid Densities Using the Taylor Dispersion Experiment," *Int. J. Thermophys.*, **8**, 363 (1987c).

Matthews, M. A., J. B. Rodden, and A. Akgerman, "High- Temperature Diffusion, Viscosity, and Density Measurements in n-Hexadecane," *J. Chem. Eng. Data*, **32**, 317 (1987a).

Matthews, M. A., J. B. Rodden, and A. Akgerman, "High-Temperature Diffusion of Hydrogen, Carbon Monoxide, and Carbon Dioxide in Liquid n-Heptane, n-Dodecane, and n-Hexadecane," *J. Chem. Eng. Data*, **32**, 319 (1987b).

McArdle, J. C., M. J. Humbach, M. W. Schoonover, and F. G. Padrta, *Fischer–Tropsch Wax Characterization and Upgrading*, Department of Energy Contract DE-AC22-85PC80017, Proceedings of Indirect Liquefaction Contractors' Review Meeting, Pittsburgh, December, 1986.

McCall D. W., D. C. Douglass, and E. W. Anderson, "Self-Diffusion in Liquids: Paraffin Hydrocarbons," *Phys. Fluids*, **2**, 87 (1959).

Moore, J. W., and R. M. Wellek, "Diffusion Coefficients of n–Heptane and n–Decane in n–Alkanes and n–Alcohols at Several Temperatures," *J. Chem. Eng. Data*, **19**, 136 (1974).

Nunge, R. J., T. S. Lin, and W. N. Gill, "Laminar dispersion in curved tubes and channels," *J. Fluid Mech.*, **51**, 363 (1972).

Orwoll, R. A., and P. J. Flory, "Equation of State Parameters for Normal Alkanes. Correlation with Chain Length," *J. Am. Chem. Soc.*, **89**, 6814 (1967).

Peter S., and M. Weinert, "Uber die Loslichkeit von H_2, CO, CO_2, und Wasserdampf in flussigen Kohlenwasserstoffen," *Z. Phys. Chem., Neue Folge*, **5**, 114 (1955).

Peter S., and M. Weinert, "Die Diffusiongeschwindigkeit des Wasserstoffs in Kohlenwasserstoffen bei hohen Drucken," *Z. Phys. Chem., Neue Folge*, **9**, 49 (1956).

Prigogine, I., N. Trappeniers, and V. Mathot, "Statistical Thermodynamics of r-mers and r-mer Solutions," *Disc. Faraday Soc.*, **15**, 93 (1953).

Radeke, K. H., "Critical Remarks on Using the Moment Method," *I. & E. C. Fund.*, **20**, 302 (1981).

Riekena, M. L., A. G. Vickers, E. C. Haun, and R. C. Koltz, "A Comparison of Fischer-Tropsch Reactors," *Chem. Eng. Prog.*, 4, 86 (1982).

Rossi, C., and E. Bianchi, "Diffusion of Small Molecules," *Nature*, **189**, 822 (1961).

Satterfield C. H., and G. A. Huff, "Effects of Mass Transfer on Fischer-Tropsch Synthesis in Slurry Reactors," *Chem. Eng. Sci.*, **35**, 195 (1980).

Shieh, J. C., and P. A. Lyons, "Transport Properties of Liquid n–Alkanes," *J. Phys. Chem.*, **73**, 3258 (1969).

Sun, C. K. J., and S.–H. Chen, "Diffusion of Benzene, Toluene, Naphthalene, and Phenanthrene in Supercritical Dense 2,3–Dimethylbutane," *A. I. Ch. E. J.*, **31**, 1904 (1985).

Taylor, G. I., "Dispersion of soluble matter in solvent flowing slowly through a tube," *Proc. Roy. Soc.*, **A219**, 186 (1953).

Taylor, G. I., "Diffusion and Mass Transport in Tubes (38th Guthrie Lecture)," *Proc. Phys. Soc. B*, **67**, 857 (1954a).

Taylor, G. I., "Conditions under which dispersion of a solute in a stream of solvent can be used to measure molecular diffusion," *Proc. Roy. Soc.*, **A225**, 473 (1954b).

TRC Thermodynamic Tables–Hydrocarbons, Thermodynamics Research Center, Texas A&M University, College Station, 1986.

Tyrrell, H. J. V., and K. R. Harris, *Diffusion in Liquids*, Butterworths, London, 1984.

Van Geet, A. L. and A. W. Adamson, "Diffusion in Liquid Hydrocarbon Mixtures," *J. Phys. Chem.*, **68**, 238 (1964).

Wilke, C. R., and P. Chang, "Correlations of Diffusion Coefficients in Dilute Solutions," *A. I. Ch. E. J.*, **1**, 264 (1955).

