

Interpolation of gas-liquid multicomponent fluid properties for piping fluid flow analysis

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Abstract. The article proposes the use of bicubic spline interpolation to optimize hydraulic and thermal calculations while processing thermodynamic library data. Research was carried out both in single-phase gas and liquid regions, as well as in the two-phase gas-liquid region. The accuracy of bicubic spline interpolation was tested for various thermodynamic libraries on multi-component mixtures. Various coordinate systems (P, x), (P, T), (P, H), (P, S) were tested, optimal coordinates and interpolation grids were selected based on the nature of changes in various thermophysical properties. Experiments were conducted in the range of up to 80% of critical pressure, since in the near-critical region the properties behavior changes sharply. Plots of properties and interpolation absolute and relative errors were also produced for a more detailed study and determination of problem areas where property functions undergo sharp changes that make interpolation difficult. The results obtained demonstrate an acceptable level of accuracy for engineering calculations in the approximation of data from thermodynamic libraries.

To perform hydraulic and thermal calculations for pipelines during the design and reconstruction of objects in various industrial sectors, numerous calculations are necessary. Programs such as "Hydrosystem" [1], "Safety valve" [2] and others are used for such calculations. When performing such analysis, it is necessary to calculate the thermodynamic and transport thermophysical properties (TTP), as well as calculate phase equilibrium (PE) of different phases, with changing parameters in the process of calculation, including nested cycles of iterations. Thermodynamic libraries are used for TTP and PE calculations, including libraries like "STARS", "Simulis Thermodynamics", GERG-2008, REFPROP, and others. These programs contain databases that include a total of over 5000 individual substances, and it is possible to calculate the content and composition of phases for any input pairs of thermodynamic parameters.

The number of subroutine calls from thermodynamic libraries increases with the complexity of the product composition, the branching of the considered pipeline, and the complexity of the calculations being performed. In some cases, this leads to a sharp increase in calculation time. From the practice of using libraries, it is apparent that up to 90% of program execution time for complex calculations is spent specifically on the calculation of

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TTP and PE! Therefore, the task was set to rationalize (speed up) the calculation process through optimization of the number of program queries to the libraries.

One of the standard methods of solving this problem is to replace numerous queries to thermodynamic libraries with a relatively small number of queries to a pre-determined or dynamically generated set of points, with subsequent interpolation of results over the entire region of interest (so-called Spline-Based table look-up method). In this case, the necessary interpolation accuracy should be ensured that is adequate to the accuracy of the computational models and methods used in the calling programs, as well as to the accuracy of the thermodynamic libraries themselves.

Based on previous results [3-5], the use of cubic interpolation for dependency on one parameter and the use of bicubic spline interpolation for single-component and multi-component substances in single-phase and two-phase regions was found to be effective, as the relative errors were within acceptable limits.

1. Relevance and scientific novelty

Currently, the methods of interpolation are quite well developed. Despite this, there are quite few studies in the field of interpolation application for the calculation of TTP and PE, and the results obtained mainly relate to single-phase or single-component products. Approaches to the implementation of two-dimensional interpolation are studied to a lesser extent than for one-dimensional one. Another feature of the case under consideration is the explicit division of the region and parameters in which interpolation is required into zones with curved boundaries (regions of the liquid phase, gas phase, supercritical region, and two-phase region bounded by boiling and dew lines).

2. Problem definition and applied methods

This article discusses the use of bicubic spline interpolation to determine the TTP and PE of various multicomponent mixtures of real gases and liquids, including in the two-phase region, depending on temperature and pressure, the vapour fraction and pressure, pressure and enthalpy, pressure and entropy.

Two types of bicubic splines were considered: spline (not-a-knot) [5, 7] and makima (Akima) [8]. It is natural to expect that bicubic splines (which give a doubly differentiable smooth interpolation) provide very high interpolation accuracy for properties that change smoothly and uniformly in the interpolation domain. At the same time, monotonicity-preserving makima splines may have an advantage when interpolating functions with different rates of change in different parts of the interpolation domain.

