

Interactive comment on “Numerical implementation and oceanographic application of the Gibbs thermodynamic potential of seawater” **by R. Feistel**

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The editor of Ocean Science Discussion encourages the author(s) of a paper to write a final response, covering all previously published comments. So I will take this opportunity here.

In his second comment, David Webb is asking: Why the Gibbs function? He gives an excellent answer by listing a number of very plausible reasons. I can only underline his arguments by some additional remarks.

Thermodynamic potential functions are indeed well-known in physics and chemistry since the works of e.g. Clausius (1822-88), Gibbs (1839-1903), Helmholtz (1821-94) or Maxwell (1831-79). It was always the aim of theoretical physics to find ways to condense the wealth of experimental findings into very few compact mathematical expres-

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sions. As a famous example, the various laws of electricity, conduction, magnetism, induction, polarisation etc. were described in the 19th century in extended textbooks giving separate equations for all the particular observations; the famous partial differential equations known today by Maxwell's name finally replaced this variety by a compact and comprehensive theoretical formulation, later even triggering additional discoveries like Hertz' waves or Einstein's relativity.

Thermodynamic potential functions are similar "canonical" tools for describing the equilibrium properties of a substance. 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 formulation is consistent because no mutually contradicting conclusions can be derived from it. It is independent because no part of it can be deduced from other parts. And it is complete as all equilibrium properties can be obtained from it. The classical EOS-80 formulation of seawater, consisting of separate equations for density ρ , heat capacity c_P and sound speed U , violates all three of these elementary principles. It is not independent because these three quantities are related to each other by the thermodynamic identity

$$T \left[\left(\frac{d\rho}{dT} \right)_P \right]^2 = \left[\left(\frac{d\rho}{dP} \right)_T - \left(\frac{1}{U^2} \right) \right] \rho^2 c_P$$

It is inconsistent because one can compute by this equation e.g. heat capacity from ρ and U in an alternative way and gets contradicting results, especially for low temperatures and salinities. And it is incomplete because you cannot even properly quantify the First Law, i.e. energy conservation in the ocean, by the EOS-80 equations, since internal energy, enthalpy or entropy cannot be derived from the equations given.

The use of a seawater Gibbs function in oceanography is not a new idea; it was already proposed more than 40 years ago by Nicholas Fofonoff in 1962. The actual January

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2005 issue of J. Mar. Res. is dedicated to him. Among other papers, it contains a new Gibbs potential of ice, providing significantly improved freezing points of water and seawater up to high pressures. The numerical implementation of this function has been submitted to Ocean Science but is not yet accepted for publication at the time this comment is written. With this formulation, four aqueous phases (liquid water, vapour, ice, and seawater) are described now in a comprehensive and consistent way, and beyond the properties of these 4 single-phase states, all 6 mutual phase equilibria properties are available now, too (vapour pressure over water, ice, and seawater, freezing points of water and seawater, and osmotic pressure of seawater), as well as the properties of their possible phase mixtures (e.g. seawater + ice = sea ice, seawater + vapour = sea spray, ice + vapour = cirrus clouds), without any additional formula or measurement required.

The various possibilities for choosing a potential function, as explained in detail in Alberty's (2001) review article, are all mathematically equivalent but not equally well suited for a particular application purpose. Different potential functions can be converted into each other by so-called Legendre transforms. The IAPWS-95 formulation for pure water uses free energy (Helmholtz energy), $f(T, \rho) = g - T^*(dg/dT)_P$, as a potential function of temperature and density. At given temperature and pressure, water may be liquid or vapour or both, but at given temperature and density the state is unique. For seawater, free enthalpy (Gibbs function) $g(T, P)$ is preferred because it depends on temperature and pressure, directly available from CTD data. For processes in the ocean, which are often adiabatic or proceed on isopycnals, internal energy (depending on entropy and density), $e(\sigma, \rho) = g - T^*(dg/dT)_P - P * (dg/dP)_T$, or enthalpy (depending on pressure and entropy) may perhaps prove more appropriate theoretical formulations. So far, to my knowledge, only enthalpy, $h(\sigma, P) = g - T^*(dg/dT)_P$, was constructed once (together with the 1995 Gibbs function) in form of an explicit numerical expression, but appeared somewhat clumsy in the chosen mathematical structure.

