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

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ABSTRACT

An automated system for calculating thermophysical properties of gases and liquids in wide region of parameters is developed. On the basis of values of properties the processes of isothermal compression, adiabatic throttling, polytropic expansion, heat exchange in two- and multi-stream heat exchangers, division of vapor-liquid mixture in the vessel of liquid, rectification in the air separation plant can be calculated. For the certain structure scheme of cryogenic plant the optimization of corresponding thermodynamic cycle can be fulfilled.

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

1. INTRODUCTION

For designing and investigation of cryogenic plants reliable information on thermophysical properties in wide range of density and temperature is necessary. Therefore we created an automated system ProCSys for **c**alculating thermophysical properties of fluids and most important thermal processes of cryogenic plants. By means of this system the process of rectification in the air separation plant can be calculated also.

2. CHARACTERISTIC OF SYSTEM

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

The user has an opportunity to choose 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 processes the names of working substances, the values of flow-rate and a set of other necessary initial data are given. For processes of isothermal compression in compressor or polytropic expansion in expander the values of initial pressure and initial temperature and the efficiency of mentioned machines are introduced. At calculating the adiabatic throttling the values of initial and final pressure and initial temperature (or enthalpy) are given and corresponding regime of calculation is chosen (on the basis of pressure and temperature or pressure and enthalpy).

At calculating processes in two and three-stream heat exchangers the values of pressure and temperature (or enthalpy) in necessary points of input in apparatus and in 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 calculation that corresponds the initial data is chosen. The heat exchanger may be divided by 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 three-stream heat exchanger the amount of heated and cooled streams is indicated.

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

For calculation of processes the data on thermophysical properties of working substances at different independent variables are necessary. By means of developed system the properties of monatomic and diatomic gases, 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 pressures up to 100 MPa at nine combinations of independent variables: *T*,ρ*; T,p; T,s; T,x; p*,ρ*; p,h; p,s; p,x; h,s*. The system allows to calculate temperature, pressure, density, enthalpy, entropy, isochoric and isobaric specific heats, speed of sound, Joule-Thomson coefficient, heat of vaporization, fugacity, viscosity, thermal conductivity, Prandtl number, surface tension and some other properties.

Unified equations of state for gas and liquid are used for calculating thermodynamic properties in wide intervals of density and temperature. The most part of them are accurate reference equations. For increasing the reliability of calculated values of properties 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

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

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

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

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

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

The 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 equation of state. The equations for calculating ideal-gas functions and the saturated vapor pressure and melting pressure are also used for each substance.

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

On the basis of calculated values of properties the parameters of stream in points of input in machines and apparatus and in points of output, and also energy and material balances of processes are determined. On the Figures 1 the state of working window at calculating the processes in multi-stream heat exchanger is shown.

The rectification column is the principal apparatus of the separation assembly of the air separation plants. Working process in this column is based on interaction of descending liquid phase of the separated mixture with vapor phase. Driving force of process is a nonequilibrium difference in concentrations of the components of 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. At calculations the constructive features of column and varying properties of vapor and liquid are taken into account. Generalized flow diagram covers many possible variants of the upper and lower columns. The parameters of all incoming and leaving streams (composition, flow rate, mixture state), heat loads of condensers and evaporators, 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. At calculation of process of rectification air is considered as a mixture nitrogen-oxygen-argon.

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

The calculation of a rectification column can be executed as for nominal regime of operations corresponding to the technical project on designing and for other regimes (in view of temperature conditions of environment, deterioration of the equipment at operation etc.). The calculations for the maximal and minimal flow-rates specified by the user may be fulfilled simultaneously. In such case the system creates on the display the window with three tables for different variants of calculations. On the Figures 2 and 3 correspondingly the state of screen forms for input data and results of calculation the process of rectification are shown.

Complex decision of described tasks for the certain structure scheme of cryogenic plant makes possible to determine parameters and basic characteristics of the thermodynamic cycle.

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

The described systems can be used by the specialists in cryogenic engineering at the decision of practical tasks, in particular, at 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 is effectively used at calculating the 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 be successfully used for training students of universities.

