

Literatur

- [1] Mulder, M.: *Basic Principles of Membrane Technology*, Kluwer Academic Publishers, Dordrecht, Boston, London, second edition, **1998**.
- [2] Staude, E.: *Membranen und Membranprozesse*, VCH, Weinheim, **1992**.
- [3] Nick, B.; Suter, U. W.: Solubility of water in polymers — atomistic simulations, *Computational and Theoretical Polymer Science*, 11(1):49–55, **2001**.
- [4] Boulougouris, G. C.; Economou, I. G.; Theodorou, D. N.: On the calculation of the chemical potential using the particle deletion scheme, *Molecular Physics*, 96(6):905–913, **1999**.
- [5] Boulougouris, G. C.; Voutsas, E. C.; Economou, I. G.; Theodorou, D. N.; Tsasios, D. P.: Henry's constant analysis for water and nonpolar solvents from experimental data, macroscopic models, and molecular simulation, *Journal of Physical Chemistry B*, 105(32):7792–7798, **2001**.
- [6] Boulougouris, G. C.; Economou, I. G.; Theodorou, D. N.: Calculation of the chemical potential of chain molecules using the staged particle deletion scheme, *The Journal of Chemical Physics*, 115(17):8231–8237, **2001**.
- [7] Boulougouris, G. C.: *Study of Water-Hydrocarbon Phase Equilibria Through Molecular Simulation and Molecular Theory*, Ph.D. Thesis, NTU – National Technical University of Athens, Greece, **2001** in greek.
- [8] Hofmann, D.; Heuchel, M.; Yampolskii, Y.; Shantarovich, V.: Free volume distribution in ultrahigh and lower free volume polymers: Comparison between molecular modeling and positron lifetime studies, *Macromolecules*, 35(6):2129–2140, **2002**.
- [9] Hofmann, D.; Entrialgo Castaño, M.; Lerbret, A.; Heuchel, M.; Yampolskii, Y.: Molecular modeling investigation of free volume distributions in stiff chain polymers with conventional and ultrahigh free volume: Comparison between molecular modeling and positron lifetime studies, *Macromolecules*, 36(22):8528–8538, **2003**.
- [10] Wijmans, J. G.; Baker, R. W.: The solution-diffusion model: a review, *Journal of Membrane Science*, 107(1):1–21, **1995**.
- [11] Stern, S. A.; Frisch, H. L.: The selective permeation of gases through polymers, *Annual Review Materials Science*, 11:523–550, **1981**.
- [12] Stern, S. A.: Polymers for gas separations: the next decade, *Journal of Membrane Science*, 94(1):1–65, **1994**.
- [13] Matson, S. L.; Lopez, J.; Quinn, J. A.: Separation of gases with synthetic membranes, *Chemical Engineering Science*, 38(4):503–524, **1983**.

- [14] Robeson, L. M.: Correlation of separation factor versus permeability for polymeric membranes, *Journal of Membrane Science*, 62(2):165–185, **1991**.
- [15] Dhoot, S. N.; Freeman, B. D.; Steward, M. E.; Hill, A. J.: Sorption and transport of linear alkane hydrocarbons in biaxially oriented polyethylene terephthalate, *Journal of Polymer Science, Part B, Polymer Physics*, 39(14):1160–1172, **2001**.
- [16] Berendsen, H. J. C.; Postma, J. P. M.; van Gusteren, W. F.; DiNola, A.; Haak, J. R.: Molecular dynamics with coupling to an external bath, *The Journal of Chemical Physics*, 81(8):3684–3890, **1984**.
- [17] Kotelyansii, M. J.; Wagner, N. J.; Paulaitis, M. E.: Building large amorphous polymer structures: Atomistic simulation of glassy polystyrene, *Macromolecules*, 29(26):8497–8506, **1996**.
