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COMPUTER SUBROUTINES FOR THE CALCULATION OF THERMOPHYSICAL PROPERTIES OF WORKING FLUIDS USED IN ENERGY ENGINEERING

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INTRODUCTION

The application of electronic computers also in the field of energetics requires increasingly corresponding software for computer-aided design and optimization as well as automated operating of plants. According to these tendencies, scientific work for the mechanical placing at disposal of substance data for all thermodynamic and thermohydraulic modellings of processes had been started at the beginning of the seventies.

This paper represents the working situation of 1985 as a summary and shows some selected scientific results.

SYMBOLS, INDEXES AND ABBREVIATIONS

nomenclature		sense
with dimension	dimensionless	
n		material parameter
p	Π	pressure
t	Θ	temperature
v	χ	specific volume
s	σ	specific entropy
h	ϵ	specific enthalpy
u	ζ	specific internal energy
x		dryness fraction
c	φ	specific heat capacity
a_s		isentropic sonic speed
η		dynamic viscosity
λ		thermal conductivity
σ_d		surface tension
index		sense
k		critical state
t		triple state
d		saturated state
l		saturated liquid
"		dry saturated vapour
SP		SUBPROGRAMM
PS		programme set

ASPECTS OF MODERN PLACING AT DISPOSAL OF SUBSTANCE DATA

Statements following are focussed on the problems of energetics and by that on the mostly used working fluids (pure substances).

New problems in preparing and making available thermophysical substance data have come out by microelec-

tronics and the fast availability of all-size computers connected by terminals and long-distance data transmission plants:

- complex placing at disposal of substance data by medium and large-size computers;
- simplified calculation of substance data by small-size and microcomputers and microprocessors respectively as well as developing of processes for the automated generation of such algorithmus (also for unsteady modellings by medium and large-size computers;
- establishment of data banks and attached dialog programmes for substance data by all-size computers;
- generation of equilibrium diagrammes on dieplays and plotters as working means;
- generation of printable vapour charts.

Fig. 1 shows how to realize these tasks at the Thermodynamics Department.