Bicubic piecewise spline interpolation is used to solve the interpolation problem in a rectangle in the x ; y plane, with boundaries $a \leq x \leq b$, $c \leq y \leq d$, with uniform grid points $(x_i; y_j)$ of size $n \times m$. The bicubic interpolating spline must pass through the grid points values. The coefficients of the splines of the surface $S(x, y)$ are determined by $16 \times n \times m$ coefficients; in this case, the continuity of the function itself and its first partial derivatives is usually required. Thus, the smoothness of the entire surface is ensured, for which $S(x, y)$ must satisfy the conditions of equality of the values of the function itself, the first and mixed second derivatives at the nodes of the grid. Or the first and mixed second derivatives of splines in the grid points are calculated by some finite difference method from the values of the interpolated function at the nodes [5, 9-12].

3. Literature analysis

An analysis of the literature shows that this topic was discussed, but at the moment it has not been studied enough.

In works [13, 14], bicubic spline interpolation is used to calculate the range of thermodynamic properties of refrigerants through Helmholtz energy interpolation. This method has three particularly useful characteristics: it is much faster than standard EOS methods, it is quite accurate, and the calculations of the properties are consistent. Also, an important point described in these works is that the calculation process time was reduced by 33%!

Articles [15-17] consider the use of bicubic interpolation depending on (P, T). The object of the study was water vapour. As a result, the use of interpolation has reduced time and computational costs.

An interesting work turned out to be [18], where complex mixtures were considered: nitrogen and carbon dioxide; and a mixture of hydrogen, methane, carbon dioxide, and kerosene. The use of spline interpolation gave acceptable results of errors in the range of 0.1%, which is more than enough for engineering calculations, also, in addition to reducing time costs to 68%, the cost of storing these properties decreased to 80%.

The work of J. Bonilla [19] is also important, since the two-phase region was considered depending on (P, H). Phase transitions and density discontinuities of some substances were studied.

The use of bicubic spline interpolation to predict the thermodynamic properties and phase equilibria of complex mixtures (a mixture of hydrogen, oxygen, carbon dioxide, nitrogen, methane) is considered in [20-22]. The analysis was carried out on mixtures with different amounts of components. This type of interpolation has shown good results in terms of accuracy, with the exception of the vapour-liquid curve and the supercritical state. The interpolation error increases significantly near the critical point.

Thus, the application of this method can potentially make it possible to perform complex numerical simulation of the flow in dynamics without significant loss of accuracy. The error in calculating the physical properties is no more than 0.5% compared to the interpolated values.

Research results. Bicubic interpolation of TTP and PE of multicomponent mixtures in two-phase and single-phase regions, depending on (P,T), (P,H), (P,S), (P,x)

In this article, the subject of discussion is the use of bicubic spline interpolation to determine the TTP and PE of real gases and liquids representing multicomponent mixtures on a uniform grid with a constant mixture composition. Our task is to find a universal approach for various libraries, various mixtures, taking into account the behavior of all the necessary properties. For testing, the compositions of hydrocarbon mixtures were selected from the real engineering practice of designing oil processing and petrochemical facilities (see Table No. 1).

Hydraulic and thermal calculations require an extensive list of properties. The following properties were investigated: molar mass of gas, volume expansion coefficient, dynamic viscosity, thermal conductivity, liquid density, compressibility coefficient, enthalpy, entropy, specific heat, isentropy coefficients, speed of sound, Joule-Thompson coefficient, surface tension coefficient and other properties. The following thermodynamic libraries were used: "STARS" and "Simulis Thermodynamics".

Table 1. Compositions of the mixtures used for the study

№	Composition of the mixture	Molar content of mixtures
1	Methane, ethane, propane	0.3 0.3 0.4
2	Methane, propane, 1-butene-2-methyl, ethane, nitrogen, carbon dioxide, pentane	0.2275 0.072 0.0322 0.049 0.0333 0.006 0.58
3	Ethane, methane, propane, carbon dioxide	0.9688 0.0204 0.0093 0.0015
4	Methane, ethane, propane, butane, isobutane, isobutane, pentane, hexane, methanol	0.02 0.01 0.15 0.15 0.15 0.12 0.15 0.15 0.1
5	Methane, ethane, propane, isobutane, butane, isopentane, pentane, cyclohexane, hexane, isoheptane, benzene, heptane, isooctane, toluene, octane, isononane, nonane, isodecane, decane, carbon dioxide, nitrogen	0.456094 0.163140 0.211402 0.051382
		0.070745 0.014431 0.013521 0.007539
		0.002825 0.001321 0.000061 0.000753
		0.000193 0.000679 0.000026 0.000003
		0.000012 0.000100 0.000160 0.001083
		0.004530

The MATLAB application software package was used to analyze the obtained data of thermodynamic libraries.

