UNIVERSITY OF PANNONIA

SUBJECT DATASHEET

Semester:	2010/11/2
Subject:	Program Solving Practice In Physical Chemistry III.
Code:	VEMKFKM122A
Responsible department:	Department of Physical Chemistry
Responsible department code:	MKFK
Responsible lecturer:	dr. Dezső Boda

Educational objectives:

Teach physical chemistry from molecular (particle) point of view. Interpretation of physicochemical phenomena within the framework of statistical mechanics via numerical examples.

Detailed content of the subject:

Summary of classical thermodynamics. Molecular interpretation of thermodynamic concepts. Energy distribution. Macrostate, microstate. The most probable distribution. Maxwell-Boltzmann distribution. Molecular partition function. Molecular partition function and thermodynamic properties. Elements of ensemble theory. Phase space of classical systems. Canonical ensemble. Fluctuations. Grand canonical ensemble. Adiabatic ensembles. Partition functions and characteristic thermodynamic functions. Hamilton function. Modelling intermolecular interactions: Born-Oppenheimer approximation, holonomic constraints. Intermolecular interaction potentials. Correlation functions, configurational properties. Statistical derivation of the virial and the van der Waals equation. Equation of state for the hard sphere fluid. Determination of thermodynamic properties on the basis of statistical mechanical models: 1. p-V-T and other thermochemical-thermophysical properties of pure substances. 2. Properties of mixing. Models for mixtures. 3. Phase equilibria of pure systems and mixtures. 4. Statistical thermodynamics of adsorption. Statistical derivation of the Langmuir isotherm. Multilayer adsorption. 5. Modelling electrolytes. Electrochemical double layer. 6. Modelling colloid systems. DLVO theory. 7. Transport properties of fluids in statistical mechanics. 8. Statistical thermodynamics of chemical equilibria. 9. Statistical modelling of chemical kinetics. Calculation of structural and thermodynamic properties by molecular simulations: ergodicity, ensemble and time average. Monte Carlo simulations. Molecular dynamics of equilibrium and nonequilibrium systems. Molecular simulations and industrial applications (technological aspects, design of materials). Determination of thermodynamic properties in chemical engineering: modern estimation methods based on statistical mechanical approximations. Summary and special questions.

Requirements:

The students must write a test at the end of the term.

Required and suggested references:

1. Atkins, P. W.: Fizikai kémia I-III., Tankönyvkiadó, Budapest, 1992. 2. Lucas, K.: Applied Statistical

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Required and suggested references:

Thermodynamics, Springer-Verlag, Berlin, Heidelberg, 1991. 3. Liszi, J., Ruff, I., Schiller, R., Varsányi, Gy.: Bevezetés a fizikai kémiába, Műszaki Könyvkiadó, Budapest, 1983. 4. Liszi, J.: Fizikai kémia, Veszprém, 1993. Kézirat. 5. Reed, T. M., Gubbins, K. E.: Gázok és folyadékok statisztikus termodinamikája, Műszaki Könyvkiadó, Budapest, 1978.