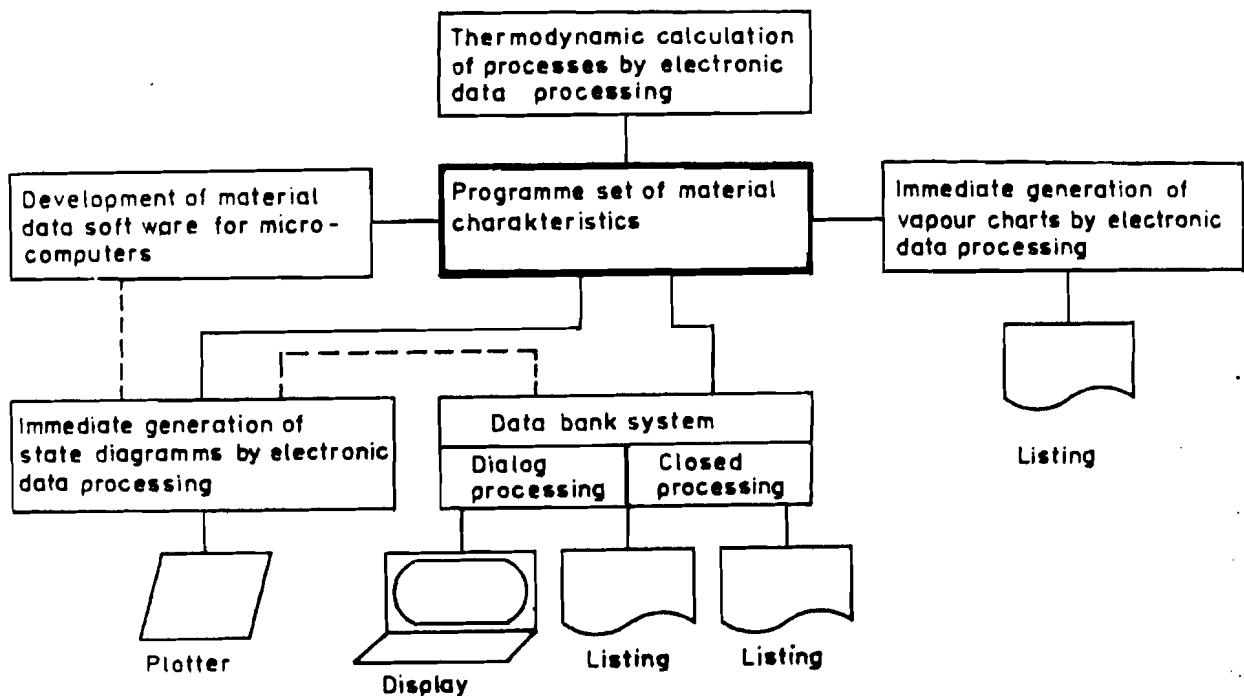


Fig. 1 Illustration of research objectives at the Thermodynamics Department

First of all, the central programme set for placing at disposal of substance data had been designed for calculating substance data for thermodynamic process calculations by large-size computers (1,2,3). The other working directions arranged radially in fig. 1 have been started later on. They use computable information by the programme set.

A SUBSTANCE DATA PROGRAMME SET FOR MEDIUM AND LARGE-SIZE COMPUTERS

As it is known, the quality of thermodynamic process calculations depend decisively upon substance data available. The concept of the programme system for comprehensive substance data computation is determined by:

- placing at disposal of substance data for the most important working fluids of energetics;
- computation of many thermophysical properties and their derivatives;
- realization of implicate thermodynamic functions with any pairs of the given quantities p, T, v, s, h, u by substance-independent calculations;
- acquisition of the largest-possible range of state and fluid one and two-phase regions;
- selection of several equations of state (formulation) of different complexity and precision for the most important substances;
- guarantee of thermodynamic consistency between functions and especially at interphases.

WORKING FLUIDS

At present, working fluids as shown in fig 2 may be computed.

substance	equation of state	material parameter
water	IAPS 1984	8
	IFC 1968	9
	IFC 1967	2
	IFC 1967 (techn.region)	4
	RIVKIN and KREMENEVSKAJA /4/	11
	VDI 1963	10
ammonia	MARTIN-HOU-equation (ILKA-calculation catalogue)	20
R11	/5/	21
R12		22
R13		23
R22		24
R13 B1		25
R113		26
R114		27
R502		28
R12	BAEHR and HICKEN	3
carbondioxide	ALTUNIN,IUPAC resp.	5
helium	ZEDERBERG	6
sodium	PEE /6/	7
nitrogen	unified state equation /7/	12
helium		13
oxigen		14
air		15
methane		16
ethane		17
ethylene		18
15 substances	model of the semi ideal gas	1

Fig. 2 Working fluids contained in the programme set of the Thermodynamics Department at Dresden University of Technology (1985)

According to manifold application, five formulations have been considered for water as the mostly used working fluid at energetics. Experiences with different equations from the point of view of thermodynamic process calculation shows /8/. Furthermore, some refrigerants and especially cooling fluids for nuclear reactors and gases for combustion computation are available.

FUNCTIONS

The wide range of thermodynamic functions of state, transport quantities and derivatives (see fig. 3) of the programme set results from requirements of different process computations at energetics. Especially inverse functions for any given pairs of quantities p, T, v, s, h, u are placed at disposal. The dryness fraction x contained in relations indicates the functional capability of subprogrammes at fluid one and two-phase regions. The substance data programme set may be used in the shape of subprogrammes for each function shown in chart 1. Through a characteristic number, the desired substance and equation of state respectively may be chosen.

