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A METHOD FOR GENERATING INTERPOLATION TABLES WITH OPTIMIZED DATA DENSITY FOR FAST INTERPOLATIONS OF THERMODYNAMIC PROPERTIES IN PROCESS MODELING

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ABSTRACT

The paper presents an algorithm which is able to generate interpolation tables with optimized data density

- for the required interpolation accuracy (absolute or relative)
- for the required thermodynamic functions, including backward functions, and
- for a given interpolation method (linear interpolation, spline interpolation - with or without coordinate transformations).

The generated tables may be used for the interpolation of thermodynamic properties in process modeling. The optimization of the data density is realized by a flexible strategy of condensing the data grid. Ranges of state where the required interpolation accuracy is already fulfilled are sorted out step by step. Furthermore, the data density is decreased by transforming the properties concerned in the interpolation. The transformations differ in the liquid and vapor regions and, also, for linear and spline interpolations.

The findings show that the number of data points necessary for accurate interpolations is considerably fewer than expected.

INTRODUCTION

The interpolation of thermodynamic properties in process modeling is becoming more and more attractive due to the availability of computers with large memories and modern spline algorithms. The advantages of interpolation are:

- Simple mathematical operations requiring very brief computing times.
- Fast application of the calculations to other fluids, other functions, or other ranges of state, by merely replacing the interpolation data tables.
- Interpolation of both forward and backward thermodynamic functions, such as $h=f(T,p)$ and $T=f(h,p)$, with the extremely high numerical consistency required in process modeling.

A very important issue in all interpolations is the density of the data tables. As is well known, the data density depends on:

- the demanded interpolation accuracy
- the interpolation method used.

However, the data density may be decreased, provided the variables upon which the interpolation is based are first mathematically transformed.

This investigation advances the authors' earlier works (Kretschmar, 1990) and (Nabel, 1991) and describes the present state of research.

INTERPOLATION METHODS AND DATA TABLE STRUCTURE

In the work presented here, linear and spline interpolations have been applied. The procedure for generating the corresponding, optimized data tables can also be used for other interpolation methods.

As shown in Fig. 1, the data tables for supercooled liquid and superheated vapour are divided by the saturation line $p_s = f(T)$ and by the critical isotherm $T_{cr} = \text{const}$ above the critical pressure and have an isobaric structure.

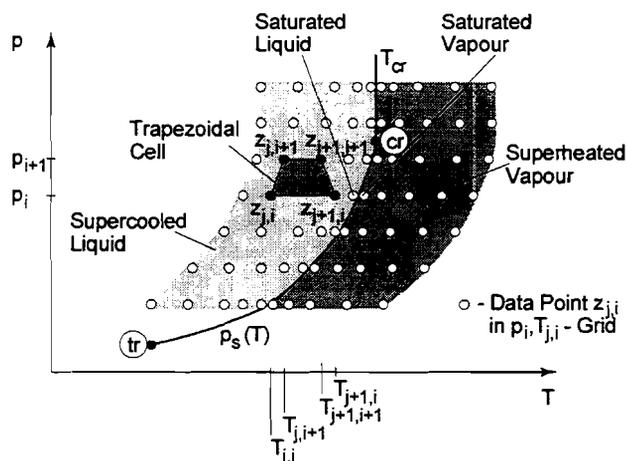


FIGURE 1. Isobaric Structure of Interpolation Data Tables with Trapezoidal Cells

The data points along the isobars correspond to different temperatures and include the saturation temperature in the case that the saturation line is part of the required range of state. This means that the data tables do not have an isotherm structure. For every property z ($z = v, h, s, c_p, a_s, \lambda$ or η , etc.) to be interpolated in process modeling, a data table consisting of data point $(p_i, T_{j,i}, z_{j,i})$ is stored. Therefore, points on adjacent isobars display a trapezoidal geometry (see Fig. 1). This data structure has the advantage that thermodynamic variables arbitrarily close to the saturation line need not be interpolated as special cases.

The spline interpolation is here achieved by using one-dimensional, cubic spline polynomials of the form

$$z_{j,i}(T) = a_{j,i} + b_{j,i}(T - T_{j,i}) + c_{j,i}(T - T_{j,i})^2 + d_{j,i}(T - T_{j,i})^3 \quad (1)$$

for each isobar p_i , and for T between $T_{j,i}$ and $T_{j+1,i}$. For calculation of the polynomial coefficients $a_{j,i}, \dots, d_{j,i}$, the derivatives $(dz/dT)_p$ at both ends of the isobar p_i are determined numerically from the base equation (Späth, 1978).