APPENDIX A

FORTRAN CODE FOR TAYLOR DISPERSION MODEL

```
c-----------------------------------------------------------------------
c--------------TAYMOD (Taylor Dispersion Peak Model)--------------------
c--------------Developed by: J.B. Rodden (Dec. 1987)--------------------
c-----------------------------------------------------------------------
c
c TAYMOD is a interactive FORTRAN program which determines diffusion
c coefficients from raw Taylor dispersion data (voltage vs. time).
c Data is fit to a 5 parameter model based on the analytical solution
c originally given by Taylor.  The code was developed specifically
c for use on an HP9000 computer.
c
c-----------------------------------------------------------------------
      double precision l,eps,b(5),t(999),v(999),mod(999),res(999)
      double precision a,u,root1,root2,rad,pt(999),pv(999),time1
      double precision aberr(999),res2(999),sab,sres2,sres,bfull(5)
      double precision svolt,smod,ares2,ares,av,amod,aaerr,stder
      double precision requ,diff,exvar,totvar,ebig,d12
      double precision tayk,totk,totk4
      dimension pmod(999),pres(999)
      integer ind(5),fo,hr,min,sec,ten,hrc,minc,secc
      character*20 datfile
      character*30 outfile
      character*60 title,solv
      character*80 tx(60)
      character*1 q,prb
      common /mntay/ l,kk,time1
      common /mnpeak/ bistp,bline
c
c Function to convert clock time to seconds:
      time(hr,min,sec)=3600.*hr+60.*min+sec
c
c Radius and length of diffusion tube (meters at 21 C):
      data a/5.23d-04/
      l=4.355d+01
c
      time2=-9999.
      prb='B'
c
c Text variables used for output:
      tx(1)=' TAYMOD (Taylor Dispersion Peak Model) '
      tx(2)=' Developed by: J.B. Rodden (Dec. 1987) '
      tx(3)='HP9000 data filename: '
      tx(4)='Solvent name: '
      tx(5)='Peak description: '
      tx(6)='Temperature :'
      tx(7)='Temperature compensated diffusion tube length: '
      tx(8)='Temperature compensated diffusion tube radius: '
      tx(9)='Injection time: '
      tx(10)='Peak start time: '
      tx(11)='Peak end time: '
      tx(12)='Peak maximum at: '
      tx(13)='Peak start value: '
      tx(14)='Peak end value: '
      tx(15)='Peak max value: '
      tx(16)='Peak width at half height: '
      tx(17)='Preliminary estimate of D12 (see Sun and Chen, 1985): '
      tx(18)='The model is:'
      tx(19)='v(i)=B1/SQRT(t(i))*exp(-(L-B4*t(i))**2/(B2*t(i))+B3+B5*(t(
     *i)-t(1))'
      tx(20)='B1=pre-exp constant (v*s**0.5)'
      tx(22)='B2=4*K (m**2/s)'
      tx(24)='B3=baseline voltage (v)'
      tx(26)='B4=u; avg. fluid velocity (m/s)'
      tx(21)='B5=baseline drift (v/s)'
      tx(23)='K=D12+(a*u)**2/48/D12 (m**2/s)'
      tx(25)='a=diffusion tube radius (m)'
      tx(27)='L=diffusion tube length (m)'
      tx(28)='Drift included in model? '
```

```
      tx(29)='B1             B2             B3             B4             B5'
      tx(30)='Initial values:'
      tx(31)='User override:'
      tx(32)='Final iteration:'
      tx(33)='NOTE: The following parameters were fit by the model: '
      tx(34)='       All other parameters were held constant.'
      tx(35)='Convergence criteria:  (1) epsilon ='
      tx(36)=';  (2) max # of iterations ='
      tx(37)='Model converged following'
      tx(38)='Model did NOT converge.  Maximum number of iterations exce
     *eded.'
      tx(39)='D12 (final model result): '
      tx(40)='Taylor-Hunt criteria: D12/(u*a)='
      tx(41)=' ?>>? a/(4*L)='
      tx(42)='No. of points : '
      tx(43)='Sum of sq res : '
      tx(44)='Avg sq error  : '
      tx(45)='Std err of est: '
      tx(46)='r-squared     : '
      tx(47)='Average error  : '
      tx(48)='Avg abs error  : '
      tx(49)='Max abs error  : '
      tx(50)='Avg observation: '
      tx(51)='Avg prediction : '
      tx(52)='B1                B2                B3                B4
     *     B5'
      tx(53)='COMPUTER GENERATED INITIAL VALUES'
      tx(54)='b(1)              D12               bline             u
     *     bslp'
      tx(55)='ACTUAL PEAK DATA AND MODEL RESULTS'
      tx(56)='PT  ACT TIME  TIME FROM INJECT.  OBSERVATION  PREDICTION
     *RESIDUAL  SQ. RESID.'
      tx(57)='#   Hr Mi Se  Hr Mi Se  (sec)       (volts)      (volts)
     *(volts)   (volts**2)'
      tx(58)='-- -------- ---------------- ----------- -----------
     *-------- ----------'
  900 format(t2,a17,2(i2,1h:),i2,2h (,f6.0,3h s),/)
  901 format(t2,a17,2(i2,1h:),i2,2h (,f6.0,3h s),15h - inj. time = ,
     *2(i2,1h:),i2,2h (,f6.0,3h s))
  902 format(/,t2,a18,i3,t46,a17,e15.9,2h v)
  903 format(t2,a16,e15.9,5h v**2,t46,a17,e15.9,2h v)
  904 format(t2,a16,e15.9,2h v,t46,a17,e15.9,2h v)
  905 format(t2,a16,f11.9,t46,a17,e15.9,2h v)
  906 format(t2,a26,f8.4,12h E-09 m**2/s)
  907 format(/,t2,a32,e8.3,a14,e8.3)
  908 format(t2,'D12 (top',f5.1,'% of peak; ',i3,' pts; ',2(i2,1h:),
     *i2,' thru ',2(i2,1h:),i2,'):',f9.4,' E-09 m**2/s')
  909 format(/,t2,'Retention time, (L/B4): ',2(i2,1h:),i2,2h (,f7.1,
     *' s)')
      write(6,'(79(1h-),/,2(20(1h-),a39,20(1h-),/),79(1h-),/)')
     *tx(1),tx(2)
c
c Data file containing raw time and voltage data is in main directory:
      write(6,*)'Enter name of data file:'
      read(5,'(a20)')datfile
c
c Output is written both to the screen (Unit=6) and to a file in the
c directory 'tayout' (Unit=9):
      outfile='tayout/'//datfile
      open(9,file=outfile)
c
      write(6,*)'Enter solvent name:'
      read(5,'(a60)')solv
      write(6,*)'Enter the temperature of the experiment (Centigrade):'
c
c Corrections for thermal expansion of the diffusion tube:
      read(5,*)temp
      alpha=(16.46+0.00424*(temp-21.))*1.e-06
```

```
      a=a*(1.d0+alpha*(temp-21.))
      l=l*(1.d0+alpha*(temp-21.))
c
    5 continue
      write(9,'(1h1,///,t2,79(1h-),/,2(t2,20(1h-),a39,20(1h-),/),
     *t2,79(1h-))')tx(1),tx(2)
      write(9,'(t2,a22,a20,)')tx(3),datfile
      write(9,'(1h0,t2,a14,a60)')tx(4),solv
      write(6,*)'Enter peak description (50 characters max):'
      read(5,'(a60)')title
      write(9,'(1h0,t2,a18,a60)')tx(5),title
      write(9,'(t2,79(1h-))')
      write(9,'(t2,a13,f7.2,2h C)')tx(6),temp
      write(9,'(t2,a47,f6.2,2h m)')tx(7),l
      write(9,'(t2,a47,e11.5,2h m)')tx(8),a
      write(9,'(t2,79(1h-))')
      write(6,*)'Enter injection time (HrMiSe):      example: 010510'
      read(5,'(3i2)')hr,min,sec
      tinj=time(hr,min,sec)
      write(9,900)tx(9),hr,min,sec,tinj
      write(6,*)'Do you wish to enter peak endpoints using distances'
      write(6,*)'measured directly from the chart? (answer y or n):'
      read(5,'(a1)')q
      if(q.eq.'y')go to 10
      write(6,*)'Enter peak start time (HrMiSe):      example: 010510'
      read(5,'(3i2)')hr,min,sec
      st=time(hr,min,sec)
      write(6,*)'Enter peak end time (HrMiSe):      example: 010510'
      read(5,'(3i2)')hr,min,sec
      et=time(hr,min,sec)
      go to 20
   10 write(6,*)'Enter recorder chart speed (in/hr):'
      read(5,*)cspd
      write(6,*)'Enter chart dist. from inj. time to peak start (cm):'
      read(5,*)st
      st=tinj+1417.323/cspd*st
      write(6,*)'Enter chart dist. from inj. time to peak end (cm):'
      read(5,*)et
      et=tinj+1417.323/cspd*et
   20 continue
      write(6,*)'Do you want voltage drift included in the model? (y/n)'
      read(5,'(a1)')q
c
c Program has the ability to reread data that has already been read:
      if(time2.lt.-9000.)go to 22
      if((st-tinj).gt.time2)go to 23
c
c Unit 8 is the main directory file containing the raw data:
      close(8)
   22 open(8,file=datfile)
c
   23 continue
c
c Call routine to locate and read peak from input data file:
      call peak(st,et,tinj,q, t,v,n,ipmax,ihalf1,ihalf2)
c
      time1=t(1)
      tm=time1
      call clock(tm, hr,min,sec)
      ctime=time1+tinj
      call clock(ctime, hrc,minc,secc)
      write(9,901)tx(10),hrc,minc,secc,ctime,hr,min,sec,time1
      time2=t(n)
      call clock(time2, hr,min,sec)
      ctime=time2+tinj
      call clock(ctime, hrc,minc,secc)
      write(9,901)tx(11),hrc,minc,secc,ctime,hr,min,sec,time2
      tm=t(ipmax)
```

```
      call clock(tm, hr,min,sec)
      ctime=t(ipmax)+tinj
      call clock(ctime, hrc,minc,secc)
      write(9,901)tx(12),hrc,minc,secc,ctime,hr,min,sec,tm
      write(9,'(1h0,t2,a18,f7.5,2h v)')tx(13),v(1)
      write(9,'(t2,a18,f7.5,2h v)')tx(14),v(n)
      write(9,'(t2,a18,f7.5,2h v)')tx(15),v(ipmax)
      write(9,'(t2,79(1h-))')
      write(6,'(t2,a18,f7.5,2h v)')tx(13),v(1)
      write(6,'(t2,a18,f7.5,2h v)')tx(14),v(n)
      write(6,'(t2,a18,f7.5,2h v)')tx(15),v(ipmax)
c
c Compute peak width at half height:
      thalf=t(ihalf2)-t(ihalf1)
c
      write(6,'(/,t2,a27,f6.1,2h s)')tx(16),thalf
      write(9,'(t2,a27,f6.1,2h s)')tx(16),thalf
c
c-----------------------------------------------------------------------
c Preliminary estimates of the 5 model parameters (b(1) thru b(5)):
c
      u=l/t(ipmax)
c
c Half height method of Sun and Chen (1985):
      h=l*thalf**2/(5.54*t(ipmax)**2)
      d12=u/4.*(h-sqrt(h*h-a*a/3))
c
      d12=d12*1.e09
      write(9,'(1h0,t2,a54,f8.4,12h E-09 m**2/s)')tx(17),d12
      write(9,'(t2,79(1h-))')
      d12=d12/1.e09
      write(9,'(t2,a37,/,t2,a67)')tx(18),tx(19)
      write(9,'(1h0,3(t2,a36,t43,a35,/),t2,a36,t43,a35)')(tx(i),i=20,27)
      b(1)=(v(ipmax)-bislp*(t(ipmax)-time1)-bline)*dsqrt(t(ipmax))
      b(3)=bline
      b(4)=u
      tayk=(a*b(4))**2/48.d0/d12
      b(2)=4.d0*(tayk+d12)
      b(5)=bislp
c-----------------------------------------------------------------------
c
      npar=5
      do 25 i=1,5
   25 ind(i)=i
      if(q.ne.'y')npar=4
      if(q.ne.'y')q='n'
      write(9,'(1h0,t2,a25,1x,a1)')tx(28),q
      write(9,'(1h0,t25,a51)')tx(29)
      write(9,'(t2,a16,t20,5(e11.5,1x))')tx(30),(b(i),i=1,5)
      write(6,'(/,23(1h-),a33,23(1h-))')tx(53)
      write(6,'(t7,a71)')tx(54)
      d12=d12*1e09
      write(6,'(e15.9,1x,f11.7,4hE-09,1x,2(e15.9,1x),e15.9)')
     *b(1),d12,b(3),b(4),b(5)
      d12=d12/1e09
c
c Program provides option of user entered initial parameter estimates:
      write(6,*)'Do you want to enter your own initial guesses?'
      write(6,*)'(enter y or n)'
      read(5,'(a1)')q
      if(q.eq.'y')go to 27
c
c Any number of parameters may be fixed at their initial values, thus
c reducing the order of the model (default is full 5 parm. model):
      write(6,*)'Do you want the program to fit all of the parameters?'
      write(6,*)' NOTE: By answering no, you can choose to fit only'
      write(6,*)'       certain parameters, while holding the others'
      write(6,*)'       fixed at their initial guesses.'
```

```
      read(5,'(a1)')q
      if(q.ne.'n')go to 30
      go to 28
c
   27 write(6,*)'Enter guesses for the following parameters:'
      write(6,*)'  b(1)  = pre-exponential constant'
      write(6,*)'  D12   = diffusion coef. (m**2/sec)'
      write(6,*)'  bline = baseline value (volts). (Baseline value at'
      write(6,*)'          start of peak when drift is included.)'
      write(6,*)'  u     = average velocity in tube (m/sec)'
      write(6,*)'  blslp = baseline slope or driftrate (volts/sec)'
      write(6,*)
      write(6,*)'NOTE: Enter as follows: b(1) , D12, bline, u, blslp'
      read(5,*)b(1),d12,b(3),b(4),b(5)
      tayk=(a*b(4))**2/48.d0/d12
      b(2)=4.d0*(tayk+d12)
      write(9,'(t2,a16,t20,5(e11.5,1x))')tx(31),(b(i),i=1,5)
   28 continue
      write(6,*)'Enter the total no. of parameters to be fit (max=5):'
      write(6,*)
      write(6,*)'NOTE: The remainder of the parameters will be'
      write(6,*)'      fixed at their initial guesses.'
      read(5,*)npar
      write(6,*)'Enter indices of the ',npar,' parameters to be fit:'
      write(6,*)' 1 = b(1), 2 = D12, 3 = blint, 4 = u, 5 = blslp'
      write(6,*)' eg. type: 1 2 4  (to fit b(1), D12, and u)'
      read(5,*)(ind(i),i=1,npar)
   30 continue
c
c Convergence criteria:
      eps=1.d-09
      imax=20
      write(6,*)'Do you want to enter your own convergence criteria?'
      write(6,*)' DEFAULT: epsilon = 1.e-09, max iterations = 20'
      read(5,'(a1)')q
      if(q.ne.'y')go to 31
      write(6,*)'Enter epsilon:'
      read(5,*)eps
      write(6,*)'Enter the maximum number of iterations:'
      read(5,*)imax
   31 continue
c
      write(6,'(t8,a70)')tx(52)
c
c Call Newton-Raphson routine to determine best fit set of b's:
      call tayfit(n,t,v,b,npar,ind,eps,imax, mod,res)
c
      write(9,'(t2,a16,t20,5(e11.5,1x))')tx(32),(b(i),i=1,5)
      do 32 i=1,5
      bfull(i)=b(i)
   32 continue
      if(npar.gt.4)go to 33
      write(9,'(1h0,t2,a54,5(a1,i1,1x))')tx(33),(prb,ind(i),i=1,npar)
      write(9,'(t2,a65)')tx(34)
   33 write(9,'(1h0,t2,a36,e8.2,a28,i3)')tx(35),eps,tx(36),imax
      if(kk.le.imax)go to 34
      write(9,'(1h0,t2,a76)')tx(38)
      write(6,*)tx(38)
      write(6,*)'Do you want to enter new initial values? (y/n)'
      read(5,'(a1)')q
      if(q.eq.'n')go to 75
      write(9,'(1h0,t25,a51)')tx(29)
      go to 27
   34 write(9,'(1h0,t2,a25,i3,12h iterations.)')tx(37),kk
   35 continue
c
c Statistical section:
      sres2=0.
```

```
      sab=0.
      sres=0.
      svolt=0.
      smod=0.
      exvar=0.
      totvar=0.
      do 40 i=1,n
      aberr(i)=dabs(res(i))
      res2(i)=res(i)*res(i)
      pmod(i)=mod(i)
      pres(i)=res(i)
   39 sab=sab+aberr(i)
      sres2=sres2+res2(i)
      sres=sres+res(i)
      svolt=svolt+v(i)
      smod=smod+mod(i)
   40 continue
      aaerr=sab/float(n)
      ares2=sres2/float(n)
      ares=sres/float(n)
      av=svolt/float(n)
      amod=smod/float(n)
      stder=dsqrt(sres2/dfloat(n-2))
      ebig=0.d0
      do 41 l=1,n
      diff=mod(i)-av
      exvar=exvar+diff*diff
      diff=v(i)-av
      totvar=totvar+diff*diff
      if(aberr(i).lt.ebig)go to 41
      iebig=i
      ebig=aberr(i)
   41 continue
      rsqu=exvar/totvar
c
c Compute D12 using quadratic formula:
      rad=dsqrt(b(2)**2/16.d0-(a*b(4))**2/12.d0)
      d12=b(2)/8.d0-rad/2.d0
c
c Hunt(1976) criteria:
      hunt1=d12/b(4)/a
      hunt2=a/4./l
c
      d12=d12*1.e09
      rtime=l/b(4)
      call clock(rtime, hr,min,sec)
      do 44 fo=6,9,3
      write(fo,902)tx(42),n,tx(47),ares
      write(fo,903)tx(43),sres2,tx(48),aaerr
      write(fo,903)tx(44),ares2,tx(49),aberr(iebig)
      write(fo,904)tx(45),stder,tx(50),av
      write(fo,905)tx(46),rsqu,tx(51),amod
      write(fo,'(t2,79(1h-))')
      write(fo,906)tx(39),d12
      write(fo,907)tx(40),hunt1,tx(41),hunt2
      write(fo,909)hr,min,sec,rtime
      write(fo,'(t2,79(1h-))')
   44 continue
      d12=d12/1.e09
   45 continue
c
c This section allows user the option of using only a percentage of the
c peak to determine the diffusion coefficient.  Baseline and drift
c terms are fixed at their initial values.
      write(6,*)'Do you want to analyze the peak using only the points'
      write(6,*)'which are greater than a certain percentage of the'
      write(6,*)'difference between the peak maximum and the baseline?'
      write(6,*)'(Enter y or n)'
```

```
      read(5,'(a1)')q
      if(q.ne.'y')go to 70
      write(6,*)'Enter percentage:'
      read(5,*)per
      call perc(per,n,ipmax, iper1,iper2)
      j=0
      do 50 i=iper1,iper2
      pt(j+1)=t(i)
      pv(j+1)=v(i)
      j=j+1
   50 continue
      ind(1)=1
      ind(2)=2
      ind(3)=4
      write(6,'(t8,a70)')tx(52)
      call tayfit(j,pt,pv,b,3,ind,eps,imax, mod,res)
      if(kk.gt.imax)go to 68
   60 rad=dsqrt(b(2)**2/16.d0-(a*b(4))**2/12.d0)
      d12=b(2)/8.d0-rad/2.d0
      ctime=pt(1)+tinj
      call clock(ctime, hr,min,sec)
      ctime=pt(j)+tinj
      call clock(ctime, hrc,minc,secc)
      d12=d12*1.e09
      write(9,908)per,j,hr,min,sec,hrc,minc,secc,d12
      write(6,*)
      write(6,908)per,j,hr,min,sec,hrc,minc,secc,d12
      write(6,*)
      d12=d12/1.e09
      go to 45
   68 write(9,'(t2,12hPERCENTAGE= ,f5.0)')per
      write(9,'(t2,a76)')tx(38)
      write(6,'(t2,a76,/)')tx(38)
   70 continue
c
c All peak data and residuals may be printed:
      write(6,*)'Do you want to print the list of observations,'
      write(6,*)'model predictions, and residuals for the full peak '
      write(6,*)'analysis to the output file? (y/n)'
      read(5,'(a1)')q
      if(q.ne.'y')go to 75
      write(9,'(1h1,t2,21(1h-),a34,24(1h-))')tx(55)
      write(9,'(1h0,t2,a22,a20)')tx(3),datfile
      write(9,'(t2,a14,a60)')tx(4),solv
      write(9,'(t2,a18,a60)')tx(5),title
      write(9,'(1h0,t25,a51)')tx(29)
      write(9,'(t2,a16,t20,5(e11.5,1x))')tx(32),(bfull(i),i=1,5)
      write(9,'(1h0,t2,a78)')tx(56)
      write(9,'(t2,a78)')tx(56)
      write(9,'(t2,a78,/,t2,a78)')tx(57),tx(58)
      do 73 i=1,n
      ctime=t(i)+tinj
      call clock(ctime, hr,min,sec)
      tm=t(i)
      call clock(tm, hrc,minc,secc)
      write(9,'(t2,i3,1x,2(i2,1h:),i2,2x,2(i2,1h:),i2,2h (,f6.0,1h),
     *t36,f8.5,t49,f8.5,t60,f8.5,t69,e11.5)')i,hr,min,sec,hrc,minc,
     *secc,tm,v(i),pmod(i),pres(i),res2(i)
   73 continue
      write(9,'(1h0,t2,11hEND OF DATA)')
   75 continue
c
      write(6,*)'Do you want to analyze any more peaks? (y or n)'
      read(5,'(a1)')q
      if(q.ne.'n')go to 5
c
      close(8)
      write(9,'(1h1)')
```

```
      close(9)
      stop
      end
c
c*********************************************************************
c
c Subroutine PEAK reads in voltage and time data from the input file.
c All data including the total no. of points in the peak, n, is returned
c to MAIN. This subroutine also uses a search technique to determine
c the two voltage values at the peak half height.  The indices of
c these two points are returned to MAIN to be used in the calculation
c of the initial guess for D12.
c
      subroutine peak(st,et,tinj,q, t,v,n,ipmax,ihalf1,ihalf2)
      double precision t(999),v(999)
      dimension abv(999)
      character*1 q
      integer hr,min,sec,ten
      common /peper/ abv
      common /mnpeak/ bslp,bline
      time(hr,min,sec,ten)=3600.*hr+60*min+sec+float(ten)/10.
  100 format(d8.5,t10,3i2,i1)
    5 read(8,100)v(1),hr,min,sec,ten
      t(1)=time(hr,min,sec,ten)
      if(t(1).lt.st)go to 5
      n=2
   10 read(8,100)v(n),hr,min,sec,ten
      t(n)=time(hr,min,sec,ten)
      if(t(n).ge.et)go to 20
      n=n+1
      go to 10
   20 continue
      if(q.ne.'y')go to 22
      bslp=(v(n)-v(1))/(t(n)-t(1))
      bline=v(1)
      go to 25
   22 bslp=0.
      bline=(v(1)+v(n))/2.
   25 continue
      vbig=0.0
      do 30 i=1,n
      abv(i)=dabs(v(i)-bslp*(t(i)-t(1))-bline)
      if(abv(i).lt.vbig)go to 30
      ipmax=i
      vbig=abv(i)
   30 continue
      vhalf=abv(ipmax)/2.d0
      do 40 i=ipmax,1,-1
      ihalf1=i
      if(abv(i).le.vhalf)go to 45
   40 continue
   45 continue
      do 60 i=ipmax,n
      ihalf2=i
      if(abv(i).le.vhalf)go to 65
   60 continue
   65 continue
      do 80 i=1,n
      t(i)=t(i)-tinj
   80 continue
      return
      end
c
c*********************************************************************
c
c Subroutine PERC searches the peak to determine the voltage values at
c a given percentage (per) of the peak height.  The indices of these
c two values (one on each side of the peak) are returned to MAIN.
```

```
c
      subroutine perc(per,n,ipmax, iper1,iper2)
      dimension abv(999)
      common /peper/abv
      vper=abv(ipmax)*(1.-per/100.)
      do 10 i=ipmax,1,-1
      iper1=i
      if(abv(i).le.vper)go to 15
   10 continue
   15 continue
      do 20 i=ipmax,n
      iper2=i
      if(abv(i).le.vper)go to 25
   20 continue
   25 continue
      return
      end
c
c***********************************************************************
c
c Subroutine TAYFIT uses the Newton-Raphson method to determine the
c best fit (least squares) parameters for the model.  All derivatives
c are calculated from analytical expressions.  The routine has
c the ability to be used as a 5, 4, 3, 2, or 1 parameter fit,
c with any of the model parameters fixed at their initial value(s).
c
      subroutine tayfit(n,t,v,b,npar,ind,eps,imax, mod,res)
      double precision arg1,arg2,arg3,arg4,c1,c2,c3,ex,l,lut,term,eps,
     * pf(5,5),f(5),b(5),dm(5),ddm(5,5),pfdum(10,10),fdum(10),del(10),
     * bold(5),t(999),v(999),mod(999),res(999),time1
      dimension ind(5)
      common /mntay/ l,kk,time1
      kk=0
c
c Increment number of iterations and check if imax is exceeded:
    5 kk=kk+1
      if(kk.gt.imax)go to 90
c
      do 8 i=1,5
      f(i)=0.d0
      do 7 j=1,5
      pf(i,j)=0.d0
    7 continue
    8 continue
      do 20 i=1,n
      lut=l-b(4)*t(i)
      term=lut**2/t(i)
      ex=dexp(-term/b(2))
      arg1=1.d0/t(i)**0.5d0*ex
      arg2=arg1*term
      arg3=arg2*term
      arg4=arg1*lut
      c1=b(1)/b(2)**2
      c2=b(2)*c1
      c3=c1/b(1)
c
c The Taylor dispersion model and residuals:
      mod(i)=b(1)*arg1+b(3)+b(5)*(t(i)-time1)
      res(i)=v(i)-mod(i)
c
c Partial derivatives of model with respect to each parameter:
      dm(1)=arg1
      dm(2)=c1*arg2
      dm(3)=1.d0
      dm(4)=2.d0*c2*arg4
      dm(5)=t(i)-time1
c
c Partial derivatives of least sq. function with respect to each parameter:
```

```
      f(1)=f(1)+res(i)*dm(1)
      f(2)=f(2)+res(i)*dm(2)
      f(3)=f(3)+res(i)
      f(4)=f(4)+res(i)*dm(4)
      f(5)=f(5)+res(i)*dm(5)
c
c Second partial derivatives of model with respect to each parameter:
      ddm(1,2)=c3*arg2
      ddm(1,4)=2.d0/b(2)*arg4
      ddm(2,2)=c1*c3*arg3-2.d0*c2*c3*arg2
      ddm(2,4)=2.d0*(c2*c3*arg2*lut-c1*arg4)
      ddm(4,4)=4.d0*c1*arg4*lut-2.d0*c2*arg1*t(i)
c
c Second part. derivatives of least sq. func. with respect to each parameter:
      pf(1,1)=pf(1,1)-dm(1)*dm(1)
      pf(1,2)=pf(1,2)+res(i)*ddm(1,2)-dm(1)*dm(2)
      pf(1,3)=pf(1,3)-dm(1)
      pf(1,4)=pf(1,4)+res(i)*ddm(1,4)-dm(1)*dm(4)
      pf(1,5)=pf(1,5)-dm(1)*dm(5)
      pf(2,2)=pf(2,2)+res(i)*ddm(2,2)-dm(2)*dm(2)
      pf(2,3)=pf(2,3)-dm(2)
      pf(2,4)=pf(2,4)+res(i)*ddm(2,4)-dm(2)*dm(4)
      pf(2,5)=pf(2,5)-dm(2)*dm(5)
      pf(3,4)=pf(3,4)-dm(4)
      pf(3,5)=pf(3,5)-dm(5)
      pf(4,4)=pf(4,4)+res(i)*ddm(4,4)-dm(4)*dm(4)
      pf(4,5)=pf(4,5)-dm(4)*dm(5)
      pf(5,5)=pf(5,5)-dm(5)*dm(5)
   20 continue
      pf(3,3)=-n
      pf(2,1)=pf(1,2)
      pf(3,1)=pf(1,3)
      pf(3,2)=pf(2,3)
      pf(4,1)=pf(1,4)
      pf(4,2)=pf(2,4)
      pf(4,3)=pf(3,4)
      pf(5,1)=pf(1,5)
      pf(5,2)=pf(2,5)
      pf(5,3)=pf(3,5)
      pf(5,4)=pf(4,5)
c
      do 30 i=1,5
      f(i)=-f(i)
   30 continue
c
c These loops allow model to be fit using less than 5 free parameters
c (npar parameters).  The 'ind' array stores the Index of each parameter
c to be fit.  Remaining parameters are fixed at their initial value(s).
      do 40 i=1,npar
      fdum(i)=f(ind(i))
      do 35 j=1,npar
      pfdum(i,j)=pf(ind(i),ind(j))
   35 continue
   40 continue
c
c Call matrix solver for Newton-Raphson iteration:
      call doolu(npar,pfdum,fdum, del)
c
c Increment parameters:
      do 50 i=1,npar
      bold(i)=b(ind(i))
      b(ind(i))=b(ind(i))+del(i)
   50 continue
c
      write(6,'(4(e15.9,1x),e15.9)')(b(i),i=1,5)
c
c Check for convergence:
      do 55 i=1,npar
```

```
      if(dabs(del(i)/bold(i)).gt.eps)go to 5
   55 continue
c
   90 return
      end
c
c************************************************************************
c
c Subroutine CLOCK converts clock time in seconds to clock time in
c hours, minutes, and seconds.
c
      subroutine clock(tm,hr,min,sec)
      integer hr,min,sec
      hr=tm/3600.
      min=(tm-float(hr)*3600.)/60.
      sec=tm-float(hr)*3600.-float(min)*60.
      return
      end
c************************************************************************
c************************************************************************
c
c DOOLU solves the nxn system of equations: cx=b, using the Doolittle
c LU decomposition method (see Ralston and Rabinowitz).
c The routine uses implicit equilibration and partial (row)
c pivoting.  The original version of DOOLU was developed as
c part of an assignment for MATH 609 (Prof.: Dr. Allen) at TAMU.
c Developer: J.B. Rodden
c
c DOOLU consists of the following subroutines:
c DOOLU (main), SCFAC, PVCRIT, PIVOT, and SOLVE.
c
      subroutine doolu(n,c,b,x)
      double precision pin,c(10,10)
      double precision b(10),s(10),d(10),x(10),a
      integer v(10)
      common /lucom/ a(10,10)
      do 5 i=1,n
      do 5 j=1,n
    5 a(i,j)=c(i,j)
      do 10 i=1,n
      v(i)=i
   10 continue
c
c Find scale factors (elements of max magnitude in each row).
      call scfac(n,d)
c
c 'ir' is the step of the Doolittle decomposition.
      do 60 ir=1,n
c
c Calculate s, which is used together with d, to formulate the pivot
c criteria:
      call pvcrit(ir,n,v, s)
c
      if(ir.eq.n)go to 15
c
c Call pivot to determine whether the pivot vector needs to be rearranged.
c This implicitly equilibrates the matrix:
      call pivot(ir,n,s,d, v)
c
c Write diagonal term of U, the upper triangular matrix, over a:
   15 a(v(ir),ir)=s(v(ir))
c
      if(ir.eq.1)go to 45
      if(ir.eq.n)go to 60
      irp1=ir+1
      do 40 j=irp1,n
      pin=0.d0
      irm1=ir-1
```

```
c
c Calculate inner product:
      do 30 k=1,irm1
      pin=pin+a(v(ir),k)*a(v(k),j)
   30 continue
c
c Calc. row ir of U, the upper triangular matrix, and write over a:
      a(v(ir),j)=a(v(ir),j)-pin
   40 continue
c
   45 irp1=ir+1
c
c Calc. column ir of L, the lower triangular matrix, and write over a:
      do 50 i=irp1,n
      a(v(i),ir)=s(v(i))/a(v(ir),ir)
   50 continue
   60 continue
c
c Determine solution vector, x:
      call solve(n,b,v, x)
      return
      end
c***********************************************************************
c
c Subroutine SCFAC locates the element of largest magnitude in
c each row and stores it in the vector d.
c
      subroutine scfac(n, d)
      double precision d(10),a,big,anext
      common /lucom/ a(10,10)
      do 20 i=1,n
      big=dabs(a(i,1))
      do 10 j=2,n
      anext=dabs(a(i,j))
      if(anext.gt.big)big=anext
   10 continue
      d(i)=big
   20 continue
      return
      end
c***********************************************************************
c
c Subroutine PVCRIT calculates the values s(i) (see Ralston and
c Rabinowitz).  Both s and d are used to determine whether or not
c to pivot.
c
      subroutine pvcrit(ir,n,v, s)
      double precision pin,s(10),a
      integer v(10)
      common /lucom/ a(10,10)
      if(ir.gt.1)go to 15
      do 10 i=1,n
      s(v(i))=a(v(i),1)
   10 continue
      go to 50
   15 do 40 i=ir,n
      pin=0.d0
      irm1=ir-1
      do 30 k=1,irm1
      pin=pin+a(v(i),k)*a(v(k),ir)
   30 continue
      s(v(i))=a(v(i),ir)-pin
   40 continue
   50 continue
      return
      end
c***********************************************************************
c
```

```
c Subroutine PIVOT determines whether or not to switch elements of the
c pivot vector, v, which implicitly equilibrates the matrix.
c (See pages 428-429 of Ralston and Rabinowitz for clarification.)
c
      subroutine pivot(ir,n,s,d, v)
      double precision s(10),d(10),a,big,sbyd
      integer v(10)
      common /lucom/ a(10,10)
      ibig=ir
      big=dabs(s(v(ir))/d(v(ir)))
      irp1=ir+1
      do 20 i=irp1,n
c
c The pivot criteria is to pivot on the max abs(s(v(i))/d(v(i))):
      sbyd=dabs(s(v(i))/d(v(i)))
c
      if(sbyd.le.big)go to 20
      big=sbyd
c
c Save the index of the largest sbyd:
      ibig=i
c
   20 continue
c
c Switch elements of the v array. If ibig=ir, no effective switch
c is made.
      i=v(ibig)
      v(ibig)=v(ir)
      v(ir)=i
c
      return
      end
c***********************************************************************
c
c Subroutine SOLVE determines the solution vector x, following the
c completion of the Doolittle LU decomposition.  Forward decomposition
c is used to solve Ly=b for Y.  Backward substitution is then used
c to solve Ux=y for the solution vector, x.
c
      subroutine solve(n,b,v, x)
      double precision pin
      double precision y(10),b(10),x(10),a
      integer v(10)
      common /lucom/ a(10,10)
c
c Forward substitution process:
      y(1)=b(v(1))
      do 30 i=2,n
      pin=0.d0
      im1=i-1
      do 20 j=1,im1
      pin=pin+a(v(i),j)*y(j)
   20 continue
      y(i)=b(v(i))-pin
   30 continue
c
c Backward substitution process:
      x(n)=y(n)/a(v(n),n)
      nm1=n-1
      do 50 l=1,nm1
      j=n-l
      pin=0.d0
      jp1=j+1
      do 40 i=jp1,n
      k=n+jp1-i
      pin=pin+a(v(j),k)*x(k)
   40 continue
      x(j)=(y(j)-pin)/a(v(j),j)
```

```
   50 continue
      return
      end
c*****************************************************************
c*****************************************************************
```

