Full Paper _____ *Thematic Section:* Physicochemical Research.
Reference Object Identifier – ROI: jbc-02/17-49-2-96 *Subsection:* Supercritical Fluids.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Submitted on February 15, 2017.

Thermal effects dissolution main tea components in supercritical carbon dioxide

© **Zufar I. Zaripov**,[1] **Lenar Yu. Yarullin**,[1+] **Farid M. Gumerov**,[1]* **Truong Nam Hung**,[2] **Farizan R. Gabitov**,[1] and **Venera A. Kayumova**[1]

[1] *Department of Theoretical Foundations of Heat Engineering. Kazan National Research Technological University. Karl Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia.*
Phone: +7 (843) 231-42-11. E-mail: yarul.lenar@gmail.com
[2] *Hanoi.Electric Power University. Hanoi. Vietnam.*

*Supervising author; [+]Corresponding author

Keywords: caffeine, supercritical carbon dioxide, cellulose, tea leaves, mixing enthalpy.

Abstract

In example pretreatment of tea leaves with supercritical carbon dioxide showed a significant (30%) increase in the extractable substances of natural physiologically active material for subsequent solvent extraction. The composition of tea leaves include cellulose, amino acids and other. Cellulose – a natural polymer structure which is full of physiologically active substances of natural material. The interaction with the polymeric material in fluid sub- and supercritical fluids (SCF), usually of swelling occurs, whereby the molecular structure and dynamics of a local free volume of these polymers may undergo very significant changes. Thus, the local molecular dynamics of polymers is of great theoretical and practical interest because of the types of molecular motion, which are in the polymer depend essentially on its mechanical, thermal, dielectric and diffusion properties. In particular, the local dynamics defines secondary relaxation transitions in glassy polymers. Molecular mobility in the polymer is closely related to its free volume and free volume distribution. In this article, we show the results of measurement of thermal effects depending on different temperatures and pressures encountered in the processing of the main components of tea (caffeine, cellulose, leaf tea) with supercritical carbon dioxide. Research has set a different behavior of the heat of the dissolution of the considered substances and supercritical carbon dioxide. The greatest enthalpy change intensity with changes in temperature occur in the pressure range 8-20 MPa. Studies of thermal effects of dissolution of the major tea components in the supercritical carbon dioxide, is carried out by heat-conducting calorimeter. Submitted control measurements of the enthalpy of mixing of CO_2-H_2O binary system. Confidence limits the total measurement uncertainty (P = 0.95) heat of solution do not exceed ±3%. The comparison of the heat of solution in the supercritical carbon dioxide is the main component of tea leaf, from which it is clear that the value of the enthalpy of caffeine and cellulose are practically identical values.

References

[1] L.Y. Yarullin, F.M. Gumerov, Truong Nam Hung, I.I. Gilmutdinov, Z.I. Zaripov, F.R. Gabitov, and A.B. Remizov. The composition and structure of the tea leaves, processed in supercritical carbon dioxide. *Butlerov Communications.* **2016**. Vol.48. No.11. P.88-100. ROI: jbc-02/16-48-11-88
[2] V.F. Khairutdinov, F.R. Gabitov, F.M. Gumerov, and P.R. Khusnutdinov. Nanodispersion of polystyrene with the use of the method of supercritical fluid anti-solvent. *Butlerov Communications*. **2009**. Vol.15. No.1. P.34-39. ROI: jbc-02/09-15-1-34
[3] I.Sh. Khabriev, V.F. Khairutdinov, Z.I. Zaripov, F.M. Gumerov, V.A. Petrov, N.V. Kuznetsova, and R.M. Huzahanov. Dispersion paracetamol using the method of SAS. *Butlerov Communications.* **2016**. Vol.48. No.11. P.71-87. ROI: jbc-02/16-48-11-71
[4] D. Koschel. Enthalpy and solubility data of CO_2 in water and NaCl (aq) at conditions of interest for geological sequestration. *Fluid Phase Equilibria*. **2006**. Vol.247. P.107.
[5] D. Koschel, J.-Y. Coxam, V. Majer. Enthalpy and Solubility Data of H_2S in Water at Conditions of Interest for Geological Sequestration. *Ind. Eng. Chem. Res*. **2007**. Vol.46. P.1421.
[6] C. Mathonat, V. Majer, A.E. Mather, J-P. Grolier. Enthalpies of absorption and solubility of CO_2 in aqueous solutions of methyldiethanolamine. *Fluid Phase Equilib*. **1997**. Vol.40. P.171.