$p_s = p_s(T_s)$ $T_s = T_s(p_s)$	$\eta = \eta(p, T, v^*, x)$ $\lambda = \lambda(p, T, v^*, x)$ $\sigma_s = \sigma_s(T)$
$v = v(p, T, x)$ $p, x = p, x(T, v)$ $T, x = T, x(p, v)$	$c_p = c_p(p, T, v^*, x)$ $a_s = a_s(p, T, v^*, x)$
$s = s(p, T, v^*, x)$ $h = h(p, T, v^*, x)$	$\left(\frac{\partial p}{\partial T}\right)_v = \left(\frac{\partial p}{\partial T}\right)_v(p, T, v^*, x)$
$p, v, x = p, v, x(T, s)$ $p, v, x = p, v, x(T, h)$	$\left(\frac{\partial T}{\partial v}\right)_p = \left(\frac{\partial T}{\partial v}\right)_p(p, T, v^*, x)$
$T, v, x = T, v, x(p, s)$ $T, v, x = T, v, x(p, h)$	$\left(\frac{\partial v}{\partial p}\right)_T = \left(\frac{\partial v}{\partial p}\right)_T(p, T, v^*, x)$
$p, T, x = p, T, x(v, s)$ $p, T, x = p, T, x(s, h)$ $p, T, x = p, T, x(v, u)$	$\left(\frac{\partial s}{\partial T}\right)_v = \left(\frac{\partial s}{\partial T}\right)_v(p, T, v^*, x)$
$p, T, v, x = p, T, v, x(s, h)$	<p>* - There is no necessity of the input of v as a given quantity</p>

Fig. 3 Relations for thermodynamic quantities in the substance data programme set (1985)

CALCULATION

All thermodynamic functions and derivatives are calculated substance-independently by means of iteration and numerical differentiation in subprogrammes of plane III. To do so, it is departed from substance-specific equations of state in reduced shape ($v, s, h = f(p, T)$) at engineering formulation and $p, s, h = f(T, v)$ at physical formulation as well as the vapour pressure function $P_d = P_d(T_d)$ and their derivatives (see fig. 4, plane 3). This line of action has proved a success because of the possibility for controlling the thermodynamic consistency of calculated functions between each other and especially at interphases.

As an example, fig. 5 shows the internal calculation of the SP TVPSRE for functions $p, T, x = f(p, s)$.

Departing from the pressure given, the attached limit cycle entropies are calculated and compared to the attached entropy in the phase test at first. After that, the actual calculations take place in the one and two-phase region. To avoid ineffective and confound iterations, algorithms have been written separately for engineering and physical formulations of equations of state (Those interested will find detailed description in /10/).

