PROPERTIES OF WATER AND STEAM

Proceedings of the 11th International Conference

Edited by

M. Píchal
O. Šifner
Institute of Thermomechanics
Czechoslovak Academy of Sciences

HEMISPHERE PUBLISHING CORPORATION
A member of the Taylor & Francis Group

New York Washington Philadelphia London

Computer Code for the Generation of Optimized Algorithms to Calculate Thermophysical Properties of Water and Steam

A. DITTMAN, T. ZSCHUNKE, and J. KLINGER
Technische Universität Dresden
Mommsenstrasse 13, Dresden 8027, DDR

H.-J. KRETZSCHMAR
Zentrum für Forschung und Technik
Institut für Energieversorgung Dresden des Kombinates Verbundnetze Energie, Zeunerstrasse 83, Dresden 8027, DDR

INTRODUCTION

Formulations of the properties of water and steam , such as the 1967 IFC or the 1984 IAPS formulation, for many applications are not required in their exactness and have a too high need in computation time. This paper is a contribution to the development of "minor" equations of state (with an exactness as good as demanded and for minimized ranges of state.)

THERMODYNAMIC TASK

For practical use equation sets are needed which work without iterations and represent the thermophysical properties in predefined parameter ranges with predefined exactness [1]. Basic data for their construction are taken from international formulations, in the general form $z=z(x,y)$.

MATHEMATICAL TASK

The mathematical task may be formulated in two levels:

1. On the bottom level free parameters of a given function are to be determined so, that a norm will be a minimum. Approximating to "exact" functions the maximum difference is the more important norm than the usually taken sum of squares of differences.
2. On the top level the smallest function is to be found, which fulfills a predefined criterion like
   - a value for the maximum difference from the original equation or
   - the fulfilment of the International Skeleton Tables.

CONSISTENCY

A set of independent equations cannot be consistent. So numerical problems may appear in practical iterative or stepwise calculations. To prevent such events, relations between approximated equations should be controlled to derive conclusions about minimum parameter step widths.

MATHEMATICAL SOLUTION

The search for optimal functions is made by the help of a modification of WAGNERs stepwise linear regression analysis [2,3,4]. (Parameter determination occurs here under minimization of the sum of error squares.)
A new method for nonlinear Chebyshev approximation (minimization of maximum error) by JING and FAM [5] was extended and it is used now for the improvment of the function parameters.

The original version of JING's and FAM's method considers the following Chebyshev approximation problem. Find a parameter vector

$$\underline{a}^b = (a_1^b, a_2^b, \ldots, a_n^b) \tag{1}$$

with linear and nonlinear parameters of an approximating function $f(\underline{a},x)$ to minimize max[$E(\underline{a},x)$] (superscript "b") where

$$E(\underline{a},x) = |f(\underline{a},x) - F(x)| \tag{2}$$

with the original function $F(x)$.

The problem is designed in a form improving the parameter vector by a linear optimization.

But for the thermodynamic relation $0=F(x,y,z)$ up to three approximating functions (superscript "*") are necessary :

$$\begin{aligned} z^* &= z^*(\underline{a}_z, x, y) \\ y^* &= y^*(\underline{a}_y, x, z) \\ x^* &= x^*(\underline{a}_x, y, z) \,. \end{aligned} \tag{3}$$

Instead of (2) now several error functions E_N may be taken in consideration to control relations between functions.
A choice of important ones is shown in Tab. 1 . Error function E_{VIII} is formulated to fit equations to the International Skeleton Tables (subscript "ST"). Error function E_{IX} allows to fit other functions with the same parameter vector (point above the symbol) like

$$\dot{z}^* = \left(\frac{\partial z^*}{\partial x}\right)_y \tag{4}$$

simultaneously.