APPENDIX B

EXAMPLE OUTPUT FROM TAYLOR DISPERSION MODEL

B.1 CARBON DIOXIDE IN N-EICOSANE AT 222°C

B.2 N-DODECANE IN N-EICOSANE AT 222°C

B.3 N-OCTANE IN N-OCTACOSANE AT 100°C

APPENDIX B.1

CARBON DIOXIDE IN N-EICOSANE AT 222°C

```
------------------- TAYMOD (Taylor Dispersion Peak Model) -------------------
------------------- Developed by: J.B. Rodden (Dec. 1987) -------------------

HP9000 data filename: 031087c

Solvent name: n-eicosane

Peak description: #2 CO2, sat. liquid, 20 sec. inj.
-----------------------------------------------------------------------------
Temperature : 222.00 C
Temperature compensated diffusion tube length:  43.70 m
Temperature compensated diffusion tube radius:  .52482E-03 m
-----------------------------------------------------------------------------
Injection time:   0:23:10 ( 1390. s)

Peak start time:  3:15: 0 (11700. s) - inj. time =  2:51:50 (10310. s)
Peak end time:    3:31: 0 (12660. s) - inj. time =  3: 7:50 (11270. s)
Peak maximum at:  3:22:40 (12160. s) - inj. time =  2:59:30 (10770. s)

Peak start value: -.00141 v
Peak end value:   -.00154 v
Peak max value:   -.09453 v
-----------------------------------------------------------------------------
Peak width at half height:  220.0 s

Preliminary estimate of D12 (see Sun and Chen, 1985):  14.1781 E-09 m**2/s
-----------------------------------------------------------------------------
The model is:
v(i)=B1/SQRT(t(i))*exp(-(L-B4*t(i))**2/(B2*t(i))+B3+B5*(t(i)-t(1))

B1=pre-exp constant (v*s**0.5)          B5=baseline drift (v/s)
B2=4*K (m**2/s)                         K=D12+(a*u)**2/48/D12 (m**2/s)
B3=baseline voltage (v)                 a=diffusion tube radius (m)
B4=u; avg. fluid velocity (m/s)         L=diffusion tube length (m)

Drift included in model?  y

                        B1          B2          B3          B4          B5
Initial values:    -.96574E+01  .26712E-04 -.14100E-02  .40577E-02 -.13537E-06
Final iteration:   -.96839E+01  .25200E-04 -.13636E-02  .40583E-02 -.17073E-06

Convergence criteria:  (1) epsilon = .10E-06;  (2) max # of iterations = 20

Model converged following  5 Iterations.

No. of points :   192                   Average error   :  .146254356E-16 v
Sum of sq res :  .202709765E-05 v**2    Avg abs error   :  .765973148E-04 v
Avg sq error  :  .105578003E-07 v**2    Max abs error   :  .316759227E-03 v
Std err of est:  .103290537E-03 v       Avg observation: -.231360417E-01 v
r-squared     :  .999988933             Avg prediction : -.231360417E-01 v
-----------------------------------------------------------------------------
D12 (final model result):  15.0372 E-09 m**2/s

Taylor-Hunt criteria: D12/(u*a)=.706E-02 ?>>? a/(4*L)=.300E-05

Retention time, (L/B4):  2:59:28 (10768.5 s)
-----------------------------------------------------------------------------
D12 (top 95.0% of peak;  90 pts;  3:18:55 thru  3:26:25):  15.0361 E-09 m**2/s
D12 (top 90.0% of peak;  78 pts;  3:19:25 thru  3:25:55):  15.0251 E-09 m**2/s
D12 (top 85.0% of peak;  72 pts;  3:19:40 thru  3:25:40):  15.0137 E-09 m**2/s
D12 (top 80.0% of peak;  66 pts;  3:19:55 thru  3:25:25):  14.9957 E-09 m**2/s
D12 (top 60.0% of peak;  50 pts;  3:20:35 thru  3:24:45):  14.9248 E-09 m**2/s
D12 (top 40.0% of peak;  38 pts;  3:21: 5 thru  3:24:15):  14.8694 E-09 m**2/s
D12 (top 20.0% of peak;  25 pts;  3:21:35 thru  3:23:40):  14.8019 E-09 m**2/s
D12 (top 10.0% of peak;  19 pts;  3:21:55 thru  3:23:30):  14.6987 E-09 m**2/s
D12 (top  5.0% of peak;  14 pts;  3:22: 5 thru  3:23:10):  14.4873 E-09 m**2/s
D12 (top  2.0% of peak;  10 pts;  3:22:15 thru  3:23: 0):  14.3689 E-09 m**2/s
```

ACTUAL PEAK DATA AND MODEL RESULTS

HP9000 data filename: 031087c
Solvent name: n-eicosane
Peak description: #2 CO2, sat. liquid, 20 sec. inj.

	B1	B2	B3	B4	B5
Final iteration:	-.96839E+01	.25200E-04	-.13636E-02	.40583E-02	-.17073E-06

PT #	ACT TIME Hr Mi Se	TIME FROM INJECT. Hr Mi Se	(sec)	OBSERVATION (volts)	PREDICTION (volts)	RESIDUAL (volts)	SQ. RESID. (volts**2)
1	3:15: 0	2:51:50	(10310.)	-.00141	-.00136	-.00005	.21396E-08
2	3:15: 5	2:51:55	(10315.)	-.00141	-.00136	-.00005	.20549E-08
3	3:15:10	2:52: 0	(10320.)	-.00140	-.00137	-.00003	.11838E-08
4	3:15:15	2:52: 5	(10325.)	-.00139	-.00137	-.00002	.55117E-09
5	3:15:20	2:52:10	(10330.)	-.00141	-.00137	-.00004	.18863E-08
6	3:15:25	2:52:15	(10335.)	-.00142	-.00137	-.00005	.26507E-08
7	3:15:30	2:52:20	(10340.)	-.00143	-.00137	-.00006	.36479E-08
8	3:15:35	2:52:25	(10345.)	-.00142	-.00137	-.00005	.24228E-08
9	3:15:40	2:52:30	(10350.)	-.00142	-.00137	-.00005	.23118E-08
10	3:15:45	2:52:35	(10355.)	-.00140	-.00137	-.00003	.71647E-09
11	3:15:50	2:52:40	(10360.)	-.00140	-.00137	-.00003	.64110E-09
12	3:15:55	2:52:45	(10365.)	-.00140	-.00138	-.00002	.56029E-09
13	3:16: 0	2:52:50	(10370.)	-.00140	-.00138	-.00002	.47861E-09
14	3:16: 5	2:52:55	(10375.)	-.00141	-.00138	-.00003	.88700E-09
15	3:16:10	2:53: 0	(10380.)	-.00140	-.00138	-.00002	.29932E-09
16	3:16:15	2:53: 5	(10385.)	-.00141	-.00139	-.00002	.60055E-09
17	3:16:20	2:53:10	(10390.)	-.00141	-.00139	-.00002	.44377E-09
18	3:16:25	2:53:15	(10395.)	-.00141	-.00139	-.00002	.29337E-09
19	3:16:30	2:53:20	(10400.)	-.00143	-.00140	-.00003	.10379E-08
20	3:16:35	2:53:25	(10405.)	-.00144	-.00140	-.00004	.13350E-08
21	3:16:40	2:53:30	(10410.)	-.00147	-.00141	-.00006	.35288E-08
22	3:16:45	2:53:35	(10415.)	-.00148	-.00142	-.00006	.37349E-08
23	3:16:50	2:53:40	(10420.)	-.00148	-.00143	-.00005	.25901E-08
24	3:16:55	2:53:45	(10425.)	-.00149	-.00144	-.00005	.23543E-08
25	3:17: 0	2:53:50	(10430.)	-.00150	-.00146	-.00004	.18684E-08
26	3:17: 5	2:53:55	(10435.)	-.00151	-.00148	-.00003	.11742E-08
27	3:17:10	2:54: 0	(10440.)	-.00154	-.00150	-.00004	.19045E-08
28	3:17:15	2:54: 5	(10445.)	-.00156	-.00152	-.00004	.13534E-08
29	3:17:20	2:54:10	(10450.)	-.00157	-.00155	-.00002	.24948E-09
30	3:17:25	2:54:15	(10455.)	-.00160	-.00159	-.00001	.51035E-10
31	3:17:30	2:54:20	(10460.)	-.00164	-.00164	.00000	.76309E-11
32	3:17:35	2:54:25	(10465.)	-.00169	-.00169	.00000	.51281E-11
33	3:17:40	2:54:30	(10470.)	-.00175	-.00176	.00001	.25760E-10
34	3:17:45	2:54:35	(10475.)	-.00183	-.00183	.00000	.71003E-12
35	3:17:50	2:54:40	(10480.)	-.00192	-.00192	.00000	.77192E-13
36	3:17:55	2:54:45	(10485.)	-.00202	-.00203	.00001	.30244E-10
37	3:18: 0	2:54:50	(10490.)	-.00213	-.00215	.00002	.35644E-09
38	3:18: 5	2:54:55	(10495.)	-.00227	-.00229	.00002	.53179E-09
39	3:18:10	2:55: 0	(10500.)	-.00244	-.00246	.00002	.43973E-09
40	3:18:15	2:55: 5	(10505.)	-.00265	-.00267	.00002	.34035E-09
41	3:18:20	2:55:10	(10510.)	-.00285	-.00289	.00003	.97236E-09
42	3:18:25	2:55:15	(10515.)	-.00311	-.00314	.00003	.95290E-09
43	3:18:30	2:55:20	(10520.)	-.00344	-.00345	.00001	.29376E-10
44	3:18:35	2:55:25	(10525.)	-.00375	-.00378	.00003	.91395E-09
45	3:18:40	2:55:30	(10530.)	-.00413	-.00417	.00004	.15349E-08
46	3:18:45	2:55:35	(10535.)	-.00457	-.00461	.00004	.16793E-08
47	3:18:50	2:55:40	(10540.)	-.00504	-.00511	.00007	.50391E-08
48	3:18:55	2:55:45	(10545.)	-.00559	-.00567	.00008	.71899E-08
49	3:19: 0	2:55:50	(10550.)	-.00622	-.00631	.00009	.77779E-08
50	3:19: 5	2:55:55	(10555.)	-.00692	-.00702	.00010	.94349E-08
51	3:19:10	2:56: 0	(10560.)	-.00771	-.00781	.00010	.95377E-08
52	3:19:15	2:56: 5	(10565.)	-.00865	-.00869	.00004	.12854E-08
53	3:19:20	2:56:10	(10570.)	-.00955	-.00966	.00011	.11607E-07
54	3:19:25	2:56:15	(10575.)	-.01069	-.01073	.00004	.15371E-08
55	3:19:30	2:56:20	(10580.)	-.01179	-.01191	.00012	.13440E-07

56	3:19:35	2:56:25	(10585.)	-.01307	-.01319	.00012	.15189E-07
57	3:19:40	2:56:30	(10590.)	-.01448	-.01460	.00012	.13465E-07
58	3:19:45	2:56:35	(10595.)	-.01600	-.01615	.00015	.22566E-07
59	3:19:50	2:56:40	(10600.)	-.01765	-.01780	.00015	.22134E-07
60	3:19:55	2:56:45	(10605.)	-.01945	-.01957	.00012	.15296E-07
61	3:20: 0	2:56:50	(10610.)	-.02136	-.02148	.00012	.13646E-07
62	3:20: 5	2:56:55	(10615.)	-.02340	-.02347	.00007	.45266E-08
63	3:20:10	2:57: 0	(10620.)	-.02558	-.02563	.00005	.20851E-08
64	3:20:15	2:57: 5	(10625.)	-.02790	-.02791	.00001	.12520E-09
65	3:20:20	2:57:10	(10630.)	-.03034	-.03032	-.00002	.36575E-09
66	3:20:25	2:57:15	(10635.)	-.03287	-.03285	-.00002	.38956E-09
67	3:20:30	2:57:20	(10640.)	-.03553	-.03549	-.00004	.13432E-08
68	3:20:35	2:57:25	(10645.)	-.03831	-.03824	-.00007	.45509E-08
69	3:20:40	2:57:30	(10650.)	-.04118	-.04109	-.00009	.83532E-08
70	3:20:45	2:57:35	(10655.)	-.04414	-.04408	-.00006	.36138E-08
71	3:20:50	2:57:40	(10660.)	-.04715	-.04703	-.00012	.15304E-07
72	3:20:55	2:57:45	(10665.)	-.05024	-.05009	-.00015	.22091E-07
73	3:21: 0	2:57:50	(10670.)	-.05339	-.05320	-.00019	.35962E-07
74	3:21: 5	2:57:55	(10675.)	-.05652	-.05634	-.00018	.33742E-07
75	3:21:10	2:58: 0	(10680.)	-.05970	-.05948	-.00022	.47971E-07
76	3:21:15	2:58: 5	(10685.)	-.06282	-.06268	-.00014	.20390E-07
77	3:21:20	2:58:10	(10690.)	-.06592	-.06578	-.00014	.19738E-07
78	3:21:25	2:58:15	(10695.)	-.06896	-.06877	-.00019	.36343E-07
79	3:21:30	2:58:20	(10700.)	-.07190	-.07181	-.00009	.89123E-08
80	3:21:35	2:58:25	(10705.)	-.07475	-.07469	-.00006	.40803E-08
81	3:21:40	2:58:30	(10710.)	-.07749	-.07745	-.00004	.16546E-08
82	3:21:45	2:58:35	(10715.)	-.08010	-.08007	-.00003	.68886E-09
83	3:21:50	2:58:40	(10720.)	-.08255	-.08254	-.00001	.13141E-09
84	3:21:55	2:58:45	(10725.)	-.08480	-.08478	-.00002	.40035E-09
85	3:22: 0	2:58:50	(10730.)	-.08686	-.08687	.00001	.11279E-09
86	3:22: 5	2:58:55	(10735.)	-.08870	-.08875	.00005	.20644E-08
87	3:22:10	2:59: 0	(10740.)	-.09030	-.09039	.00009	.78288E-08
88	3:22:15	2:59: 5	(10745.)	-.09165	-.09179	.00014	.18399E-07
89	3:22:20	2:59:10	(10750.)	-.09275	-.09292	.00017	.30575E-07
90	3:22:25	2:59:15	(10755.)	-.09358	-.09380	.00022	.46777E-07
91	3:22:30	2:59:20	(10760.)	-.09412	-.09439	.00027	.74218E-07
92	3:22:35	2:59:25	(10765.)	-.09445	-.09471	.00026	.66718E-07
93	3:22:40	2:59:30	(10770.)	-.09453	-.09474	.00021	.43762E-07
94	3:22:45	2:59:35	(10775.)	-.09431	-.09449	.00018	.33076E-07
95	3:22:50	2:59:40	(10780.)	-.09378	-.09395	.00017	.28551E-07
96	3:22:55	2:59:45	(10785.)	-.09301	-.09314	.00013	.16698E-07
97	3:23: 0	2:59:50	(10790.)	-.09198	-.09206	.00008	.67988E-08
98	3:23: 5	2:59:55	(10795.)	-.09069	-.09073	.00004	.14933E-08
99	3:23:10	3: 0: 0	(10800.)	-.08915	-.08915	.00000	.61146E-14
100	3:23:15	3: 0: 5	(10805.)	-.08737	-.08734	-.00003	.87621E-09
101	3:23:20	3: 0:10	(10810.)	-.08535	-.08532	-.00003	.11593E-08
102	3:23:30	3: 0:20	(10820.)	-.08079	-.08074	-.00005	.22395E-08
103	3:23:35	3: 0:25	(10825.)	-.07826	-.07819	-.00007	.55046E-08
104	3:23:40	3: 0:30	(10830.)	-.07561	-.07549	-.00012	.14413E-07
105	3:23:45	3: 0:35	(10835.)	-.07282	-.07262	-.00020	.40416E-07
106	3:23:50	3: 0:40	(10840.)	-.06990	-.06977	-.00013	.18114E-07
107	3:23:55	3: 0:45	(10845.)	-.06692	-.06678	-.00014	.19838E-07
108	3:24: 0	3: 0:50	(10850.)	-.06388	-.06374	-.00014	.20103E-07
109	3:24: 5	3: 0:55	(10855.)	-.06081	-.06066	-.00015	.21606E-07
110	3:24:10	3: 1: 0	(10860.)	-.05789	-.05757	-.00032	.10034E-06
111	3:24:15	3: 1: 5	(10865.)	-.05459	-.05449	-.00010	.10468E-07
112	3:24:20	3: 1:10	(10870.)	-.05167	-.05142	-.00025	.60487E-07
113	3:24:25	3: 1:15	(10875.)	-.04861	-.04840	-.00021	.44591E-07
114	3:24:30	3: 1:20	(10880.)	-.04560	-.04543	-.00017	.29875E-07
115	3:24:35	3: 1:25	(10885.)	-.04267	-.04252	-.00015	.21686E-07
116	3:24:40	3: 1:30	(10890.)	-.03981	-.03970	-.00011	.12590E-07
117	3:24:45	3: 1:35	(10895.)	-.03702	-.03696	-.00006	.32478E-08
118	3:24:50	3: 1:40	(10900.)	-.03434	-.03428	-.00006	.40852E-08
119	3:24:55	3: 1:45	(10905.)	-.03177	-.03180	.00003	.83742E-09
120	3:25: 0	3: 1:50	(10910.)	-.02915	-.02934	.00019	.34747E-07
121	3:25: 5	3: 1:55	(10915.)	-.02696	-.02704	.00008	.65338E-08
122	3:25:10	3: 2: 0	(10920.)	-.02478	-.02487	.00009	.74300E-08
123	3:25:15	3: 2: 5	(10925.)	-.02268	-.02281	.00013	.18069E-07