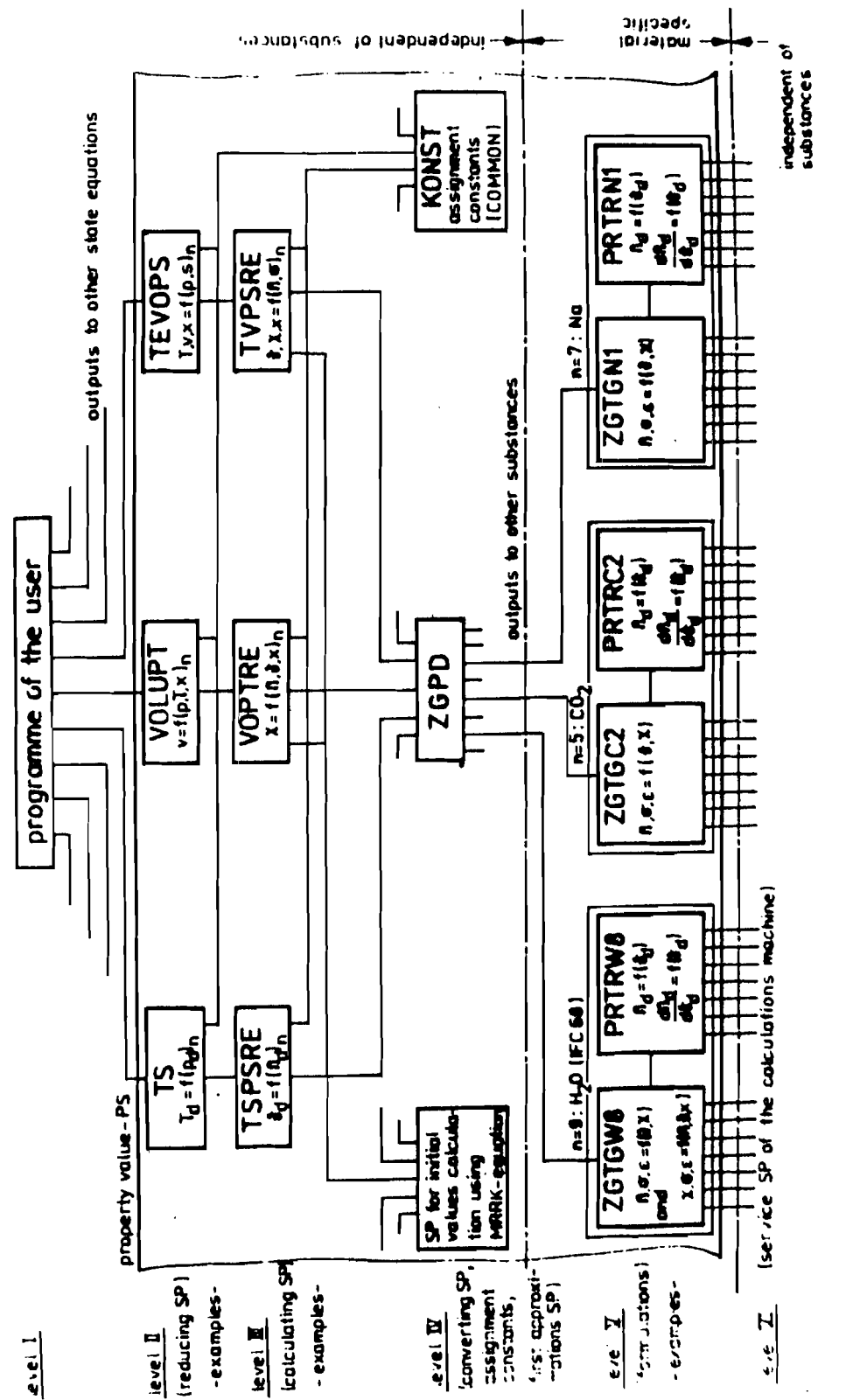
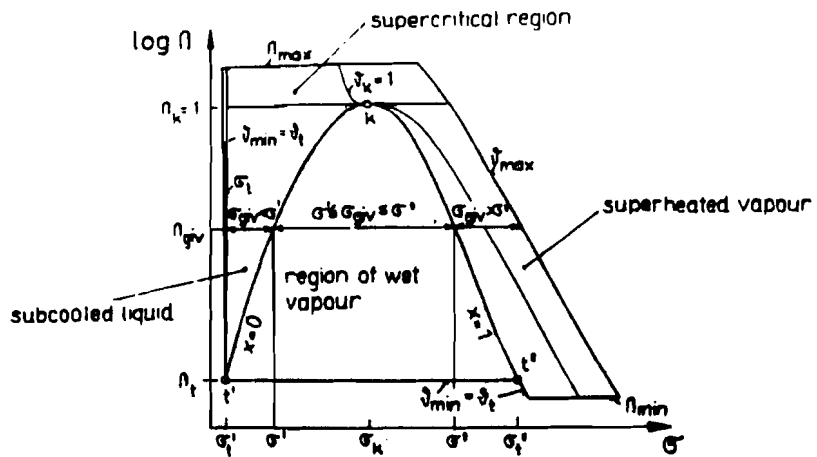


Fig. 4 Part of the substance data programme set.



physical formulation
 $(\rho, \sigma, \varepsilon = \rho, \sigma, \varepsilon(\vartheta, \chi))$

technical formulation
 $(\chi, \sigma, \varepsilon = \chi, \sigma, \varepsilon(\rho, \vartheta, \chi))$

Test of phases

- $\rho_{giv} < \rho_t$ — vapour
 - $\rho_{giv} \geq 1$ — supercritical
 - $\sigma_{giv} < \sigma_t'$ — liquid
 - $\sigma_{giv} > \sigma_t''$ — vapour
 - $\rho_{giv} < 1 \wedge \sigma_{giv} < \sigma'$ — liquid
 - $\wedge \sigma_{giv} > \sigma''$ — vapour
 - $\wedge \sigma'' \leq \sigma_{giv} \leq \sigma'$ — wet vapour
- with $\vartheta_s = \vartheta_s(\rho_{giv})$