If an isobar has only two data points, linear interpolation is used. If only three data points are present, quadratic Lagrange interpolation (Engeln-Müllges, 1993) is used. Cubic spline interpolation requires at least four data points. Linear interpolation takes place between the polynomials

along the adjacent isobars. While this procedure allows arbitrary trapezoidal data sets to be handled, a certain loss of accuracy in comparison with direct, two-dimensional spline interpolation does have to be accepted.

FUNCTIONAL DEPENDENCIES FOR INTERPOLATION

In Fig. 2, the functional dependencies to be interpolated in calculations of thermodynamic properties are summarized.

One-dimensional interpolations $z = f(x)$ are sufficient for calculating properties for the saturation states ($x, z = p, T, v, h, s, c_p, a_s, \lambda$ or η , etc.). The backward function $x = f(z)$ can be interpolated with exact numerical consistency with the respect to the related forward function $z = f(x)$ using the same data points (x_j, y_j) . When using cubic spline polynomials for $z = f(x)$, the backward function may be calculated by the analytic solution algorithm for cubic equations (Bronstein and Semendjajev, 1984) with, however, an increase in calculation time because of the transcendent functions that have to be computed.

Two-dimensional interpolations are necessary for calculating properties in the single phase regions. In the first instance, shown in Fig. 2, one property z ($z = v, h, s, c_p, a_s, \lambda$ or η , etc.) is linked to the grid variables pressure and temperature. Both the forward function $z = f(T, p)$ and backward functions $T = f(z, p)$, $p = f(z, T)$ can be interpolated using the same data points $(p_i, T_{j,i}, z_{j,i})$. For example, the functions $h = f(T, p)$ and $T = f(h, p)$, both very important in process modeling, are interpolated in this way. The numerical consistency between the forward and backward functions obtained is extremely high.

In the second instance, two properties z and w ($z, w = v, h, s, c_p, a_s, \lambda$ or η , etc.), both of which provide interpolation data tables over the p, T -grid, have to be handled. Here, besides z and w , only one grid variable is involved: either p or T . The functions $p = f(s, h)$ and $h = f(s, p)$ required in process modeling are frequently seen in two-property interpolations. Again, the related forward functions $h = f(T, p)$, $s = f(T, p)$ are interpolated over the same $(p_i, T_{j,i}, h_{j,i})$ and $(p_i, T_{j,i}, s_{j,i})$ data tables.

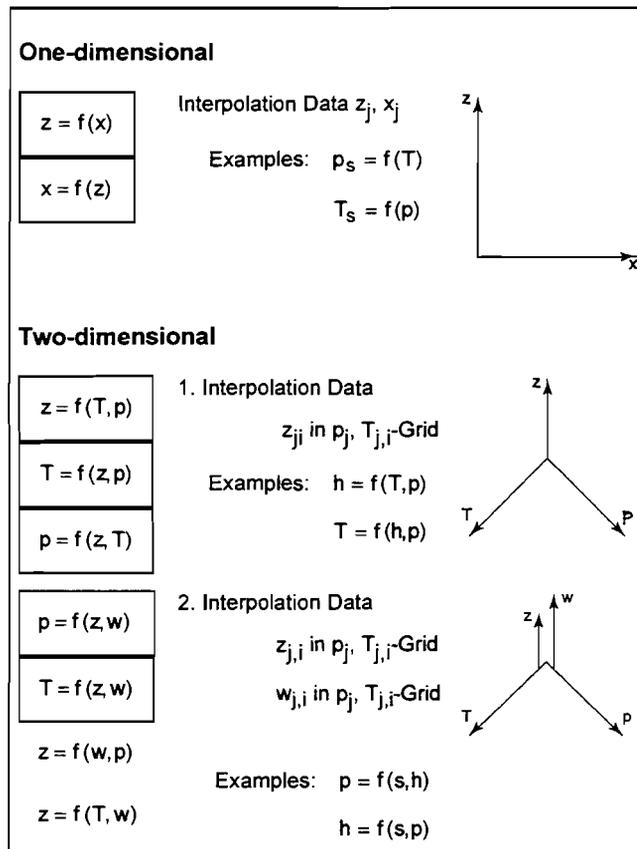


FIGURE 2. Functional Dependencies of Thermodynamic Properties to be Interpolated in Process Modeling

TRANSFORMATION OF COORDINATES

The accuracy of every interpolation can be increased by transforming the properties concerned in the interpolation (transformation of coordinates). The following two examples show the increase in accuracy obtained by using suitable transformations. In the upper part of Table 1, values of vapour pressure p_s and calculated values for saturation temperature T_s and the saturated vapour volume v'' of water are listed (using the IFC 67 Formulation (Grigull, 1989 and Meyer, 1967)).