- [18] Müller, M.; Nievergelt, J.; Santos, S.; Suter, U. W.: A novel geometric embedding algorithm for efficiently generation dense polymer structures, *The Journal of Chemical Physics*, 114(22):9764–9771, **2001**.
- [19] van der Vegt, N. F. A.; Briels, W. J.; Wessling, M.; Strathmann, H.: Free energy calculations of small molecules in dense amorphous polymers. Effect of the initial guess configuration on molecular dynamics studies, *The Journal of Chemical Physics*, 105(19):8849–8857, **1996**.
- [20] Theodorou, D. N.; Suter, U. W.: Detailed molecular structure of a vinyl polymer glass, *Macromolecules*, 18(7):1467–1478, **1985**.
- [21] Theodorou, D. N.; Suter, U. W.: Atomistic modeling of mechanical properties of polymeric glasses, *Macromolecules*, 19(1):139–154, **1986**.
- [22] Lechner, M. D.; Gehrke, K.; Nordmeier, E. H.: *Makromolekulare Chemie*, Birkhäuser Verlag, Basel, **1993**.
- [23] Flory, P. J.: *Statistical Mechanics of Chain Molecules*, Hanser, New York, **1989**.
- [24] Metropolis, N.; Rosenbluth, A. W.; Rosenbluth, M. N.; Teller, A. H.; Teller, E.: Equation of state calculations by fast computing machines, *The Journal of Chemical Physics*, 21(6):1087–1092, **1953**.
- [25] Widom, B.: Some topics in the theory of fluids, *The Journal of Chemical Physics*, 39(11):2808–2812, **1963**.
- [26] Gusev, A. A.; Arizzi, S.; Suter, U. W.; Moll, D. J.: Dynamics of light gases in rigid matrices of dense polymers, *The Journal of Chemical Physics*, 99(3):2221–2227, **1993**.
- [27] Gusev, A. A.; Suter, U. W.: Dynamics of small molecules in dense polymers subject to thermal motion, *The Journal of Chemical Physics*, 99(3):2228–2234, **1993**.

- [28] Gusev, A. A.; Suter, U. W.: A model for transport of diatomic molecules through elastic solids, *Journal of Computer-Aided Materials Design*, 1(1):63–73, **1993**.
- [29] Snurr, R. Q.; June, R. L.; Bell, A. T.; Theodorou, D. N.: Molecular simulation of methane adsorption in silicalite, *Molecular Simulation*, 8:73–92, **1991**.
- [30] Snurr, R. Q.; Bell, A. T.; Theodorou, D. N.: Prediction of adsorption of aromatic hydrocarbons in silicalite from grand canonical Monte Carlo simulation with biased insertions, *Journal of Physical Chemistry*, 97(51):13742–13752, **1993**.
- [31] Mezei, M.: A cavity-biased (T, V, μ) Monte-Carlo method for the computer-simulation of fluids, *Molecular Physics*, 40(4):901–906, **1980**.
- [32] Snurr, R. Q.; Bell, A. T.; Theodorou, D. N.: A hierarchical atomistic/lattice simulation approach for the prediction of adsorption thermodynamics of benzene in silicalite, *Journal of Physical Chemistry*, 98(19):5111–5119, **1994**.
- [33] Siepmann, J. I.; Frenkel, D.: Configurational bias Monte-Carlo: A new sampling scheme for flexible chains, *Molecular Physics*, 75(1):59–70, **1992**.
- [34] Frenkel, D.; Mooij, G. C. A. M.; Smit, B.: Novel scheme to study structural and thermal properties of continuously deformable molecules, *Journal of Physics: Condensed Matter*, 4(12):3053–3076, **1992**.
- [35] de Pablo, J. J.; Laso, M.; Suter, U. W.: Estimation of the chemical potential of chain molecules by simulation, *The Journal of Chemical Physics*, 96(8):6157–6162, **1992**.
