

NUMERICALLY CONSISTENT EQUATIONS OF STATE
FOR THE FUNCTIONS $T=T(P,H)$ AND $T=T(P,S)$
FOR WATER AND STEAM

○Th. Willkommen*, J. Trübenbach*, H.-J. Kretschmar**, A. Dittmann*

*Technische Universität Dresden, Institut für Thermodynamik und TGA,
01062 Dresden, Germany

**Hochschule Zittau/Görlitz (FH), Fachgebiet Technische Thermodynamik,
02755 Zittau, Germany

ABSTRACT

A new Industrial Formulation for the thermodynamic properties of water is to replace the IFC 67 formulation currently in use. It is expected to be more precise and at least 3 times faster when used in process modeling.

The paper presents equations for the so called backward functions $T=T(p,h)$ and $T=T(p,s)$. The equations fit the corresponding forward equations $h=h(T,p)$ and $s=s(T,p)$ developed previously within the international task group "New Industrial Formulation" extremely well. Their maximum deviation from the corresponding forward equations is less than $\Delta T=0.025$ K. Calculating backward functions using these equations requires 5 to 14 times less computing time than iterating them from the IFC 67 forward equations.

In order to set up the equations with minimal manual expenditure, a special algorithm was developed. The algorithm connects sophisticated methods for optimizing the structure of thermodynamic correlation equations with a method for simultaneous steady approximation.

The accuracy of the backward equations can be improved by an iteration procedure developed for this purpose.

NOMENCLATURE

a_i	coefficients
a_s	speed of sound
c_p	specific isobaric heat capacity
c_v	specific isochoric heat capacity
f	specific free energy
g	specific free enthalpy
h	specific enthalpy
I, J	integer exponents

p	pressure
R	ideal gas constant of water
s	specific entropy
T	Temperature
v	specific volume
Δ	difference
π	reduced pressure ($\pi=p/p_{cr}$)
τ	reduced temperature ($\tau=T_{cr}/T$)

SUBSCRIPTS

cr	critical
m	mean value
n	normalization factor (divisor)
r	reduced
s	saturated, saturation
tr	triple

SUPERSCRIPTS

con	consistency
it	iterated

CONSTANTS

h_{cr}	= 2085.1246 kJ/kg
h_n	= 2000 kJ/kg
p_{cr}	= 22.064 MPa
p_n	= 22 MPa
R	= 0.46152 kJ/kg K
s_{cr}	= 4.4237 kJ/kg K
s_n	= 4.41 kJ/kg K
T_{cr}	= 647.096 K
T_n	= 1 K

INTRODUCTION

Currently, the International Association for the Properties of Water and Steam (IAPWS) is working on

a new Industrial Formulation for calculating the thermodynamic properties of water and steam. For that purpose, an international task group termed the "Task Group New Industrial Formulation" was founded. The project is described in detail by *Wagner and Rukes* in [1].

The new Industrial Formulation is to have an accuracy commensurable with the current state of measurement technology and a considerably reduced computing time compared to the existing IFC 67 formulation when used in process modeling. In order to achieve such a fast equation package, explicit equations for the most important backward functions $T=T(p,h)$, $T=T(p,s)$ and $T_s=T_s(p)$, calculated iteratively until now, will be set up. The backward equations have to fit the corresponding forward equations $h=h(T,p)$, $s=s(T,p)$ and $p_s=p_s(T)$ extremely well, i.e. they have to be numerically consistent. If they are not, process modeling may fail.

IAPWS asked many turbine manufacturers to test their algorithms for calculating power cycles, to determine the least acceptable level of numerical consistency. The results of these investigations were then included in the specifications for the new Industrial Formulation, as set forth by the IAPWS Subcommittee on Industrial Calculations (SIC).

This paper presents equations $T=T(p,h)$ and $T=T(p,s)$ for both liquid and vapour states.

For the case in which the consistency criterion set by IAPWS and to be held by the equations does not meet the requirements of a particular process modeling, an iteration algorithm, here further refined from its original version [2], was developed. With this algorithm, the numerical consistency can be improved by two orders of magnitude with one iteration step.

THE NEW INDUSTRIAL FORMULATION

Range of validity and functions

The new Industrial Formulation will be valid in the pressure range 0.6112 kPa to 100 MPa and in the temperature range 273.15 K to 1073.15 K (see Fig. 1). The liquid range (1) corresponds to Region 1 of IFC 67 and covers temperatures up to 623.15 K. The vapour range (2) coincides with Region 2 of IFC 67; the new Industrial Formulation will use the same quadratic boundary equation $p_L(T)$ as IFC 67. For both, liquid and vapour ranges, the equations for the specific free enthalpy $g=g(T,p)$ and for the backward functions $T=T(p,h)$ as well as $T=T(p,s)$ are to be set up. The critical range (3) is equivalent to Region 3 and 4 of IFC 67. In this region only one equation $f=f(T,v)$ will be established. Also equations $p_s=p_s(T)$ and $T_s=T_s(p)$ for the saturation line will be included in the new Industrial Formulation.