124	3:25:20	3: 2:10	(10930.)	-.02073	-.02089	.00016	.24400E-07
125	3:25:25	3: 2:15	(10935.)	-.01890	-.01908	.00018	.32814E-07
126	3:25:30	3: 2:20	(10940.)	-.01721	-.01740	.00019	.35281E-07
127	3:25:35	3: 2:25	(10945.)	-.01564	-.01586	.00022	.50160E-07
128	3:25:40	3: 2:30	(10950.)	-.01419	-.01441	.00022	.50247E-07
129	3:25:45	3: 2:35	(10955.)	-.01285	-.01308	.00023	.51546E-07
130	3:25:50	3: 2:40	(10960.)	-.01162	-.01185	.00023	.52124E-07
131	3:25:55	3: 2:45	(10965.)	-.01050	-.01072	.00022	.49826E-07
132	3:26: 0	3: 2:50	(10970.)	-.00948	-.00970	.00022	.46947E-07
133	3:26: 5	3: 2:55	(10975.)	-.00856	-.00876	.00020	.41341E-07
134	3:26:10	3: 3: 0	(10980.)	-.00775	-.00792	.00017	.28110E-07
135	3:26:15	3: 3: 5	(10985.)	-.00701	-.00715	.00014	.20757E-07
136	3:26:20	3: 3:10	(10990.)	-.00637	-.00647	.00010	.94006E-08
137	3:26:25	3: 3:15	(10995.)	-.00573	-.00584	.00011	.11914E-07
138	3:26:30	3: 3:20	(11000.)	-.00518	-.00530	.00012	.14395E-07
139	3:26:35	3: 3:25	(11005.)	-.00472	-.00481	.00009	.79841E-08
140	3:26:40	3: 3:30	(11010.)	-.00431	-.00437	.00006	.40648E-08
141	3:26:45	3: 3:35	(11015.)	-.00396	-.00399	.00003	.80042E-09
142	3:26:50	3: 3:40	(11020.)	-.00365	-.00364	-.00001	.64447E-10
143	3:26:55	3: 3:45	(11025.)	-.00336	-.00335	-.00001	.11159E-09
144	3:27: 0	3: 3:50	(11030.)	-.00311	-.00309	-.00002	.50398E-09
145	3:27: 5	3: 3:55	(11035.)	-.00288	-.00285	-.00003	.64614E-09
146	3:27:10	3: 4: 0	(11040.)	-.00269	-.00266	-.00003	.91736E-09
147	3:27:15	3: 4: 5	(11045.)	-.00254	-.00249	-.00005	.28153E-08
148	3:27:20	3: 4:10	(11050.)	-.00241	-.00233	-.00008	.56615E-08
149	3:27:25	3: 4:15	(11055.)	-.00229	-.00221	-.00008	.66092E-08
150	3:27:30	3: 4:20	(11060.)	-.00218	-.00210	-.00008	.70581E-08
151	3:27:35	3: 4:25	(11066.)	-.00208	-.00199	-.00009	.79001E-08
152	3:27:40	3: 4:30	(11070.)	-.00201	-.00192	-.00009	.76847E-08
153	3:27:45	3: 4:35	(11075.)	-.00194	-.00185	-.00009	.74794E-08
154	3:27:50	3: 4:40	(11080.)	-.00188	-.00179	-.00009	.73775E-08
155	3:27:55	3: 4:45	(11085.)	-.00183	-.00174	-.00009	.72273E-08
156	3:28: 0	3: 4:50	(11090.)	-.00180	-.00170	-.00010	.91401E-08
157	3:28: 5	3: 4:55	(11095.)	-.00176	-.00167	-.00009	.81721E-08
158	3:28:10	3: 5: 0	(11100.)	-.00172	-.00164	-.00008	.63994E-08
159	3:28:15	3: 5: 5	(11105.)	-.00169	-.00162	-.00007	.54255E-08
160	3:28:20	3: 5:10	(11110.)	-.00168	-.00160	-.00008	.71881E-08
161	3:28:25	3: 5:15	(11115.)	-.00167	-.00158	-.00009	.81409E-08
162	3:28:30	3: 5:20	(11120.)	-.00164	-.00157	-.00007	.54809E-08
163	3:28:35	3: 5:25	(11125.)	-.00161	-.00155	-.00006	.30312E-08
164	3:28:40	3: 5:30	(11130.)	-.00158	-.00155	-.00003	.11556E-08
165	3:28:45	3: 5:35	(11135.)	-.00157	-.00154	-.00003	.97285E-09
166	3:28:50	3: 5:40	(11140.)	-.00154	-.00153	-.00001	.46688E-10
167	3:28:55	3: 5:45	(11145.)	-.00154	-.00153	-.00001	.13164E-09
168	3:29: 0	3: 5:50	(11150.)	-.00155	-.00153	-.00002	.62258E-09
169	3:29: 5	3: 5:55	(11155.)	-.00154	-.00152	-.00002	.31603E-09
170	3:29:10	3: 6: 0	(11160.)	-.00152	-.00152	.00000	.70831E-13
171	3:29:15	3: 6: 5	(11165.)	-.00152	-.00152	.00000	.15048E-11
172	3:29:20	3: 6:10	(11170.)	-.00152	-.00152	.00000	.51223E-11
173	3:29:25	3: 6:15	(11175.)	-.00153	-.00152	-.00001	.16764E-09
174	3:29:30	3: 6:20	(11180.)	-.00154	-.00152	-.00002	.54243E-09
175	3:29:35	3: 6:25	(11185.)	-.00154	-.00152	-.00002	.54792E-09
176	3:29:40	3: 6:30	(11190.)	-.00152	-.00152	.00000	.11072E-10
177	3:29:45	3: 6:35	(11195.)	-.00153	-.00152	-.00001	.17129E-09
178	3:29:50	3: 6:40	(11200.)	-.00154	-.00152	-.00002	.51584E-09
179	3:29:55	3: 6:45	(11205.)	-.00154	-.00152	-.00002	.49510E-09
180	3:30: 0	3: 6:50	(11210.)	-.00154	-.00152	-.00002	.47087E-09
181	3:30: 5	3: 6:55	(11215.)	-.00154	-.00152	-.00002	.44451E-09
182	3:30:10	3: 7: 0	(11220.)	-.00152	-.00152	.00000	.17267E-12
183	3:30:15	3: 7: 5	(11225.)	-.00153	-.00152	-.00001	.94226E-10
184	3:30:20	3: 7:10	(11230.)	-.00154	-.00152	-.00002	.35972E-09
185	3:30:25	3: 7:15	(11235.)	-.00155	-.00152	-.00003	.79526E-09
186	3:30:30	3: 7:20	(11240.)	-.00154	-.00152	-.00002	.30327E-09
187	3:30:35	3: 7:25	(11245.)	-.00154	-.00152	-.00002	.27547E-09
188	3:30:40	3: 7:30	(11250.)	-.00151	-.00152	.00001	.20183E-09
189	3:30:45	3: 7:35	(11255.)	-.00152	-.00153	.00001	.25225E-10
190	3:30:50	3: 7:40	(11260.)	-.00153	-.00153	.00000	.17066E-10
191	3:30:55	3: 7:45	(11265.)	-.00154	-.00153	-.00001	.17721E-09

192 3:31: 0 3: 7:50 (11270.) -.00154 -.00153 -.00001 .15430E-09

END OF DATA

APPENDIX B.2

N-DODECANE IN N-EICOSANE AT 222°C

TAYMOD (Taylor Dispersion Peak Model)
Developed by: J.B. Rodden (Dec. 1987)

HP9000 data filename: 0420871a

Solvent name: n-eicosane

Peak description: #2 C12, 20 sec. injection

Temperature : 220.00 C
Temperature compensated diffusion tube length: 43.70 m
Temperature compensated diffusion tube radius: .52480E-03 m

Injection time: 0:30:10 (1810. s)

Peak start time: 3:15: 0 (11700. s) - inj. time = 2:44:50 (9890. s)
Peak end time: 3:39: 0 (13140. s) - inj. time = 3: 8:50 (11330. s)
Peak maximum at: 3:27:15 (12435. s) - inj. time = 2:57: 5 (10625. s)

Peak start value: -.00138 v
Peak end value: -.00133 v
Peak max value: -.03227 v

Peak width at half height: 384.9 s

Preliminary estimate of D12 (see Sun and Chen, 1985): 4.5607 E-09 m**2/s

The model is:
v(i)=B1/SQRT(t(i))*exp(-(L-B4*t(i))**2/(B2*t(i))+B3+B5*(t(i)-t(1))

B1=pre-exp constant (v*s**0.5)
B2=4*K (m**2/s)
B3=baseline voltage (v)
B4=u; avg. fluid velocity (m/s)
B5=baseline drift (v/s)
K=D12+(a*u)**2/48/D12 (m**2/s)
a=diffusion tube radius (m)
L=diffusion tube length (m)

Drift included in model? y

	B1	B2	B3	B4	B5
Initial values:	-.31867E+01	.85147E-04	-.13800E-02	.41129E-02	.34722E-07
Final iteration:	-.31914E+01	.83861E-04	-.13520E-02	.41126E-02	.33807E-07

Convergence criteria: (1) epsilon = .10E-08; (2) max # of iterations = 20

Model converged following 4 iterations.

No. of points : 287
Sum of sq res : .227765983E-06 v**2
Avg sq error : .793609698E-09 v**2
Std err of est: .282697522E-04 v
r-squared : .999993108

Average error : -.635204209E-15 v
Avg abs error : .216654737E-04 v
Max abs error : .841796136E-04 v
Avg observation: -.101013240E-01 v
Avg prediction : -.101013240E-01 v

D12 (final model result): 4.6299 E-09 m**2/s

Taylor-Hunt criteria: D12/(u*a)=.215E-02 ?>>? a/(4*L)=.300E-05

Retention time, (L/B4): 2:57: 5 (10625.9 s)

D12 (top 95.0% of peak;	160 pts;	3:20:45 thru 3:34: 0):	4.6290 E-09 m**2/s
D12 (top 90.0% of peak;	141 pts;	3:21:30 thru 3:33:10):	4.6291 E-09 m**2/s
D12 (top 85.0% of peak;	128 pts;	3:22: 0 thru 3:32:35):	4.6294 E-09 m**2/s
D12 (top 80.0% of peak;	118 pts;	3:22:25 thru 3:32:10):	4.6310 E-09 m**2/s
D12 (top 60.0% of peak;	90 pts;	3:23:35 thru 3:31: 0):	4.6325 E-09 m**2/s
D12 (top 40.0% of peak;	67 pts;	3:24:30 thru 3:30: 0):	4.6209 E-09 m**2/s
D12 (top 20.0% of peak;	45 pts;	3:25:25 thru 3:29: 5):	4.5873 E-09 m**2/s
D12 (top 10.0% of peak;	32 pts;	3:26: 0 thru 3:28:35):	4.5780 E-09 m**2/s
D12 (top 5.0% of peak;	23 pts;	3:26:20 thru 3:28:10):	4.5501 E-09 m**2/s
D12 (top 2.0% of peak;	15 pts;	3:26:40 thru 3:27:50):	4.4812 E-09 m**2/s

ACTUAL PEAK DATA AND MODEL RESULTS

HP9000 data filename: 0420871c
Solvent name: n-eicosane
Peak description: #2 C12, 20 sec. injection

	B1	B2	B3	B4	B5
Final iteration:	-.31914E+01	.83861E-04	-.13520E-02	.41126E-02	.33807E-07

PT #	ACT TIME Hr Mi Se	TIME FROM INJECT. Hr Mi Se	(sec)	OBSERVATION (volts)	PREDICTION (volts)	RESIDUAL (volts)	SQ. RESID. (volts**2)
1	3:15: 0	2:44:50	(9890.)	-.00138	-.00135	-.00003	.75625E-09
2	3:15: 5	2:44:55	(9895.)	-.00137	-.00135	-.00002	.30916E-09
3	3:15:10	2:45: 0	(9900.)	-.00137	-.00135	-.00002	.31166E-09
4	3:15:15	2:45: 5	(9905.)	-.00137	-.00135	-.00002	.31353E-09
5	3:15:20	2:45:10	(9910.)	-.00136	-.00135	-.00001	.59960E-10
6	3:15:25	2:45:15	(9915.)	-.00136	-.00135	-.00001	.60196E-10
7	3:15:30	2:45:20	(9920.)	-.00136	-.00135	-.00001	.60072E-10
8	3:15:35	2:45:25	(9925.)	-.00136	-.00135	-.00001	.59549E-10
9	3:15:40	2:45:30	(9930.)	-.00137	-.00135	-.00002	.31160E-09
10	3:15:45	2:45:35	(9935.)	-.00137	-.00135	-.00002	.30811E-09
11	3:15:50	2:45:40	(9940.)	-.00136	-.00135	-.00001	.54976E-10
12	3:15:55	2:45:45	(9945.)	-.00135	-.00135	.00000	.76652E-11
13	3:16: 0	2:45:50	(9950.)	-.00135	-.00135	.00000	.90148E-11
14	3:16: 5	2:45:55	(9955.)	-.00135	-.00135	.00000	.10891E-10
15	3:16:10	2:46: 0	(9960.)	-.00135	-.00135	.00000	.13322E-10
16	3:16:15	2:46: 5	(9965.)	-.00135	-.00135	.00000	.16720E-10
17	3:16:20	2:46:10	(9970.)	-.00135	-.00135	.00000	.21087E-10
18	3:16:25	2:46:15	(9975.)	-.00135	-.00136	.00001	.27018E-10
19	3:16:30	2:46:20	(9980.)	-.00135	-.00136	.00001	.35098E-10
20	3:16:35	2:46:25	(9985.)	-.00135	-.00136	.00001	.45399E-10
21	3:16:40	2:46:30	(9990.)	-.00135	-.00136	.00001	.59601E-10
22	3:16:45	2:46:35	(9995.)	-.00135	-.00136	.00001	.77616E-10
23	3:16:50	2:46:40	(10000.)	-.00135	-.00136	.00001	.10175E-09
24	3:16:55	2:46:45	(10005.)	-.00135	-.00136	.00001	.13341E-09
25	3:17: 0	2:46:50	(10010.)	-.00135	-.00136	.00001	.17575E-09
26	3:17: 5	2:46:55	(10015.)	-.00135	-.00137	.00002	.22998E-09
27	3:17:10	2:47: 0	(10020.)	-.00135	-.00137	.00002	.29882E-09
28	3:17:15	2:47: 5	(10025.)	-.00137	-.00137	.00000	.69772E-13
29	3:17:20	2:47:10	(10030.)	-.00138	-.00137	-.00001	.56177E-10
30	3:17:25	2:47:15	(10035.)	-.00138	-.00138	.00000	.18536E-10
31	3:17:30	2:47:20	(10040.)	-.00139	-.00138	-.00001	.11783E-09
32	3:17:35	2:47:25	(10045.)	-.00139	-.00138	-.00001	.47653E-10
33	3:17:40	2:47:30	(10050.)	-.00140	-.00139	-.00001	.15319E-09
34	3:17:45	2:47:35	(10055.)	-.00139	-.00139	.00000	.67467E-11
35	3:17:50	2:47:40	(10060.)	-.00138	-.00140	.00002	.33834E-09
36	3:17:55	2:47:45	(10065.)	-.00139	-.00140	.00001	.20261E-09
37	3:18: 0	2:47:50	(10070.)	-.00141	-.00141	.00000	.16399E-11
38	3:18: 5	2:47:55	(10075.)	-.00142	-.00142	.00000	.14050E-11
39	3:18:15	2:48: 5	(10085.)	-.00144	-.00144	.00000	.10153E-10
40	3:18:20	2:48:10	(10090.)	-.00144	-.00145	.00001	.53323E-10
41	3:18:25	2:48:15	(10095.)	-.00145	-.00146	.00001	.83728E-10
42	3:18:30	2:48:20	(10100.)	-.00146	-.00147	.00001	.13758E-09
43	3:18:35	2:48:25	(10105.)	-.00149	-.00149	.00000	.14635E-10
44	3:18:40	2:48:30	(10110.)	-.00150	-.00150	.00000	.21611E-11
45	3:18:45	2:48:35	(10115.)	-.00151	-.00152	.00001	.74468E-10
46	3:18:50	2:48:40	(10120.)	-.00153	-.00154	.00001	.56095E-10
47	3:18:55	2:48:45	(10125.)	-.00154	-.00156	.00002	.33097E-09
48	3:19: 0	2:48:50	(10130.)	-.00157	-.00158	.00001	.12912E-09
49	3:19: 5	2:48:55	(10135.)	-.00159	-.00161	.00002	.24777E-09
50	3:19:10	2:49: 0	(10140.)	-.00162	-.00163	.00001	.18178E-09
51	3:19:15	2:49: 5	(10145.)	-.00164	-.00166	.00002	.51062E-09
52	3:19:20	2:49:10	(10150.)	-.00167	-.00169	.00002	.62363E-09
53	3:19:25	2:49:15	(10155.)	-.00168	-.00173	.00005	.25245E-08
54	3:19:30	2:49:20	(10160.)	-.00171	-.00177	.00006	.34367E-08
55	3:19:35	2:49:25	(10165.)	-.00176	-.00181	.00005	.25334E-08