- [36] Laso, M.; de Pablo, J. J.; Suter, U. W.: Simulation of phase equilibria for chain molecules, *The Journal of Chemical Physics*, 97(4):2817–2819, **1992**.
- [37] de Pablo, J. J.; Laso, M.; Suter, U. W.: Continuum configurational bias Monte Carlo studies of alkanes and polyethylene, *Fluid Phase Equilibria*, 83:323–331, **1993**.
- [38] de Pablo, J. J.; Laso, M.; Suter, U. W.: Simulation of the solubility of alkanes in polyethylene, *Macromolecules*, 26(23):6180–6183, **1993**.
- [39] de Pablo, J. J.; Laso, M.; Suter, U. W.: Simulation of polyethylene above and below the melting point, *The Journal of Chemical Physics*, 96(3):2395–2403, **1992**.
- [40] de Pablo, J. J.; Laso, M.; Siepmann, I.; Suter, U. W.: Continuum-configurational-bias Monte Carlo simulations of long-chain alkanes, *Molecular Physics*, 80(1):55–63, **1993**.
- [41] Leontidis, E.; de Pablo, J. J.; Laso, M.; Suter, U. W.: A critical evaluation of novel algorithms for the off-lattice Monte Carlo simulation of condensed polymer phases, *Advances in Polymer Science*, 116:283–318, **1994**.

- [42] Consta, S.; Wilding, N. B.; Frenkel, D.; Alexandrowicz, Z.: Recoil growth: An efficient simulation method for multi-polymer systems, *The Journal of Chemical Physics*, 110(6):3220–3228, **1999**.
- [43] Consta, S.; Vlugt, T. J. H.; Hoeth, J. W.; Smit, B.; Frenkel, D.: Recoil growth algorithm for chain molecules with continuous interactions, *Molecular Physics*, 97(12):1243–1254, **1999**.
- [44] Swope, W. C.; Andersen, H. C.: A molecular dynamics method for calculating the solubility of gases in liquids and the hydrophobic hydration of inert-gas atoms in aqueous solution, *Journal of Physical Chemistry*, 88(26):6548–6556, **1984**.
- [45] Lyubartsev, A. P.; Martsinovski, A. A.; Shevkunov, S. V.; Vorontsov-Velyaminov, P. N.: A new approach to Monte Carlo calculation of the free energy: Method of expanded ensemble, *The Journal of Chemical Physics*, 96(3):1776–1783, **1992**.
- [46] Lyubartsev, A. P.; Laaksonen, A.; Vorontsov-Velyaminov, P. N.: Free energy calculations for Lennard-Jones systems and water using the expanded ensemble method, *Molecular Physics*, 83(3):455–471, **1994**.
- [47] Åberg, K. M.; Lyubartsev, A. P.; Jacobsson, S. P.; Laaksonen, A.: Determination of solvation free energies by adaptive expanded ensemble molecular dynamics, *The Journal of Chemical Physics*, 120(8):3770–3776, **2004**.
- [48] Khare, A. A.; Rutledge, G. C.: Chemical potential of aromatic compounds in pure *n*-alkanes using expanded ensemble Monte Carlo simulations, *Journal of Physical Chemistry B*, 104(15):3639–3644, **2000**.
- [49] Khare, A. A.; Rutledge, G. C.: Chemical potential of model benzene fluids using expanded ensemble Monte Carlo simulations, *The Journal of Chemical Physics*, 110(6):3063–3069, **1999**.
- [50] Boulougouris, G. C.; Errington, J. R.; Economou, I. G.; Panagiotopoulos, A. Z.; Theodorou, D. N.: Molecular simulation of phase equilibria for water–*n*-butane and water–*n*-hexane mixtures, *Journal of Physical Chemistry B*, 104(20):4958–4963, **2000**.
- [51] van der Vegt, N. F. A.; Briels, W. J.: Efficient sampling of solvent free energies in polymers, *The Journal of Chemical Physics*, 109(17):7578–7582, **1998**.
