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IMPROVED EQUATIONS FOR BACKWARD FUNCTIONS
 $T=f(p,h)$, $T=f(p,s)$, $T_s=f(p)$
- A CONTRIBUTION TO THE IAPWS PROJECT
„NEW INDUSTRIAL FORMULATION“

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ABSTRACT: The paper presents improved equation structures for $g=f(T,p)$, $T=f(p,h)$ and $T=f(p,s)$ in the steam region, equation structures for $T=f(p,h)$ and $T=f(p,s)$ in the liquid region and various equation pairs $p_s=f(T)$ and $T_s=f(p)$ on the saturation curve which are the subject of the current IAPWS project "New Industrial Formulation".

The established equations fall within the uncertainty limits set by the IAPWS 1985 Skeleton Tables when compared to the *Saul/Wagner* equation converted to the new Temperature Scale ITS 90. The numerical consistency of the backward equations meets the demands of process modeling which were set by the IAPWS Subcommittee on Industrial Calculations. Using these equations in process modeling eliminates the otherwise necessary iterations in calculating backward functions.

The structures of the equations have been optimized with the Algorithm of *Setzmann and Wagner*. After that equations have been made numerically consistent with the simultaneous approximation method developed by *Zschunke* and advanced by *Willkommen*.

INTRODUCTION

At present equations of state for the New Industrial Formulation (NIF) are being developed in the IAPWS Task Group, New Industrial Formulation. This new equation set is expected to replace the IFC 1967 Formulation for Industrial Use in 1997.

The requirements for the new formulation were formulated by the IAPWS Subcommittee on Industrial Calculations (SIC) in 1991 [1] and corrected in 1992 [2] and 1993 [3]. The most important requirements are:

- The range of state and the functional dependencies of the equations to be set up in the subregions ①, ②, ③ and on saturation line are shown in Fig. 1.
- The accuracy of the equations will be given by the New Scientific Formulation. It has to be within the tolerances of the IAPWS Skeleton Tables 1985 (Revision 1994) [4] with the exception of some corrections in the liquid region.

forward equations $h=f(T,p)$, $s=f(T,p)$, both derived from $g=f(T,p)$ and $p_s=f(T)$ follows from process calculations. It will be explained later.

- The main requirement of the industry is that, the new formulation must be 3 times faster than the IFC 1967 Formulation in energy process modeling

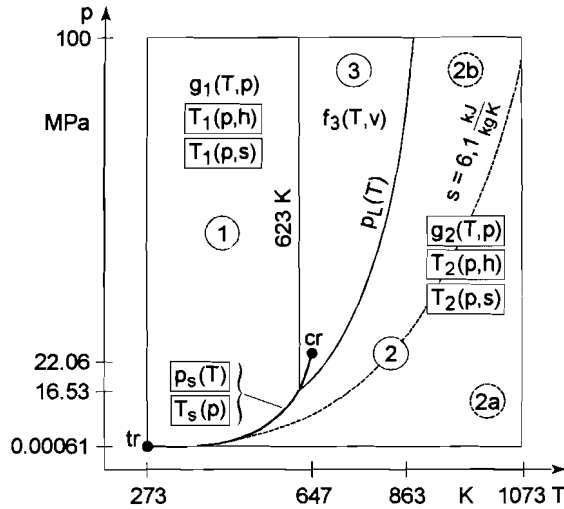


Figure 1. Range of State, Subregions and Functions of the New Industrial Formulation

In this work equation structures for the framed functional dependencies in Figure 1 are presented. They have been developed using the structure optimization methods of *Wagner* [5,6], the simultaneous steady approximation method of *Zschunke* [7] and the new algorithm to improve the numerical consistency of *Willkommen* [8,9]. Because the New Scientific Formulation is not issued yet the *Saul/Wagner Equation* [10] was the basis for the approximations. Therefore the following equations are preliminary and their coefficients are not added. In case there is an interest one can receive the coefficients from the authors.

