A presentation method of the thermophysical properties of matter in the form of spreadsheets

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Abstract. The research of methods to reduce CO₂ emissions into the atmosphere has led to formation of new thermodynamic cycles in which oxygen is separated from the air before combustion. Fuel, pure oxygen and some recirculating substances, from which it is easy to separate CO₂ formed during the combustion, are fed into the combustion chamber. Usually, CO₂, H₂O or a mixture of thereof are used in the form of recirculated flue gas. The parameters in such cycles are chosen at different points in the cycle, where the working fluid can be in liquid, gaseous or supercritical states. The computational study of such cycles requires a convenient presentation of the thermophysical properties of different substances that can be part of the working fluid in a wide range of parameters. The aim of this work is to develop a data array and a computational module (spreadsheet) considering the dependence of the basic thermophysical properties of various substances. A conversion method of variables that allowed the formation of a compact interpolation grid with minimal loss of accuracy during subsequent interpolation was proposed, where the use of integers for the nodal values of the independent variables saved computational resources during interpolation significantly.

1. Problem Statement

The research of methods to reduce CO₂ emissions into the atmosphere has led to formation of new thermodynamic cycles in which oxygen is separated from the air before combustion. Fuel, pure oxygen and some recirculating substances, from which it is easy to separate the CO₂ formed during the combustion, are fed into the combustion chamber [1]-[4]. Usually, CO₂, H₂O or a mixture of thereof are used in the form of recirculated flue gas. The parameters in such cycles are chosen at different points in the cycle, where the working fluid can be in liquid, gaseous or supercritical states [5]-[7]. The composition of the working fluid is also variable, for example, at some points the working fluid is a pure substance, while at others it is a mixture of substances. The computational study of such cycles requires a convenient presentation of the thermophysical properties of different substances that can be part of the working fluid in a wide range of parameters, covering the supercritical, gaseous, and liquid states. A great deal of attention was paid to the study of the thermophysical properties of various substances. All substances that can be part of the working fluid of new cycles are well studied in sufficient ranges of variation of parameters. The thermophysical properties of most substances can be found in reference literature in a tabular form. To develop such tables, there are approximating systems of equations based on experimental data; however, the use of such forms of representation of thermophysical properties is extremely inconvenient in software-computing complexes. The reference literature is not adapted to processing using computer technology, and the systems of equations are too
bulky and require enormous calculations. For instance, when the range is not very wide, as in traditional gas turbine cycles where only the gaseous phase is covered, the properties are approximated by the power of polynomials. However, using simple polynomials for wider ranges of variation of the calculation domain would not give a sufficiently accurate presentation.

The aim of this work is to develop a data array and a computational module (spreadsheet) considering the dependence of the basic thermophysical properties of various substances, which can be effectively used in computational programs and software-computing complexes.

2. The presentation method of the thermophysical properties of matter in the form of spreadsheets

The state of all substances of interest, for the studied cycles, in the single-phase region is simply determined by two independent parameters, most often, temperature and pressure. For equilibrium states, when several phases are simultaneously present, for clarity, one more parameter is required to determine the phase condition. For all substances, there are extensive zones in which the laws of variation of the properties can be considered linear; however, when the state of substances is close to a phase change, it is extremely difficult to select an approximating dependence. One of the presentation methods is grids with parameter values at nodal points (a tabular form), where the values in the intervals between the nodes are determined by interpolation between the nearest nodes. The required accuracy of such a representation can always be achieved due to the density of the grid. If we consider temperature and pressure as the independent variables, then a small zone will be present, which will dictate a very dense grid, whereas for the most of the considered range, the mesh density will be excessively redundant. To avoid this problem, replacing the variables is proposed. The source function is:

\[ Z = f(P, T) \]  

where \( Z \) represents vector values of the properties of interest; \( P \) is pressure; \( T \) is temperature.

The equation (1) is converted into the following form:

\[ Z = f(IP, IT) \]  

where \( IP \) and \( IT \) are new variables.

The new variables are expressed in terms of pressure and temperature as follows:

\[ IP = \ln \left( \left( \frac{P}{P_0} \right)^a \right) \]  
\[ IT = \ln \left( \left( \frac{T}{T_0} \right)^b \right) \]

where \( P_0 \) is reference pressure, taken equal to the pressure at the critical point; \( T_0 \) is reference temperature, which depends on the pressure (if the pressure is above critical, it is taken equal to the temperature at the critical point; if the pressure is below critical, it is taken equal to the equilibrium phase transition temperature at the corresponding pressure); \( a \) and \( b \) are coefficients determining the density of the grid.