- [52] Iba, Y.: Extended ensemble Monte Carlo, *International Journal of Modern Physics C*, 12(5):623–656, **2001**.
- [53] Zervopoulou, E.; Mavrantzas, V. G.; Theodorou, D. N.: A new Monte Carlo simulation approach for the prediction of sorption equilibria of oligomers in

- polymer melts: Solubility of long alkanes in linear polyethylene, *The Journal of Chemical Physics*, 115(6):2860–2875, **2001**.
- [54] Kumar, S. K.; Szleifer, I.; Panagiotopoulos, A. Z.: Determination of the chemical potential of polymeric systems from Monte Carlo simulation, *Physical Review Letters*, 66(22):2935–2938, **1991**.
- [55] Shing, K. S.; Gubbins, K. E.: The chemical potential in dense fluids and fluid mixtures via computer simulation, *Molecular Physics*, 46(5):1109–1128, **1982**.
- [56] Shing, K. S.; Gubbins, K. E.: The chemical potential from computer simulation. Test particle method with umbrella sampling, *Molecular Physics*, 43(3):717–721, **1981**.
- [57] Parsonage, N. G.: Computation of the chemical potential in high density fluids by a Monte Carlo method, *Molecular Physics*, 89(4):1133–1144, **1996**.
- [58] Parsonage, N. G.: Determination of the chemical potential by the particle insertion method and by its inverse, *Journal of the Chemical Society Faraday Transactions*, 91:2971–2973, **1995**.
- [59] Parsonage, N. G.: Chemical-potential paradoxon in molecular simulation. Explanation and Monte Carlo results for a Lennard-Jones fluid, *Journal of the Chemical Society Faraday Transactions*, 92(7):1129–1134, **1996**.
- [60] Dodd, L. R.; Theodorou, D. N.: Analytical treatment of the volume and surface area of molecules formed by an arbitrary collection of unequal spheres intersected by planes, *Molecular Physics*, 72(6):1313–1345, **1991**.
- [61] Kofke, D. A.; Cummings, P. T.: Quantitative comparison and optimization of methods for evaluating the chemical potential by molecular simulation, *Molecular Physics*, 92(6):973–996, **1997**.
- [62] Boulougouris, G. C.: persönliche Mitteilung, **2003**.
- [63] Theodorou, D. N.: Final technical report for EU-project PERMOD, Section 4, Workpackage 3, March **2004**.
- [64] Sun, H.: COMPASS: An ab initio force-field optimized for condensed-phase application — Overview with details on alkane and benzene compounds, *Journal of Physical Chemistry B*, 102(38):7338–7364, **1998**.
- [65] Ousterhout, J. K.: *Tcl and the Tk toolkit*, Addison Wesley, Readings, Mass., **1994**.
- [66] Swope, W. C.; Andersen, H. C.; Berens, P. H.; Wilson, K. R.: A computer simulation method for the calculation of equilibrium constants for the formation of physical clusters of molecules: Application to small water clusters, *The Journal of Chemical Physics*, 76(1):637–649, **1982**.

- [67] Flyvbjerg, H.; Petersen, H. G.: Error estimates on averages of correlated data, *The Journal of Chemical Physics*, 91(1):461–466, **1989**.
- [68] Bondi, A.: van der Waals volumes and radii, *Journal of Physical Chemistry*, 68(3):441–451, **1964**.
- [69] Stapleton, M. R.; Panagiotopoulos, A. Z.: Application of excluded volume map sampling to phase equilibrium calculations in the Gibbs ensemble, *The Journal of Chemical Physics*, 92(2):1285–1293, **1990**.
- [70] Kamiya, Y.; Naito, Y.; Hirose, T.; Mizoguchi, K.: Sorption and partial molar volume of gases in poly(dimethyl siloxane), *Journal of Polymer Science, Part B, Polymer Physics*, 28(8):1297–1308, **1990**.