The main criterion for the success of interpolation in the problem of calculating a set of thermodynamic properties and phase equilibria is the required error of properties. Interpolation of thermodynamic properties is desirable with an accuracy of up to fractions of percent, and for transport properties an accuracy of about 1% is quite acceptable for the purposes of thermohydraulic calculations of pipelines [3]. The error was estimated by the relative error of interpolation on the interpolated area, as well as by the ratio of the error to the maximum difference of the property on the interpolated area (the latter is important when the property can take small or even zero values, such as entropy).

3.1. On some features of interpolation in the two-phase domain. Problems and solutions.

At the initial stage of the study, the coordinates of the two-phase region were $\ln(P_r)$ (where $P_r = P/P_c$ is reduced pressure) and vapour fraction. At this stage, some specific behavior of the "Simulis Thermodynamics" library were discovered. The values of liquid density, viscosity and thermal conductivity of the liquid phase calculated from the library, as well as the surface tension coefficient in the two-phase region behaved poorly - they experienced jumps of its values or its first derivatives. As it turned out, this behavior is due to the default "classical" methods used in the library for calculating these properties (Ideal mixture, "CLASSIC" mixing rules), which calculate the properties of the mixture based on the properties of individual components. In this case, the saturation lines of individual components fall into the zone of the two-phase region of the mixture, which leads such effects on these lines. This behavior of the function, of course, immediately leads to a deterioration in the quality of interpolation in the vicinity of places of such behavior. After analyzing the available calculation methods, "smooth" methods were chosen for further use, — Modified Rackett (mixtures) for calculating the density of the liquid, Ely-Hanley model (TRAPP method) for the viscosity and thermal conductivity of the liquid, Loo and Chien for the surface tension coefficient.

The fact that it makes sense to use spline interpolation only in areas of smooth variation of the interpolated functions was obvious in advance. However, as it turned out, thermodynamic libraries do not always provide such smoothness, and the behavior features of a particular library are not always obvious initially, and may depend both on the chosen

calculation methods and on the programming implementation in a particular library. This means that a successful application of spline interpolation requires a good understanding of the operation of specific thermodynamic libraries!

Three interpolation grids were investigated (10*10, 15*15, 20*20 points) with a pressure coordinate – a uniform grid along $\ln(1/P_r - 1)$. At the same time, several variants of pressure coordinates were considered, $\ln(P_r)$, $1/\ln(P_r)$, $\ln(P_r - 1/P_r)$, $\ln(1/P_r - 1)$ in order to ensure optimal grid density in various areas of pressure change without significantly number of points increasing, and to cover in the same time as large interpolation area as possible. As it is known, at low pressures, properties practically do not change or change quite slowly, and at high P_r , a rapid change in property values begins. Instead of using an uneven grid, it was proposed to modify the pressure coordinate so that a uniform grid for this coordinate automatically takes into account the behavior of the properties. The uniform interpolation by $\ln(1/P_r - 1)$ turned out to be the most optimal, while the interpolation grid by P_r is automatically found out compact for high pressures and sparse for low ones.

Another thermodynamic specific aspect to be taken in account is the behavior of the isentropy coefficient (inverse number to well-known parameter ω in Leung ω method) of a gas-liquid mixture in a two-phase region. As is known, at low pressures, the isentropy coefficient has a zone of rapid change in the asymptotic width of the order of P_r in terms of vapour fraction x near the boiling line, in which it increases from small values to values of the order of 1. In this zone, the accuracy of interpolation in x drops sharply. Unfortunately, this zone is of the greatest interest for calculating critical and near-critical flow in pipelines and safety valves. Therefore, to calculate the isentropy coefficient, an attempt was also made to find a suitable coordinate that provides acceptable interpolation accuracy in the entire two-phase region under consideration. It turned out that a coordinate $eps = x/(x + (1 - x)\sqrt{P_r})$ can serve for this purpose, a uniform grid along which provides the required accuracy of interpolation of the isentropy coefficient.