56	3:19:40	2:49:30	(10170.)	-.00180	-.00186	.00006	.33056E-08
57	3:19:45	2:49:35	(10175.)	-.00186	-.00190	.00004	.19965E-08
58	3:19:50	2:49:40	(10180.)	-.00192	-.00196	.00004	.14305E-08
59	3:19:55	2:49:45	(10185.)	-.00199	-.00202	.00003	.70109E-09
60	3:20: 0	2:49:50	(10190.)	-.00205	-.00208	.00003	.74836E-09
61	3:20: 5	2:49:55	(10195.)	-.00213	-.00214	.00001	.20489E-09
62	3:20:15	2:50: 5	(10205.)	-.00228	-.00229	.00001	.19862E-09
63	3:20:20	2:50:10	(10210.)	-.00237	-.00238	.00001	.56807E-10
64	3:20:25	2:50:15	(10215.)	-.00247	-.00247	.00000	.10763E-11
65	3:20:30	2:50:20	(10220.)	-.00256	-.00256	.00000	.99552E-11
66	3:20:35	2:50:25	(10225.)	-.00266	-.00267	.00001	.36030E-10
67	3:20:40	2:50:30	(10230.)	-.00277	-.00278	.00001	.68375E-10
68	3:20:45	2:50:35	(10235.)	-.00288	-.00289	.00001	.18245E-09
69	3:20:50	2:50:40	(10240.)	-.00302	-.00302	.00000	.21180E-11
70	3:20:55	2:50:45	(10245.)	-.00315	-.00315	.00000	.60867E-11
71	3:21: 0	2:50:50	(10250.)	-.00332	-.00329	-.00003	.64282E-09
72	3:21: 5	2:50:55	(10255.)	-.00345	-.00345	.00000	.12514E-11
73	3:21:10	2:51: 0	(10260.)	-.00363	-.00361	-.00002	.29421E-09
74	3:21:15	2:51: 5	(10265.)	-.00379	-.00378	-.00001	.10323E-09
75	3:21:20	2:51:10	(10270.)	-.00399	-.00396	-.00003	.88764E-09
76	3:21:25	2:51:15	(10275.)	-.00416	-.00415	-.00001	.16726E-09
77	3:21:30	2:51:20	(10280.)	-.00439	-.00435	-.00004	.17340E-08
78	3:21:35	2:51:25	(10285.)	-.00458	-.00457	-.00001	.22288E-09
79	3:21:40	2:51:30	(10290.)	-.00480	-.00478	-.00002	.24046E-09
80	3:21:45	2:51:35	(10295.)	-.00506	-.00502	-.00004	.16019E-08
81	3:21:50	2:51:40	(10300.)	-.00528	-.00527	-.00001	.15696E-09
82	3:21:55	2:51:45	(10305.)	-.00559	-.00553	-.00006	.39363E-08
83	3:22: 0	2:51:50	(10310.)	-.00587	-.00581	-.00006	.42045E-08
84	3:22: 5	2:51:55	(10315.)	-.00615	-.00608	-.00007	.42591E-08
85	3:22:10	2:52: 0	(10320.)	-.00645	-.00638	-.00007	.45050E-08
86	3:22:15	2:52: 5	(10325.)	-.00678	-.00670	-.00008	.63115E-08
87	3:22:20	2:52:10	(10330.)	-.00711	-.00704	-.00007	.50690E-08
88	3:22:25	2:52:15	(10335.)	-.00743	-.00736	-.00007	.53180E-08
89	3:22:30	2:52:20	(10340.)	-.00775	-.00771	-.00004	.16961E-08
90	3:22:35	2:52:25	(10345.)	-.00813	-.00807	-.00006	.31151E-08
91	3:22:40	2:52:30	(10350.)	-.00849	-.00845	-.00004	.13539E-08
92	3:22:45	2:52:35	(10355.)	-.00891	-.00885	-.00006	.41156E-08
93	3:22:50	2:52:40	(10360.)	-.00930	-.00925	-.00005	.22992E-08
94	3:22:55	2:52:45	(10365.)	-.00971	-.00968	-.00003	.88802E-09
95	3:23: 0	2:52:50	(10370.)	-.01015	-.01010	-.00005	.20562E-08
96	3:23: 5	2:52:55	(10375.)	-.01058	-.01055	-.00003	.85870E-09
97	3:23:10	2:53: 0	(10380.)	-.01104	-.01101	-.00003	.92556E-09
98	3:23:15	2:53: 5	(10385.)	-.01152	-.01148	-.00004	.15216E-08
99	3:23:20	2:53:10	(10390.)	-.01197	-.01197	.00000	.18833E-10
100	3:23:25	2:53:15	(10395.)	-.01248	-.01246	-.00002	.40217E-09
101	3:23:30	2:53:20	(10400.)	-.01300	-.01297	-.00003	.11147E-08
102	3:23:35	2:53:25	(10405.)	-.01350	-.01349	-.00001	.30459E-10
103	3:23:40	2:53:30	(10410.)	-.01401	-.01401	.00000	.30161E-11
104	3:23:45	2:53:35	(10415.)	-.01455	-.01455	.00000	.10079E-11
105	3:23:50	2:53:40	(10420.)	-.01509	-.01510	.00001	.26668E-10
106	3:23:55	2:53:45	(10425.)	-.01564	-.01565	.00001	.90374E-10
107	3:24: 0	2:53:50	(10430.)	-.01618	-.01621	.00003	.97571E-09
108	3:24: 5	2:53:55	(10435.)	-.01676	-.01679	.00003	.95462E-09
109	3:24:10	2:54: 0	(10440.)	-.01730	-.01735	.00005	.28574E-08
110	3:24:15	2:54: 5	(10445.)	-.01792	-.01793	.00001	.14681E-09
111	3:24:21	2:54:11	(10451.)	-.01866	-.01865	-.00001	.27442E-10
112	3:24:25	2:54:15	(10455.)	-.01912	-.01912	.00000	.96284E-11
113	3:24:30	2:54:20	(10460.)	-.01964	-.01969	.00005	.21524E-08
114	3:24:35	2:54:25	(10465.)	-.02022	-.02027	.00005	.28827E-08
115	3:24:40	2:54:30	(10470.)	-.02085	-.02086	.00001	.10783E-09
116	3:24:45	2:54:35	(10475.)	-.02141	-.02146	.00005	.22020E-08
117	3:24:50	2:54:40	(10480.)	-.02204	-.02205	.00001	.10934E-09
118	3:24:55	2:54:45	(10485.)	-.02262	-.02260	-.00002	.22598E-09
119	3:25: 0	2:54:50	(10490.)	-.02320	-.02319	-.00001	.13027E-09
120	3:25: 5	2:54:55	(10495.)	-.02374	-.02375	.00001	.19634E-09
121	3:25:10	2:55: 0	(10500.)	-.02429	-.02430	.00001	.10842E-09
122	3:25:15	2:55: 5	(10505.)	-.02483	-.02485	.00002	.35137E-09
123	3:25:20	2:55:10	(10510.)	-.02536	-.02539	.00003	.70438E-09

124	3:25:25	2:55:15	(10515.)	-.02593	-.02592	-.00001	.50789E-10
125	3:25:30	2:55:20	(10520.)	-.02642	-.02643	.00001	.29473E-10
126	3:25:35	2:55:25	(10525.)	-.02694	-.02692	-.00002	.25586E-09
127	3:25:40	2:55:30	(10530.)	-.02741	-.02741	.00000	.88997E-11
128	3:25:45	2:55:35	(10535.)	-.02786	-.02788	.00002	.50028E-09
129	3:25:50	2:55:40	(10540.)	-.02829	-.02832	.00003	.99513E-09
130	3:25:55	2:55:45	(10545.)	-.02872	-.02875	.00003	.94476E-09
131	3:26: 0	2:55:50	(10550.)	-.02916	-.02916	.00000	.76015E-13
132	3:26: 5	2:55:56	(10555.)	-.02951	-.02955	.00004	.14021E-08
133	3:26:10	2:56: 0	(10560.)	-.02988	-.02991	.00003	.10815E-08
134	3:26:15	2:56: 5	(10565.)	-.03023	-.03026	.00003	.62922E-09
135	3:26:20	2:56:10	(10570.)	-.03055	-.03057	.00002	.53535E-09
136	3:26:25	2:56:15	(10575.)	-.03086	-.03087	.00001	.13881E-09
137	3:26:30	2:56:20	(10580.)	-.03109	-.03113	.00004	.18924E-08
138	3:26:35	2:56:25	(10585.)	-.03133	-.03137	.00004	.19647E-08
139	3:26:40	2:56:30	(10590.)	-.03156	-.03159	.00003	.10249E-08
140	3:26:45	2:56:35	(10595.)	-.03176	-.03178	.00002	.30595E-09
141	3:26:50	2:56:40	(10600.)	-.03189	-.03193	.00004	.20067E-08
142	3:26:55	2:56:45	(10605.)	-.03202	-.03206	.00004	.18942E-08
143	3:27: 0	2:56:50	(10610.)	-.03212	-.03216	.00004	.17339E-08
144	3:27: 5	2:56:55	(10615.)	-.03221	-.03223	.00002	.57696E-09
145	3:27:10	2:57: 0	(10620.)	-.03225	-.03227	.00002	.61751E-09
146	3:27:15	2:57: 5	(10625.)	-.03227	-.03229	.00002	.30169E-09
147	3:27:20	2:57:10	(10630.)	-.03224	-.03227	.00003	.93677E-09
148	3:27:25	2:57:15	(10635.)	-.03220	-.03222	.00002	.60052E-09
149	3:27:30	2:57:20	(10640.)	-.03213	-.03215	.00002	.30602E-09
150	3:27:35	2:57:25	(10645.)	-.03204	-.03204	.00000	.80478E-11
151	3:27:40	2:57:30	(10650.)	-.03192	-.03191	-.00001	.54966E-10
152	3:27:45	2:57:35	(10655.)	-.03176	-.03175	-.00001	.13530E-09
153	3:27:50	2:57:40	(10660.)	-.03159	-.03156	-.00003	.70277E-09
154	3:27:55	2:57:45	(10665.)	-.03138	-.03134	-.00004	.13322E-08
155	3:28: 0	2:57:50	(10670.)	-.03113	-.03110	-.00003	.83386E-09
156	3:28: 5	2:57:55	(10675.)	-.03086	-.03084	-.00002	.45705E-09
157	3:28:10	2:58: 0	(10680.)	-.03056	-.03054	-.00002	.39990E-09
158	3:28:15	2:58: 5	(10685.)	-.03024	-.03022	-.00002	.29382E-09
159	3:28:20	2:58:10	(10690.)	-.02989	-.02987	-.00002	.46687E-09
160	3:28:25	2:58:15	(10695.)	-.02958	-.02953	-.00005	.27797E-08
161	3:28:30	2:58:20	(10700.)	-.02919	-.02914	-.00005	.21392E-08
162	3:28:35	2:58:25	(10705.)	-.02878	-.02873	-.00005	.23331E-08
163	3:28:40	2:58:30	(10710.)	-.02839	-.02831	-.00008	.65726E-08
164	3:28:45	2:58:35	(10715.)	-.02796	-.02788	-.00008	.70862E-08
165	3:28:50	2:58:40	(10720.)	-.02749	-.02742	-.00007	.52192E-08
166	3:28:55	2:58:45	(10725.)	-.02700	-.02693	-.00007	.43154E-08
167	3:29: 0	2:58:50	(10730.)	-.02648	-.02646	-.00002	.60318E-09
168	3:29: 5	2:58:55	(10735.)	-.02599	-.02595	-.00004	.13266E-08
169	3:29:10	2:59: 0	(10740.)	-.02547	-.02544	-.00003	.92860E-09
170	3:29:15	2:59: 5	(10745.)	-.02494	-.02491	-.00003	.64987E-09
171	3:29:20	2:59:10	(10750.)	-.02439	-.02437	-.00002	.44111E-09
172	3:29:25	2:59:15	(10755.)	-.02385	-.02383	-.00002	.59797E-09
173	3:29:30	2:59:20	(10760.)	-.02333	-.02327	-.00006	.30465E-08
174	3:29:35	2:59:25	(10765.)	-.02279	-.02273	-.00006	.37066E-08
175	3:29:40	2:59:30	(10770.)	-.02220	-.02217	-.00003	.10584E-08
176	3:29:45	2:59:35	(10775.)	-.02163	-.02159	-.00004	.15309E-08
177	3:29:50	2:59:40	(10780.)	-.02106	-.02103	-.00003	.67503E-09
178	3:29:55	2:59:45	(10785.)	-.02048	-.02046	-.00002	.24084E-09
179	3:30: 0	2:59:50	(10790.)	-.01984	-.01986	.00002	.41456E-09
180	3:30: 5	2:59:55	(10795.)	-.01934	-.01933	-.00001	.21884E-09
181	3:30:11	3: 0: 1	(10801.)	-.01863	-.01863	.00000	.91172E-11
182	3:30:15	3: 0: 5	(10805.)	-.01818	-.01818	.00000	.16555E-11
183	3:30:20	3: 0:10	(10810.)	-.01760	-.01761	.00001	.74956E-10
184	3:30:25	3: 0:15	(10815.)	-.01706	-.01707	.00001	.19771E-09
185	3:30:30	3: 0:20	(10820.)	-.01650	-.01652	.00002	.50145E-09
186	3:30:35	3: 0:25	(10825.)	-.01596	-.01597	.00001	.36639E-10
187	3:30:40	3: 0:30	(10830.)	-.01540	-.01544	.00004	.14595E-08
188	3:30:45	3: 0:35	(10835.)	-.01486	-.01491	.00005	.22234E-08
189	3:30:50	3: 0:40	(10840.)	-.01436	-.01438	.00002	.59379E-09
190	3:30:55	3: 0:45	(10845.)	-.01385	-.01386	.00001	.10646E-09
191	3:31: 0	3: 0:50	(10850.)	-.01332	-.01337	.00005	.21161E-08

192	3:31: 5	3: 0:55 (10855.)	-.01283	-.01287	.00004	.17223E-08
193	3:31:10	3: 1: 0 (10860.)	-.01236	-.01239	.00003	.75241E-09
194	3:31:15	3: 1: 5 (10865.)	-.01189	-.01190	.00001	.22180E-09
195	3:31:20	3: 1:10 (10870.)	-.01143	-.01145	.00002	.49303E-09
196	3:31:25	3: 1:15 (10875.)	-.01097	-.01100	.00003	.10078E-08
197	3:31:30	3: 1:20 (10880.)	-.01054	-.01056	.00002	.53401E-09
198	3:31:35	3: 1:25 (10885.)	-.01011	-.01014	.00003	.70376E-09
199	3:31:40	3: 1:30 (10890.)	-.00969	-.00971	.00002	.57917E-09
200	3:31:45	3: 1:35 (10895.)	-.00929	-.00932	.00003	.91542E-09
201	3:31:50	3: 1:40 (10900.)	-.00888	-.00893	.00005	.25826E-08
202	3:31:55	3: 1:45 (10905.)	-.00849	-.00855	.00006	.40802E-08
203	3:32: 0	3: 1:50 (10910.)	-.00815	-.00819	.00004	.15756E-08
204	3:32: 5	3: 1:55 (10915.)	-.00778	-.00784	.00006	.33677E-08
205	3:32:10	3: 2: 0 (10920.)	-.00743	-.00750	.00007	.47520E-08
206	3:32:15	3: 2: 5 (10925.)	-.00712	-.00717	.00005	.27386E-08
207	3:32:20	3: 2:10 (10930.)	-.00682	-.00685	.00003	.10235E-08
208	3:32:25	3: 2:15 (10935.)	-.00654	-.00656	.00002	.26224E-09
209	3:32:30	3: 2:20 (10940.)	-.00624	-.00627	.00003	.69603E-09
210	3:32:35	3: 2:25 (10945.)	-.00598	-.00598	.00000	.96275E-11
211	3:32:40	3: 2:30 (10950.)	-.00567	-.00572	.00005	.27463E-08
212	3:32:45	3: 2:35 (10955.)	-.00543	-.00547	.00004	.14310E-08
213	3:32:50	3: 2:40 (10960.)	-.00521	-.00522	.00001	.21184E-09
214	3:32:55	3: 2:45 (10965.)	-.00499	-.00499	.00000	.47567E-11
215	3:33: 0	3: 2:50 (10970.)	-.00478	-.00477	-.00001	.82708E-10
216	3:33: 5	3: 2:55 (10975.)	-.00457	-.00456	-.00001	.10015E-09
217	3:33:10	3: 3: 0 (10980.)	-.00434	-.00436	.00002	.37285E-09
218	3:33:15	3: 3: 5 (10985.)	-.00416	-.00417	.00001	.73318E-10
219	3:33:20	3: 3:10 (10990.)	-.00399	-.00398	-.00001	.36748E-10
220	3:33:25	3: 3:15 (10995.)	-.00381	-.00381	.00000	.54557E-11
221	3:33:30	3: 3:20 (11000.)	-.00363	-.00365	.00002	.27432E-09
222	3:33:35	3: 3:25 (11005.)	-.00350	-.00350	.00000	.17253E-10
223	3:33:40	3: 3:30 (11010.)	-.00334	-.00335	.00001	.17288E-09
224	3:33:45	3: 3:35 (11015.)	-.00319	-.00322	.00003	.65213E-09
225	3:33:50	3: 3:40 (11020.)	-.00308	-.00308	.00000	.10046E-10
226	3:33:55	3: 3:45 (11025.)	-.00296	-.00296	.00000	.10852E-10
227	3:34: 0	3: 3:50 (11030.)	-.00284	-.00285	.00001	.33075E-10
228	3:34: 5	3: 3:55 (11035.)	-.00273	-.00274	.00001	.90515E-10
229	3:34:10	3: 4: 0 (11040.)	-.00265	-.00264	-.00001	.15450E-09
230	3:34:15	3: 4: 5 (11045.)	-.00256	-.00254	-.00002	.39987E-09
231	3:34:20	3: 4:10 (11050.)	-.00246	-.00245	-.00001	.63071E-10
232	3:34:25	3: 4:15 (11055.)	-.00237	-.00237	.00000	.43574E-11
233	3:34:30	3: 4:20 (11060.)	-.00228	-.00229	.00001	.83420E-10
234	3:34:35	3: 4:25 (11065.)	-.00220	-.00221	.00001	.19689E-09
235	3:34:40	3: 4:30 (11070.)	-.00213	-.00215	.00002	.27548E-09
236	3:34:45	3: 4:35 (11075.)	-.00207	-.00208	.00001	.12290E-09
237	3:34:50	3: 4:40 (11080.)	-.00201	-.00202	.00001	.15314E-09
238	3:34:55	3: 4:45 (11085.)	-.00196	-.00197	.00001	.29849E-10
239	3:35: 0	3: 4:50 (11090.)	-.00191	-.00191	.00000	.20437E-10
240	3:35: 5	3: 4:55 (11095.)	-.00185	-.00187	.00002	.23207E-09
241	3:35:10	3: 5: 0 (11100.)	-.00180	-.00182	.00002	.45061E-09
242	3:35:15	3: 5: 5 (11105.)	-.00176	-.00178	.00002	.38082E-09
243	3:35:20	3: 5:10 (11110.)	-.00173	-.00174	.00001	.11723E-09
244	3:35:25	3: 5:15 (11115.)	-.00169	-.00170	.00001	.22435E-09
245	3:35:30	3: 5:20 (11120.)	-.00166	-.00167	.00001	.12442E-09
246	3:35:35	3: 5:25 (11125.)	-.00163	-.00164	.00001	.12302E-09
247	3:35:40	3: 5:30 (11130.)	-.00160	-.00161	.00001	.16184E-09
248	3:35:45	3: 5:35 (11135.)	-.00158	-.00159	.00001	.36319E-10
249	3:35:50	3: 5:40 (11140.)	-.00155	-.00156	.00001	.15283E-09
250	3:35:55	3: 5:45 (11145.)	-.00152	-.00154	.00002	.38666E-09
251	3:36: 0	3: 5:50 (11150.)	-.00150	-.00152	.00002	.38325E-09
252	3:36: 5	3: 5:55 (11155.)	-.00150	-.00150	.00000	.11717E-12
253	3:36:10	3: 6: 0 (11160.)	-.00149	-.00148	-.00001	.44225E-10
254	3:36:15	3: 6: 5 (11165.)	-.00148	-.00147	-.00001	.16627E-09
255	3:36:20	3: 6:10 (11170.)	-.00148	-.00145	-.00003	.74104E-09
256	3:36:25	3: 6:15 (11175.)	-.00146	-.00144	-.00002	.43686E-09
257	3:36:30	3: 6:20 (11180.)	-.00144	-.00143	-.00001	.16739E-09
258	3:36:35	3: 6:25 (11185.)	-.00143	-.00142	-.00001	.20159E-09
259	3:36:40	3: 6:30 (11190.)	-.00141	-.00141	.00000	.20263E-10

260	3:36:45	3: 6:35	(11195.)	-.00141	-.00140	-.00001	.19382E-09
261	3:36:50	3: 6:40	(11200.)	-.00141	-.00139	-.00002	.51494E-09
262	3:36:55	3: 6:45	(11205.)	-.00140	-.00138	-.00002	.42795E-09
263	3:37: 0	3: 6:50	(11210.)	-.00139	-.00137	-.00002	.30824E-09
264	3:37: 5	3: 6:55	(11215.)	-.00138	-.00137	-.00001	.19864E-09
265	3:37:10	3: 7: 0	(11220.)	-.00137	-.00136	-.00001	.10102E-09
266	3:37:15	3: 7: 5	(11225.)	-.00136	-.00135	-.00001	.29982E-10
267	3:37:20	3: 7:10	(11230.)	-.00136	-.00135	-.00001	.10843E-09
268	3:37:25	3: 7:15	(11235.)	-.00135	-.00135	.00000	.24053E-10
269	3:37:30	3: 7:20	(11240.)	-.00135	-.00134	-.00001	.80787E-10
270	3:37:35	3: 7:25	(11245.)	-.00134	-.00134	.00000	.76730E-11
271	3:37:40	3: 7:30	(11250.)	-.00134	-.00133	-.00001	.36852E-10
272	3:37:45	3: 7:35	(11255.)	-.00134	-.00133	-.00001	.84488E-10
273	3:37:50	3: 7:40	(11260.)	-.00134	-.00133	-.00001	.14194E-09
274	3:37:55	3: 7:45	(11265.)	-.00134	-.00133	-.00001	.20845E-09
275	3:38: 0	3: 7:50	(11270.)	-.00133	-.00132	-.00001	.45274E-10
276	3:38: 5	3: 7:55	(11275.)	-.00133	-.00132	-.00001	.78270E-10
277	3:38:10	3: 8: 0	(11280.)	-.00134	-.00132	-.00002	.42827E-09
278	3:38:15	3: 8: 5	(11285.)	-.00135	-.00132	-.00003	.10503E-08
279	3:38:20	3: 8:10	(11290.)	-.00134	-.00132	-.00002	.57565E-09
280	3:38:25	3: 8:15	(11295.)	-.00133	-.00131	-.00002	.23642E-09
281	3:38:30	3: 8:20	(11300.)	-.00134	-.00131	-.00003	.71076E-09
282	3:38:35	3: 8:25	(11305.)	-.00135	-.00131	-.00004	.14309E-08
283	3:38:40	3: 8:30	(11310.)	-.00135	-.00131	-.00004	.15125E-08
284	3:38:45	3: 8:35	(11315.)	-.00132	-.00131	-.00001	.97925E-10
285	3:38:50	3: 8:40	(11320.)	-.00131	-.00131	.00000	.57536E-12
286	3:38:55	3: 8:45	(11325.)	-.00133	-.00131	-.00002	.46565E-09
287	3:39: 0	3: 8:50	(11330.)	-.00133	-.00131	-.00002	.49665E-09

END OF DATA

APPENDIX B.3

N-OCTANE IN N-OCTACOSANE AT 100°C

TAYMOD (Taylor Dispersion Peak Model)
Developed by: J.B. Rodden (Dec. 1987)

HP9000 data filename: 060187c

Solvent name: n-octacosane

Peak description: #3 C6, 20 s inj.