TABLE 1. Some error functions E_N for approximation of sets of thermodynamic equations

N	E_N	N	E_N
I	$\lvert z^*(\underline{a}_z,x,y)-z(x\,y)\rvert$	VIII	$\Delta z-1$ (if $\Delta z>1$) 0 (if $\Delta z<0$) $\left[\Delta z=\left\lvert\frac{z^*(\underline{a}_z,x,y)-z_{ST}(x,y)}{\Delta z_{ST}}\right\rvert\right]$
II	$\lvert y^*(\underline{a}_y,x,z)-y\rvert$		
III	$\lvert x^*(\underline{a}_x,y,z)-x\rvert$		
IV	$\lvert y^*(\underline{a}_y,x,z^*(\underline{a}_z,x,y))-y\rvert$		
V	$\lvert x^*(\underline{a}_x,y,z^*(\underline{a}_z,x,y))-x\rvert$	IX	$\lvert\dot{z}^*(\underline{a}_z,x,y)-\dot{z}(x,y)\rvert$
⋮		⋮	

The extension on JING's approximation method allows to consider two or more error functions of two independent variables simultaneously and to weight them against each other. The flow chart (fig. 1) shows the simultaneous minimization of error functions E_I and E_{IV}. In every iteration step at first all local maxima of all chosen error functions are determined. Before starting the linear optimization for the calculation of improved parameters the maxima of every observed error function E_N are weighted with the empirical factor w_N and their derivations to the parameters are calculated. The iteration will stop if no further improvment of the maximum weighted error is possible.

COMPUTER PROGRAM

The developed algorithm is a part of the program ECOFIT concerning also modules for

- minimization of the sum of error squares (Gauss approximation) for functions with nonlinear parameters,
- approximation with Chebyshev polynomials for two undependent variables,
- approximation with functions of the type

$$\left.\begin{aligned} z^* &= \sum_{i=1}^{l} b_i \cdot x^{c_i} \cdot y^{d_i} \quad , \\ z^* &= \sum_{i=1}^{l} b_i \cdot \exp(c_i \cdot x + d_i \cdot y) \end{aligned}\right\} \quad (b_i, c_i, d_i \in R) \qquad (5)$$

with special algorithms for starting value estimation.

Direct data transfer from the programs PROLIB and WAREG is realized.
PROLIB is our program package evaluating the thermophysical properties of pure substances, including the 1967 IFC and 1984 IAPS and other formulations [7,8].

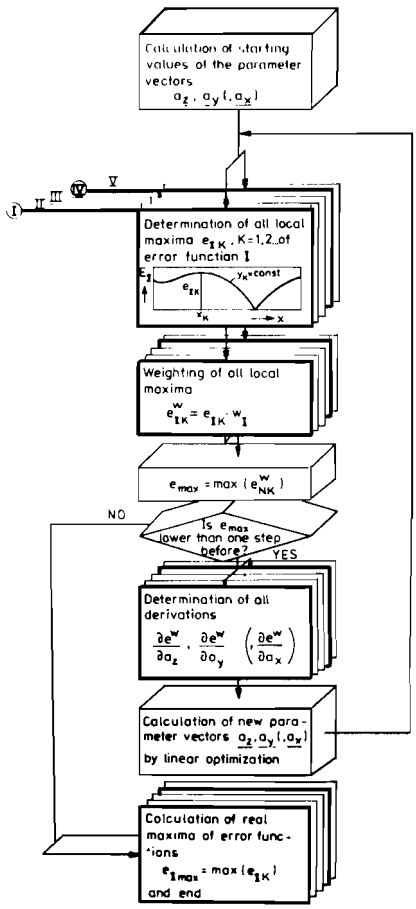


FIGURE 1. Simultaneous Chebyshev approximation for a set of functions of two undependend variables

In WAREG is implemented a modification of WAGNER's stepwise regression method with simultaneous optimization [4] characterized by a significant decrease of computation time and memory demand. By the help of this program the search for the "best" equations occurs independently for every function. Then the parameter vectors are improved by ECOFIT. WAREG is also directly linked to PROLIB.
All these programs are compatible to personal computers and are written in FORTRAN 77.

EXAMPLE

To illustrate the effects of the new simultaneous approximation method an example was constructed. The chosen

parameter range is approximately bordered by pressures of about 5...18 MPa and entropies of about 6.2 ... 6.6 kJ/(kg*K). (see fig. 2) Following functions were approximated :

$$h^* = h^*(\underline{a_h}, \rho, T)$$
$$T^* = T^*(\underline{a_T}, \rho, h)\ . \qquad (6)$$

As basic data discrete values were used calculated from the 1967 IFC formulation [8] in a lnp - T - grid with distances of 0.2 ... 0.8 MPa and 10 K. Functions (6) were approximated on three ways:

A. By the search procedure the following functions were found:

$$h^* = \sum_{k=1}^{5} a_{hk} \cdot \{\rho/(0{,}1\ MPa)\}^{i(k)} \cdot \{T/(647{,}3\ K)\}^{j(k)} \cdot kJ/kg$$
$$i(k) = (0;0;1;1;2 \mid k=1,5)$$
$$j(k) = (0;1;-3;4;4 \mid k=1,5) \qquad (7)$$

$$T^* = \sum_{k=1}^{7} a_{Tk} \{exp[0{,}01 \cdot (\rho/(0{,}1\ MPa))^{0{,}3}] - 1{,}0311711\}^{i(k)} \cdot$$
$$\cdot \{h/(70{,}1204\ kJ/kg) - 26\}^{j(k)} \cdot K$$
$$i(k) = (0;0;1;3;4;5;6 \mid k=1,7) \qquad (8)$$
$$j(k) = (1;-3;-2;0;1;0;0 \mid k=1,7)\ .$$

The terms of (7) were chosen from 50 terms with the exponents 0...4 for i and -5...4 for j. The final equation (8) represents the "best" from 53 of MEYER-PITTROFF's and GRIGULL's terms [9].

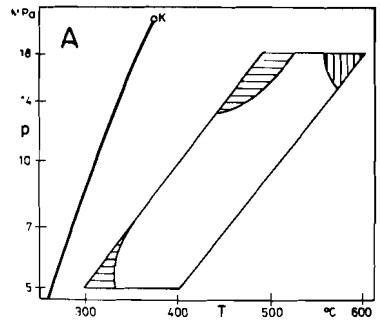
B. The enthalpy equation (7) was fitted to the 1967 IFC formulation and after that the temperature equation (8) was fitted to the approximated version of (7). That means, in a sequential Chebyshev approximation error function E_I was first minimized for (7) and then for (8) regarding to (7).

C. Using error functions E_I and E_{IV} the enthalpy equation (7) was fitted to the original function and simultaneously the temperature function (8) to (7). Weighting factors w_I and w_{IV} were 1. and 2.

In B and C relativ values of E were minimized. Fig. 2 shows the unweighted differences between given temperatures and temperatures calculated from the fitted temperature equation using the enthalpy calculated from the fitted enthalpy equation, for variants A , B and C. Table 2 shows the parameters for the fitted functions of variants B and C refered to those of A.

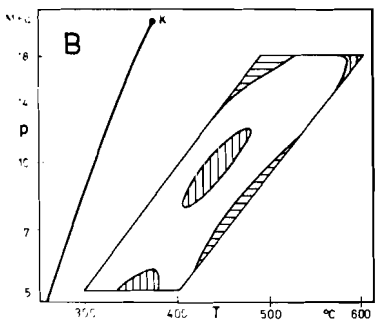
$$\frac{T^*[a_T^b, \rho, h^*(a_h^b, \rho, T)] - T}{T} \text{ in \%}$$

-0,8 -0,6 -0,4 -0,2 0,2 0,4 0,6 0,8



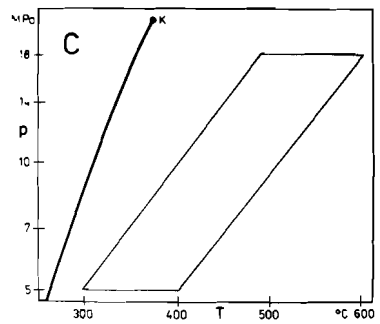
$$\sum \{h^*[a_h, \rho, T] - h[\rho, T]\}^2 \longrightarrow \min$$

$$\sum \{T^*[a_T, \rho, h] - T[\rho, h]\}^2 \longrightarrow \min$$



$$\max\{h^*[a_h, \rho, T] - h[\rho, T]\} \longrightarrow \min$$

$$\max\{T^*[a_T, \rho, h^*(a_h^b, \rho, h)] - T\} \longrightarrow \min$$



$$\left\{ \begin{array}{l} w_I \cdot \max\{h^*[a_h, \rho, T] - h[\rho, T]\} \\ w_{IV} \cdot \max\{T^*[a_T, \rho, h^*(a_h, \rho, T)] - T\} \end{array} \right\} \longrightarrow \min$$