The accuracy required of the equations must

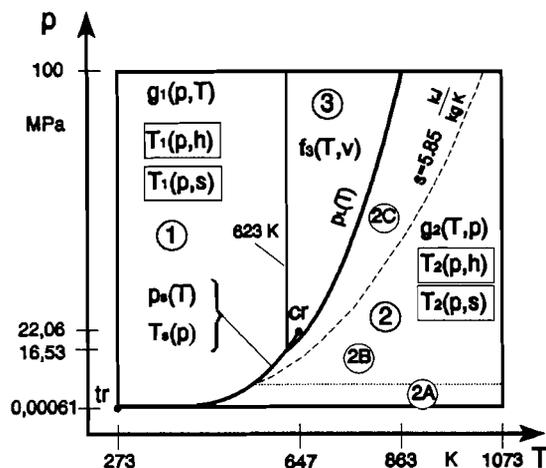


Fig. 1 Functions of the new Industrial Formulation and their ranges of validity

satisfy two important criteria: First, the equations must represent physical truth within definite tolerances. Second, they have to be numerically consistent.

Accuracy

Data Base and Permissible Tolerances. The forthcoming new Scientific Formulation will be used as the data base for establishing the new Industrial Formulation, thus enabling it to more closely represent physical truth. The new Scientific Formulation is expected to become the best available representation of the thermodynamic properties of water.

The permissible deviation from the new Scientific Formulation is defined as follows: From the $g=g(T,p)$ and $f=f(T,v)$ equations all other thermodynamic properties such as v , h , s , c_p , c_v and a_s must be derivable, such that the tolerance of v and h shall not exceed their respective tolerances in the International Skeleton Table, IST 85, in the Caller's 1994 revised form [3]. The deviations of c_p and a_s have to be generally less than 0.5%, and in difficult regions less than 1.0%.

Essentially, the Skeleton Tables IST 85 represent the current status of measurement technology. Therefore, the new Industrial Formulation will hold to the tolerances of measured data.

Numerical Consistency. Numerical consistency is defined by the maximum distance between the state surfaces described by two different equations with the same three variables. The difference between the values obtained from the two equations is the numerical consistency error. For instance, the numerical consistency error ΔT^{con} between $h=h(T,p)$ and $T=T(p,h)$ is equal to the maximum difference between T calculated directly from $T=T(p,h)$ and T^{it} calculated iteratively from $h=h(T,p)$.

$$\Delta T^{\text{con}} = \text{MAX}(|T - T^{\text{it}}|) \quad (1)$$

Investigations of the SIC (see above) have proved that the following conditions are to be met in order to ensure numerical consistency for the forward and backward equations and to avoid failures in process modeling: The difference between $h=h(T,p)$ and $T=T(p,h)$ as well as between $s=s(T,p)$ and $T=T(p,s)$ must not exceed

$$\begin{aligned} \Delta T^{\text{con}} &= 0.025\text{K for } s \leq 5.85 \text{ kJ/kg K} \\ &\text{and} \\ \Delta T^{\text{con}} &= 0.010\text{K for } s > 5.85 \text{ kJ/kg K.} \end{aligned} \quad (2)$$

The dashed line in Fig. 1 represents constant s , equal to 5.85 kJ/kg K.

NUMERICALLY CONSISTENT EQUATIONS

Liquid Range

The equations presented in this section have been fitted to the higher accurate equation $f=f(T,v)$ of *Saul and Wagner* [4] with 58 coefficients. They are the results of a search for efficient equation structures able to fulfill the IAPWS demands. It is expected that such or similar equation structures will be numerically consistent with respect to the forward equation $g_1=g_1(T,p)$ of the new Industrial Formulation, as well.

The numerical consistency criterion $\Delta T^{\text{con}} \leq 0.025\text{K}$ with respect to the Saul-Wagner-equation can be met with equation structures as follows:

$$T_1(p,h) = T_n \sum_{i=1}^{20} a_i p_r^{I_i} h_r^{J_i} \quad (3)$$

where $p_r=p/p_n$, $h_r=h/h_n+0.1$, $I_i=-2...5$ and $J_i=-5...27$

and

$$T_1(p,s) = T_n \sum_{i=1}^{19} a_i p_r^{I_i} s_r^{J_i} \quad (4)$$

where $p_r=p/p_n$, $s_r=s/s_n+0.1$, $I_i=-4...4$ and $J_i=-5...31$

Equations (3) and (4) are about 14 times faster than the functions iterated from the IFC 67 equations.

Vapour Range

The equations for region 2 have been fitted to data calculated from the equation $g_2=g_2(T,p)$ by *Kruse and Wagner* [5]. This is a very fast equation with simple polynomials, and it is to be expected that a similar equation structure will be part of the new Industrial Formulation. Therefore, using this equation as the forward equation is a good basis in searching

for equation structures for the backward equations.

In region 2, there has been no success in meeting the criteria of numerical consistency while using only one equation for each backward function. This region has therefore been split into subregions. Subregion 2C is for entropies less than 5.85 kJ/kg K (see Fig. 1), subregions 2B and 2A are for higher entropies. The border between subregions 2B and 2A is defined by a constant pressure of 6.5 MPa (dotted line in Fig. 1). Subregion 2B is for higher pressures; subregion 2A for lower.