Starting from the middle temperature $T_s = 457.217$ K, the related value of vapour pressure is first calculated using linear interpolation and the two adjacent data points. The result is shown in the middle part of Table 1. Linear interpolation without coordinate transformation yields a deviation of 0.3%. Using linear interpolation with the coordinate transformation $\ln(p)$, $1/T$, the absolute value of the error decreases to 0.008%, for an overall increase in interpolation accuracy of more than one order of magnitude.

TABLE 1. Interpolation of Vapour Pressure and Saturated Vapour Volume of Water With and Without Transformation of Coordinates

IFC 1967 Formulation for Water		
P_s kPa	T_s K	v'' $\frac{m^3}{kg}$
1000.00	453.034	0.194293
1100.00	$\leftarrow 457.217 \rightarrow$	0.177384
1200.00	461.111	0.163200
Linear Interpolation $p_s = f(T_s = 457.217K)$		Relative deviation
Without transformation:	$p_s = 1103.58$ kPa	0.3 %
With transformation $\ln(p_s), \frac{1}{T_s}$:	$p_s = 1099.91$ kPa	-0.008 %
Linear Interpolation $v'' = f(T_s = 457.217K)$		Relative deviation
Without transformation:	$v'' = 0.178190$ $\frac{m^3}{kg}$	0.5%
With transformation $\ln(v''), T_s$:	$v'' = 0.177514$ $\frac{m^3}{kg}$	0.07%
With transformation $\ln(v''), \frac{1}{T_s}$:	$v'' = 0.177378$ $\frac{m^3}{kg}$	-0.003%

The reason for this can be seen in Figure 3. While the vapour pressure function is exponential in the ordinary p, T -plane, i.e. in the general z, x -plane, in the transformed Z, X -plane, where $Z = \ln(p)$, $X = 1/T$, it is almost a straight line. Therefore, a linear interpolation in the transformed plane, given by

$$Z = Z_j + \frac{X - X_j}{X_{j+1} - X_j} (Z_{j+1} - Z_j), \quad (2)$$

where j and $j+1$ are data points,

must be considerably more precise. Note, the interpolated result Z has to be retransformed into z using the inverse transformation function.

For fast interpolations, the data points (x_j, z_j) and (x_{j+1}, z_{j+1}) should be stored in the data table already transformed as (X_j, Z_j) and (X_{j+1}, Z_{j+1}) . In this way, only the given value x has to be transformed and the interpolated value Z retransformed. The computing time compared to interpolation without transformation, will admittedly increase particularly, when using the logarithm as the transformation function, as was done for pressure. But investigations have shown, that the logarithm may be replaced by the fourth root, which may then be computed by the fast square root function, without considerable loss of accuracy (Kretschmar et al., 1995).

Similar results are obtained when interpolating $v'' = f(T_s)$. The bottom part of Table 1 demonstrates the accuracies achieved by using linear interpolation without and with two different coordinate transformations. Here, the accuracy is increased from 0.5% without transformation to 0.003% with the transformation $\ln(v'')$, $1/T_s$.

Table 2 shows the transformations used for linear and spline interpolations of important properties in the supercooled/saturated liquid region and superheated/saturated vapour regions. These transformations may be also used for interpolating thermodynamic tables by hand. When the range of state to be interpolated is situated far from the saturation states, other transformations are to be preferred. They result from the thermodynamic dependencies in the ideal gas and ideal (incompressible) liquid regions, respectively.

To sum up, transformation of coordinates increases interpolation accuracy and as discussed below, reduces the number of data points required for a given level of accuracy. Using coordinate transformations, the loads of data necessary in the methods of Pflieger (1988) and van der Looij (1986) could be reduced considerably. However, computing time does increase when transcendent transformation functions are used.

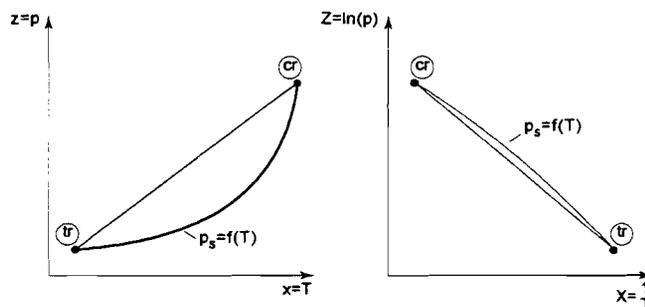


FIGURE 3. Vapour Pressure Curve of Water in the p, T - and in the $\ln(p), 1/T$ -Planes

TABLE 2. Transformations of Coordinates Used for Linear and Spline Interpolations