Additional features of mixtures 4 and 5 are the presence in an extremely small percentage of low- or high-boiling components. In mixture 4, low-boiling components of extremely low content (methane and ethane) are boiled off first, and in mixture 5 there are also high-boiling components of low content (hexane and heavier), which are boiled off last. In this regard, in the zones adjacent to the boiling and dew curves, where there is a rapid change in the content of these components in liquid and vapour phases (from almost 0 to 1), there is a rapid change in the composition and properties of the liquid and / or gas phase. As it turned out, in this case it is also possible to apply a universal approach, since the width of such zones, as it turned out, depends primarily not on the content of the components, but on the magnitude of the reduced pressure. Because of this, for such mixtures with such zones, the coordinates $eps = x/(x + (1 - x)P_r)$ describes such zones for mixture 4, and $eps = x/(x + (1 - x)/P_r)$ for mixture 5. After that, during further research, it was concluded that it is necessary to smoothly "stitch" two interpolations along the second coordinate (x , eps) by multiplying by the corresponding smoothly varying weighted coefficients, which is a non-trivial way. The stitching helped to reduce the error, since each of the coordinates (x/eps) take into account the peculiarities of changing the function along the axis, each coordinate works for a certain edge. A similar approach can be used for the isentropy coefficient, however, the single coordinate described above is also suitable for it, since its value does not change very much in almost the entire region and begins to change rapidly only near the boiling line ($x=0$).

3.2. Two-phase area. Results of interpolation in (P,x) coordinates

When interpolating in the two-phase region, the subcritical region of the mixture was considered, up to about $0.8*P_c$. Some mixtures have a narrow two-phase region in the

coordinates P, T. It is inefficient to interpolate such a region in these coordinates, hence the interpolation by pressure and vapour fraction was tested. In addition, the interpolation grid becomes rectangular, and there is no need to resort to additional coordinate transformation operators.

After conducting studies for coordinates $(\ln(1/P_r - 1), x)$ (or ϵ), the results were satisfactory, since an error of 1% or even smaller was achieved. Figures 1, 2 show graphs of the property of the isentropic coefficient before the coordinate transformation and after transformation.

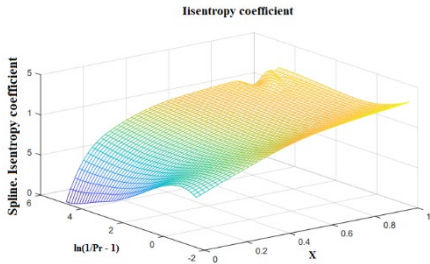


Figure 1. Plot of the isentropic coefficient before coordinate transformations

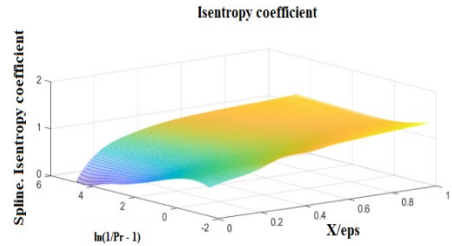


Figure 2. Plot of the isentropic coefficient after coordinate transformations

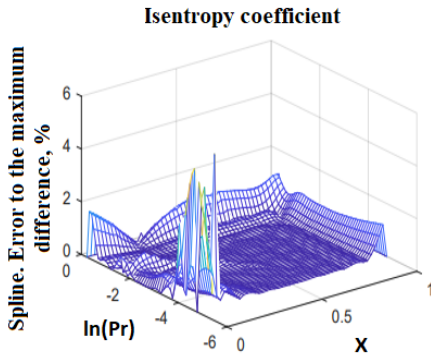


Figure 3. Plot of the error of the isentropic coefficient before coordinate transformations

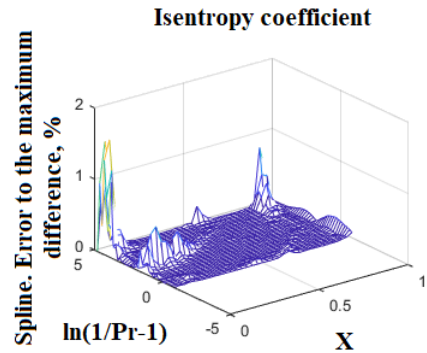


Figure 4. Plot of the error of the isentropic coefficient after coordinate transformations

Plots 3, 4 illustrate the interpolation error of the isentropic coefficient before the coordinate transformation and after transformation.