As of the date of preparation of this paper the demands on numerical consistency ($\Delta T^{\text{con}} \leq 0.025\text{K}$ and $\Delta T^{\text{con}} \leq 0.010\text{K}$ respectively) have best been met by the following equation structures in subregions 2A, 2B and 2C respectively:

$$T_{2A}(p,h) = T_{\text{cr}} \sum_{i=1}^{30} a_i p_r^{I_i} h_r^{J_i} \quad (5)$$

where $p_r=(p/p_{\text{cr}})^{1/4}$, $h_r=h/h_{\text{cr}}-2.5$, $I_i=0...44$, $J_i=0...52$

$$T_{2B}(p,h) = T_{\text{cr}} \sum_{i=1}^{35} a_i p_r^{I_i} h_r^{J_i} \quad (6)$$

where $p_r=p/p_{\text{cr}}+1$, $h_r=h/h_{\text{cr}}-2.2$, $I_i=-24...16$, $J_i=0...60$

$$T_{2C}(p,h) = T_{\text{cr}} \sum_{i=1}^{35} a_i p_r^{I_i} h_r^{J_i} \quad (7)$$

where $p_r=p/p_{\text{cr}}+1$, $h_r=h/h_{\text{cr}}-2.2$, $I_i=-24...16$, $J_i=0...60$

$$T_{2A}(p,s) = T_{\text{cr}} \ln(p_r) \sum_{i=1}^{40} a_i p_r^{I_i} s_r^{J_i} \quad (8)$$

where $p_r=p/p_{\text{cr}}$, $s_r=s/s_{\text{cr}}$, $I_i=0...16$, $J_i=-56...64$

$$T_{2B}(p,s) = T_{\text{cr}} \sum_{i=1}^{38} a_i p_r^{I_i} s_r^{J_i} \quad (9)$$

where $p_r=p/p_{\text{cr}}+1$, $s_r=s/s_{\text{cr}}-2.3$, $I_i=-32...4$, $J_i=0...44$

$$T_{2C}(p,s) = T_{\text{cr}} \sum_{i=1}^{38} a_i p_r^{I_i} s_r^{J_i} \quad (10)$$

where $p_r=p/p_{\text{cr}}+1$, $s_r=s/s_{\text{cr}}-2.3$, $I_i=-12...24$, $J_i=0...64$

Use of equations (5) through (10), including the necessary algorithms for switching between subregions, is from 5 to 6 times faster than iterating the corresponding functions from the equations of IFC 67.

APPROXIMATION PROCEDURE

For setting up all of the above equations an algorithm developed by *Willkommen* [6,7] was used. The algorithm finds numerically consistent equations with a

minimized total number of terms automatically and with hardly any subjective influence. It connects the structure optimization method of *Setzmann and Wagner* [8] with the simultaneous steady approximation method of *Zschunke* [9]. The disadvantages of the one method are thus compensated by the advantages of the other.

The structure optimization method is a least squares method for setting up regression equations. With respect to the sum of the squares, it selects the best combination of only a few terms from a large number of possible mathematical terms. That is, the root-mean-square is minimized. In order to minimize the maximum error the simultaneous steady approximation method is used. With it, the maximum error of several independent equations, such as the forward and backward equations, can be minimized. The structure of these equations is determined previously by structure optimization methods.

Sub-algorithms for optimizing the distribution of the regression input data and for optimizing their weightings have been developed in order to obtain good equations automatically. Optimization of data distribution and weighting is important, because it influences not only the coefficients, but the selection of terms, too.

IMPROVED ITERATION PROCEDURE

Via the following procedure, the numerical consistency of equations $h=h(T,p)$ and $T=T(p,h)$ can be improved by about two orders of magnitude with one iteration step (i.e. two calls of the forward equation).

First, the starting value T_1 is calculated for given p and h :

$$T_1=T(p,h) \quad (11)$$

Then

$$h_1=h(T_1,p) \quad (12)$$

is determined. The temperature T_2 is estimated from an average $c_{p,m}$ adjusted separately for region 1 as well as for subregions 2A, 2B and 2C:

$$T_2=T_1+(h-h_1)/c_{p,m} \quad (13)$$

After that

$$h_2=h(T_2,p) \quad (14)$$

is calculated. The iterated temperature T^{it} is computed now according to:

$$T^{it}=T_1+(h-h_1)(T_2-T_1)/(h_2-h_1) \quad (15)$$

A similar procedure can be used for improving the numerical consistency of equations $s=s(T,p)$ and $T=T(p,s)$. In this case Eq. (13) must be written:

$$T_2=T_1+T_1(s-s_1)/c_{p,m} \quad (16)$$

CONCLUSION

Equation structures for the backward functions $T=T(p,h)$ and $T=T(p,s)$ capable of meeting the demanding requirements of numerical consistency for process modeling are presented. The backward equations consume much less computing time than the iteration of these functions from corresponding forward equations $h=h(T,p)$ and $s=s(T,p)$.

Furthermore, an effective iteration procedure for process modeling under the most extreme requirements of numerical consistency is presented.

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