REFERENCES

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Figure Captions

Fig. 1. The working window at calculating the process in multi-stream heat exchanger

Fig. 2. The dialog windows for input data at calculating the process of rectification

Fig. 3. The results of calculating the process of rectification

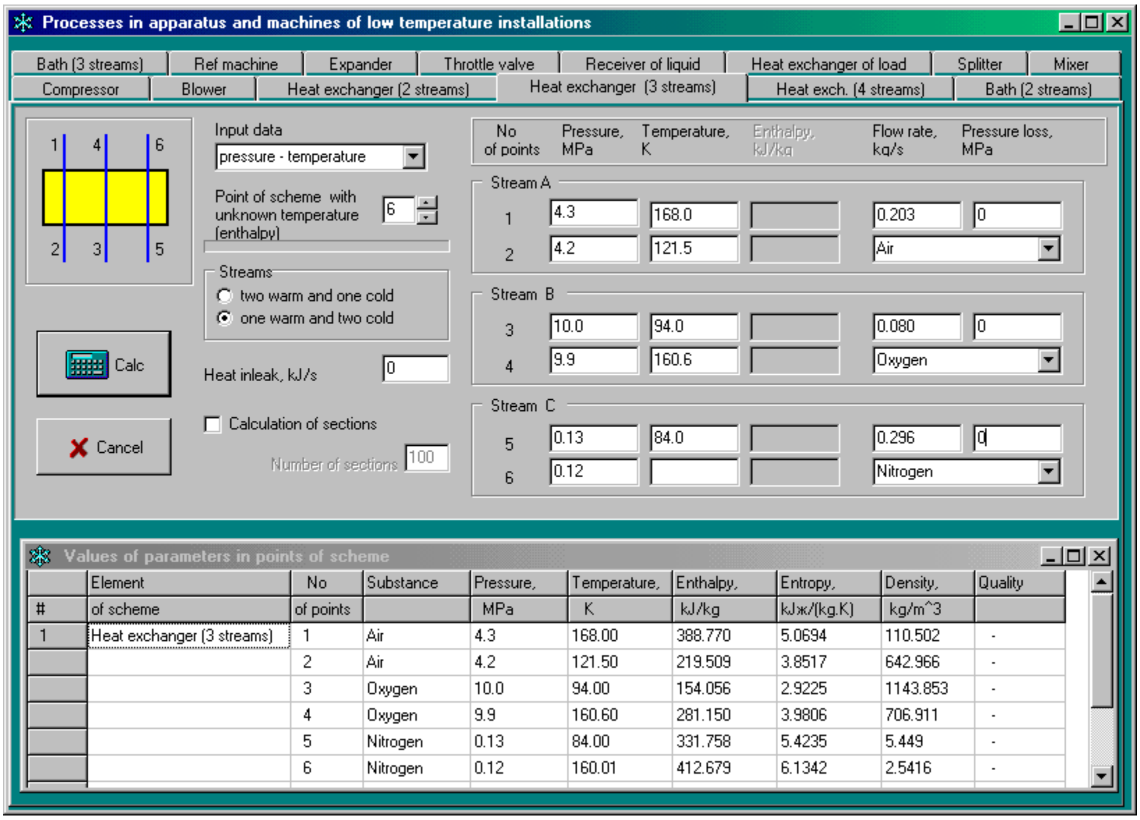
Processes in apparatus and machines of low temperature installations
Bath (3 streams)
Ref machine
Expander
Throttle valve
Receiver of liquid
Heat exchanger of load
Splitter
Mixer
Compressor
Blower
Heat exchanger (2 streams)
Heat exchanger (3 streams)
Heat exch. (4 streams)
Bath (2 streams)
1 4 6
2 3 5
Input data
pressure - temperature
Point of scheme with unknown temperature (enthalpy)
6
Streams
two warm and one cold
one warm and two cold
Calc
Cancel
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
Values of parameters in points of scheme
| 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