- one-dimensional iteration of χ' and χ'' out of $\rho = \rho(\vartheta_s, \chi)$, compensation to ρ_{giv}
- $\sigma' = \sigma'(\vartheta_{it}, \chi')$ $\sigma'' = \sigma''(\vartheta_{it}, \chi'')$
- $\sigma', \sigma'' = \sigma', \sigma''(\rho_{giv}, \vartheta_s)$

One phase region

- two-dimensional iteration of ϑ_{it} and χ_{it} out of $\rho = \rho(\vartheta, \chi)_{it}$, compensation to ρ_{giv} ; $\sigma = \sigma(\vartheta, \chi)$, compensation to σ_{giv}
- one-dimensional iteration of ϑ_{it} out of $\sigma = \sigma(\rho_{giv}, \vartheta)$, compensation to σ_{giv}
- $\chi_{it} = \chi(\rho_{giv}, \vartheta_{it})$

Two phase region

$$\vartheta_{it} = \vartheta_s(\rho_{giv}) \quad x_k = \frac{\sigma_{gv} - \sigma'}{\sigma'' - \sigma'} \quad x_{it} = \chi + x_{it}(\chi'' - \chi')$$

with

- χ', χ'' and σ', σ'' out of the test of phases
- σ', σ'' out of the test of phases
- $\chi', \chi'' = \chi', \chi''(\rho_{giv}, \vartheta_{it})$

Fig. 5 Illustration of test of phases and iterative calculation at the example $T, v, x = f(p, e)$

Redlich-Kwong equation and linear setups for the vapour-pressure relation in the $\log p_D : 1/T_D$ -plane. They are transposable to other substances without the use of chart data and regression.

USE OF THE SUBSTANCE DATA PROGRAMME SET

At present, the use of the programme set for modelling and optimizations of power plant processes is in the first place. The storage location needed depends upon substance data functions called-in as well as substances to be calculated:

properties out of the function of p and T :	14 K Byte
inverse functions:	60 K Byte
derivatives:	5 K Byte
working fluids depending on the complexity of the equation of state:	2...15 K Byte

The computation time needed for one characteristic point is also determined by the complexity of the chosen equation of state. Some selected examples might be noted (CO₂ DEM 6):

properties as a function of p and T :	1.002...7.00 s
inverse functions:	0.00 ...0.2 s

For the direct and daily use, a dialog inquiry programme is available (storage location of 20 K Byte).

GENERATION OF THERMODYNAMIC EQUILIBRIUM DIAGRAMS

Because of the accomplishment of many logical and computation processes by fast available computers, visual working means as outline and test diagrams for thermodynamic calculations have an increasing significance. It has come out a necessary task to generate them with the most different state parameters and also in coordinates unusual up to now on plotters and graphical screens.

Departing from many programmes being already in

existence for thermophysical state parameters, a programme system for medium and large-size computers has been developed with using the substance data programme set at Thermodynamics Department of the Dresden University of Technology. The possibilities are as follows:

- representation of any quantities in any coordinates with different axis graduations in closed curves;
- substance-independent diagram computation and selective representation of several substances and equations of state respectively in one diagram for the purpose of comparison;
- drawing of any cut-outs and enlargements inclusive one and two-phase regions;
- interpolation of all coordinate values only out of supporting values to be computed
in the one-phase region in the frame of temperature and pressure (isothermal),
in the two-phase region in the frame of temperature and dryness fraction (isothermal);
- production of diagrams for the purpose of comparison as well as reading off with high precision.

Fig. 7 illustrates the principle of diagram generation.

A detailed description of algorithms contains /9/.

Fig. 8 represents a photo copy of a h s-diagram of water according to IFC '68 drawn by the DIGIGRAF-plotter / 12 / as part of steam turbine calculation (original size 100 cm x 80 cm, ball-point pen drawing).

