International Journal of Thermophysics, Vol. 25, No. 2, March 2004 (© 2004)

Automated System for Calculating Thermophysical Properties of Fluids and Thermal Processes of Cryogenic Plants[1]

A. A. Vasserman,[2,3] S. V. Bodyul,[4] and E. S. Bodyul[4]

An automated system for calculating thermophysical properties of gases and liquids over a wide range of parameters has been developed. On the basis of values of the properties, the processes of isothermal compression, adiabatic throttling, polytropic expansion, heat exchange in two- and multi-stream heat exchangers, separation of vapor-liquid mixtures in the liquid vessel, and rectification in an air separation plant can be analyzed. For a specified structure scheme of a cryogenic plant, optimization of a corresponding thermodynamic cycle can be fulfilled.

KEY WORDS: automated system; cryogenic plants; fluids; processes; thermophysical properties.

1. INTRODUCTION

For the design and analysis of cryogenic plants, reliable information on thermophysical properties over wide ranges of density and temperature is necessary. Therefore, we created an automated system (ProCSys) for calculating thermophysical properties of fluids, and most importantly, thermal processes of cryogenic plants. By means of this system, the process of rectification in an air separation plant can also be analyzed.

---

[1] Paper presented at the Fifteenth Symposium on Thermophysical Properties, June 22–27, 2003, Boulder, Colorado, U.S.A.

[2] Odessa National Maritime University, Mechnikova Str. 34, Odessa 65029, Ukraine.

[3] To whom correspondence should be addressed. E-mail: avas@paco.net

[4] Odessa State Academy of Refrigeration, Dvoryanskaya Str. 1/3, Odessa 65026, Ukraine.

2. CHARACTERISTICS OF SYSTEM

Determination of substances' parameters for isobaric cooling or heating, condensation, evaporation, cooling or heating of a stream in heat exchanger channels with losses of pressure, and mixing of streams of the same substance at different temperatures is required for designing cryogenic equipment. The automated system ProCSys allows calculations of these processes and also isothermal compression, adiabatic throttling, polytropic expansion, heat exchange in two- and multi-stream apparatus, separation of vapor-liquid mixtures in a liquid vessel, rectification in an air separation plant, and any other processes.

The user has an opportunity to choose a device or apparatus, for which the process is calculated. According to a choice of the user on the screen forms, there are necessary fields for input of the initial information about parameters of streams and other data.

For calculation of process parameters the names of working substances, the values of flow-rates, and a set of other necessary initial data are provided. For processes of isothermal compression in a compressor or polytropic expansion in an expander, the values of initial pressure and initial temperature and the efficiency of mentioned machines are introduced. On calculating the adiabatic throttling, the values of initial and final pressure and initial temperature (or enthalpy) are given and the corresponding regime of calculation is chosen (on the basis of pressure and temperature or pressure and enthalpy).

For calculations for processes in two- and three-stream heat exchangers, the values of pressure and temperature (or enthalpy) for necessary points of input in an apparatus and for points of output are used as initial data. The user selects the point for which the equation of the energy balance must be solved. The regime of calculations that corresponds to the initial data is chosen. The heat exchanger may be divided into many sections for determination of differences of temperatures in each section. It is necessary for verification of observance of the second law of thermodynamics in these sections. For a three-stream heat exchanger the amount of heated and cooled streams is indicated.

For determination of parameters of vapor, liquid, and their mixture in a liquid vessel, in addition to the name of the substance and the value of the flow-rate, the values of pressure and enthalpy for the point of input must be given. For calculations for the process of rectification, many initial data indicated later are used.

For calculations for processes, data on thermophysical properties of working substances for different independent variables are necessary. By means of a developed system, the properties of helium, argon, krypton, hydrogen, nitrogen, oxygen, air, carbon dioxide, and some hydrocarbons (methane, ethane, ethylene, propane, and *n*-butane) can be calculated. These properties can be determined in the single-phase and two-phase regions, and on the saturation and melting lines at temperatures from the triple point to 1500 K and at pressures up to 100 MPa for nine combinations of independent variables: T, ρ; T, p; T, s; T, x; p, ρ; p, h; p, s; p, x; and h, s. The system allows calculations of temperature, pressure, density, specific volume, compressibility factor, internal energy, enthalpy, entropy, Gibbs energy, Helmholtz energy, isochoric and isobaric specific heats, adiabatic index, speed of sound, Joule–Thomson coefficient, isothermal throttling coefficient, coefficients of thermal expansion and isothermal compression, heat of vaporization, fugacity, dynamic and kinematic viscosities, thermal conductivity, Prandtl number, and surface tension.