VARIOUS EQUATION STRUCTURES FOR $p_s=f(T)$ AND $T_s=f(p)$

Three equation pairs $p_s=f(T)$ and $T_s=f(p)$ could be found each with its pros and cons. They are shown in Table 1.

Convertible Equation $f(T_s, p_s)=0$

The first equation pair $p_s=f(T)$ and $T_s=f(p)$ which fulfills all requirements results from an approximated implicit equation $f(p_{rs}, T_{rs})=0$.

It has the following form:

$$a_1 T_{rs} + a_2 p_{rs}^2 + a_3 T_{rs}^2 + a_4 p_{rs} T_{rs} + a_5 p_{rs} T_{rs}^2 + a_6 p_{rs}^2 T_{rs} + a_7 p_{rs}^2 T_{rs}^2 - p_{rs} = 0$$

$$\text{with } T_{rs} = \frac{T_{cr}}{T_s} - 1 \quad \text{and } p_{rs} = \ln\left(\frac{p_s}{p_{cr}}\right)$$

Table 1. Equation Pairs $p_s=f(T)$ and $T_s=f(p)$

Convertible Equation Pair			
$p_s = f(T)$		$T_s = f(p)$	
$p_s = p_{cr} \cdot \exp \left\{ \frac{A - \sqrt{A^2 - B \cdot C}}{B} \right\}$ $A = -\frac{1}{2} (a_4 \cdot T_r + a_5 \cdot T_r^2 - 1)$ $B = a_2 + a_6 \cdot T_r + a_7 \cdot T_r^2$ $C = a_1 \cdot T_r + a_3 \cdot T_r^2$ with $T_r = \frac{T_{cr}}{T} - 1$		$T_s = T_{cr} \cdot \frac{E}{D + E - \sqrt{D^2 - D \cdot F}}$ $D = -\frac{1}{2} (a_1 + a_4 \cdot p_r + a_6 \cdot p_r^2)$ $E = a_3 + a_5 \cdot p_r + a_7 \cdot p_r^2$ $F = a_2 \cdot p_r^2 - p_r$ with $p_r = \ln \left(\frac{p}{p_{cr}} \right)$	
7 Coefficients $a_1 \dots a_7$			
Polynomial Equation Pair			
$p_s = p_n \cdot \sum_{m=1}^{11} a_m \cdot T_r^{k_m}$ with $T_r = \frac{T - T_{tr}}{T_n}$		$T_s = T_n \cdot \sum_{m=1}^9 b_m \cdot p_r^{l_m}$ with $p_r = \frac{p}{p_n}$	
11 Coefficients $a_1 \dots a_{11}$		9 Coefficients $b_1 \dots b_9$	
m	k_m	m	l_m
1	0	1	-8
2	1	2	-4
3	2	3	-3
4	3	4	-2
5	4	5	-1
6	5	6	0
7	6	7	1
8	7	8	3
9	8	9	12
10	9		
11	15		
Short Equation Pair			
$p_s = p_{cr} \cdot \exp \left\{ \sum_{m=1}^5 a_m \cdot T_r^{\frac{k_m}{2}} \right\}$ with $T_r = \frac{T_{cr}}{T} - 1$		$T_s = T_{cr} \left[1 - \sum_{m=1}^4 b_m \cdot p_r^{\frac{l_m}{2}} \right]$ with $p_r = 1 - \frac{1}{1 - 0.136 \ln \left(\frac{p}{p_{cr}} \right)}$	
5 Coefficients $a_1 \dots a_5$		4 Coefficients $b_1 \dots b_4$	
m	k_m	m	l_m
1	2	1	2
2	3	2	3
3	4	3	5
4	7	4	9
5	10		
$T_{cr} = 647.096 \text{ K} \quad , \quad p_{cr} = 22.064 \text{ MPa} \quad , \quad T_{tr} = 273.16 \text{ K} \quad , \quad T_n = 1 \text{ K} \quad , \quad p_n = 1 \text{ MPa}$			

Table 1 contains the solutions of this equation for p_s and T_s in the upper part. Both equations have the same 7 coefficients $a_1...a_7$.