Property	Transformation Functions Used			
	Supercooled and saturated liquid		Superheated and saturated vapour	
	Linear Interpolation	Spline Interpolation	Linear Interpolation	Spline Interpolation
p	$\ln(p)$	$\ln(p)$	$\ln(p)$	$\ln(p)$
T	$\frac{1}{T}$	T	$\frac{1}{T}$	T
v	v	v	$\ln(v)$	$\ln(v)$
h	$\frac{1}{h}$	h	h	h
s	$\ln(s)$	s	s	s
c_p	$\frac{1}{c_p}$	$\frac{1}{c_p}$	$\frac{1}{c_p}$	$\frac{1}{c_p}$
w	w	w	w	w
λ	$\ln(\lambda)$	λ	$\frac{1}{\lambda}$	$\frac{1}{\lambda}$
η	$\ln(\eta)$	η	$\frac{1}{\eta}$	η
r	r^1	r^1		
σ_s	σ_s^1	σ_s^1		

¹ Saturation state

GENERATION OF THE INTERPOLATION DATA TABLES

From the foregoing, it is clear that the accuracy of an interpolation can be increased by

1. More complicated interpolation methods

- Enhancement of the complexity of the algorithm by incorporating more data points (Parabolic or rational interpolations)
- Using more complicated functions between data points (Spline interpolations)

and by

2. Suitable transformations of the coordinates.

Furthermore, the accuracy of every interpolation increases with

3. Increasing density of the data tables.

In consideration of this basic situation, an algorithm has been developed which is able to generate interpolation tables with optimized data density for the interpolation method used either with or without transformation of the coordinates, and for the interpolation accuracy required in the respective process modeling.

In the following, the principle of this algorithm will be explained briefly by means of an example. A data table, using the transformations $\ln(v)$, $\ln(p)$ and $1/T$, is to be generated for linear interpolation of the function $v = f(T,p)$ in the steam region from 5 MPa ($T_s \dots 573$ K) up to 10 MPa ($T_s \dots 623$ K), shown by the shaded area in Fig. 4. (The right boundary of the range of state, i.e. the curve connecting the points (2,1) and (2,2), is straight line in the $\ln(p), 1/T$ -plane.) The interpolation accuracy to be met is $\Delta v/v = 0.2\%$. The basis of the interpolation data table is the IFC 1967 Formulation for steam.