Unified equations of state for the gas and liquid are used for calculating thermodynamic properties over wide intervals of density and temperature. Most of them are accurate reference equations. For increasing the reliability of calculated values of properties, the user has the possibility to select equations compiled by different authors for the same substance. In particular, for nitrogen, oxygen, and air, unified equations of state [1–3] are used having a simple polynomial form,

$$Z = 1 + \sum_{i=1}^{m} \sum_{j=0}^{s_i} b_{i,j} \frac{\omega^i}{\tau^j}, \tag{1}$$

where $Z = pv/(RT)$ is the compressibility factor, $\omega = \rho/\rho_{\text{cr}}$ is the reduced density, and $\tau = T/T_{\text{cr}}$ is the reduced temperature.

For the same substances additional equations of state [4–6] are used having a more complicated so-called fundamental form,

$$\Phi = \frac{A}{RT} = \alpha_0(\omega, \tau) + \alpha(\omega, \tau), \tag{2}$$

where $A/(RT)$ is the dimensionless Helmholtz energy, $\alpha_0(\omega, \tau)$ is the ideal-gas part of Φ, and $\alpha(\omega, \tau)$ is the real part of Φ.

The function $\alpha(\omega, \tau)$ may be represented in a form containing a polynomial part and exponents with different powers of ω. The advantages of Eq. (2) are the possibility to calculate all thermodynamic properties by differentiation of the function $\Phi(\omega, \tau)$ and higher precision in the critical region in comparison with Eq. (1).

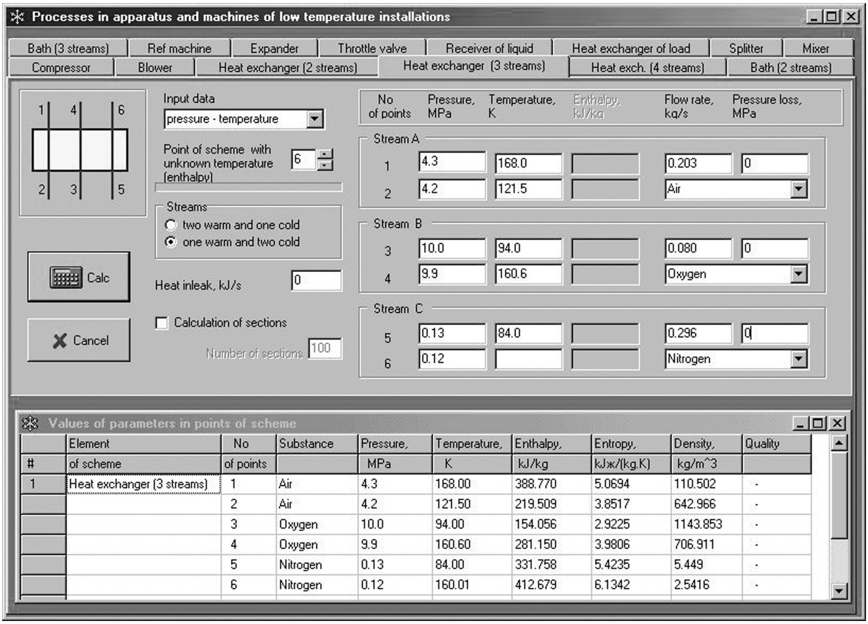
Equations describing the dependence of viscosity and thermal conductivity on temperature and density are used for calculating transport properties. If other initial parameters are given, the necessary values of temperature or density are calculated by means of an equation of state. Equations for calculating ideal-gas functions and the saturated vapor pressure and melting pressure are also used for each substance.

Software for calculating properties was taken from the thermophysical property databank developed earlier by the authors from this study [7]. In this paper the literature sources for all equations of state and equations for transport properties used in this system are provided.

It should be noted that calculations of the thermophysical properties for all combinations of independent variables, except for T and ρ, are based on iteration procedures, because the equations of state were developed for temperature and density as independent variables.

On the basis of calculated values of properties, the parameters of streams for points of input in machines and apparatus and for points of output, and also for energy and material balances of processes, are determined. In Fig. 1 the state of a working window for calculations for processes in multi-stream heat exchangers is shown.