Polynomial Equations $p_s=f(T)$ and $T_s=f(p)$

The next equation pair consists of fast polynomials $p_s=f(T)$ and $T_s=f(p)$. The middle part of Table 1 shows the equation structures with altogether 20 coefficients.

Short Equations $p_s=f(T)$ and $T_s=f(p)$

The last equation pair $p_s=f(T)$ and $T_s=f(p)$ consists of short equations with more complicated structures and just 9 coefficients altogether. It is shown in the lower part of Table 1.

Discussion of the 3 Equation Pairs $p_s=f(T)$ and $T_s=f(p)$

The convertible equation pair, the polynomial equations and the short equations meet the *Saul/Wagner* Equation within the corrected skeleton table pressure tolerance of 0.025% between triple point and critical point. Table 2 contains weighted state errors in % relating to the Skeleton Table Tolerances. The short equation pair is most accurate.

All equations also meet the requirements on numerical consistency. Table 2 shows weighted numerical consistency errors in % relating to the value 0.003% given by SIC. Of course the convertible equation has a consistency error of zero. The polynomial equation pair comes up to 83%, i.e. it almost exhausts the required numerical consistency.

Table 2. Results of the Equation Pairs $p_s=f(T)$ and $T_s=f(p)$

		Convertible Equations	Polynomial Equations	Short Equations
Weighted state error relating to 0.025 %		68 %	84 %	44 %
Weighted numerical consistency error relating to 0.003 %		0	83 %	17 %
Factor of computing time improvement in comparison with IFC 67 (IAPWS Program NIFBENCH)	p_s (T)	1.0	3.1	1.1
	T_s (p)	6.3	8.3	7.1
Factor of computing time improvement of a complete NIF with equation pair $p_s=f(T)$ and $T_s=f(p)$ (other functions estimated)		3.3	3.5	3.3

A very important criterion for choosing the final equation pair is the necessary computing time. The IAPWS Program, NIFBENCH was used to measure it. The next rows of Table 2 show factors of computing time improvements of $p_s=f(T)$ and $T_s=f(p)$ in comparison with IFC 67. The computing times of the convertible and the short equation $p_s=f(T)$ are almost similar to IFC 67. The polynomial equation $p_s=f(T)$ is 3.1 times faster.

The equations $T_s=f(p)$ are between 6.3 and 8.3 times faster than with IFC 67. The reason is, the saturation temperature has to be iterated using the IFC 67 Formulation whereas explicit equations $T_s=f(p)$ are available now. Again the polynomial equation is faster than the other 2 equations. The differences between the three saturation temperature equations are not so great because of their nearly similar structure and the much higher computing time of IFC 67.

In order to judge the influence on the whole package it is necessary to do a forecasting of the computing time of a complete New Industrial Formulation (NIF) with these saturation equation pairs. The last row in Table 2 contains the results. A NIF with the convertible equation pair would be 3.3 times faster than IFC 67, a NIF with the polynomial equation pair 3.5 times faster and a NIF with the short equation pair again 3.3 times faster. So the factor of computing time improvement using the polynomial equations would just increase by 0.2 in comparison with the other equation pairs.

Since the difference of the influence of the 3 equation pairs on the computing time of the complete formulation is small the advantage of the convertible equation pair to have an exact numerical consistency overweighs. Therefore the convertible equation pair is recommended as part of the New Industrial Formulation.

A SHORT EQUATION STRUCTURE $g_2=f(T,p)$ FOR STEAM

In order to set up backward equations $T_2=f(p,h)$, $T_2=f(p,s)$ in the steam region ② (Figure 1) it was necessary to establish also the related forward equation $g_2=f(T,p)$. The reason was, the *Saul/Wagner* Equation converted to ITS 90 could not be used because of the sharp extreme value at 903.15 K in the conversion algorithm.