Temperature : 100.00 C
Temperature compensated diffusion tube length: 43.61 m
Temperature compensated diffusion tube radius: .52369E-03 m

Injection time: 1:32:10 (5530. s)

Peak start time: 3: 0: 0 (10800. s) - inj. time = 1:27:50 (5270. s)
Peak end time: 3:31: 0 (12660. s) - inj. time = 1:58:50 (7130. s)
Peak maximum at: 3:15: 0 (11700. s) - inj. time = 1:42:50 (6170. s)

Peak start value: .00061 v
Peak end value: .00081 v
Peak max value: -.00614 v

Peak width at half height: 575.0 s

Preliminary estimate of D12 (see Chen, 1985): 1.1820 E-09 m**2/s

The model is:
v(i)=B1/SQRT(t(i))*exp(-(L-B4*t(i))**2/(B2*t(i))+B3+B5*(t(i)-t(1))

B1=pre-exp constant (v*s**0.5)
B2=4*K (m**2/s)
B3=baseline voltage (v)
B4=u; avg. fluid velocity (m/s)
B5=baseline drift (v/s)
K=D12+(a*u)**2/48/D12 (m**2/s)
a=diffusion tube radius (m)
L=diffusion tube length (m)

Drift included in model? y

	B1	B2	B3	B4	B5
Initial values:	-.53782E+00	.96578E-03	.61000E-03	.70674E-02	.10753E-06
Final iteration:	-.53901E+00	.95483E-03	.64578E-03	.70737E-02	.11073E-06

Convergence criteria: (1) epsilon = .10E-06; (2) max # of iterations = 20

Model converged following 4 iterations.

No. of points : 371
Sum of sq res : .487650280E-06 v**2
Avg sq error : .131442124E-08 v**2
Std err of est: .363530669E-04 v
r-squared : .999774656

Average error : -.271905865E-14 v
Avg abs error : .292854012E-04 v
Max abs error : .944403503E-04 v
Avg observation: -.148234501E-02 v
Avg prediction : -.148234501E-02 v

D12 (final model result): 1.1977 E-09 m**2/s

Taylor-Hunt criteria: D12/(u*a)=.323E-03 ?>>? a/(4*L)=.300E-05

Retention time, (L/B4): 1:42:44 (6164.8 s)

D12 (top 95.0% of peak;	230 pts;	3: 5:35 thru	3:24:45):	1.1960 E-09 m**2/s
D12 (top 90.0% of peak;	205 pts;	3: 6:35 thru	3:23:40):	1.1949 E-09 m**2/s
D12 (top 85.0% of peak;	188 pts;	3: 7:15 thru	3:22:45):	1.1909 E-09 m**2/s
D12 (top 80.0% of peak;	173 pts;	3: 7:45 thru	3:22:10):	1.1865 E-09 m**2/s
D12 (top 60.0% of peak;	132 pts;	3: 9:25 thru	3:20:25):	1.1820 E-09 m**2/s
D12 (top 40.0% of peak;	99 pts;	3:10:45 thru	3:19: 0):	1.1875 E-09 m**2/s
D12 (top 20.0% of peak;	65 pts;	3:12:10 thru	3:17:35):	1.2078 E-09 m**2/s
D12 (top 10.0% of peak;	45 pts;	3:13: 0 thru	3:16:45):	1.2413 E-09 m**2/s
D12 (top 5.0% of peak;	31 pts;	3:13:35 thru	3:16:10):	1.2574 E-09 m**2/s
D12 (top 2.0% of peak;	18 pts;	3:14: 5 thru	3:15:35):	1.4066 E-09 m**2/s

ACTUAL PEAK DATA AND MODEL RESULTS

HP9000 data filename: 060187c
Solvent name: n-octacosane
Peak description: #3 C8, 20 sec. injection

	B1	B2	B3	B4	B5
Final iteration:	-.53901E+00	.95483E-03	.64578E-03	.70737E-02	.11073E-06

PT #	ACT TIME Hr Mi Se	TIME FROM INJECT. Hr Mi Se (sec)	OBSERVATION (volts)	PREDICTION (volts)	RESIDUAL (volts)	SQ. RESID. (volts**2)
1	3: 0: 0	1:27:50 (5270.)	.00061	.00064	-.00003	.11011E-08
2	3: 0: 5	1:27:55 (5275.)	.00061	.00064	-.00003	.11202E-08
3	3: 0:10	1:28: 0 (5280.)	.00060	.00064	-.00004	.19140E-08
4	3: 0:15	1:28: 5 (5285.)	.00061	.00064	-.00003	.11548E-08
5	3: 0:20	1:28:10 (5290.)	.00062	.00064	-.00002	.58576E-09
6	3: 0:25	1:28:15 (5295.)	.00061	.00064	-.00003	.11822E-08
7	3: 0:30	1:28:20 (5300.)	.00062	.00064	-.00002	.60212E-09
8	3: 0:35	1:28:25 (5305.)	.00062	.00064	-.00002	.60791E-09
9	3: 0:40	1:28:30 (5310.)	.00061	.00064	-.00003	.12063E-08
10	3: 0:45	1:28:35 (5315.)	.00060	.00064	-.00004	.20041E-08
11	3: 0:50	1:28:40 (5320.)	.00061	.00064	-.00003	.12082E-08
12	3: 0:55	1:28:45 (5325.)	.00062	.00064	-.00002	.61028E-09
13	3: 1: 0	1:28:50 (5330.)	.00062	.00064	-.00002	.60499E-09
14	3: 1: 5	1:28:55 (5335.)	.00063	.00064	-.00001	.20823E-09
15	3: 1:10	1:29: 0 (5340.)	.00062	.00064	-.00002	.58597E-09
16	3: 1:15	1:29: 5 (5345.)	.00061	.00064	-.00003	.11505E-08
17	3: 1:20	1:29:10 (5350.)	.00061	.00064	-.00003	.11265E-08
18	3: 1:25	1:29:15 (5355.)	.00063	.00064	-.00001	.17250E-09
19	3: 1:30	1:29:20 (5360.)	.00063	.00064	-.00001	.15940E-09
20	3: 1:35	1:29:25 (5365.)	.00061	.00064	-.00003	.10261E-08
21	3: 1:40	1:29:30 (5370.)	.00064	.00064	.00000	.18610E-11
22	3: 1:45	1:29:35 (5375.)	.00064	.00064	.00000	.32526E-12
23	3: 1:50	1:29:40 (5380.)	.00062	.00064	-.00002	.38762E-09
24	3: 1:55	1:29:45 (5385.)	.00064	.00064	.00000	.18122E-11
25	3: 2: 0	1:29:50 (5390.)	.00064	.00064	.00000	.58238E-11
26	3: 2: 5	1:29:55 (5395.)	.00065	.00064	.00001	.18554E-09
27	3: 2:10	1:30: 0 (5400.)	.00066	.00064	.00002	.62427E-09
28	3: 2:15	1:30: 5 (5405.)	.00067	.00063	.00004	.13316E-08
29	3: 2:20	1:30:10 (5411.)	.00066	.00063	.00003	.80599E-09
30	3: 2:25	1:30:15 (5415.)	.00065	.00063	.00002	.39841E-09
31	3: 2:30	1:30:20 (5420.)	.00066	.00063	.00003	.10204E-08
32	3: 2:35	1:30:25 (5425.)	.00067	.00063	.00004	.19454E-08
33	3: 2:40	1:30:30 (5430.)	.00065	.00062	.00003	.70814E-09
34	3: 2:45	1:30:35 (5435.)	.00065	.00062	.00003	.84493E-09
35	3: 2:50	1:30:40 (5440.)	.00065	.00062	.00003	.10136E-08
36	3: 2:55	1:30:45 (5445.)	.00065	.00062	.00003	.12136E-08
37	3: 3: 0	1:30:50 (5450.)	.00066	.00061	.00005	.23111E-08
38	3: 3: 5	1:30:55 (5455.)	.00067	.00061	.00006	.37898E-08
39	3: 3:10	1:31: 0 (5460.)	.00067	.00060	.00007	.42650E-08
40	3: 3:15	1:31: 5 (5465.)	.00065	.00060	.00005	.24353E-08
41	3: 3:20	1:31:10 (5470.)	.00065	.00060	.00005	.28812E-08
42	3: 3:25	1:31:15 (5475.)	.00064	.00059	.00005	.23344E-08
43	3: 3:30	1:31:20 (5480.)	.00061	.00059	.00002	.53728E-09
44	3: 3:35	1:31:25 (5485.)	.00060	.00058	.00002	.34156E-09
45	3: 3:40	1:31:30 (5490.)	.00061	.00058	.00003	.11658E-08
46	3: 3:45	1:31:35 (5495.)	.00059	.00057	.00002	.40739E-09
47	3: 3:50	1:31:40 (5500.)	.00057	.00056	.00001	.43837E-10
48	3: 3:55	1:31:45 (5505.)	.00057	.00056	.00001	.18153E-09
49	3: 4: 0	1:31:50 (5510.)	.00057	.00055	.00002	.43182E-09
50	3: 4: 5	1:31:55 (5515.)	.00054	.00054	.00000	.13836E-11
51	3: 4:10	1:32: 0 (5520.)	.00053	.00053	.00000	.10740E-10
52	3: 4:15	1:32: 5 (5525.)	.00053	.00052	.00001	.29581E-10
53	3: 4:20	1:32:10 (5530.)	.00053	.00052	.00001	.22092E-09
54	3: 4:25	1:32:15 (5535.)	.00051	.00051	.00000	.19807E-10
55	3: 4:30	1:32:20 (5540.)	.00050	.00049	.00001	.27221E-10

56	3: 4:35	1:32:25	(5545.)	.00049	.00048	.00001	.35324E-10
57	3: 4:40	1:32:30	(5550.)	.00047	.00047	.00000	.75108E-11
58	3: 4:45	1:32:35	(5555.)	.00047	.00046	.00001	.89020E-10
59	3: 4:50	1:32:40	(5560.)	.00047	.00045	.00002	.49600E-09
60	3: 4:55	1:32:45	(5565.)	.00045	.00043	.00002	.24942E-09
61	3: 5: 0	1:32:50	(5570.)	.00043	.00042	.00001	.11259E-09
62	3: 5: 5	1:32:55	(5575.)	.00043	.00040	.00003	.64019E-09
63	3: 5:10	1:33: 0	(5580.)	.00042	.00039	.00003	.94431E-09
64	3: 5:15	1:33: 5	(5585.)	.00041	.00037	.00004	.14130E-08
65	3: 5:20	1:33:10	(5590.)	.00041	.00036	.00005	.29804E-08
66	3: 5:25	1:33:15	(5595.)	.00038	.00034	.00004	.18617E-08
67	3: 5:30	1:33:20	(5600.)	.00034	.00032	.00002	.47659E-09
68	3: 5:35	1:33:25	(5605.)	.00031	.00030	.00001	.15879E-09
69	3: 5:40	1:33:30	(5610.)	.00028	.00028	.00000	.70782E-11
70	3: 5:45	1:33:35	(5615.)	.00025	.00026	-.00001	.25653E-10
71	3: 5:50	1:33:40	(5620.)	.00021	.00023	-.00002	.51529E-09
72	3: 5:55	1:33:45	(5625.)	.00019	.00021	-.00002	.35658E-09
73	3: 6: 0	1:33:50	(5630.)	.00015	.00018	-.00003	.11241E-08
74	3: 6: 5	1:33:55	(5635.)	.00010	.00016	-.00006	.33171E-08
75	3: 6:10	1:34: 0	(5640.)	.00006	.00013	-.00007	.49807E-08
76	3: 6:15	1:34: 5	(5645.)	.00006	.00010	-.00004	.18011E-08
77	3: 6:20	1:34:10	(5650.)	.00004	.00007	-.00003	.10999E-08
78	3: 6:25	1:34:15	(5655.)	.00003	.00004	-.00001	.16196E-09
79	3: 6:30	1:34:20	(5660.)	.00001	.00001	.00000	.12051E-11
80	3: 6:35	1:34:25	(5665.)	.00000	-.00002	.00002	.44429E-09
81	3: 6:40	1:34:30	(5670.)	-.00005	-.00006	.00001	.26340E-10
82	3: 6:45	1:34:35	(5675.)	-.00009	-.00009	.00000	.13502E-11
83	3: 6:50	1:34:40	(5680.)	-.00012	-.00013	.00001	.49554E-10
84	3: 6:55	1:34:45	(5685.)	-.00017	-.00016	-.00001	.25655E-10
85	3: 7: 0	1:34:50	(5690.)	-.00021	-.00020	-.00001	.34205E-10
86	3: 7: 5	1:34:55	(5695.)	-.00025	-.00024	-.00001	.28007E-10
87	3: 7:10	1:35: 0	(5700.)	-.00028	-.00029	.00001	.43843E-10
88	3: 7:15	1:35: 5	(5705.)	-.00035	-.00033	-.00002	.36923E-09
89	3: 7:20	1:35:10	(5710.)	-.00038	-.00037	-.00001	.29340E-10
90	3: 7:25	1:35:15	(5715.)	-.00041	-.00042	.00001	.11363E-09
91	3: 7:30	1:35:20	(5720.)	-.00048	-.00047	-.00001	.11859E-09
92	3: 7:35	1:35:25	(5725.)	-.00054	-.00052	-.00002	.52610E-09
93	3: 7:40	1:35:30	(5730.)	-.00061	-.00057	-.00004	.18140E-08
94	3: 7:45	1:35:35	(5735.)	-.00066	-.00062	-.00004	.16652E-08
95	3: 7:50	1:35:40	(5740.)	-.00071	-.00067	-.00004	.13325E-08
96	3: 7:55	1:35:45	(5745.)	-.00077	-.00073	-.00004	.18406E-08
97	3: 8: 0	1:35:50	(5750.)	-.00081	-.00078	-.00003	.71713E-09
98	3: 8: 5	1:35:55	(5755.)	-.00088	-.00084	-.00004	.15373E-08
99	3: 8:10	1:36: 0	(5760.)	-.00092	-.00090	-.00002	.36114E-09
100	3: 8:15	1:36: 5	(5765.)	-.00098	-.00096	-.00002	.38969E-09
101	3: 8:20	1:36:10	(5770.)	-.00106	-.00102	-.00004	.13402E-08
102	3: 8:25	1:36:15	(5775.)	-.00112	-.00109	-.00003	.11937E-08
103	3: 8:30	1:36:20	(5780.)	-.00117	-.00115	-.00002	.34342E-09
104	3: 8:35	1:36:25	(5785.)	-.00123	-.00122	-.00001	.18839E-09
105	3: 8:40	1:36:30	(5790.)	-.00131	-.00128	-.00003	.68846E-09
106	3: 8:45	1:36:35	(5795.)	-.00137	-.00135	-.00002	.30254E-09
107	3: 8:50	1:36:40	(5800.)	-.00142	-.00142	.00000	.77672E-11
108	3: 8:55	1:36:45	(5805.)	-.00151	-.00149	-.00002	.24716E-09
109	3: 9: 0	1:36:50	(5810.)	-.00158	-.00157	-.00001	.13187E-09
110	3: 9: 5	1:36:55	(5815.)	-.00165	-.00164	-.00001	.79513E-10
111	3: 9:10	1:37: 0	(5820.)	-.00174	-.00172	-.00002	.49087E-09
112	3: 9:15	1:37: 5	(5825.)	-.00183	-.00179	-.00004	.13861E-08
113	3: 9:20	1:37:10	(5830.)	-.00193	-.00187	-.00006	.33744E-08
114	3: 9:25	1:37:15	(5835.)	-.00201	-.00195	-.00006	.37155E-08
115	3: 9:30	1:37:20	(5840.)	-.00212	-.00203	-.00009	.83173E-08
116	3: 9:35	1:37:25	(5845.)	-.00218	-.00211	-.00007	.47342E-08
117	3: 9:40	1:37:30	(5850.)	-.00226	-.00219	-.00007	.47171E-08
118	3: 9:45	1:37:35	(5855.)	-.00234	-.00228	-.00006	.41425E-08
119	3: 9:50	1:37:40	(5860.)	-.00241	-.00236	-.00005	.27552E-08
120	3: 9:55	1:37:45	(5865.)	-.00247	-.00244	-.00003	.70040E-09
121	3:10: 0	1:37:50	(5870.)	-.00255	-.00253	-.00002	.53202E-09
122	3:10: 5	1:37:55	(5875.)	-.00265	-.00261	-.00004	.12655E-08
123	3:10:10	1:38: 0	(5880.)	-.00273	-.00270	-.00003	.95393E-09