The rectification column is the principal apparatus of the separation assembly of air separation plants. The working process in this column is based on an interaction of the descending liquid phase of the separated



Input data: pressure - temperature

Point of scheme with unknown temperature (enthalpy): 6

Streams
○ two warm and one cold
● one warm and two cold

Heat inleak, kJ/s: 0

☐ Calculation of sections

Number of sections: 100

	No of points	Pressure, MPa	Temperature, K	Enthalpy, kJ/kg	Flow rate, kg/s	Pressure loss, MPa
Stream A	1	4.3	168.0		0.203	0
	2	4.2	121.5		Air	
Stream B	3	10.0	94.0		0.080	0
	4	9.9	160.6		Oxygen	
Stream C	5	0.13	84.0		0.296	0
	6	0.12			Nitrogen	

#	Element of scheme	No of points	Substance	Pressure, MPa	Temperature, K	Enthalpy, kJ/kg	Entropy, kJж/(kg.K)	Density, kg/m^3	Quality
1	Heat exchanger (3 streams)	1	Air	4.3	168.00	388.770	5.0694	110.502	-
		2	Air	4.2	121.50	219.509	3.8517	642.966	-
		3	Oxygen	10.0	94.00	154.056	2.9225	1143.853	-
		4	Oxygen	9.9	160.60	281.150	3.9806	706.911	-
		5	Nitrogen	0.13	84.00	331.758	5.4235	5.449	-
		6	Nitrogen	0.12	160.01	412.679	6.1342	2.5416	-

Fig. 1. Working window for calculating the process in a multi-stream heat exchanger.

mixture with the vapor phase. The driving force of the process is a nonequilibrium difference in concentrations of the components of the separated mixture.

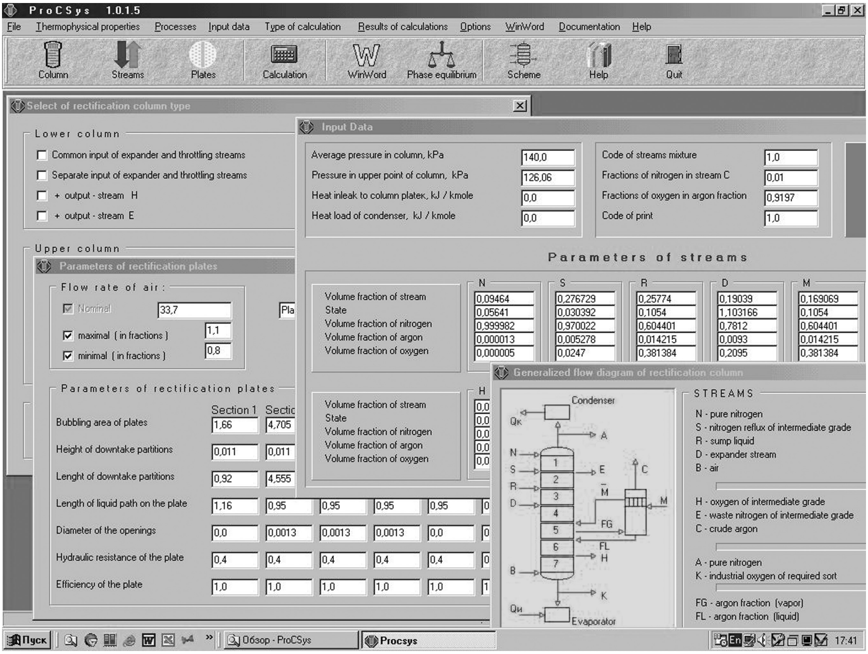
For calculating the process of rectification, the method of Lewis and Matheson [8] was used. This method is based on finding the real changes in stream composition on each plate and along the column height. For calculations the constructive features of the column and varying properties of the vapor and liquid are taken into account. A generalized flow diagram covers many possible variants of the upper and lower columns. The parameters of all incoming and exiting streams (composition, flow rate, mixture state), heat loads of condensers and evaporators, and constructive features of the plates in every section (area, length of liquid path, opening diameter, perforation pitch, and other necessary data) should be prescribed among the initial process parameters. For calculations for the process of rectification, air is considered as a mixture of nitrogen-oxygen-argon.

The system can be used to carry out thermodynamic and technological calculations for numerous variants of columns. The user selects on the screen form a type of rectification column with an indication of necessary streams of the top or bottom column, thus generating one from 20 possible variants of the scheme.

Calculations for a rectification column can be executed as for a nominal regime of operations corresponding to the technical project under design and for other regimes (in view of temperature conditions of environment, deterioration of the equipment at operation conditions, etc.). Calculations for the maximum and minimum flow-rates specified by the user may be carried out simultaneously. In such cases the system creates on the display a window with three tables for different variants of calculations. In Fig. 2 the state of screen forms for input data for calculating the process of rectification is shown.

The complex decision of described tasks for the specified structure scheme of cryogenic plants makes it possible to determine parameters and basic characteristics of the thermodynamic cycle.

After the end of calculations the system ProCSys presents on the screen results as a set of tables containing the initial data and estimated values (parameters of streams, data on phase equilibria, material balances, etc.). The system creates simultaneously text files with the data received for different variants of calculations. The results of calculations presented on the display may be saved as a Word document. Before printing these results, the user has the possibility to edit files or tables and to create corresponding technical documents. The realization of similar methods promotes acceleration of design and allows one to create the design documentation directly in the automated system.