[7] J.R. Kim, J.B. Kyong. Thermodynamic Properties of Caffeine in Compressed Gas. *Bul. Korean Chem. Soc*. **1995**. Vol.16. No.5. P.432.
[8] J.P. Grolier, E. Wilhelm. *Pure & Appl.Chem*. **1991**. Vol.63. No.10. P.1427-1434.
[9] S.M. Walas. Phase Equilibria in Chemical Engineering. *Butterworth-Heinemann. Boston*. **1985**. P.671.
[10] C. Sanchez, R.H. Lacombe. An Elementary Molecular Theory of Classical Fluids. *Pure Fluids The Journal of Physical Chemistry*. **1976**. Vol.80. No.21. P.2352-2362.
[11] C. Sanchez, R.H. Lacombe. Thermodynamics of Polymer Solutions. *Macromolecules*. **1978**. Vol.11. No.6. P.1145-1155.
[12] J.S. Vrentad, C.M. Vrentas. Sorption in Glassy Polymers. *Macromolecules*. **1991**. No.24. P.2404-2412.
[13] E. Calvet, A. Prat. Microcalorimetry. Implementation in physical chemistry and biology. *Foreign. lit. Moscow*. **1963**.P.477.
[14] Z.I. Zaripov, S.A. Burtsev, A.V. Gavrilov, G.Kh. Mukhamedzyanov. Thermal Properties of n-Hexane at Temperatures of 298.15–363.5 K and Pressures of 0.098-147 MPa. *Theoretical Foundations of Chemical Engineering*. **2002**. Vol.36. No.4. P.400-405.
[15] Z.I. Zaripov, S.A. Burtsev, A.V. Gavrilov, G.Kh. Mukhamedzyanov. Determination of the Thermophysical Properties of Halogenated Hydrocarbons in a Heat-Conducting Calorimeter. *High Temperature*. **2004**. Vol.42. No.2. P.282-289.
[16] Z.I. Zaripov, S.A. Burtsev, S.A. Bulaev, G.Kh. Mukhamedzyanov. The Heat Capacity and Thermal Diffusivity of Aqueous Solutions of Alkali Metal Salts in a Wide Pressure Range. *J. Phys. Chem*. **2004**. Vol.78. No.5. P.697-700.
[17] Z.I. Zaripov, G.Kh. Mukhamedzyanov. Thermophysical properties of liquids and solutions: *Kazan.: Kazan State Technological University*. **2008**. P.376. (russian)
[18] Liu L., Peng Q., Y Li. *Inorganic Chem*. **2008**. Vol.47. P.5022-5028.
[19] E. Bayer, A. Hiltner. *High-Molecular Compounds*. **1996**. A series. Vol.38. 549p. (russian)
[20] V.I. Kovalenko. Crystalline cellulose: structure and hydrogen bonds. *Chemical Success*. **2010**. Vol.79. No.3. P.261-272. (russian)
[21] R.A. Usmanov, F.N. Shamsetdinov, R.R. Gabitov and others. The effect of SC-CO_2 treatment procedures on content and structure of a tea leaf and cellulose. *Supercritical Fluids: Theory and Practice*. **2011**. Vol.6. No.2. P.83-91. (russian)
[22] V.F. Uriyash, V.N. Larina, N.Y. Kokurina, N.V. Novoselova. Thermochemical characteristics of cellulose and its aqueous mixtures. *Journal of Physical Chemistry*. **2010**. Vol.84. No.6. P.1023-1029. (russian)
[23] M.Ya. Eoyelovich. Enthalpy of formation and dissolution of cellulose. Union conference on chemical thermodynamics and calorimetry(thesis). *Gorkiy GGU*. **1988**. Vol.2. P.189-191. (russian)