Calculation of methane hydrate thermodynamic properties

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Gas hydrate question is very actual for today. By the present time we aren't know classical thermodynamic properties of gas hydrates. In the hydrate literature overviews are resulted only enthalpy of dissociation (ΔH), heat conductivity (λ) and thermal capacity (Cp) [2, 3]. Application of this data for the decision of variuos problems is very inconveniently in comparison with classical physical properties. Therefore the great value is to calculate classical thermodynamic functions - $\Delta_f G°$(free Gibbs energy), $\Delta_f H°$(enthalpy) and S°(enthropy).

We calculate of methane hydrate thermodynamic properties by the semiempirical methods which well proved themselves at preparation and coordination of thermodynamic properties for different geochemical databases. The equation of a thermal capacity and the first time calculated thermodynamic properties of methane gas hydrate are presented in this work and shown below (Table 1):

Thermodynamic potential	Calculated value
Entropy, S° ($CH_4 \cdot 6H_2O$; 298,15K)	455,7096 $J \cdot K^{-1} \cdot mol^{-1}$
Free Gibbs energy, $\Delta_f G°$ ($CH_4 \cdot 6H_2O$; 298,15K)	-1 470 018 $J \cdot mol^{-1}$
Enthalpy, $\Delta_f H°$ ($CH_4 \cdot 6H_2O$; 298,15K)	-1 831 056 $J \cdot mol^{-1}$

Table 1. Calculated thermodynamic potentials

All the obtained data have been used for calculation of physical and chemical model of the Baikal Lake including ice, water solution, gases and gas hydrate. SELEKTOR program complex has been used for modelling this expirement. Results of the calculation have shown good conformity to the real expirement data of other researches [1, 3]. Results of our research are unequivocally specify that hydrate free energy ΔfG and enthalpy ΔfH have admissible error values of thermodynamic potentials and can be used in different calculations.

[1] Istomin (1992) Gazovie gidrati v prirodnih uslovijah, 236. [2] Max (2003) Natural gas hydrate in oceanic and permafrost environments, **392**. [3] Sloan (2008) Clathrate hydrates of natural gases. 3d ed., 721.

Influence of ship emissions on ozone and PM concentrations around coastal areas during springs and summers of 2005-2006

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Methods

In this study, the temporal and spatial distributions of O_3 and the related pollutants (PM, etc), P with meteorological variables were analyzed in a coastal city (i.e., Busan), Korea during springs and summers of 2005-2006. The ship emissions around the port areas, Korea were estimated to evaluate their environmental impact on ambient concentration levels of particulate matter (PM) and O_3. The relative contribution of ship emissions to the change in O_3 and PM concentrations will be also examined based on the modeling analysis. The models used in this study were the PSU/NCAR no-hydrostatic meteorological model (i.e., MM5) and the Comprehensive Air Quality Model (CAMx).

Discussion of Results

A statistical summary of pollutant species (e.g., O_3, NO_2, NO, PM_{10}, etc.) for coastal area (CA) during the study period are provided in Table 1.

A compelete discussion of the importance of the results will be begun once we have completed model simulation and analysis. Further results may be obtained if the model simulation is finished before the conference.

	Pollutant species						
Season	O_3	NO_2	NO	NO_x	NO_2/NO	PM_{10}	CO
Spr.	40±17[a]	23±16	7.7±15	30±27	6.3±6.5	69±58	404±182
	6410[b]	6377	6377	6377	6377	6271	6488
Sum.	31±21	19±13	9.2±15	28±24	4.2±4.3	53±28	373±186
	7943	7887	7887	7887	7887	7965	8073

Table 1: statistical summary of pollutant species (in ppb) for coastal areas in Busan during springs and summers of 2005-2006. Area CA