- [71] Heuchel, M.; Hofmann, D.; Pullumbi, P.: Molecular modeling of small-molecule permeation in polyimides and its correlation to free-volume distributions, *Macromolecules*, 37(1):201–214, **2004**.
- [72] Hagler, A. T.; Lifson, S.; Dauber, P.: Consistent force field studies of intermolecular forces in hydrogen-bonded crystals. 2. A benchmark for the objective comparison of alternative force fields, *Journal of the American Chemical Society*, 101(18):5122–5130, **1979**.
- [73] Hagler, A. T.; Dauber, P.; Lifson, S.: Consistent force field studies of intermolecular forces in hydrogen-bonded crystals: 3. The C=O...H–O hydrogen bond and the analysis of the energetics and packing of carboxylic acids, *Journal of the American Chemical Society*, 101(18):5131–5141, **1979**.
- [74] Timmermans, J.: *Physico-chemical constants of pure organic compounds*, Chapter E: Aromatic Hydrocarbons, pages 140–145 (Benzene), 193–195 (Cyclohexane), Elsevier Publishing Company, Inc., New York, Amsterdam, London, Brussels, **1950**.
- [75] Goodwin, R. D.: Benzene thermophysical properties from 279 to 900 K at pressures to 1000 bar, *Journal of Physical and Chemical Reference Data*, 17(3):1541–1636, **1988** Table 21.
- [76] Paterson, R.; Yampolskii, Y.: IUPAC-NIST solubility data series 70. Solubility of gases in glassy polymers, *Journal of Physical and Chemical Reference Data*, 25(5):1255–1450, **1999**.
- [77] Martos, P. A.; Pawliszyn, J.: Calibration of solid phase microextraction for air analyses based on physical chemical properties of the coating, *Anal. Chem.*, 69(2):206–215, **1997**.
- [78] Tian, M.; Munk, P.: Characterization of polymer–solvent interactions and their temperature dependence using inverse gas chromatography, *Journal of Chemical Engineering Data*, 39(4):742–755, **1994**.

- [79] Lichtenthaler, R. N.; Liu, D. D.; Prausnitz, J. M.: Thermodynamics of poly(dimethylsiloxane) solutions. Combinatorial entropy and molecular interactions, *Berichte der Bunsen-Gesellschaft — Physical Chemistry Chemical Physics*, 78(5):470–477, **1974**.
- [80] Grate, J. W.; Kaganove, S. N.; Bhethanabotla, V. R.: Examination of mass and modulus contribution to thickness shear mode and surface acoustic wave vapour sensor responses using partition coefficients, *Faraday Discussions*, 107:259–283, **1997**.
- [81] Frahn, J.: Messungen bei der GKSS im Rahmen des DBU-Projektes [82], persönliche Mitteilung, **2004**.
- [82] Frahn, J.; Schwarz, H.-H.; Weigel, T.; Matuschewski, H.; Schedler, U.: Optimierung und Anwendung von Pervaporationstrennmembranen für die Aromaten-Aliphaten-Trennung in einer Pilotanlage, DBU-Abschlussbericht, Deutsche Bundesstiftung Umwelt, **2005**.
- [83] Böhning, M.: *Untersuchungen der Gaspermeationseigenschaften von Polymeren und dabei auftretender Wechselwirkungs- und Quellungsphänomene*, Dissertation, TUB – Technische Universität Berlin, **1997**.
- [84] Heuchel, M.; Böhning, M.; Hölck, O.; Siegert, M. R.; Hofmann, D.: Atomistic packing models for experimentally investigated swelling states induced by CO₂ in glassy polysulfone and poly(ether sulfone), *Journal of Polymer Science, Part B, Polymer Physics*, **2006** submitted.
- [85] McHattie, J. S.; Koros, W. J.; Paul, D. R.: Gas transport properties of polysulphones: 1. Role of symmetry of methyl group placement on bisphenol rings, *Polymer*, 32(5):840–851, **1991**.