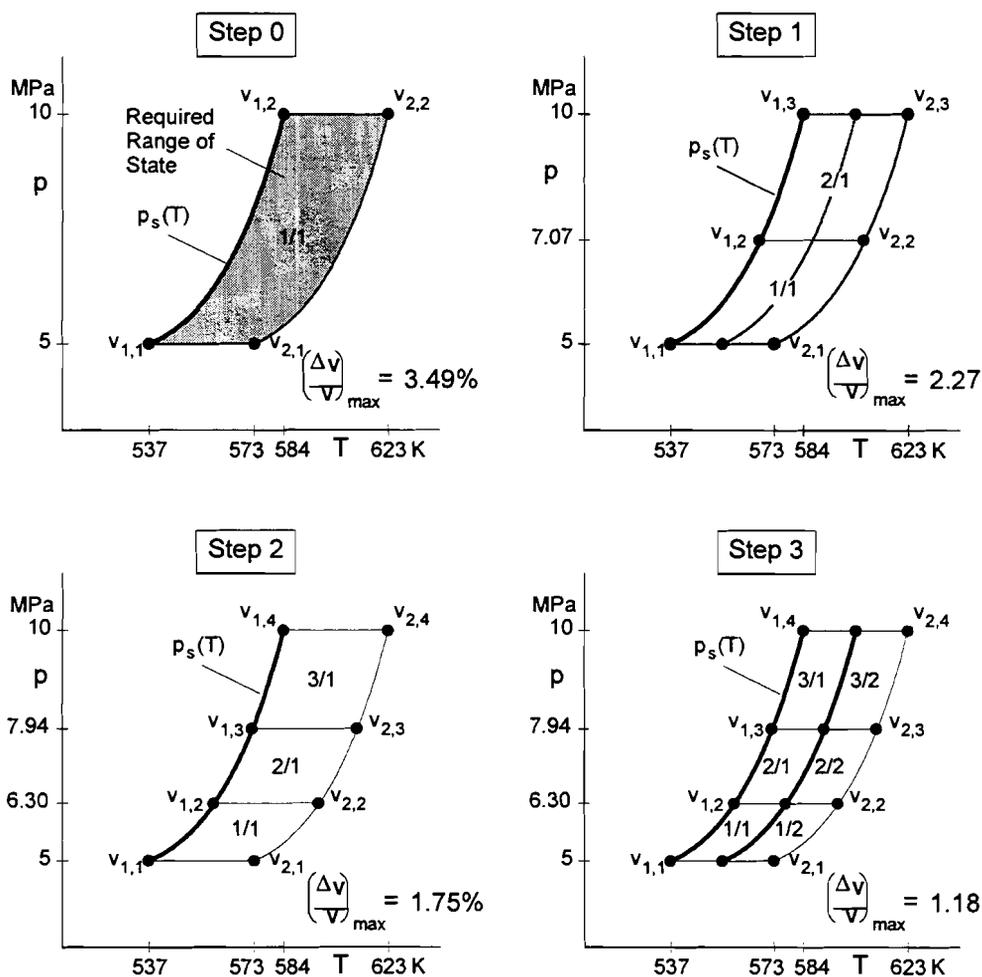


FIGURE 4. Generation of Interpolation Tables with Optimization for $v = f(T,p)$ of Steam

Starting with the cell 1/1 comprising the four corner points and equal to the required range of state (Fig. 4, Step 0), the algorithm tests whether the interpolation with these data points leads to values of v which do not deviate more than 0.2% from the simultaneously calculated IFC 67 values. In order to check this, a test grid of isobars (logarithmic division) and temperatures along each isobar (hyperbolic division) is generated in every cell. Since the number of test points has a considerable influence on the computing time needed for the generation of the interpolation tables the number of isobars and the number of temperatures can be set by the user.

For example, Figure 5 shows the test grid for the first cell. It consists of 25 (5x5) test points. As may be seen, the maximum resulting relative error $\Delta v/v$ is 3.49 %, that is, the four data points are not enough to interpolate v within the required accuracy. Therefore the cell size has to be decreased. (The test point at which the maximum error occurs depends on the topology of the property's surface. In Fig. 5, the central point coincidentally has the greatest error.)

First, the algorithm inserts an isobar (logarithmic middle value) and checks the obtained interpolation accuracy in the resulting upper and lower cells by using test grids in every cell (Fig. 4, Step 1). The maximum deviation is stored. After that, instead of this test isobar, a temperature (hyperbolic middle value) is inserted on every original isobar (dashed line). The resulting left and right cells are tested for the interpolation accuracy thus obtained. Now, the maximum deviation is compared with that of the previous isobar narrowing. Only the narrowing yielding the greatest increase of interpolation accuracy is retained. In the example, the insertion of an isobar lead to a more accurate interpolation. The deviation 2.27 %, however, was once again too high, and so the narrowing procedure had to be repeated. The insertion of two isobars again increased the interpolation accuracy more than the temperature narrowing had, but the required accuracy still was not obtained (Fig. 4, Step 2). Temperature narrowing was first realized in the next step (Fig. 4, Step 3). In fact, all the narrowings given in Table 3 are necessary to obtain the required accuracy of $\Delta v/v = 0.2$ %.

In order to show the effectiveness of this simple optimization, Table 4 contains both the sequence of narrowings with optimization and the sequence without optimization.

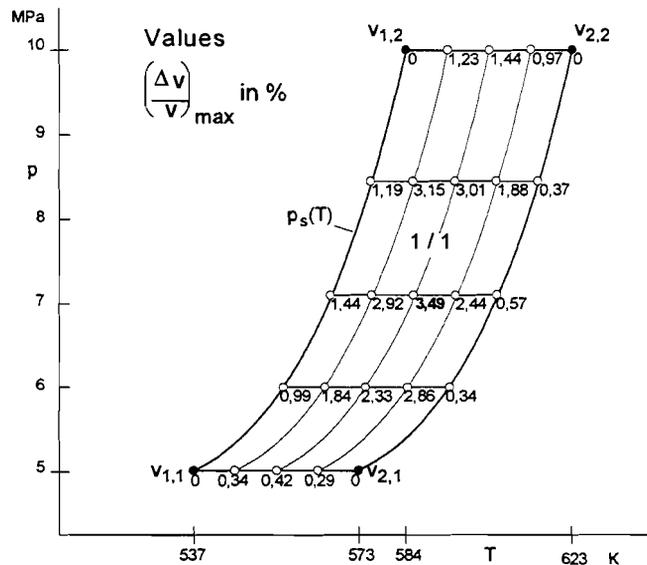


FIGURE 5. Test Grid with Test Points for the First Cell of Step 0 in Fig. 4

TABLE 3. Narrowing Steps to Optimize the Data Grid for $v = f(T,p)$ of Steam (Required Accuracy $\Delta v/v = 0.2$ %)

Step Number	Narrowed Property	Obtained Accuracy $\left \frac{\Delta v}{v} \right $
0	-	3.49 %
1	p	2.27 %
2	p	1.75 %
3	T	1.18 %
4	p	0.87 %
5	p	0.73 %
6	T	0.55 %
7	p	0.46 %
8	p	0.41 %
9	T	0.34 %
10	p	0.29 %
11	p	0.26 %
12	T	0.23 %
13	p	0.196 %