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The recent equation of state by David Jackett et al. in JAOT (2005, in press) considers the adiabatic aspect by using potential temperature as independent variable in a fast and elegant way but does not explicitly include all thermo-chemical properties. This code is available from the revised numerical supplement in a folder called JAOT2005 together with its predecessor (Trevor McDougall et al. in J. Atm. Ocean. Techn. 20(2003)730-741), which is in a folder JAOT2003. The older version is based on the 1995 Gibbs potential and is already implemented in numerical models like MOM-3. The newer one is derived from the 2003 Gibbs potential and is thus consistent with all other pieces of code in this package. Both express (besides various conversion formulas) density in terms of potential temperature. The 2005 version additionally includes an explicit freezing point formula, derived from the 2005 Gibbs potential of ice. For better performance, both contain much less coefficients than the original Gibbs functions and are valid only for an 'oceanographic funnel' of S-T-P combinations encountered in the sea. Both are given in FORTRAN and MATLAB, compressed in ZIP for Windows and TAR for UNIX users. Problems or questions regarding these implementations should be addressed to Trevor McDougall (Trevor.McDougall@csiro.au) or David Jackett (David.Jackett@csiro.au).

The emphasis of the actual paper is clearly on providing the source code examples. The accompanying oceanographic formulas as given in section 3 are only useful context but no original research results and are recommended to be omitted in referee's #1 comment. They are intended to easily see some application examples in terms oceanographers are familiar with, especially under the aspect of the 'new' thermal properties like entropy or enthalpy. Who - without searching textbooks - knows by heart e.g. the way enthalpy appears in hydrostatic or geostrophic balances, or the energy continuity equation? These formulas are not inevitable for the article but may be helpful for the reader. In the revised paper version, gravity and z coordinate will be defined to be pointing into opposite directions, thus returning to the widespread sign convention as requested. I have no Solomonic solution, unfortunately, to escape from the dilemma concerning the desired use of the symbol g for both gravity acceleration

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and the Gibbs function. In thermodynamics, the rule is that G is the extensive Gibbs energy (in J) while g is the specific, intensive Gibbs function (in J/kg) as given in the source code. We could use, say, g_E for gravity instead of G , but does that really make any difference?

The technical issues mentioned by referee #2 are considered as follows: 1) is meant as headline for the formula, 2) is done in the revision, see referee #1, 3) can be understood as first iteration step, mentioned so in the revision, 4) eq. (25) does neither assume $\text{div}(\rho \cdot u) = 0$ nor $\text{div}(u) = 0$ but only mass conservation in general, $\text{d}\rho/\text{d}t + \text{div}(\rho \cdot u) = 0$, however, eq. (26) uses $\text{div}(\rho \cdot u) = 0$, mentioned in the revision, 5) eq. (27) assumes f-plane, mentioned in the revision, 6) thanks.

The MATLAB code described by Jan Reissmann in his discussion will be attached to the revised supplement, as supplements provided along with OS discussion contributions are not yet supported. This extension of available source code examples is very welcome as many oceanographers use MATLAB. Problems or questions regarding this implementation should be addressed to Jan Reissmann (jan.reissmann@io-warnemuende.de).

MATLAB code, as well as Visual Basic, is some proprietary computer language, supported by a certain company. It is not at all clear how long software will be available which is capable of reading, compiling or executing such kind of code. Many years ago, I wrote my very first scientific program in ALGOL, but where are ALGOL compilers found today? FORTRAN and C are perhaps languages with better chances of survival. This takes us to the very general and basic questions raised by David Webb's discussion #1.

Church books are important information sources for genealogists. These books are keeping European civil records for centuries in hand-written form. When I visited such an archive recently I was wondering how they are using computers now. Who will be able to read today's diskettes or CDs after 100 or 200 years? They showed me that

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they print on paper every new record, bind these pages to books, and place them in the shelves beside the old hand-written tomes. Is that the solution for scientific data, too? Hopefully not, or at least not only. In a project called Historical Data Rescue we recently had to spend significant efforts on the conversion of older hydrographic data from punched cards and tapes to recent formats and storage media, and these data were already in (obsolete) digital form!

Not only ZIP compression, but also PDF is a proprietary format, although with open documentation. Should we better avoid nicely formatted electronic pages and use ASCII text, or HTML instead? Should we better develop a scientific, open source document format and use only this for now and the future? These are important questions, relevant for everybody who intends to maintain a long-term database. I believe that one should, as far as possible, separate the contents from the form. Documents and data should be stored in a way that an automatic, lossless conversion to future formats will be possible at any later time. I am not an expert of PDF internals, but when I copy and paste texts from PDF to other files, this is mostly not error-free and requires manual post-processing. Equations and formulas appear in PDF as images only, as far as I know, not convertible at all.

Returning to the question of compression techniques to be used for OS supplements this leads to the following proposal. Authors pack their files using any common compression tool. The editor unpacks the files and stores them into an appropriate folder on his hardware. It is an internal technical problem of the editor to use compression, backups etc. to maintain these folders. There exist even error-correction techniques like those used on audio CDs if bit loss is suspected for the long run. A read.me file containing the tree structure can automatically be generated in every root folder, if necessary. If a reader wants access to a certain supplement, the unpacked folder is offered to him, to be optionally compressed for download by a tool of his choice. This concept would imply that every supplement is expected to come as a folder, not just a file. It would not require any kind of ‘compression standard’.

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