124	3:10:15	1:38: 5	(5885.)	-.00280	-.00279	-.00001	.14847E-09
125	3:10:20	1:38:10	(5890.)	-.00288	-.00287	-.00001	.41824E-10
126	3:10:25	1:38:15	(5895.)	-.00298	-.00296	-.00002	.34556E-09
127	3:10:30	1:38:20	(5900.)	-.00307	-.00305	-.00002	.22685E-09
128	3:10:35	1:38:25	(5905.)	-.00315	-.00314	-.00001	.14059E-09
129	3:10:40	1:38:30	(5910.)	-.00325	-.00323	-.00002	.45726E-09
130	3:10:45	1:38:35	(5915.)	-.00334	-.00332	-.00002	.59171E-09
131	3:10:50	1:38:40	(5920.)	-.00343	-.00341	-.00002	.56095E-09
132	3:10:55	1:38:45	(5925.)	-.00352	-.00349	-.00003	.70872E-09
133	3:11: 0	1:38:50	(5930.)	-.00360	-.00358	-.00002	.32072E-09
134	3:11: 5	1:38:55	(5935.)	-.00366	-.00367	.00001	.11239E-09
135	3:11:10	1:39: 0	(5940.)	-.00373	-.00376	.00003	.93497E-09
136	3:11:15	1:39: 5	(5945.)	-.00381	-.00385	.00004	.13448E-08
137	3:11:20	1:39:10	(5950.)	-.00387	-.00393	.00006	.41036E-08
138	3:11:25	1:39:15	(5955.)	-.00395	-.00402	.00007	.50268E-08
139	3:11:30	1:39:20	(5960.)	-.00405	-.00411	.00006	.32610E-08
140	3:11:35	1:39:25	(5965.)	-.00414	-.00419	.00005	.29465E-08
141	3:11:40	1:39:30	(5970.)	-.00422	-.00428	.00006	.32783E-08
142	3:11:45	1:39:35	(5975.)	-.00432	-.00436	.00004	.16830E-08
143	3:11:50	1:39:40	(5980.)	-.00440	-.00445	.00005	.20650E-08
144	3:11:55	1:39:45	(5985.)	-.00449	-.00453	.00004	.12606E-08
145	3:12: 0	1:39:50	(5990.)	-.00458	-.00461	.00003	.76350E-09
146	3:12: 5	1:39:55	(5995.)	-.00466	-.00469	.00003	.64115E-09
147	3:12:10	1:40: 0	(6000.)	-.00476	-.00476	.00000	.10640E-10
148	3:12:15	1:40: 5	(6005.)	-.00482	-.00484	.00002	.39110E-09
149	3:12:20	1:40:10	(6010.)	-.00489	-.00491	.00002	.61401E-09
150	3:12:25	1:40:15	(6015.)	-.00495	-.00499	.00004	.14582E-08
151	3:12:30	1:40:20	(6020.)	-.00502	-.00506	.00004	.15933E-08
152	3:12:35	1:40:25	(6025.)	-.00508	-.00513	.00005	.24887E-08
153	3:12:40	1:40:30	(6030.)	-.00518	-.00520	.00002	.32469E-09
154	3:12:45	1:40:35	(6035.)	-.00524	-.00527	.00003	.65201E-09
155	3:12:50	1:40:40	(6040.)	-.00529	-.00533	.00004	.14792E-08
156	3:12:55	1:40:45	(6045.)	-.00535	-.00539	.00004	.17503E-08
157	3:13: 0	1:40:50	(6050.)	-.00542	-.00545	.00003	.93893E-09
158	3:13: 5	1:40:55	(6055.)	-.00547	-.00551	.00004	.15672E-08
159	3:13:10	1:41: 0	(6060.)	-.00553	-.00556	.00003	.11563E-08
160	3:13:15	1:41: 5	(6065.)	-.00559	-.00562	.00003	.74053E-09
161	3:13:20	1:41:10	(6070.)	-.00565	-.00567	.00002	.40032E-09
162	3:13:25	1:41:15	(6075.)	-.00569	-.00572	.00003	.69593E-09
163	3:13:30	1:41:20	(6080.)	-.00577	-.00576	-.00001	.60437E-10
164	3:13:35	1:41:25	(6085.)	-.00580	-.00581	.00001	.30341E-10
165	3:13:40	1:41:30	(6090.)	-.00583	-.00585	.00002	.26175E-09
166	3:13:45	1:41:35	(6095.)	-.00587	-.00588	.00001	.20139E-09
167	3:13:50	1:41:40	(6100.)	-.00590	-.00592	.00002	.38039E-09
168	3:13:55	1:41:45	(6105.)	-.00593	-.00595	.00002	.48738E-09
169	3:14: 0	1:41:50	(6110.)	-.00596	-.00598	.00002	.47852E-09
170	3:14: 5	1:41:55	(6115.)	-.00600	-.00601	.00001	.87906E-10
171	3:14:10	1:42: 0	(6120.)	-.00602	-.00603	.00001	.16961E-09
172	3:14:15	1:42: 5	(6125.)	-.00605	-.00605	.00000	.22235E-10
173	3:14:20	1:42:10	(6130.)	-.00609	-.00607	-.00002	.29803E-09
174	3:14:25	1:42:15	(6135.)	-.00611	-.00609	-.00002	.47285E-09
175	3:14:30	1:42:20	(6140.)	-.00611	-.00610	-.00001	.79510E-10
176	3:14:35	1:42:25	(6145.)	-.00611	-.00611	.00000	.29947E-12
177	3:14:45	1:42:35	(6155.)	-.00612	-.00612	.00000	.12873E-11
178	3:14:50	1:42:40	(6160.)	-.00613	-.00612	-.00001	.63430E-10
179	3:14:55	1:42:45	(6165.)	-.00614	-.00612	-.00002	.39943E-09
180	3:15: 0	1:42:50	(6170.)	-.00614	-.00611	-.00003	.64056E-09
181	3:15: 5	1:42:55	(6175.)	-.00611	-.00611	.00000	.76020E-11
182	3:15:10	1:43: 0	(6180.)	-.00608	-.00610	.00002	.26501E-09
183	3:15:15	1:43: 5	(6185.)	-.00608	-.00608	.00000	.69519E-11
184	3:15:20	1:43:10	(6190.)	-.00607	-.00607	.00000	.12187E-10
185	3:15:25	1:43:15	(6195.)	-.00605	-.00605	.00000	.98873E-11
186	3:15:30	1:43:20	(6200.)	-.00603	-.00603	.00000	.22646E-10
187	3:15:35	1:43:25	(6205.)	-.00598	-.00600	.00002	.39773E-09
188	3:15:40	1:43:30	(6210.)	-.00595	-.00597	.00002	.52778E-09
189	3:15:45	1:43:35	(6215.)	-.00593	-.00594	.00001	.14837E-09
190	3:15:50	1:43:40	(6220.)	-.00589	-.00591	.00002	.40051E-09
191	3:15:55	1:43:45	(6225.)	-.00585	-.00587	.00002	.57126E-09

192	3:16: 0	1:43:50	(6230.)	-.00583	-.00584	.00001	.45087E-10
193	3:16: 5	1:43:55	(6235.)	-.00582	-.00580	-.00002	.60108E-09
194	3:16:10	1:44: 0	(6240.)	-.00576	-.00575	-.00001	.42507E-10
195	3:16:15	1:44: 5	(6245.)	-.00569	-.00571	.00002	.33393E-09
196	3:16:20	1:44:10	(6250.)	-.00565	-.00566	.00001	.95702E-10
197	3:16:25	1:44:15	(6255.)	-.00558	-.00561	.00003	.95962E-09
198	3:16:30	1:44:20	(6260.)	-.00554	-.00556	.00002	.32240E-09
199	3:16:35	1:44:25	(6265.)	-.00551	-.00550	-.00001	.25778E-10
200	3:16:40	1:44:30	(6270.)	-.00546	-.00545	-.00001	.12599E-09
201	3:16:45	1:44:35	(6275.)	-.00538	-.00539	.00001	.89524E-10
202	3:16:50	1:44:40	(6280.)	-.00532	-.00533	.00001	.11206E-09
203	3:16:55	1:44:45	(6285.)	-.00525	-.00527	.00002	.30398E-09
204	3:17: 0	1:44:50	(6290.)	-.00518	-.00521	.00003	.62571E-09
205	3:17: 5	1:44:55	(6295.)	-.00513	-.00514	.00001	.93010E-10
206	3:17:10	1:45: 0	(6300.)	-.00508	-.00507	-.00001	.75671E-10
207	3:17:15	1:45: 5	(6305.)	-.00502	-.00500	-.00002	.25239E-09
208	3:17:20	1:45:10	(6310.)	-.00495	-.00493	-.00002	.29941E-09
209	3:17:25	1:45:15	(6315.)	-.00489	-.00486	-.00003	.99959E-09
210	3:17:30	1:45:20	(6320.)	-.00482	-.00479	-.00003	.90023E-09
211	3:17:35	1:45:25	(6325.)	-.00473	-.00471	-.00002	.23821E-09
212	3:17:40	1:45:30	(6330.)	-.00468	-.00464	-.00004	.15249E-08
213	3:17:45	1:45:35	(6335.)	-.00461	-.00456	-.00005	.21860E-08
214	3:17:50	1:45:40	(6340.)	-.00453	-.00449	-.00004	.17979E-08
215	3:17:55	1:45:45	(6345.)	-.00447	-.00441	-.00006	.36596E-08
216	3:18: 0	1:45:50	(6350.)	-.00438	-.00433	-.00005	.24432E-08
217	3:18: 5	1:45:55	(6355.)	-.00427	-.00425	-.00002	.42931E-09
218	3:18:10	1:46: 0	(6360.)	-.00421	-.00417	-.00004	.15608E-08
219	3:18:15	1:46: 5	(6365.)	-.00415	-.00409	-.00006	.38584E-08
220	3:18:20	1:46:10	(6370.)	-.00407	-.00401	-.00006	.38464E-08
221	3:18:25	1:46:15	(6375.)	-.00398	-.00393	-.00005	.29160E-08
222	3:18:30	1:46:20	(6380.)	-.00389	-.00384	-.00005	.21495E-08
223	3:18:35	1:46:25	(6385.)	-.00381	-.00376	-.00005	.24046E-08
224	3:18:40	1:46:30	(6390.)	-.00373	-.00368	-.00005	.26987E-08
225	3:18:45	1:46:35	(6395.)	-.00363	-.00359	-.00004	.12270E-08
226	3:18:50	1:46:40	(6400.)	-.00356	-.00351	-.00005	.23239E-08
227	3:18:55	1:46:45	(6405.)	-.00345	-.00343	-.00002	.45863E-09
228	3:19: 0	1:46:50	(6410.)	-.00337	-.00335	-.00002	.60460E-09
229	3:19: 5	1:46:55	(6415.)	-.00330	-.00326	-.00004	.14184E-08
230	3:19:10	1:47: 0	(6420.)	-.00322	-.00318	-.00004	.16459E-08
231	3:19:15	1:47: 5	(6425.)	-.00315	-.00310	-.00005	.28359E-08
232	3:19:20	1:47:10	(6430.)	-.00308	-.00301	-.00007	.43101E-08
233	3:19:25	1:47:15	(6435.)	-.00302	-.00293	-.00009	.76925E-08
234	3:19:30	1:47:20	(6440.)	-.00289	-.00285	-.00004	.16798E-08
235	3:19:35	1:47:25	(6445.)	-.00279	-.00277	-.00002	.42295E-09
236	3:19:40	1:47:30	(6450.)	-.00270	-.00269	-.00001	.12685E-09
237	3:19:45	1:47:35	(6455.)	-.00260	-.00261	.00001	.73895E-10
238	3:19:50	1:47:40	(6460.)	-.00254	-.00253	-.00001	.15671E-09
239	3:19:55	1:47:45	(6465.)	-.00245	-.00245	.00000	.30311E-13
240	3:20: 0	1:47:50	(6470.)	-.00234	-.00237	.00003	.92619E-09
241	3:20: 5	1:47:55	(6475.)	-.00228	-.00229	.00001	.21115E-09
242	3:20:10	1:48: 0	(6480.)	-.00222	-.00222	.00000	.13416E-10
243	3:20:15	1:48: 5	(6485.)	-.00216	-.00214	-.00002	.32406E-09
244	3:20:20	1:48:10	(6490.)	-.00207	-.00206	-.00001	.55903E-10
245	3:20:25	1:48:15	(6495.)	-.00199	-.00199	.00000	.82594E-11
246	3:20:30	1:48:20	(6500.)	-.00193	-.00192	-.00001	.10662E-09
247	3:20:35	1:48:25	(6505.)	-.00186	-.00185	-.00001	.19616E-09
248	3:20:40	1:48:30	(6510.)	-.00179	-.00178	-.00001	.19180E-09
249	3:20:45	1:48:35	(6515.)	-.00172	-.00170	-.00002	.24050E-09
250	3:20:50	1:48:40	(6520.)	-.00164	-.00164	.00000	.11289E-10
251	3:20:55	1:48:45	(6525.)	-.00157	-.00157	.00000	.84028E-11
252	3:21: 0	1:48:50	(6530.)	-.00150	-.00150	.00000	.17649E-11
253	3:21: 5	1:48:55	(6535.)	-.00146	-.00143	-.00003	.74658E-09
254	3:21:10	1:49: 0	(6540.)	-.00140	-.00137	-.00003	.87782E-09
255	3:21:15	1:49: 5	(6545.)	-.00133	-.00131	-.00002	.60970E-09
256	3:21:20	1:49:10	(6550.)	-.00127	-.00124	-.00003	.68138E-09
257	3:21:25	1:49:15	(6555.)	-.00122	-.00118	-.00004	.15087E-08
258	3:21:30	1:49:20	(6560.)	-.00115	-.00112	-.00003	.78393E-09
259	3:21:35	1:49:25	(6565.)	-.00107	-.00106	-.00001	.51928E-10

260	3:21:40	1:49:30	(6570.)	-.00100	-.00100	.00000	.13045E-10
261	3:21:45	1:49:35	(6575.)	-.00093	-.00095	.00002	.32015E-09
262	3:21:50	1:49:40	(6580.)	-.00086	-.00089	.00003	.96780E-09
263	3:21:55	1:49:45	(6585.)	-.00080	-.00084	.00004	.14214E-08
264	3:22: 0	1:49:50	(6590.)	-.00074	-.00078	.00004	.19691E-08
265	3:22: 5	1:49:55	(6595.)	-.00067	-.00073	.00006	.38724E-08
266	3:22:10	1:50: 0	(6600.)	-.00059	-.00068	.00009	.81461E-08
267	3:22:15	1:50: 5	(6605.)	-.00054	-.00063	.00009	.78349E-08
268	3:22:20	1:50:10	(6610.)	-.00049	-.00058	.00009	.86187E-08
269	3:22:25	1:50:15	(6615.)	-.00044	-.00053	.00009	.89190E-08
270	3:22:30	1:50:20	(6620.)	-.00040	-.00049	.00009	.79330E-08
271	3:22:35	1:50:25	(6625.)	-.00035	-.00044	.00009	.86530E-08
272	3:22:40	1:50:30	(6630.)	-.00031	-.00040	.00009	.80805E-08
273	3:22:45	1:50:35	(6635.)	-.00027	-.00036	.00009	.75696E-08
274	3:22:50	1:50:40	(6640.)	-.00025	-.00031	.00006	.40430E-08
275	3:22:55	1:50:45	(6645.)	-.00019	-.00027	.00008	.70180E-08
276	3:23: 0	1:50:50	(6650.)	-.00016	-.00024	.00008	.56259E-08
277	3:23: 5	1:50:55	(6655.)	-.00016	-.00020	.00004	.13338E-08
278	3:23:10	1:51: 0	(6660.)	-.00009	-.00016	.00007	.47755E-08
279	3:23:15	1:51: 5	(6665.)	-.00003	-.00012	.00009	.84694E-08
280	3:23:20	1:51:10	(6670.)	.00000	-.00009	.00009	.76422E-08
281	3:23:25	1:51:15	(6675.)	.00001	-.00005	.00006	.39841E-08
282	3:23:30	1:51:20	(6680.)	.00003	-.00002	.00005	.24827E-08
283	3:23:35	1:51:25	(6685.)	.00005	.00001	.00004	.14081E-08
284	3:23:40	1:51:30	(6690.)	.00009	.00004	.00005	.21341E-08
285	3:23:45	1:51:35	(6695.)	.00014	.00007	.00007	.43328E-08
286	3:23:50	1:51:40	(6700.)	.00018	.00010	.00008	.58356E-08
287	3:23:55	1:51:45	(6705.)	.00019	.00013	.00006	.33500E-08
288	3:24: 0	1:51:50	(6710.)	.00019	.00016	.00003	.88380E-09
289	3:24: 5	1:51:55	(6715.)	.00022	.00019	.00003	.11253E-08
290	3:24:10	1:52: 0	(6720.)	.00024	.00021	.00003	.76651E-09
291	3:24:15	1:52: 5	(6725.)	.00025	.00024	.00001	.14848E-09
292	3:24:20	1:52:10	(6730.)	.00029	.00026	.00003	.78497E-09
293	3:24:25	1:52:15	(6735.)	.00031	.00029	.00002	.60809E-09
294	3:24:30	1:52:20	(6740.)	.00033	.00031	.00002	.48806E-09
295	3:24:35	1:52:25	(6745.)	.00036	.00033	.00003	.91785E-09
296	3:24:40	1:52:30	(6750.)	.00041	.00035	.00006	.35109E-08
297	3:24:45	1:52:35	(6755.)	.00044	.00037	.00007	.47531E-08
298	3:24:50	1:52:40	(6760.)	.00045	.00039	.00006	.35221E-08
299	3:24:55	1:52:45	(6765.)	.00045	.00041	.00004	.16662E-08
300	3:25: 0	1:52:50	(6770.)	.00046	.00043	.00003	.10386E-08
301	3:25: 5	1:52:55	(6775.)	.00048	.00044	.00004	.12257E-08
302	3:25:10	1:53: 0	(6780.)	.00052	.00046	.00006	.33728E-08
303	3:25:15	1:53: 5	(6785.)	.00054	.00048	.00006	.38150E-08
304	3:25:20	1:53:10	(6790.)	.00054	.00049	.00005	.21215E-08
305	3:25:25	1:53:15	(6795.)	.00054	.00051	.00003	.95745E-09
306	3:25:30	1:53:20	(6800.)	.00055	.00052	.00003	.69671E-09
307	3:25:35	1:53:25	(6805.)	.00055	.00054	.00001	.15378E-09
308	3:25:40	1:53:30	(6810.)	.00056	.00055	.00001	.79956E-10
309	3:25:45	1:53:35	(6815.)	.00058	.00056	.00002	.25687E-09
310	3:25:50	1:53:40	(6820.)	.00058	.00058	.00000	.12711E-10
311	3:25:55	1:53:45	(6825.)	.00059	.00059	.00000	.26072E-11
312	3:26: 0	1:53:50	(6830.)	.00061	.00060	.00001	.10271E-09
313	3:26: 5	1:53:55	(6835.)	.00063	.00061	.00002	.36519E-09
314	3:26:10	1:54: 0	(6840.)	.00061	.00062	-.00001	.13168E-09
315	3:26:15	1:54: 5	(6845.)	.00061	.00063	-.00002	.46809E-09
316	3:26:20	1:54:10	(6850.)	.00063	.00064	-.00001	.12963E-09
317	3:26:25	1:54:15	(6855.)	.00063	.00065	-.00002	.43014E-09
318	3:26:30	1:54:20	(6860.)	.00064	.00066	-.00002	.38858E-09
319	3:26:35	1:54:25	(6865.)	.00066	.00067	-.00001	.69168E-10
320	3:26:40	1:54:30	(6870.)	.00068	.00068	.00000	.11790E-10
321	3:26:45	1:54:35	(6875.)	.00069	.00068	.00001	.27209E-10
322	3:26:50	1:54:40	(6880.)	.00073	.00069	.00004	.14400E-08
323	3:26:55	1:54:45	(6885.)	.00073	.00070	.00003	.94159E-09
324	3:27: 0	1:54:50	(6890.)	.00070	.00071	-.00001	.39336E-10
325	3:27: 5	1:54:55	(6895.)	.00070	.00071	-.00001	.16734E-09
326	3:27:10	1:55: 0	(6900.)	.00072	.00072	.00000	.46430E-12
327	3:27:15	1:55: 5	(6905.)	.00074	.00073	.00001	.21227E-09