TABLE 4. Comparison of Narrowings With and Without Optimizations

Step Number	Without Optimization				With Optimization			
	Number			$\frac{ \Delta v }{v}$	Number			$\frac{ \Delta v }{v}$
	p	T	Data points		p	T	Data points	
0	2	2	4	3.49 %	2	2	4	3.49 %
1	2	3	6	3.49 %	3	2	6	2.27 %
2	3	3	9	2.04 %	4	2	8	1.75 %
3	3	4	12	1.96 %	4	3	12	1.18 %
4	4	4	16	1.16 %	5	3	15	0.87 %
5	4	5	20	1.12 %	6	3	18	0.74 %
.
.
12	10	6	60	0.23 %
13	11	6	66	0.196 %
.
15	9	10	90	0.24 %				
16	10	10	100	0.198 %				

Without optimization means that the narrowings of temperature and pressure occur alternately and independent of the change in accuracy. Whereas the procedure without optimization leads to 100 data points, the procedure with optimization leads to 66 data points and likewise fulfills the same interpolation accuracy. A further improvement of the optimization procedure results from exempting cells that already fulfill the required interpolation accuracy from subsequent narrowings. However, for simplicity's sake, the sequence of narrowings in Table 4 was performed by the algorithm without, exempting cells that already fulfilled the accuracy criterion. Had such cells been exempted, the number of required data points would have been reduced still further.

EXAMPLES OF GENERATED INTERPOLATION DATA TABLES

Data Table for Specific Volume $v = f(T,p)$ of Steam with Experimental Uncertainty

For calculating high and middle pressure steam turbine stages, the function $v = f(T,p)$ was to be interpolated. Table 5 shows, in the upper part, the range of state required. As in the previous example, the curves connecting between the corner points are straight lines in the $\ln(p), 1/T$ -plane. The required accuracy corresponds to the current experimental uncertainty $\Delta v/v = 0.02 \%$, with respect to the IFC 1967 Formulation. Whereas 270 data points are necessary to achieve the accuracy without optimization of the grid narrowing, just 68 points (= 25%) are required when using the optimization algorithm with optimization of the grid narrowing including the exemption of cells. In both cases, the transformations of Table 2 were used. Similar results have been achieved when generating data tables for $h = f(T,p)$ and $s = f(T,p)$.

TABLE 5. Interpolation Tables for $v = f(T,p)$ Generated With and Without Optimization of Grid Narrowing in the Range of State Required in Calculations of High and Middle Pressure Steam Turbine Stages

$v = f(T,p)$ of Steam With Experimental Uncertainty		
Range of validity	from 0.5 MPa (425 ... 573 K) up to 16.5 MPa (723 ... 823 K)	
Interpolation accuracy: $\frac{\Delta v}{v} = 0.2 \%$		
Basic equation: IFC 1967 Formulation		
	Generated data points	
	Without optimization	With optimization
Linear Interpolation with coordinate transformation (Table 2)	270	68 (= 25 %)

Data Tables for Vapour Pressure $p_s = f(T)$ of Water with Experimental Uncertainty

Table 6 shows the results for generated interpolation data points for the vapour pressure function $p_s = f(T)$ of water. An accuracy of $\Delta p_s/p_s = 0.025 \%$ is required by The International Association of Water and Steam (IAPWS) for the development of the forthcoming new Industrial Formulation (Wagner and Rukes 1995).

TABLE 6. Generated Data Tables for $p_s = f(T)$ of Water for Linear and Spline Interpolation With and Without Coordinate Transformation

$p_s = f(T)$ of Water With Experimental Uncertainty		
Range of validity: from triple point to critical point		
Interpolation accuracy: $\frac{\Delta p_s}{p_s} = 0.025 \%$		
Basic equation: IFC 1967 Formulation		
	Generated data points	
	Without transformation	With transformation (Table 2)
Linear interpolation	220	39 (= 18 %)
Spline interpolation	26	13 (= 50 %)