Furthermore from our experience the precondition for approximating short backward equations is a short forward equation with only a few terms. That was reached by application of the relatively complicated „spinodal-terms“ developed by *Willkommen* [9]. These terms permit an expansion of the range of validity up to 633.15 K on the saturation line. The corresponding boundary is described by a polynomial of second degree through 3 points (Table 3) similar to the L-function of IFC 67.

The developed fundamental equation $g_2=f(T,p)$, with just 20 terms, is shown in Table 4. It can be seen it has 3 terms with an approximation of the spinodal for reduced temperature as a function of reduced pressure.

Table 5 contains the main features of the derived equations $h_2=f(T,p)$, $v_2=f(T,p)$ and $s_2=f(T,p)$. The equations $h_2=f(T,p)$ and $v_2=f(T,p)$ meet the Skeleton Table Tolerances. The uncertainty of $s_2=f(T,p)$ amounts 0.2% when compared to the *Saul/Wagner* Equation.

Whereas the equation $h_2=f(p,T)$ is 3.4 times faster than IFC 67 the test of $v_2=f(p,T)$ shows just a doubling of speed. The reasons are the complicated derivation of „spinodal terms“ and the fast equation structure of IFC equation $v_2=f(p,T)$.

Table 3. Boundary Function for Expanded Subregion 2 up to 633.15 K

$\ln\left(\frac{p}{p_s(633.15K)}\right) = a_1\left(1 - \frac{633.15K}{T}\right) + a_2\left(1 - \frac{633.15K}{T}\right)^2$			
fitted to points	1	2	3
p in MPa	18.665	55.0	100.0
T in K	633.15	773.15	853.15

Table 4. Equation Structure $g_2=f(p,T)$

$g_2 = f(T,p)$			
$g_2 = R \cdot T \left\{ \sum_{m=1}^9 a_m \cdot p_r^{k_m} \cdot \left(\frac{1}{T_r} - 0.45 \right)^{l_m} + \sum_{m=10}^{12} a_m \cdot \frac{p_r}{l_m \cdot (T_r - T_r^{spin} + 0.015)^{l_m}} \right.$ $+ a_{13} + a_{14} \cdot p_r + a_{15} \cdot p_r^2 + a_{16} \cdot \ln(p_r) + a_{17} \cdot p_r [\ln(p_r) - 1] \cdot \left(\frac{1}{T_r} - 0.45 \right)$ $\left. + a_{18} \cdot T_r + a_{19} \cdot \ln(T_r) + a_{20} \left(\frac{1}{T_r} - 0.45 \right) \right\}$			
with $T_r^{spin} = \frac{1}{1 - \ln(p_r) \cdot [0.173 - 0.011 \ln(p_r) - 0.02 \cdot p_r]}$			
20 Coefficients $a_1 \dots a_{20}$			
$p_r = \frac{p}{p_{cr}} \quad , \quad T_r = \frac{T}{T_{cr}}$ $T_{cr} = 647.096 \text{ K}$ $p_{cr} = 22.064 \text{ MPa}$ $R = 0.46152 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}$	m	k_m	l_m
	1	1	2
	2	1	3
	3	1	4
	4	2	8
	5	3	6
	6	4	6
	7	6	8
	8	8	20
	9	12	12
	10		3
	11		2
12		1	

Table 5. Uncertainties and Computing Times of Equations Derived from $g_2=f(p,T)$

	$h_2 = f(T,p)$	$v_2 = f(T,p)$	$s_2 = f(T,p)$
State Error (relating to <i>Saull/Wagner</i> Equation converted into ITS 90)	within Tolerances of the IAPWS Skeleton Tables 1985 (Revision 1994)		< 0.2 %
Factor of computing time improve- ment in comparison with IFC 67 (IAPWS Program NIFBENCH)	3.4	2.1	2.2