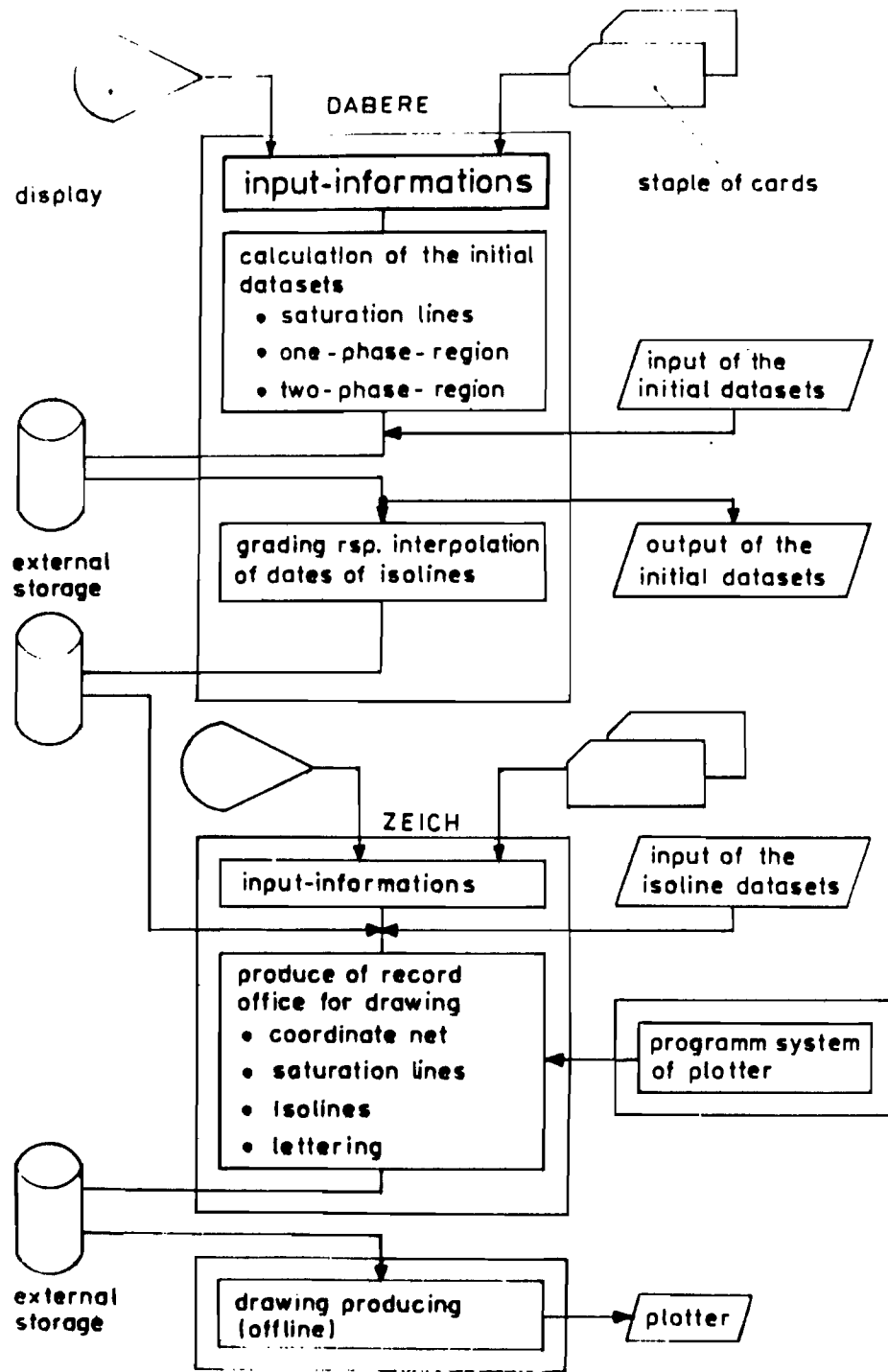


Fig. 7 Principle of computing and automated drawing of equilibrium diagrams

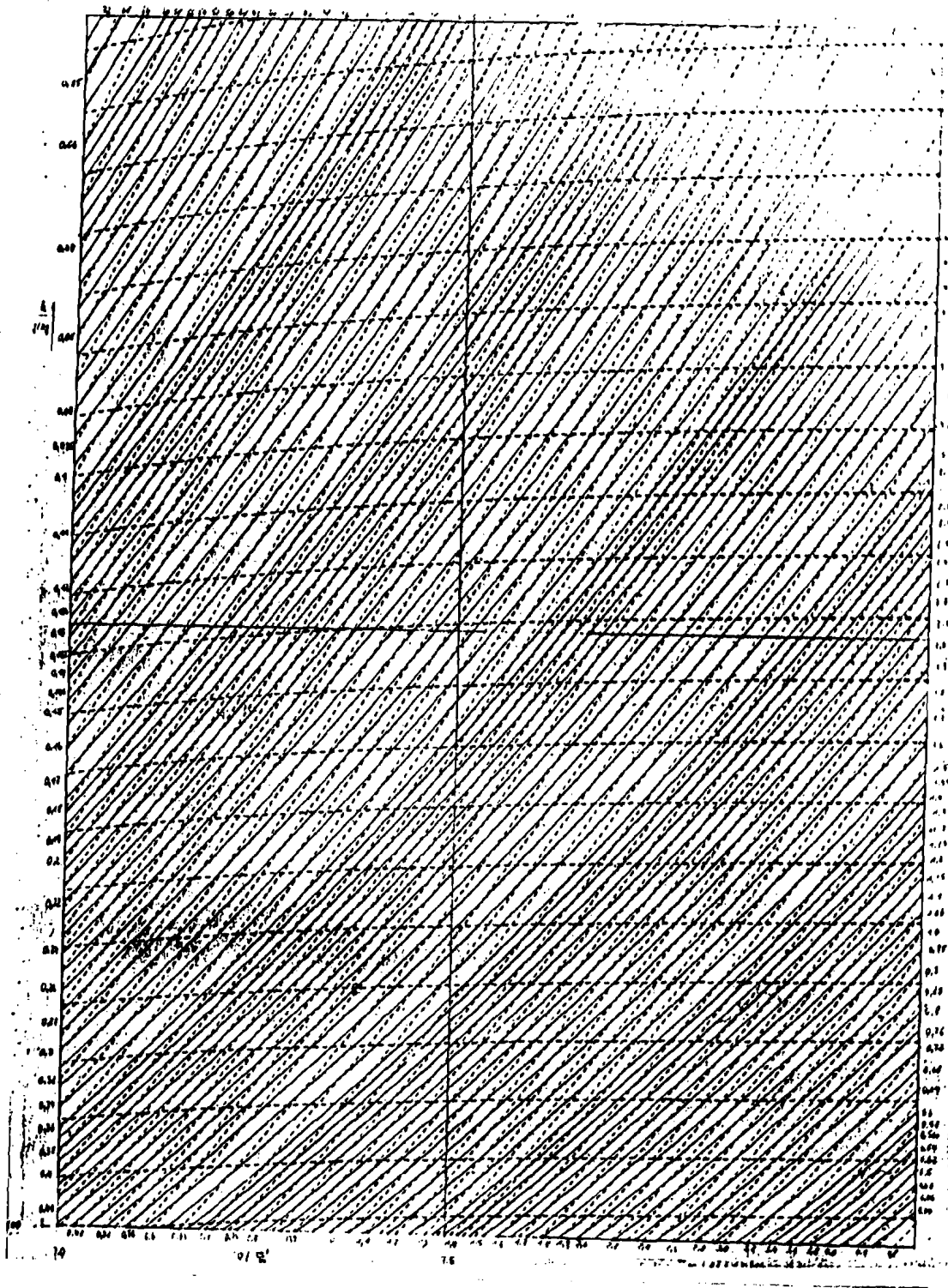


Fig. 8 Part of a h, s -diagram; region of superheated steam.

SIMPLIFIED SUBSTANCE DATA COMPUTATION ON MICROCOMPUTERS

The use of personal computers at design departments and microprocessors for operating energy plants requires software for simplified modellings of basic units and processes in a large scale. Because of limited resources of microcomputers, an effective placing at disposal of substance data is required with respect to demands of calculation time and storage location. Especially the small extension of terms has to be considered. Besides elaborating suitable and simplified algorithms for microcomputers, research work is also done with respect to their automated generation on large-size computers by use of the substance data programme set. This work is focussed on a programme system making available simplified algorithms for a given range of state at required precision and with quantitative consideration of the thermodynamic consistency.

Three traditional paths of solution are possible to compute substance data by microcomputers. They are illustrated in Fig. 9 and should be discussed shortly.