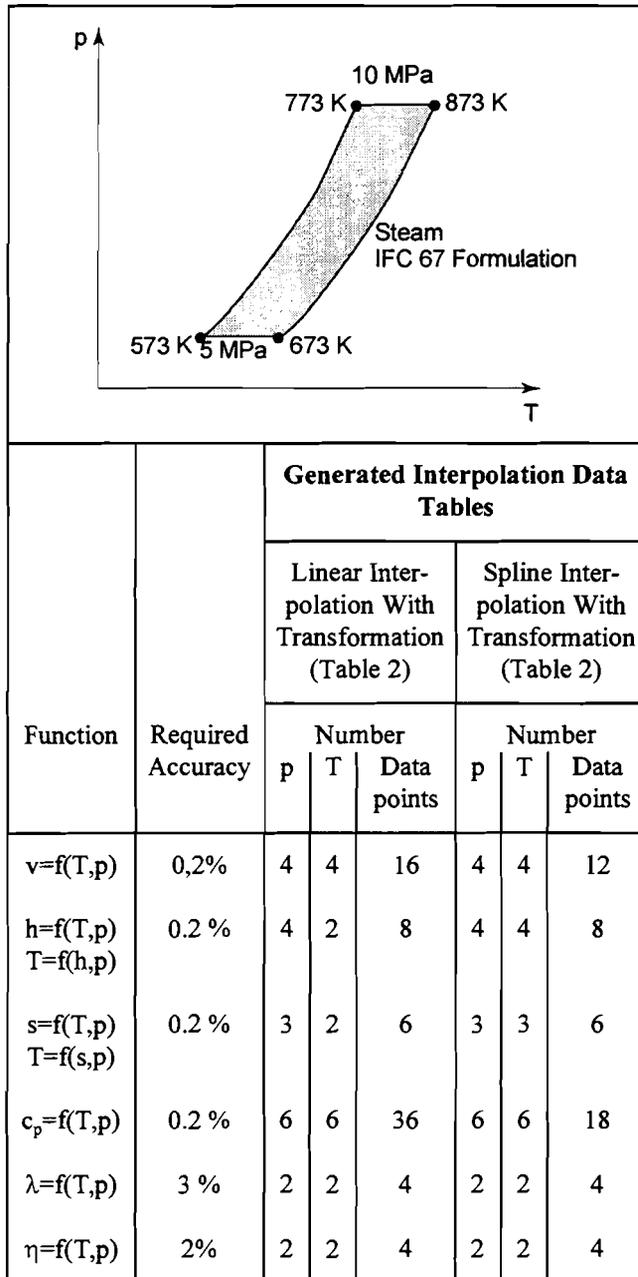
For linear interpolation with transformation, just 39 data points are necessary to achieve this high accuracy, or 18 % of the number of points required without transformation. As expected, spline interpolation with transformation required far fewer data points, namely 13. Here, the transformation lead to a decrease of 50 % in the number of the required data points.

A Set of Data Tables for Important Properties of Steam Required in Process Modeling

Table 7 summarizes the results of generated interpolation tables for properties required in calculations of steam turbine high-pressure stages. The range of validity is bordered by two isobars and the curves between the corner temperatures (straight lines in the $\ln(p), 1/T$ -plane). The accuracies shown result from requirements of the process model and were set by the user.

The data tables were generated for linear and spline interpolations with transformation of coordinates given in Table 2.

TABLE 7. A Set of Generated Interpolation Tables for Properties Necessary in Calculations of Steam Turbine High Pressure Stages



Note that, in some cases, the number of data points is not equal to the product of the number of isobars, p, and the number of temperatures, T, because each isobar can have a different number of temperatures. This results from the exemption of cells in the data density optimization algo-

rithm. In the columns for T in Table 7, only the maximum number of temperatures is given.

The interpolations of the backward functions $T = f(h,p)$ and $T = f(s,p)$ are realized using the same data tables as for the forward functions $h = f(T,p)$ and $s = f(T,p)$, respectively. The numerical consistency between backward and forward functions calculated from the same data tables is high enough for process modeling.

Because the grid generation algorithm has been developed with the principle goals of minimizing the number of interpolation data points and of obtaining a high flexibility with regard to such requirements of process modeling as functional dependency, range of state and interpolation method, minimization of computing time for applications of the algorithm was at first not in the immediate foreground of the investigation.

INTERPOLATION ALGORITHM AND GENERATED DATA TABLES

In Fig. 6, the entire procedure of generating optimized data tables and using them for interpolation of thermodynamic properties in process modeling is illustrated.

Assumed are subprograms with definite names and parameters, using specific interpolation algorithms and using interpolation data files with definite names and data structures (left boxes in fig. 6). Besides linear and spline interpolation, any other method, for example parabolic, rational, or interpolation-with-incorporation-of-derivatives (Baehr, 1974), (van der Looij, 1986) and (Hill, 1994) can be handled. The subprograms used should be the same as later provided for use in process modeling.

By using these subprograms, the interpolation tables are generated (central box in fig. 6). The data density is optimized for the interpolation accuracy required in the process modeling. In order to calculate the interpolation data, the basic equations of state and formulations for the actual working fluid are required. The interpolation tables with optimized data density resulting from the generation algorithm are stored for use in later interpolations or are output to terminal or printer.