FIGURE 2. Error diagrams for Gauss (A), sequential (B) and simultaneous (C) Chebyshev approximation

TABLE 2. Coefficients of equations (7) and (8) calculated by sequential (B) and simultaneous (C) Chebyshev approximation refered to those calculated by Gaussian regression.

i	$\frac{a_{hB}}{a_{hA}}$	$\frac{a_{hC}}{a_{hA}}$	j	$\frac{a_{TB}}{a_{TA}}$	$\frac{a_{TC}}{a_{TA}}$
1	0,931	0,944	1	0,944	0,993
2	1,097	1,081	2	1,141	1,123
3	0,941	0,958	3	1,049	1,036
4	0,207	0,268	4	0,442	0,649
5	0,225	0,126	5	0,722	0,680
			6	1,665	0,801
			7	-6,779	0,904

DISCUSSION

Simultaneous fitting of enthalpy and temperature equations effects a decrease of differences between both equations, see fig. 2 B and 2 C. That results in a small-size increase of errors of enthalpy and temperature values compared with the original equation. Relation between both errors depends on the relation between the weighting factors w_I /w_{IV}. From a greater w_{IV} a lower error between both approximated functions results, but a greater one comparing to the original formulation.
For the same function types tests show a lower maximum error using simple Chebyshev approximation in comparison to Gaussian approximation. Sequential and simultaneous Chebyshev approximation effect different values for the parameters compare tab. 2.

CONCLUSIONS

To fit equations of state to international formulations in chosen parameter ranges we recommend to use Chebyshev approximation for two independent variables with simultaneous controlling of several error functions. In this way relations between exactness and consistency may be checked for sets of thermophysical equations. Supposition for a successful determination of effectiv "minor" equations is an efficient search procedure for the structure of the equations.

REFERENCES

1. Kretzschmar,H.-J.,Klinger,J.,Schneider,S.,Dittmann,A., Zur Bereitstellung thermophysikalischer Stoffdaten für die Modellierung energiewandelnder Prozesse auf Personalcomputer, Wissenschaftliche Berichte der IH Zittau, vol. 709, no. VI/5, pp. 16-22, 1987

2. Wagner,W., Eine mathematisch statistische Methode zum Aufstellen thermodynamischer Gleichungen - gezeigt am Beispiel der Dampfdruckkurve reiner fluider Stoffe, VDI-

Fortschrittsberichte, Reihe 3, Nr. 39, 1974

3. De Reuck,K.M.,Armstrong,B., A method of Correlation Using a Search Procedure, Based on Step-wise Least Squares Technique, and its Application to an Equation of State for Propylene, Cryogenics, vol. 19, no.9, pp.505-512,1979

4. Zschunke,T.,Kretzschmar,H.-J.,Klinger,J., WAREG - Ein Programm zur nutzerorientierten Erzeugung thermophysikalischer Stoffwert-Berechnungsalgorithmen für thermodynamische und thermohydraulische Prozeßmodellierungen, Kernenergie, vol.32, no. 5, pp. 198-205, 1988

5. Jing,Z.,Fam,A.T., An Algorithm for Computing Continuous Chebyshev Approximations, Mathematics of Computation, vol. 48, no. 178, pp. 691-710, 1987

6. Kretzschmar,H.-J.,Klinger,J., Zur stoffunabhängigen Berechnung von impliziten Zustandsfunktionen - ein Beitrag zur effektiven Bereitstellung von Stoffdaten in thermodynamischen Prozeßberechnungen der Energieanlagentechnik, Energietechnik, vol. 34, no. 6, pp. 210-215, 1984

7. Dittmann,A.,Klinger,J.,Kretzschmar,H.-J., in The Properties of Steam, ed. V.V. Sychev and A.A. Aleksandrov, vol. 1, pp. 284-293, Mir, Moscow, 1986

8. Grigull,U., Proprties of Water and Steam in SI-Units, Springer, Berlin, 1982

9. Meyer-Pittroff,R.,Grigull,U., Eine Umkehrfunktion zu der "1967 IFC Formulation for Industrial Use" für die Berechnung der Temperatur von überhitztem Wasserdampf, abhängig von Druck und Enthalpie, Brennstoff-Wärme-Kraft, vol. 21, no. 12, pp. 636-638, 1969