EQUATION STRUCTURES $T_2=f(p,h)$ AND $T_2=f(p,s)$ FOR STEAM

The initial aim to set up one equation for $T_2=f(p,h)$ and for $T_2=f(p,s)$ in the steam region (2) which would fulfill the demanded numerical consistency in the whole region could not be achieved even with equation structures of considerable length and computing time. So region (2) had to be split into 2 subregions. For the boundary the isentrope $s=6.1 \text{ kJ/kgK}$ was chosen. It divides the steam region into a subregion (2a) and subregion

(2b) (Fig. 1). The splitting by an isentrope simplifies not only the fitting of equations but also the handling of the equation package in process modeling. Turbine expansion processes usually start from entropies above 6.1 kJ/kgK, so most calculations take place in subregion (2a). Furthermore it was possible to expand the range of validity of subregion (2b) up to 633.15 K on the saturation line.

In order to achieve computing speeds at least 3 times faster than those of the IFC 67 Formulation the use of terms with large computing times were avoided as far as possible. The structures of equations developed for subregions (2a) and (2b) are shown in Table 6.

Table 6. Equation Structures $T_2=f(p,h)$ and $T_2=f(p,s)$ for Steam

$T_{2a} = f(p,h)$	$T_{2b} = f(p,h)$
$T_{2a} = T_n \cdot \left\{ \sum_{m=1}^{19} a_m \cdot p_r^{k_m} \cdot h_r^{l_m} \right.$ $+ \sum_{m=20}^{24} a_m \cdot p_r^{k_m} \cdot (h_r - 1)^{l_m}$ $+ \sum_{m=25}^{28} a_m \left[0.1^{k_m} - (p_r + 0.1)^{k_m} \right] \cdot h_r^{l_m}$ $\left. + \sum_{m=29}^{31} a_m \left[0.1^{k_m} - (p_r + 0.1)^{k_m} \right] \cdot (h_r - 1)^{l_m} \right\}$	$T_{2b} = T_n \cdot \left\{ \sum_{m=1}^{23} b_m \cdot p_r^{k_m} \cdot h_r^{l_m} \right.$ $+ \sum_{m=24}^{26} b_m \cdot p_r^{k_m} \cdot (h_r - 1)^{l_m}$ $+ \sum_{m=27}^{33} b_m \left[1 + (p_r + 1)^{k_m} \right] \cdot h_r^{l_m}$ $\left. + \sum_{m=34}^{35} b_m \left[1 + (p_r + 1)^{k_m} \right] \cdot (h_r - 1)^{l_m} \right\}$
31 Coefficients $a_1 \dots a_{31}$	35 Coefficients $b_1 \dots b_{35}$
$T_{2a} = f(p,s)$	$T_{2b} = f(p,s)$
$T_{2a} = T_n \cdot \left\{ \sum_{m=1}^{19} c_m \cdot p_r^{k_m} \cdot s_r^{l_m} \right.$ $+ \sum_{m=20}^{27} c_m \cdot p_r^{k_m} \cdot (s_r - 1)^{l_m}$ $\left. + \sum_{m=28}^{40} c_m \cdot (p_r + 1)^{k_m} \cdot (s_r - 1)^{l_m} \right\}$	$T_{2b} = T_n \cdot \left\{ \sum_{m=1}^{13} d_m \cdot p_r^{k_m} \cdot s_r^{l_m} \right.$ $+ \sum_{m=14}^{30} d_m \cdot p_r^{k_m} \cdot (s_r - 1)^{l_m}$ $+ \sum_{m=31}^{35} d_m \cdot (p_r + 1)^{k_m} \cdot s_r^{l_m}$ $\left. + \sum_{m=36}^{40} d_m \cdot (p_r + 1)^{k_m} \cdot (s_r - 1)^{l_m} \right\}$
40 Coefficients $c_1 \dots c_{40}$	40 Coefficients $d_1 \dots d_{40}$
$p_r = \frac{p}{p_n}; s_r = \frac{s}{s_n}; h_r = \frac{h}{h_n}; T_n = 1 \text{ K}; p_n = 22.064 \text{ MPa}; h_n = 2085.12 \frac{\text{kJ}}{\text{kg}}; s_n = 4.42 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}$	

Equation Structures $T_2=f(p,h)$ for Steam

The manifold but still simple polynomial structures of both equations (upper part of Table 6) provide a numerical consistency higher than demanded and a high computing speed. The equations have just 31 and 35 coefficients. The exponents are divided by 2 or 4 partially and run from -14 up to 12.5 for reduced pressure and from -70 up to 20 for reduced enthalpy (Table 7, left columns).