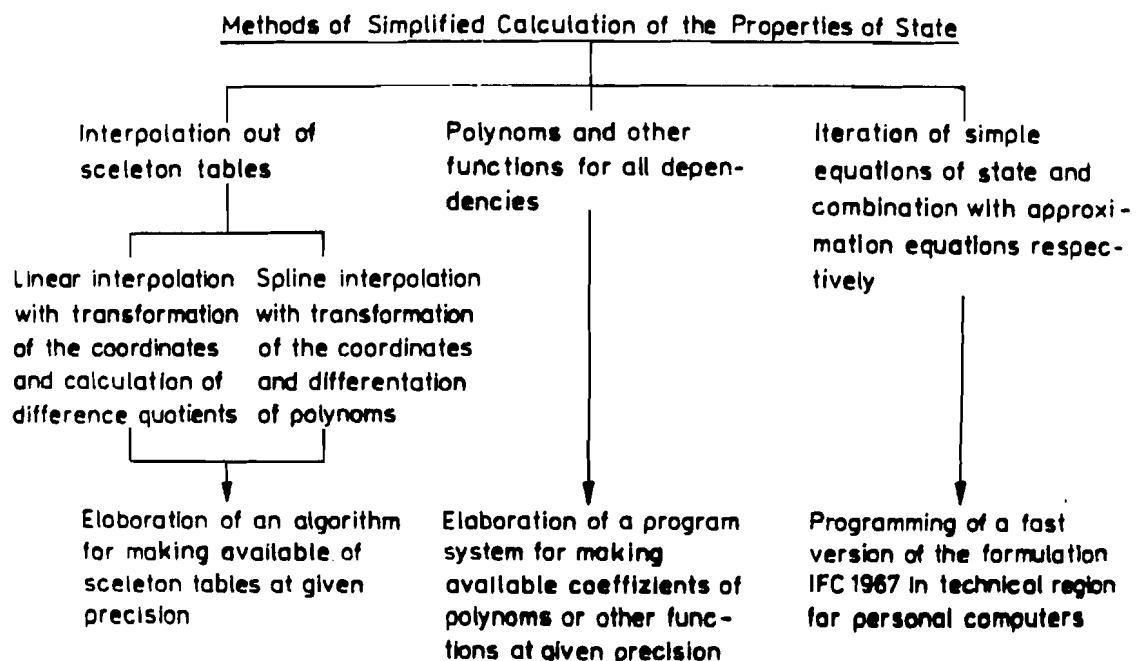


Fig. 9 Paths of solution for simplified substance data computation by microcomputers

The number of supporting values ejected in the primary store limits the range of state computable by the first method of interpolation. Because of carrying out all calculations with the same supporting data, thermodynamic consistency between functions and at interphases is well guaranteed. On account of simple mathematical operations, the interpolation is very suitable to computers. Presuming the interpolation in the primary store, computation time needed for finding of one characteristic point becomes relatively short. A few supporting values will do for calculations when adapting the transformation of coordinates in connection with spline-interpolation to the true thermodynamic behavior.

When calculating functions of state by simple functions and polynome, the region of state covered is limited by the maximum degree of polynome. It results from significant numbers needed for coefficients as well as the maximum number of coefficients for polynome in the primary store. The quantitative consideration of the thermodynamic consistency between functions and at interphases forms a special problem within this path of solution. However, very little computation time is needed when using high-performance polynome.

Referring to the third path, the computable region of state depends upon equations of state used. When determining implicate functions iteratively out of equations of state, consistency is controllable but computation time increases considerably. On the other hand, a combination of equations of state and polynome or interpolations are favourable. The altogether long computation time and relatively high demands for storage location forbid the direct use at process calculations but they are well sufficient for substance data banks on personnel computers.

SUMMARY

The represented scientific work for processing and

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making available of substance data deliver solutions for medium and large-size computers as well as microcomputers as follows:

- informations programmes for substance data;
- complex placing at disposal of substance data;
- generation of simplified substance data algorithms;
- generation of equilibrium diagrammes and printable vapour charts.

A central problem of present research work is given by the automated generation of simplified algorithms for substance data.

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