When applied to process modeling, the interpolation data are read from the file the first time the respective subprogram is called and stay in memory after that.

This procedure allows the interpolation table generation and its application to be handled almost automatically.

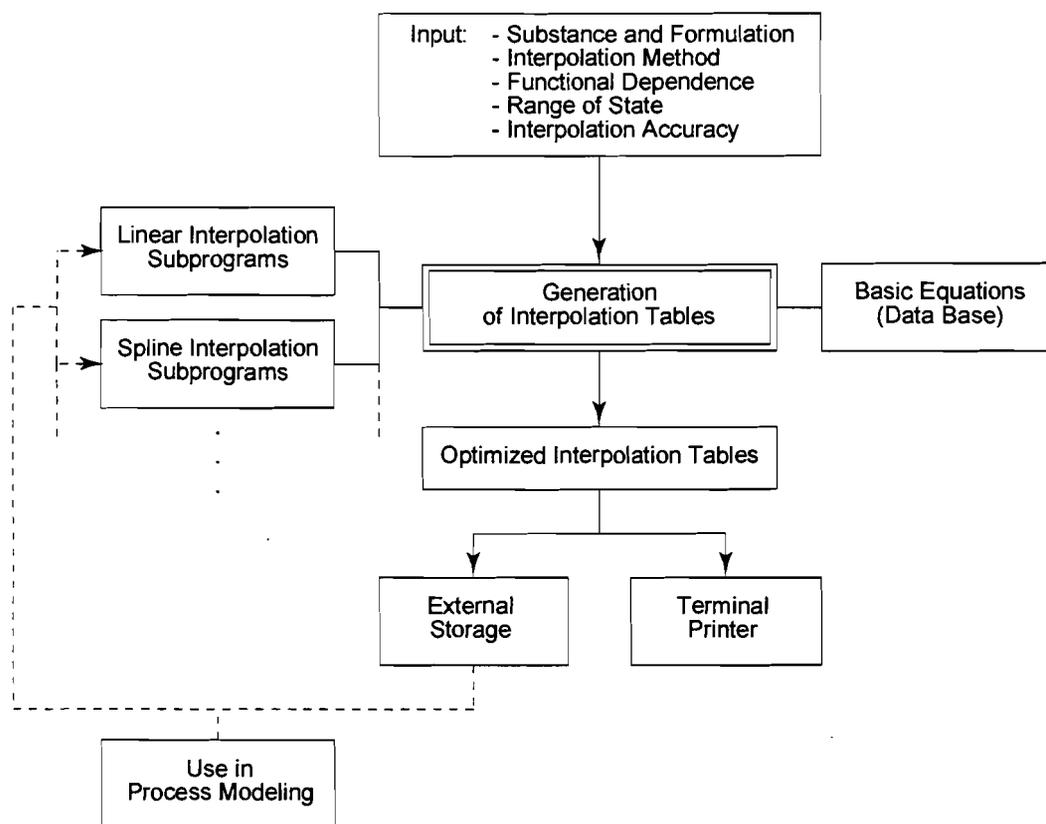


FIGURE 6. Procedure for Generating Optimized Data Tables and Using Them in Interpolations of Thermodynamic Properties in Process Modeling

CONCLUSIONS

The algorithm presented is able to generate interpolation tables with optimized data density

- for any required interpolation accuracy (absolute or relative)
- for any required thermodynamic function, including backward functions such as $T=f(h,p)$, $T=f(s,p)$ and
- for a given interpolation method (linear interpolation, spline interpolation, or any other interpolation - with or without transformation of coordinates).

The optimization of the data density is realized by means of a flexible strategy of condensing the data grid. Ranges of state in which the required interpolation accuracy is already fulfilled are exempted from further narrowing at each step of the process. The findings show, that the number of data points necessary for accurate interpolations is considerably fewer than might be expected.

By using suitable transformations of the properties to be interpolated, the number of data points can be further considerably decreased.

Users who are interested in calculating thermodynamic properties by interpolation can receive a sample interpolation subprogram and associated data table for given process modeling requirements from the authors for a nominal fee on request.

The algorithm can also be used for setting up the data grids for thermodynamic tables yet to be published, in order to minimize their size.

Presently, computing times are to be compared with several other interpolation algorithms, e. g. (Pfleger, 1988), (Caldwell and Spragg, 1977), as well as with other methods for the calculation of thermodynamic properties, e. g. (McClintock and Silvestry, 1968), (Schiebener and Straub, 1990).

Further investigations are underway to improve the algorithm for optimizing the interpolation data grid. In

particular, the search for favourable coordinate transformations shall be integrated into the optimization procedure.

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