3.3. Two-phase area. Results of interpolation in coordinates (P, H) / (P,S)

Studies have also been conducted on interpolation in coordinates (P,H) / (P,S) since these coordinates are more convenient for hydraulic calculations, and also for safety valve sizing. The coordinates $\ln(1/P_r - 1)$ and dimensionless enthalpy or entropy coordinates normalized to the enthalpy/entropy difference between the dew and boiling points depending on pressure were used:

$$\frac{H - H(\text{bubble})}{H(\text{dew}) - H(\text{bubble})}$$

Statistical analysis of relative errors shows that such coordinates provide even slightly better accuracy than vapour fraction interpolation. Plots 5, 6 illustrate the acceptable error of entropy interpolation depending on $(\ln(1/P_r - 1), H)$ and the density of the liquid on $(\ln(1/P_r - 1), S)$ by the spline method, which do not exceed 0.5%

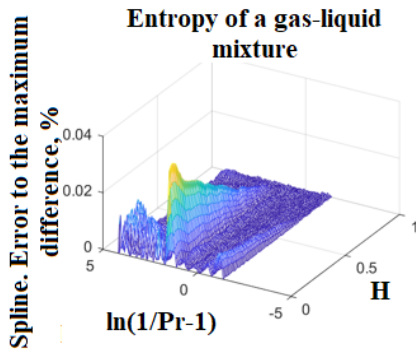


Fig. 5. Plot of the entropy error of the gas-liquid mixture depending on $(\ln(1/P_r-1), H)$

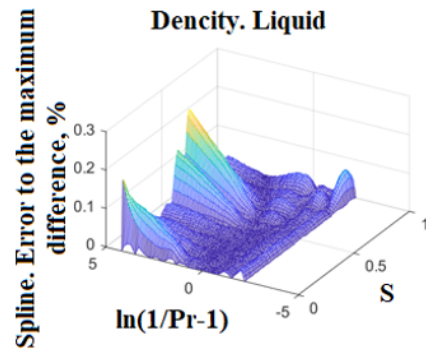


Fig. 6. Plot of liquid density error in two-phase region depending on $(\ln(1/P_r-1), S)$

3.4. Adjacent single-phase areas. Interpolation results in coordinates $(P, T)/(P,H)/(P,S)$

Since the transition of the product from a two-phase to a single-phase state and back is possible in the calculation process, it is important in this case to also have interpolation of single-phase liquid and gas regions adjacent to the boundary of the two-phase region.

To construct such an interpolation, $\ln(1/P_r - 1)$ was used as one of the coordinates in all the cases under consideration. The second coordinate was the deviation of temperature (enthalpy/entropy) from the value on the boiling line, in the case of a single-phase liquid region, and from the value on the dew line, for gas region,. This allows to convert another coordinate to a normalized one (for example, from 0 to 1) and apply interpolation on a uniform grid in a rectangle. At the same time, the interpolation error by (PH) or (PS) turns out to be significantly lower than 1%, and in average hundredths of a percent.

4. Summary and conclusion

The use of bicubic splines makes it possible to interpolate the TTP of real gases and liquids in two-phase and adjacent single-phase regions. To improve the results of interpolation, various coordinate systems have been developed that take into account the behavior of the properties being interpolated. Meshes on enthalpy/entropy were also investigated, which further reduces the error. In most cases, the ‘‘Spline’’ method gives slightly better accuracy compared to Akima splines. The grid with the number of points equal to 15×15 turned out to be optimal.

As a result, it was possible to develop approaches that allow uniform interpolation of various multicomponent mixtures based on a relatively small number of points in a very wide range: almost the entire two-phase region (except the critical region), and adjacent single-phase regions.

In the future, it is planned to test the developed approaches on more diverse mixtures, including those involving oil fractions, as well as using additional libraries GERG-2008 and REFPROP. At the same time, it is planned to develop an appropriate TTP and PE interpolation module for inclusion in the ‘‘Hydrosystem’’ and ‘‘Safety valve’’ programs.

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