Select of rectification column type

Lower column

☐ Common input of expander and throttling streams
☐ Separate input of expander and throttling streams
☐ + output - stream H
☐ + output - stream E

Upper column

Parameters of rectification plates

Flow rate of air:

☑ Nominal 33,7
☑ maximal (in fractions) 1,1
☑ minimal (in fractions) 0,8

Parameters of rectification plates

	Section 1	Sectic				
Bubbling area of plates	1,66	4,705				
Height of downtake partitions	0,011	0,011				
Lenght of downtake partitions	0,92	4,555				
Length of liquid path on the plate	1,16	0,95	0,95	0,95	0,95	0
Diameter of the openings	0,0	0,0013	0,0013	0,0013	0,0	0
Hydraulic resistance of the plate	0,4	0,4	0,4	0,4	0,4	0
Efficiency of the plate	1,0	1,0	1,0	1,0	1,0	1

Input Data

Average pressure in column, kPa	140,0
Pressure in upper point of column, kPa	126,06
Heat inleak to column platex, kJ / kmole	0,0
Heat load of condenser, kJ / kmole	0,0
Code of streams mixture	1,0
Fractions of nitrogen in stream C	0,01
Fractions of oxygen in argon fraction	0,9197
Code of print	1,0

Parameters of streams

	N	S	R	D	M
Volume fraction of stream	0,09464	0,276729	0,25774	0,19039	0,169069
State	0,05641	0,030392	0,1054	1,103166	0,1054
Volume fraction of nitrogen	0,999982	0,970022	0,604401	0,7812	0,604401
Volume fraction of argon	0,000013	0,005278	0,014215	0,0093	0,014215
Volume fraction of oxygen	0,000005	0,0247	0,381384	0,2095	0,381384

	H
Volume fraction of stream	0,0
State	0,0
Volume fraction of nitrogen	0,0
Volume fraction of argon	0,0
Volume fraction of oxygen	0,0

Generalized flow diagram of rectification column

STREAMS

N - pure nitrogen
S - nitrogen reflux of intermediate grade
R - sump liquid
D - expander stream
B - air

H - oxygen of intermediate grade
E - waste nitrogen of intermediate grade
C - crude argon

A - pure nitrogen
K - industrial oxygen of required sort

FG - argon fraction (vapor)
FL - argon fraction (liquid)

Fig. 2. Dialog windows for input data for calculating the process of rectification.

The described system can be used by specialists in cryogenic engineering for decisions of practical tasks, in particular, for calculations of the technological schemes of air separation plants.

The automated system is designed to run on any personal computer running the Microsoft Windows 95, 98, Me, 2000, or NT operating systems.

3. CONCLUSIONS

The automated system ProCSys can be effectively used for calculations for processes of cryogenic and chemical plants. On the basis of the results of these calculations, the optimization of cycles of mentioned plants can be fulfilled. The system is useful for scientists and engineers working in the field of thermophysics and cryogenics. It can also be used for training students.

REFERENCES

1. V. V. Sychev, A. A. Vasserman, A. D. Kozlov, G. A. Spiridonov, and V. A. Tsymarny, *Thermodynamic Properties of Nitrogen* (Hemisphere, New York, 1987) (originally published by Standards, Moscow, 1977).

2. V. V. Sychev, A. A. Vasserman, A. D. Kozlov, G. A. Spiridonov, and V. A. Tsymarny, *Thermodynamic Properties of Oxygen* (Hemisphere, New York, 1987) (originally published by Standards, Moscow, 1981).
3. V. V. Sychev, A. A. Vasserman, A. D. Kozlov, G. A. Spiridonov, and V. A. Tsymarny, *Thermodynamic Properties of Air* (Hemisphere, New York, 1987) (originally published by Standards, Moscow, 1978).
4. R. Span, E. W. Lemmon, R. T Jacobsen, and W. Wagner, *Int. J. Thermophys.* **19**:1121 (1998).
5. R. B. Stewart, R. T Jacobsen, and W. Wagner, *J. Phys. Chem. Ref. Data* **20**:917 (1991).
6. E. W. Lemmon, R. T Jacobsen, S. G. Penoncello, and D. G. Friend, *J. Phys. Chem. Ref. Data.* **29**:331 (2000).
7. A. A. Vasserman, A. G. Slynko, S. V. Bodyul, Yu. V. Gondarenko, and E. S. Bodyul, *Int. J. Thermophys.* **22**:477 (2001).
8. A. M. Arkharov, ed., *Cryogenic Systems, Vol. 2, Design of Apparatus, Plants, and Systems* (Bauman MSTU Press, Moscow, 2001).