The structures of these combined polynomials proved to be particularly effective in subregion (2a). In this region, which is important for turbine expansion processes, the numerical consistency error could be reduced down to 10 mK (Table 8).

Table 7. Exponents of Equations $T_2=f(p,h)$, $T_2=f(p,s)$ for Steam

m	$T_{2a} = f(p,h)$		$T_{2b} = f(p,h)$		m	$T_{2a} = f(p,s)$		$T_{2b} = f(p,s)$	
	k_m	l_m	k_m	l_m		k_m	l_m	k_m	l_m
1	0	0	0	0	1	0	2	0	-16
2	0	1	0	20	2	0	8	0	-12
3	0	4	0	-1	3	1/4	3	1/8	0
4	0	-1	0	-3	4	1/4	8	1/8	16
5	0	-3	0	-6	5	1/4	12	1/2	4
6	0	-6	0	-8	6	1/2	1	1	6
7	1/2	-1	0	-10	7	3/4	1	5/4	-1
8	3/4	0	0	-12	8	3/4	12	3/2	-4
9	1	0	1/4	0	9	1	20	2	16
10	1	-1	1/4	-4	10	3/2	10	5/2	16
11	1	-24	1/2	-8	11	5/2	20	3	-48
12	2	-2	3/4	-3	12	5/2	48	5	-40
13	2	-4	1	-4	13	3	56	9	-40
14	2	-36	1	-14	14	4	32	0	-1
15	5/2	-10	2	-3	15	0	-16	0	8
16	5/2	-24	2	-4	16	4	-16	1/8	6
17	7/2	-20	2	-8	17	0	-28	3/4	2
18	7/2	-60	2	-32	18	0	-36	5/4	-1
19	8	0	5/2	-16	19	3/2	-36	5/4	8
20	1	-4	5/2	-50	20	1/2	3	3/2	20
21	1	-5	3	-24	21	1/2	8	3/2	32
22	2	-5	4	-12	22	3/2	12	2	32
23	8	-36	25/2	-10	23	1	2	5/2	8
24	25/2	-70	2	-1	24	1	6	5/2	24
25	-1	-24	8	-28	25	3/2	3	3	12
26	-1	-50	25/2	-28	26	5/2	32	3	16
27	-2	-12	-2	-3	27	3	24	4	2
28	-5	-6	-3	0	28	-12	8	5	-24
29	-1	-5	-8	0	29	-24	4	5	-2
30	-2	-4	-8	-16	30	-32	2	7	20
31	-12	-8	-12	-1	31	-1	-1	-2	-10
32			-12	-50	32	-2	-3	-4	-2
33			-14	-50	33	-6	-3	-6	-32
34			-3	-4	34	-6	-32	-12	-48
35			-5	-6	35	-8	-2	-24	-40
36					36	-16	-2	-4	-32
37					37	-16	-16	-8	-16
38					38	-24	-1	-8	-6
39					39	-24	-32	-12	-12
40					40	-32	-8	-24	-16

For determination of the relative computing time both equations were programmed into one subroutine including a switching function $h_{2ab}=f(p)$ to handle the subregions. This equation set is 5.5 times faster than IFC 67 (Table 8). Exhausting the current allowable consistency error of 25 mK, from 2 up to 5 terms could be saved for further increasing of computing speed.