- [86] Erb, A. J.; Paul, D. R.: Gas sorption and transport in polysulfone, *Journal of Membrane Science*, 8(1):11–22, **1981**.
- [87] Chiou, J. S.; Maeda, Y.; Paul, D. R.: Gas permeation in polyethersulfone, *Journal of Applied Polymer Science*, 33(5):1823–1828, **1987**.
- [88] Kamiya, Y.; Hirose, T.; Mizoguchi, K.; Naito, Y.: Gravimetric study of high-pressure sorption of gases in polymers, *Journal of Polymer Science, Part B, Polymer Physics*, 24(7):1525–1539, **1986**.
- [89] Wang, J.-S.; Kamiya, Y.: Concurrent measurements of sorption and dilation isotherms and diffusivity for polysulfone membrane/carbon dioxide systems, *Journal of Membrane Science*, 98(1):69–76, **1995**.
- [90] Sanders, E. S.: Penetrant-induced plasticization and gas permeation in glassy polymers, *Journal of Membrane Science*, 37(1):63–80, **1988**.

- [91] Reimers, M. J.; Barbari, T. A.: Gas sorption and diffusion in hydrogen-bonded polymers. II. Polyethersulfone/polyhydroxyether blends, *Journal of Polymer Science, Part B, Polymer Physics*, 32(1):131–139, **1994**.
- [92] Singh, A.; Freeman, B. D.; Pinnau, I.: Pure and mixed gas acetone/nitrogen permeation properties of polydimethylsiloxane [PDMS], *Journal of Polymer Science, Part B, Polymer Physics*, 36(2):289–301, **1998**.
- [93] Summers, W. R.; Tewari, Y. B.; Schreiber, H. P.: Thermodynamic interaction in polydimethylsiloxane–hydrocarbon systems from gas–liquid chromatography, *Macromolecules*, 5(1):12–16, **1972**.
- [94] French, R. N.; Koplos, G. J.: Activity coefficients of solvents in elastomers measured with a quartz crystal microbalance, *Fluid Phase Equilibria*, 158–160:879–892, **1999**.
- [95] Delgado-Buscaliono, R.; Fabritis, G. D.; Coveney, P. V.: Determination of the chemical potential using energy-biased sampling, *The Journal of Chemical Physics*, 123(5):054105–1–9, **2005**.
- [96] Lyubartsev, A. P.; Laaksonen, A.; Vorontsov-Velyaminov, P. N.: Determination of free energy from chemical potentials: Application of the expanded ensemble method, *Molecular Simulation*, 18(1-2):43–58, **1996**.
- [97] Reid, R. C.; Prausnitz, J. M.; Poling, B. E.: *The Properties of Gases and Liquids*, Appendix A: Polymer Data Bank, McGraw Hill, New York, fourth edition, **1987**.
- [98] Sun, H.; Rigby, D.: Polysiloxanes: ab initio force field and structural, conformational and thermophysical properties, *Spectrochimica Acta*, 53A(8):1301–1323, **1997**.
- [99] Rigby, D.; Sun, H.; Eichinger, B. E.: Computer simulations of poly(ethylene oxide): Force field, PVT diagram and cyclization behaviour, *Polymer International*, 44(3):311–330, **1997**.
- [100] Eichinger, B. E.; Rigby, D.; Stein, J.: Cohesive properties of Ultem and related molecules from simulations, *Polymer*, 43(2):599–607, **2002**.
- [101] Hofmann, D.; Fritz, L.; Ulbrich, J.; Böhning, M.: Detailed-atomistic molecular modeling of small molecule diffusion and solution processes in polymeric membrane materials, *Macromolecular Theory and Simulation*, 9(6):293–327, **2000**.
- [102] Tiller, A. R.: GSNET and GSDIF Program; Biosym Technologies Ltd., UK (now: Accelrys Inc. San Diego, USA).