328	3:27:20	1:55:10	(6910.)	.00074	.00073	.00001	.75993E-10
329	3:27:25	1:55:15	(6915.)	.00076	.00074	.00002	.53429E-09
330	3:27:30	1:55:20	(6920.)	.00075	.00074	.00001	.60087E-10
331	3:27:35	1:55:25	(6925.)	.00075	.00075	.00000	.68540E-11
332	3:27:40	1:55:30	(6930.)	.00076	.00075	.00001	.59360E-10
333	3:27:45	1:55:35	(6935.)	.00075	.00076	-.00001	.48971E-10
334	3:27:50	1:55:40	(6940.)	.00073	.00076	-.00003	.10033E-08
335	3:27:55	1:55:45	(6945.)	.00071	.00077	-.00006	.31142E-08
336	3:28: 0	1:55:50	(6950.)	.00074	.00077	-.00003	.90529E-09
337	3:28: 5	1:55:55	(6955.)	.00074	.00077	-.00003	.11473E-08
338	3:28:10	1:56: 0	(6960.)	.00076	.00078	-.00002	.31138E-09
339	3:28:15	1:56: 5	(6965.)	.00077	.00078	-.00001	.12676E-09
340	3:28:20	1:56:10	(6970.)	.00078	.00078	.00000	.22247E-10
341	3:28:25	1:56:15	(6975.)	.00078	.00079	-.00001	.64428E-10
342	3:28:35	1:56:25	(6985.)	.00080	.00079	.00001	.33302E-10
343	3:28:40	1:56:30	(6990.)	.00077	.00080	-.00003	.73628E-09
344	3:28:45	1:56:35	(6995.)	.00076	.00080	-.00004	.15934E-08
345	3:28:50	1:56:40	(7000.)	.00077	.00080	-.00003	.10616E-08
346	3:28:55	1:56:45	(7005.)	.00077	.00081	-.00004	.12346E-08
347	3:29: 0	1:56:50	(7010.)	.00077	.00081	-.00004	.14126E-08
348	3:29: 5	1:56:55	(7015.)	.00078	.00081	-.00003	.89583E-09
349	3:29:10	1:57: 0	(7020.)	.00077	.00081	-.00004	.17792E-08
350	3:29:15	1:57: 5	(7025.)	.00078	.00081	-.00003	.11792E-08
351	3:29:20	1:57:10	(7030.)	.00080	.00082	-.00002	.26931E-09
352	3:29:25	1:57:15	(7035.)	.00078	.00082	-.00004	.14745E-08
353	3:29:30	1:57:20	(7040.)	.00076	.00082	-.00006	.36371E-08
354	3:29:35	1:57:25	(7045.)	.00076	.00082	-.00006	.38707E-08
355	3:29:40	1:57:30	(7050.)	.00077	.00082	-.00005	.29060E-08
356	3:29:45	1:57:35	(7055.)	.00077	.00083	-.00006	.30917E-08
357	3:29:50	1:57:40	(7060.)	.00079	.00083	-.00004	.13864E-08
358	3:29:55	1:57:45	(7065.)	.00080	.00083	-.00003	.82976E-09
359	3:30: 0	1:57:50	(7070.)	.00080	.00083	-.00003	.91926E-09
360	3:30: 5	1:57:55	(7075.)	.00082	.00083	-.00001	.13872E-09
361	3:30:10	1:58: 0	(7080.)	.00082	.00083	-.00001	.17530E-09
362	3:30:15	1:58: 5	(7085.)	.00080	.00083	-.00003	.11932E-08
363	3:30:20	1:58:10	(7090.)	.00080	.00084	-.00004	.12855E-08
364	3:30:25	1:58:15	(7095.)	.00078	.00084	-.00006	.32628E-08
365	3:30:30	1:58:20	(7100.)	.00077	.00084	-.00007	.46712E-08
366	3:30:35	1:58:25	(7105.)	.00077	.00084	-.00007	.48412E-08
367	3:30:40	1:58:30	(7110.)	.00079	.00084	-.00005	.25708E-08
368	3:30:45	1:58:35	(7115.)	.00080	.00084	-.00004	.17467E-08
369	3:30:50	1:58:40	(7120.)	.00079	.00084	-.00005	.27979E-08
370	3:30:55	1:58:45	(7125.)	.00079	.00084	-.00005	.29076E-08
371	3:31: 0	1:58:50	(7130.)	.00081	.00084	-.00003	.12208E-08

END OF DATA

APPENDIX C

CORRECTED DIFFUSION COEFFICIENTS IN THE SOLVENTS N-HEPTANE, N-DODECANE, AND N-HEXADECANE

Table C.1 Corrected Infinite Dilution Diffusion Coefficients for Alkanes in n–Heptane, n–Dodecane, and n–Hexadecane ($D^{o}_{12} \times 10^{9}$ m^2/s, ± 1 standard deviation)

T (K)	P (kPa)	C_8	C_{10}	C_{12}	C_{14}	C_{16}
			Solvent: n–Heptane			
298	101	2.82 ± 0.07	–	2.21 ± 0.08	1.92 ± 0.15	1.83 ± 0.04
374	3480	6.12 ± 0.14	5.45 ± 0.02	4.90 ± 0.04	4.45 ± 0.03	4.03 ± 0.02
427	710	–	8.93 ± 0.01	–	–	6.87 ± 0.01
427	3460	9.79 ± 0.09	8.69 ± 0.01	7.73 ± 0.03	6.87 ± 0.01	6.43 ± 0.01
476	1410	–	12.9 ± 0.2	–	–	10.8 ± 0.0
476	3480	15.3 ± 0.0	13.0 ± 0.0	11.9 ± 0.0	10.8 ± 0.0	10.1 ± 0.1
			Solvent: n–Dodecane			
304	1410	1.27 ± 0.02	1.09 ± 0.04	–	0.83	–
373	1410	3.33 ± 0.02	2.95 ± 0.12	–	2.05 ± 0.16	1.96 ± 0.06
373	3440	3.49 ± 0.16	–	–	–	–
443	1450	6.79 ± 0.12	5.83 ± 0.06	–	4.26 ± 0.13	4.01 ± 0.03
443	3450	6.79 ± 0.20	–	–	–	–
513	1450	11.5 ± 0.01	9.71 ± 0.00	–	7.45 ± 0.40	7.04 ± 0.13
515	3430	11.2 ± 0.1	–	–	–	–
566	1460	17.3 ± 0.1	15.1 ± 0.2	–	12.2 ± 0.1	11.2 ± 0.1
566	3440	16.2 ± 0.1	–	–	–	–
			Solvent: n–Hexadecane			
323	1420	1.19 ± 0.03	0.99 ± 0.02	0.95 ± 0.09	–	–
323	3459	1.25 ± 0.09	–	–	–	–
371	1402	2.31 ± 0.02	2.06 ± 0.03	–	–	–
371	3444	2.36 ± 0.02	–	–	–	–
443	1383	5.19 ± 0.08	4.35 ± 0.05	4.09 ± 0.11	–	–
443	3425	5.05 ± 0.07	–	–	–	–
514	1412	9.50 ± 0.44	–	7.08 ± 0.21	–	–
514	3427	9.10 ± 0.52	–	–	–	–
564	1404	13.1 ± 0.3	12.5 ± 0.7	10.4 ± 0.7	–	–
564	3408	12.7 ± 0.1	–	–	–	–

Table C.2 Corrected Infinite Dilution Diffusion Coefficients for Gases in n–Heptane, n–Dodecane, and n–Hexadecane
($D^{o}_{12} \times 10^{9}$ m^2/sec, ± 1 standard deviation)

T (K)	P (kPa)	H_2	CO	CO_2
		Solvent: n–Heptane		
298	101	20.9 ± 0.4	6.41 ± 0.30	–
427	3450	63.5 ± 0.3	24.1 ± 0.2	–
		Solvent: n–Dodecane		
304	1390	10.7 ± 0.1	4.69 ± 0.12	3.84 ± 0.01
372	1410	25.8 ± 0.1	9.69 ± 0.11	8.61 ± 0.03
372	3440	24.0 ± 0.1	9.29± 0.03	8.60 ± 0.02
445	1450	45.5 ± 0.4	17.3 ± 0.1	15.8 ± 0.1
443	3450	41.6 ± 0.1	18.0 ± 0.3	15.9 ± 0.2
513	1450	76.7 ± 0.1	28.5 ± 0.1	25.6 ± 0.1
515	3440	72.2 ± 0.4	26.5 ± 0.5	25.1 ± 0.2
567	1460	114 ± 1.0	44.3 ± 0.3	37.8 ± 0.3
567	3440	109 ± 0.2	46.2 ± 1.6	35.8 ± 0.3
		Solvent: n–Hexadecane		
323	1420	10.4 ± 0.1	4.39 ± 0.36	3.55 ± 0.01
323	3460	–	3.63 ± 0.07	3.47 ± 0.04
371	1400	19.4 ± 0.1	6.57 ± 0.15	6.52 ± 0.01
371	3440	18.5 ± 0.1	6.75 ± 0.13	6.39 ± 0.06
443	1400	34.5 ± 0.4	14.0 ± 0.1	12.6 ± 0.1
443	3430	35.7 ± 0.3	13.5 ± 0.2	12.3 ± 0.0
513	1410	55.8 ± 1.8	23.1 ± 0.4	20.5 ± 0.0
513	3430	56.1 ± 0.3	22.0 ± 0.2	20.2 ± 0.0
564	1400	79.3 ± 2.4	33.2 ± 0.4	28.3 ± 0.1
564	3410	72.4 ± 2.2	30.1 ± 0.4	27.6 ± 0.2

APPENDIX D

TABULATION OF LITERATURE DIFFUSION COEFFICIENTS VERSUS THE PREDICTIONS OF EQUATION 7.8

Table D.1. List of References for Table D.2

No.	Reference
1	Rossi and Bianchi (1961)
2	Van Geet and Adamson (1964)
3	Bidlack and Anderson (1964b)
4	Bidlack and Anderson (1964a)
5	Bidlack et al. (1969)
6	Shieh and Lyons (1969)
7	Malik and Hayduk (1968)
8	Hayduk and Cheng (1971)
9	Hayduk and Buckley (1972)
10	Hayduk et al.(1972)
11	Lo (1974)
12	Moore and Wellek (1974)
13	Hayduk and Iokimidis (1976)
14	Evans et al. (1979)
15	Chen et al. (1982)
16	Alizadeh and Wakeham (1982)

Table D.2. Predictions of n-Alkane Literature Data by Equation 7.8
($10^9 D^o_{12}$, m^2/sec; 1 = solute; 2 = solvent)
(All Data at Atmospheric Pressure)

Ref.	C#, 1	C#, 2	T (C)	$D^o_{12,\ meas.}$	$D^o_{12,\ Eq.7.8}$	% Error
1	10	7	20	2.06	2.09	1.3
1	14	7	20	1.65	1.58	-4.3
1	18	7	20	1.46	1.27	-13.0
1	28	7	20	1.08	0.83	-22.7
1	32	7	20	1.00	0.73	-27.3
2	8	8	25	2.36	2.11	-10.7
2	8	8	60	3.55	3.59	1.2
2	12	8	25	1.72	1.51	-12.0
2	12	8	60	2.72	2.67	-1.7
2	18	8	25	1.20	1.05	-12.2
2	8	12	25	1.14	0.89	-21.8
2	8	12	60	1.98	1.94	-2.0
2	12	12	25	0.81	0.58	-28.2
2	12	12	60	1.48	1.40	-5.4
2	18	12	25	0.60	0.35	-42.1
2	18	12	60	1.04	0.98	-5.4
2	18	18	60	0.53	0.47	-12.1
3	6	16	25	0.87	0.56	-35.8
3	16	6	25	2.19	2.09	-4.7
4	16	7	25	1.78	1.55	-12.9
4	7	16	25	0.76	0.47	-38.9
4	12	6	25	2.73	2.62	-4.2
4	6	12	25	1.45	1.16	-19.7
5	5	6	25	4.59	4.91	7.0
5	6	6	25	4.21	4.33	3.0
5	7	6	25	3.78	3.89	2.9
5	8	6	25	3.47	3.54	1.9
5	10	6	25	3.02	3.00	-0.6
5	12	6	25	2.74	2.62	-4.6
5	16	6	25	2.21	2.09	-5.6
5	18	6	25	2.01	1.90	-5.6
6	6	12	25	1.40	1.16	-16.8
6	12	6	25	2.72	2.62	-3.9
6	6	12	35	1.67	1.50	-10.2
6	12	6	35	3.06	3.03	-0.8
6	12	16	25	0.57	0.20	-64.3
6	16	12	25	0.95	0.41	-57.0
6	8	16	25	0.68	0.39	-42.5
6	16	8	25	1.43	1.18	-17.8
7	2	6	30	6.01	9.28	54.4
7	2	7	30	5.60	7.31	30.5
7	2	7	40	6.70	8.32	24.1
8	2	6	25	5.79	8.71	50.4
8	2	7	25	5.44	6.82	25.5
8	2	8	25	4.57	5.49	20.2

Table D.2. (continued)

Ref.	C#, 1	C#, 2	T (C)	$D^o_{12,\text{ meas.}}$	$D^o_{12,\text{ Eq.7.8}}$	% Error
8	2	12	25	2.73	2.70	-1.0
8	2	16	25	1.95	1.52	-22.0
9	1	6	25	8.64	12.54	45.2
9	1	7	25	7.52	9.90	31.1
9	1	8	25	6.49	8.02	23.6
9	1	12	25	3.94	4.08	3.5
9	1	16	25	2.66	2.40	-9.9
10	3	6	25	4.87	6.84	40.4
10	3	7	25	4.40	5.33	21.1
10	3	8	25	3.83	4.26	11.3
10	3	16	25	1.48	1.10	-25.5
11	7	10	25	1.75	1.50	-14.1
11	10	7	25	2.54	2.27	-10.5
11	7	12	25	1.35	1.01	-25.0
11	12	7	25	2.15	1.97	-8.5
11	7	14	25	0.97	0.69	-28.9
11	14	7	25	1.89	1.73	-8.2
11	8	14	25	0.88	0.60	-32.3
11	14	8	25	1.63	1.32	-18.7
12	7	7	20	3.10	2.75	-11.4
12	7	7	25	3.12	2.98	-4.5
12	7	7	30	3.22	3.22	0.0
12	7	8	20	2.33	2.13	-8.3
12	7	8	25	2.50	2.33	-6.4
12	7	8	30	2.35	2.55	8.5
12	7	8	40	2.74	2.99	9.1
12	7	9	20	1.84	1.67	-9.0
12	7	9	25	2.02	1.86	-8.1
12	7	9	30	1.97	2.04	3.8
12	7	10	20	1.52	1.33	-12.2
12	7	10	25	1.61	1.50	-6.7
12	7	10	30	1.58	1.68	6.1
12	10	6	20	4.20	2.78	-33.8
12	10	6	25	4.63	3.00	-35.2
12	10	6	30	5.00	3.23	-35.4
12	10	7	20	2.97	2.09	-29.8
12	10	7	25	3.08	2.27	-26.2
12	10	7	30	3.48	2.47	-29.1
12	10	7	40	3.82	2.87	-24.8
12	10	8	20	2.12	1.60	-24.6
12	10	8	25	2.40	1.76	-26.5
12	10	8	30	2.52	1.93	-23.3
12	10	8	40	2.96	2.29	-22.7
12	10	9	20	1.60	1.23	-23.0
12	10	9	25	1.90	1.38	-27.4
12	10	9	30	2.05	1.53	-25.3
12	10	9	40	2.22	1.85	-16.9

Table D.2. (continued)

Ref.	C#, 1	C#, 2	T (C)	$D^o_{12,\ \mathrm{meas.}}$	$D^o_{12,\ \mathrm{Eq.7.8}}$	% Error
12	10	10	20	1.44	0.96	-33.2
12	10	10	25	1.55	1.10	-29.1
12	10	10	30	1.68	1.24	-26.3
12	10	10	40	1.86	1.53	-17.9
13	12	6	25	2.72	2.62	-3.9
13	24	6	25	1.60	1.49	-6.8
13	32	6	25	1.36	1.15	-15.1
13	24	8	25	1.09	0.80	-27.0
13	32	8	25	0.92	0.58	-36.5
13	24	12	25	0.45	0.22	-51.5
14	1	6	25	8.73	12.54	44.7
14	1	10	25	4.38	5.55	26.7
14	1	14	25	2.78	3.10	11.2
15	1	8	25	6.08	8.02	31.9
15	1	8	60	9.45	12.54	32.7
15	1	8	100	14.20	18.92	33.3
15	1	8	130	18.10	24.85	37.3
15	1	10	25	4.38	5.55	26.7
15	1	10	60	7.16	9.23	28.9
15	1	10	160	18.80	24.46	30.1
15	1	14	25	2.78	3.09	11.2
15	1	14	70	5.47	6.88	25.7
15	1	14	101	7.80	10.00	28.2
15	1	14	157	13.00	16.90	30.0
16	6	7	27	3.41	3.44	0.8
16	6	7	35	3.65	3.87	5.9
16	6	7	42	4.17	4.26	2.1
16	6	7	50	4.56	4.72	3.6
16	6	7	55	4.83	5.03	4.1
16	6	7	60	5.04	5.34	6.0
16	7	6	27	3.72	4.00	7.6
16	7	6	35	4.12	4.47	8.5
16	7	6	42	4.55	4.90	7.8
16	7	6	50	4.86	5.42	11.6
16	7	6	55	5.10	5.76	13.0
16	6	8	22	2.34	2.49	6.5
16	6	8	27	2.57	2.72	5.8
16	6	8	35	2.97	3.10	4.2
16	6	8	42	3.30	3.44	4.2
16	6	8	50	3.67	3.84	4.9
16	6	8	60	4.13	4.38	6.2
16	8	6	22	3.25	3.28	4.1
16	8	6	27	3.48	3.64	4.6
16	8	6	35	3.85	4.07	5.8
16	8	6	42	4.16	4.47	7.5
16	8	6	50	4.57	4.95	8.3
16	8	6	55	4.79	5.26	9.9

Table D.2. Predictions of n-Alkane Literature Data by Equation 7.8
($10^9 D^o_{12}$, m^2/sec; 1 = solute; 2 = solvent)
(All Data at Atmospheric Pressure)

Ref.	C#, 1	C#, 2	T (C)	$D^o_{12,\ \mathrm{meas.}}$	$D^o_{12,\ \mathrm{Eq.7.8}}$	% Error
16	7	8	20	2.23	2.13	-4.3
16	7	8	35	2.88	2.77	-4.0
16	7	8	50	3.46	3.45	-0.2
16	7	8	60	3.89	3.95	1.4
16	7	8	70	4.35	4.47	2.7
16	8	7	20	2.59	2.48	-4.1
16	8	7	35	3.21	3.15	-1.9
16	8	7	50	3.82	3.87	1.3
16	8	7	60	4.24	4.39	3.5
16	8	7	70	4.74	4.94	4.3

Table D.2. Predictions of n-Alkane Literature Data by Equation 7.8
($10^9 D^o_{12}$, m^2/sec; 1 = solute; 2 = solvent)
(All Data at Atmospheric Pressure)

Ref.	C#, 1	C#, 2	T (C)	$D^o_{12,\ meas.}$	$D^o_{12,\ Eq.7.8}$	% Error
16	7	8	20	2.23	2.13	-4.3
16	7	8	35	2.88	2.77	-4.0
16	7	8	50	3.46	3.45	-0.2
16	7	8	60	3.89	3.95	1.4
16	7	8	70	4.35	4.47	2.7
16	8	7	20	2.59	2.48	-4.1
16	8	7	35	3.21	3.15	-1.9
16	8	7	50	3.82	3.87	1.3
16	8	7	60	4.24	4.39	3.5
16	8	7	70	4.74	4.94	4.3

VITA

John Bernard Rodden was born in Chicago, Illinois on November 22, 1958 to Bernard and Alice Rodden. He graduated from Fenwick High School in Oak Park, Illinois in 1976 and received a Bachelor's degree in Chemical Engineering from the University of Notre Dame in Notre Dame, Indiana in 1980. From 1978 through 1980 John spent the summers working for Sargent & Lundy Engineers in Chicago, Illinois. In 1983, he received a Master of Science degree in Chemical Engineering from Texas A&M University. Following the completion of this degree, John worked for approximately two years for the United States Environmental Protection Agency in Dallas, Texas. In 1985, he returned to Texas A&M to pursue his Ph.D. in Chemical Engineering, which will be awarded in December, 1988. While pursuing his Ph.D. degree, John met Vicki Michelle Lambert of South Haven, Michigan, whom he married on July 11, 1987. Upon the completion of his degree requirements, John accepted a full time position with the Environmental Science Department of Shell Development Company in Houston, Texas.

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