Table 8. Numerical Consistencies and Computing Times of Backward Equations for Steam

		$T_2 = f(p,h)$	$T_2 = f(p,s)$	$v_2 = f(p,h)$	$s_2 = f(p,h)$	$h_2 = f(p,s)$
Weighted numerical consistency error relating to 25 mK	2a	39 %	74 %			
	2b	67 %	100 %			
Factor of computing time improvement in comparison with IFC 67		5.5	4.8	3.8	3.7	4.4

Equation Structures $T_2=f(p,s)$ for Steam

The polynomial structures of backward equations $T_{2a}=f(p,s)$ and $T_{2b}=f(p,s)$ shown in the lower part of Table 6 are similar to the structures used for $T_{2a}=f(p,h)$ and $T_{2b}=f(p,h)$. However, in order to meet the required numerical consistency the lengths of both equations was to be increased up to 40 terms. In subregion (2a) the exponents run from -32 up to 3 for reduced pressure and from -32 up to 56 for reduced entropy and are partly divided by 2 or 4.

The structures for subregion (2b) are more complicated. The exponents run from -24 up to 7 for reduced pressure and are partly divided not only by 2 and 4 but also by 8. The exponents for reduced entropy in subregion (2b) run from -48 up to 32.

Table 8 shows the weighted numerical consistency errors relating to 25 mK. The value 100 % for $T_{2b}=f(p,s)$ points out that a relatively short equation could be achieved only by full exhausting the allowable numerical consistency error. Test calculations have shown that even by adding further terms and using much more complicated terms like the exponential function, a significant increase of accuracy, i.e. doubling or tripling, is not possible. In case of increasing the requirements on numerical consistency a splitting into more subregions would be inevitable.

The computing speed was determined in the same way as for $T_2=f(p,h)$. Because of the isentropic boundary between the subregions the switching needs no special functions. As a result the presented equations $T_{2a}=f(p,s)$ and $T_{2b}=f(p,s)$ together are 4.8 times faster than IFC 67 (Table 8).

In addition Table 8 contains computing time improvement factors of the other benchmark functions of region (2). With regard to frequencies of call the presented set of forward and backward equations for the steam region is 3.5 times faster than the IFC 67 Formulation.

EQUATION STRUCTURES $T_1=f(p,h)$ AND $T_1=f(p,s)$ FOR WATER

The backward equations $T_1=f(p,h)$ and $T_1=f(p,s)$ developed for liquid water (Subregion (1) in Fig. 1) are shown in Table 9. Both equations are simple polynomials with integer exponents between -5 and +6 for reduced pressure and between -7 and +39 for reduced enthalpy and reduced entropy

respectively. Higher and lower exponents were not chosen by the structure optimization algorithm. The $T_1=f(p,h)$ equation has 28 coefficients and $T_1=f(p,s)$ 30 coefficients.

At first exponents divided by 2, 3 and 4 were tried, but the results were not satisfying. Obviously the high exponents are more important.

Table 9. Equation Structures $T_1=f(p,h)$ and $T_1=f(p,s)$ for Liquid Water

$T_1 = f(p,h)$			$T_1 = f(p,s)$		
$T_1 = T_n \cdot \sum_{m=1}^{28} a_m \cdot p_r^{k_m} \cdot h_r^{l_m}$			$T_1 = T_n \cdot \sum_{m=1}^{30} b_m \cdot p_r^{k_m} \cdot s_r^{l_m}$		
with $p_r = \frac{p}{p_n}$, $h_r = \frac{h}{h_n} + 0$.			with $p_r = \frac{p}{p_n}$, $s_r = \frac{s}{s_n} + 0.1$		
$T_n = 1 \text{ K}$, $p_n = 22 \text{ MPa}$, $h_n = 2000 \frac{\text{kJ}}{\text{kg}}$			$s_n = 4.41 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}$		
28 Coefficients $a_1 \dots a_{28}$			30 Coefficients $b_1 \dots b_{30}$		
m	k_m	l_m	m	k_m	l_m
1	-4	39	1	-5	39
2	-2	17	2	-3	29
3	-1	10	3	-2	25
4	-1	13	4	-2	33
5	-1	15	5	-1	21
6	-1	39	6	0	-2
7	0	-1	7	0	0
8	0	0	8	0	1
9	0	1	9	0	2
10	0	2	10	0	3
11	0	3	11	0	7
12	0	4	12	0	26
13	0	19	13	1	-6
14	1	-7	14	1	-3
15	1	-6	15	1	-2
16	1	-4	16	1	1
17	1	-3	17	1	2
18	1	-2	18	1	5
19	1	-1	19	1	10
20	1	4	20	1	32
21	1	5	21	2	-1
22	1	28	22	2	0
23	2	1	23	2	2
24	2	5	24	2	5
25	2	39	25	2	12
26	3	0	26	3	-2
27	4	5	27	3	15
28	5	5	28	4	4
			29	5	2
			30	6	3

