Project Title: **CHEMICAL THERMODYNAMIC MODELING OF GEOCHEMICAL SOLUTIONS AT SUBZERO TEMPERATURES.**

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The principal structure of the computer model has been developed. That includes:

- user's interface to specify the system, temperature range and step, mass-balance etc.
- interaction of different mathematical modules, input and output.

The major efforts were focused on the development of the program code for point equilibrium computation, which is supposed to be the most challenge and key for further construction of the model of strong solutions freezing.

1. Development of the algorithm and program code for point chemical equilibria computation to be coupled with Pitzer's routine.

Because of particularities of Pitzer's model, the term of chemical potential of water differs from these of other aqueous components. According to this, the algorithm of Gibbs free energy minimization had been significantly modified. If ice is not stable in the system at current iteration, the chemical potential of the component "liquid water" is assumed to be constant (like to solid phases of constant composition) during this iteration. Its quantity and current chemical potential are calculated from mass-balance restrictions and the osmotic coefficient of the solution and molalities of species respectively. According to these changes of the algorithm, a new free energy minimization routine was written in Microsoft FORTRAN. Its validation and reliability was checked by computation of equilibria in heterogeneous ideal systems (without routines for activity coefficients and water activity calculation).

2. Calculating routines - data files interface.

It has been supposed that the used thermodynamic database should be separated from the calculating routines. So the formats of files of input

thermodynamic data on standard chemical potentials, Pitzer's parameters, and partial molal volumes as functions of temperature, were developed. The routines for search and input of needed data for point equilibrium computation routine in specified system were developed, as well as for the subroutine of calculation of activity coefficients, water activity, and partial molal volumes. □