

## ***Interactive comment on “Numerical implementation and oceanographic application of the Gibbs potential of ice” by R. Feistel et al.***

**R. Feistel et al.**

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Our disputed paper presents a new, very accurate, comprehensive, consistent, independent and complete quantitative formulation for the thermodynamic equilibrium properties of ice, and especially its numerical implementation. In an additional chapter we demonstrate to the reader some but certainly not the only possibilities of its application in oceanography, namely computation formulas for several sea ice properties. This does not turn the paper into an exhaustive description of sea ice, nor was that ever intended by the authors of the paper, who work on thermodynamic properties of ice, water, and seawater. They are neither polar oceanographers nor climate modellers. In so far, the assessment of the paper by referee #2 in this respect is correct and is not recognised as a criticism.

As has become evident already from the few discussion contributions to this article, there are at least three, rather different approaches to the problem “sea ice”. The first

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is that of numerical modellers who build ice modules for implementation into oceanographic and global circulation models, like e.g. by Hibler, W. D. III, 1979, A dynamic thermodynamic sea ice model, *J. Phys. Oceanogr.*, 9, 815-846. A second one is based on low-temperature brine chemistry, as e.g. by Marion, G.M., R.E. Farren, and A.J. Komrowski, 1999, Alternative pathways for seawater freezing, *Cold Regions Sci. Technol.* 29, 259-266. Thirdly, our own way is arising from available, comprehensive formulations for equilibrium properties of water, seawater and ice. All three of these approaches are well justified each, even though the contours of their joint part are only vaguely discernible so far. Each of them, naturally, can expect to benefit from results the others, even if or just because they are so different in their methods and perspectives.

As already outlined in the online discussion with Hajo Eicken, the latter two concepts mainly focus on two different edges of the parameter range of interest. The Gibbs functions provide comprehensive and highly accurate descriptions of sea ice but are limited yet to standard sea salt composition and relatively low brine salinities, i. e. 'high' temperatures. The brine chemistry models, however, are capable of treating high salinities up to the solubility limit, as easily encountered in natural sea ice at lower temperatures, and consider non-standard sea salt compositions, too. Both concepts rely on more or less the same theoretical tools and target on the same physical state - thermodynamic equilibrium. Thus, bridges between both may be expected for the near future and may be helpful to close the pending gap between the definitions of practical and absolute salinity in oceanography, as discussed anew by Jackett et al., 2005, cited the paper. In addition to our online discussion remarks about precipitation from freezing seawater it should be mentioned that there is the possibility of calcium carbonate precipitation just below  $-2^{\circ}\text{C}$  (G. M. Marion, 2001, Carbonate mineral solubility at low temperatures in the Na-K-Mg-Ca-H-Cl-SO<sub>4</sub>-OH-HCO<sub>3</sub>-CO<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system, *Geochim. Cosmochim. Acta* 65, 1883-1896) which would apply especially to waters like the Baltic Sea with positive calcium anomaly. We have included a comment on this into the revised paper version.

The theoretical derivation of macroscopic, equilibrium properties of a many-particle system from its microscopic interaction forces is the subject of statistical mechanics. Applying e.g. the Gibbs canonical ensemble for this purpose, only very few quantities must be considered as given. The particle number  $N$ , the volume  $V$ , the temperature  $T$  and the molecular Hamiltonian  $H$  are combined to form the partition function  $Z$ , by which the appropriate thermodynamic potential function, the Helmholtz energy  $F(N,T,V)$ , can be expressed as  $F = -kT \ln(Z)$ . From  $F$ , in turn, all other equilibrium properties become available by formal thermodynamic rules. As is obvious from this, as simple as fundamental, theoretical consideration, the physical dimension of ‘time’ is virtually not existing in equilibrium thermodynamics, and so are all related quantities like property fluxes or process rates.

Hence, thermodynamic potential formulations cannot help ocean modellers to compute any transition rates, fluxes or currents, at least not directly. In an indirect way, however, they are certainly quite helpful prerequisites for problems like the one mentioned by referee #2. To demonstrate this argument more obviously, let us consider as a simple example the Navier-Stokes equation, which governs the transport of ocean waters. If not thermodynamics provided in advance accurate relations between the equilibrium quantities “pressure” and “density” of seawater, the Navier-Stokes equation would hardly be as useful as it is in oceanographic models. Transport theories like Onsager’s linear irreversible thermodynamics are basically developed as generalisations of equilibrium state descriptions, for instance by resting on the existence of local equilibrium conditions, see e.g. P. Glansdorff and I. Prigogine, Thermodynamic theory of structure, stability and fluctuations, Wiley 1971. In this context, titles like that of Hibler’s 1979 paper sound somewhat misleading since it mainly develops empirical dynamical equations for the speed of ice formation and transition processes and hardly involves thermodynamic relations in their classical, physical sense, the way the notion was originally coined in the middle of the 19th century by scientists like Clausius, Helmholtz, or Maxwell. As we have tried to point out, “thermodynamic” is virtually not “dynamic” at all, which of course is not a new insight.

Why using the Gibbs functions instead of simple formulas we already have? What is the gain? Questions of the same kind as raised by referee #1 are asked in the oceanographic community concerning the thermodynamic potential of seawater, and need not to be answered here again in their various general aspects. Properties and advantages of the Gibbs function approach have been discussed recently in this journal in detail, see the Interactive Discussion to R. Feistel, *Ocean Science Discussion*, 1, 1-19, 2004, [http://www.cosis.net/members/journals/df/article.php?a\\_id=1317](http://www.cosis.net/members/journals/df/article.php?a_id=1317), especially in the contribution by David Webb. Moreover, we have included into the revised version a reference to the review paper of Alberty (2001) describing the generality, elegance and convenience of thermodynamic potential formulations for the theoretical and numerical description of thermodynamic equilibrium properties of arbitrary substances. Using such a formulation, all properties can be obtained from it by formal mathematical operations (partial derivatives), and vice versa, all experimentally measured such properties can be condensed into this single mathematical structure during its construction process. It obeys the important necessary conditions for a mathematical model or axiomatic system, namely consistency, independence, and completeness. The accuracy of various ice properties including freezing points derived from this formulation in comparison to experimental data is discussed in great detail by Feistel and Wagner (2005) and does not need to be repeated in the current article. We have additionally included a table of computed seawater freezing points, however.

With respect to global warming, as requested by the referees, we have added to the revised paper version the reference to P. D. Jones, 1994, Hemispheric surface air temperature variations: a reanalysis and update to 1993, *J. Climate*, 7, 1794-1802, concerning the rise of land surface temperatures. In the quoted paper of Hagen and Feistel (2005), which is in press now, this trend is compared, among other indicators, with the climatic development of the Baltic ice cover, which still deems us to suit well into the introductory remarks of our ice paper.

The removal of the implementation details from the paper, in favour of supplementary

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help files, as proposed by referee #1, is of course a question to be decided by the editor. It seems to us, however, that a paper entitled “The numerical implementation...” should contain such specifications, although perhaps in a modified form. Thanks for indicating minor errors and misprints, they have been corrected now.

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Interactive comment on Ocean Science Discussions, 2, 37, 2005.

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