Table 10 contains the weighted numerical consistency errors in comparison with the required errors for both equations. The values 56 % for $T_1=f(p,h)$ and 46 % for $T_1=f(p,s)$ point out the possibility of saving terms in the equations. Because up until now the numerical consistency errors to be met were not finally defined the search for shorter equation structures was not necessary. First calculations have shown, from 2 up to 4 terms could be saved exhausting the current errors.

The factors of computing time improvement in comparison with IFC 67 are shown in the last row of Table 10. The equation $T_1=f(p,h)$ is 11.0 times faster than IFC 67. The reason is this function has to be iterated from $h_1=f(T,p)$ when calculating the IFC 67 package.

The direct comparison of the computing time of function $T_1=f(p,s)$ is not useful because of its insignificant frequency of call in process modeling. The more important function $h_1=f(p,s)$ has the same variables p and s . So this function should be tested. That means after $T_1=f(p,s)$ the function $h_1=f(T,p)$ has to be calculated. Because there is not a final equation $h_1=f(T,p)$ for the New Industrial Formulation its computing time was estimated as up to 2 times faster than IFC 67. Together with that the comparison of $h_1=f(p,s)$ comes to a factor of 5.6.

Table 10. Numerical Consistencies and Computing Times of the Equations $T_1=f(p,h)$ and $T_1=f(p,s)$

	$T_1 = f(p, h)$	$T_1 = f(p, s)$	$h_1 = f(p, s)$
Weighted numerical consistency error relating to required value	56 % $\left(\Delta h = 0.08 \frac{\text{kJ}}{\text{kg}} \right)$ required	46 % $\left(\Delta s = 0.0001 \frac{\text{kJ}}{\text{kg} \cdot \text{K}} \right)$ required	
Relative computing time to IFC 67 (IAPWS Program NIFBENCH)	11.0		5.6 with $h_1 = f(T, p)$ 2 times faster than IFC 67

SUMMARY

The presented equation structures $p_s=f(T)$, $T_s=f(p)$ for the saturation curve, $g_2=f(T,p)$, $T_2=f(p,h)$, $T_2=f(p,s)$ for the steam region and $T_1=f(p,h)$, $T_1=f(p,s)$ for the liquid water region are proposals on how to develop the New Industrial Formulation.

In particular the convertible equation pair $p_s=f(T)$ and $T_s=f(p)$ is recommended because of its exact numerical consistency.

The equation $g_2=f(T,p)$ for steam has a relatively complicated structure but just 20 terms. The range of validity can be expanded up to 633.15 K on the saturation line without adding further terms.

In order to achieve the required numerical consistency of the backward equations $T_2=f(p,h)$, $T_2=f(p,s)$, the steam region had to be divided into 2 subregions. The minimal entropy from which turbine expansion processes usually start was used as the boundary. A significant improvement of the numerical consistency of the subregion equations $T_{2a}=f(p,s)$ and $T_{2b}=f(p,s)$ is not possible. In case of an increase in the requirements for the numerical consistency the steam region would have to be split into more subregions.

The backward equations $T_1=f(p,h)$, $T_1=f(p,s)$ for the liquid water region are simple polynomials. An improvement in their numerical consistency without splitting in subregions is possible up to 40 % of the currently required values. Doing this would not increase the computing time considerably.

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