Using the new variables, the entire considered range is conveniently divided into characteristic zones. If \( IP \) is a positive value, then the state of the substance is supercritical. If \( IP \) is a negative value, and \( IT \) is positive, then the state is gaseous. If both \( IP \) and \( IT \) are negative values, then the state is liquid. If \( IP \) is a negative value, and \( IT \) is equal to zero, then the state is equilibrium between the liquid and gaseous phases.

For the nodes of the interpolation grid, it is suggested to use integer values for the variables \( IP \) and \( IT \). The number of nodes is considered as \( N^- \) and \( N^+ \), respectively, for negative and positive values of \( IP \), and similarly, \( M^- \) and \( M^+ \) for \( IT \).
To consider the substances, data arrays were developed. For each substance, the data array should contain the following information:

- pressure and temperature values at the critical point;
- coefficients determining the density of the grid – \( a \) and \( b \);
- grid boundaries – \( N_- \), \( N^+ \), \( M_- \), and \( M^+ \);
- array \( T_e \) (equilibrium temperature values of the phase transition at \( IP = 0, -1, -2, \ldots, N^- \));
- Four property vectors arrays \( (Z^-) – \) property values in nodes \( IP = 0, -1, -2, \ldots, N^- \); \( IT = 0, -1, -2, \ldots, N^- \); \( IT = 0, 1, 2, \ldots, M^+ \); \( Z^+ \) – in nodes \( IP = 0, 1, 2, \ldots, N^+ \); \( IT = 0, -1, -2, \ldots, M^- \); \( Z^+ \) – in nodes \( IP = 0, 1, 2, \ldots, N^+ \); \( IT = 0, 1, 2, \ldots, M^+ \).

The interpolation was performed as follows:

For given values of pressure and temperature, in accordance with equation (3), \( IP \) is determined. If \( IP \) is positive, then \( T_o \) is equal to the temperature at the critical point. If \( IP \) is negative, then \( T_o \) is determined as a function of \( IP \). Therefore, the module \( IP \) is taken, and its integer \( IP_i \) and fractional \( IP_f \) parts are determined. The value of \( T_o \) will be as follows:

\[
T_o = T_e (IP_i + 1) \times (1 - IP_f) + T_e (IP_i + 2) \times IP_f
\]  (5)

After determining \( T_o \) in accordance with equation (4), \( IT \) is determined. The integer \( IT_i \) and fractional \( IT_f \) parts of the module \( IT \) are determined. The properties vector at the desired point is defined as follows:

\[
Z(P, T) = Z(IP, IT) = Z^a (IP_i + 1, IT_i + 1) \times (1 - IP_f) \times (1 - IT_f) + Z^a (IP_i + 2, IT_i + 1) \times IP_f \times ...
\]

\[
(1 - IT_f) + Z^a (IP_i + 1, IT_i + 2) \times (1 - IP_f) \times IT_f + Z^a (IP_i + 2, IT_i + 2) \times IP_f \times IT_f
\]  (6)

A data array as it is and a program that implements the above algorithm represent a spreadsheet that is convenient to use in computational calculations. Storage of data arrays requires moderate amounts of memory, and the use of integers for the nodal values of the independent variables reduces the number of computational operations for each access to a minimum. The proposed conversion makes it possible to obtain acceptable interpolation accuracy with a reasonable grid density.

In the phase transition region \( (IP < 0, IT = 0) \), another variable appears to eliminate the uncertainty, the dryness fraction of the vapor, where the properties are determined as mass-average values, based on the properties of each phase at the phase transition boundary.

A method of presenting the thermophysical properties and a computational module (spreadsheet) were developed for a software-computing complex to simulate a compressor-less combined cycle gas turbine power plant, however, the method can still be used in other computational calculations, where the thermophysical properties of various substances are required. For now, data arrays that consider \( \text{CO}_2, \text{H}_2\text{O}, \text{O}_2 \) and \( \text{CH}_4 \) in a wide range of pressure and temperature variations (from 600 Pa to 600 MPa and from 70 K to 2000 K) have already been generated and tested. Deviations of the obtained values of the considered properties from the original tables, found in the reference literature, do not exceed 1%. This range fully meets the requirements of the task set; however, further work will be aimed at expanding the range of the substances considered.

**Conclusions**

A conversion method of variables that allowed the formation of a compact interpolation grid with minimal loss of accuracy during subsequent interpolation was proposed, where the use of integers for...
the nodal values of the independent variables significantly saved computational resources during interpolation. Spreadsheets of the thermophysical properties of matter were developed for a software-computing complex to simulate a compressor-less combined cycle gas turbine power plant; however, this method can still be used in other computational calculations. The proposed method has been tested on several thermophysical properties such as enthalpy, entropy, specific volume, dynamic viscosity, thermal conductivity coefficient and heat capacity at a constant volume for the following substances: water ($H_2O$), carbon dioxide ($CO_2$), oxygen ($O_2$) and methane ($CH_4$).

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