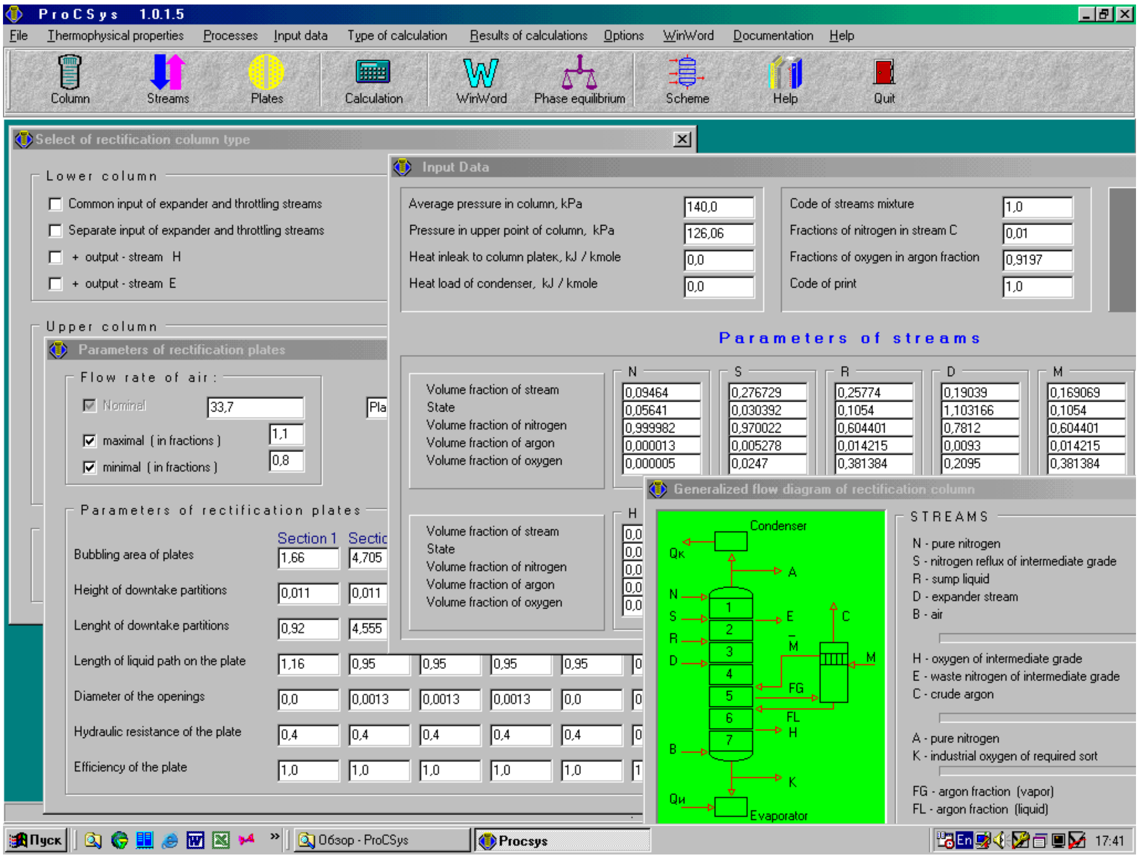
ProCSys 1.0.1.5
File
Thermophysical properties
Processes
Input data
Type of calculation
Results of calculations
Options
WinWord
Documentation
Help
Column
Streams
Plates
Calculation
WinWord
Phase equilibrium
Scheme
Help
Quit
Select of rectification column type
Lower column
Common input of expander and 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
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
Diameter of the openings
0,0
0,0013
0,0013
0,0013
0,0
Hydraulic resistance of the plate
0,4
0,4
0,4
0,4
0,4
Efficiency of the plate
1,0
1,0
1,0
1,0
1,0
Input Data
Average pressure in column, kPa
140,0
Pressure in upper point of column, kPa
126,06
Heat inleak to column platek, 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
Volume fraction of stream
State
Volume fraction of nitrogen
Volume fraction of argon
Volume fraction of oxygen
N
0,09464
0,05641
0,999982
0,000013
0,000005
S
0,276729
0,030392
0,970022
0,005278
0,0247
R
0,25774
0,1054
0,604401
0,014215
0,381384
D
0,19039
1,103166
0,7812
0,0093
0,2095
M
0,169069
0,1054
0,604401
0,014215
0,381384
H
Generalized flow diagram of rectification column
Condenser
Evaporator
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)
Пуск
Обзор - ProCSys
Procsys
17:41

Fig. 2

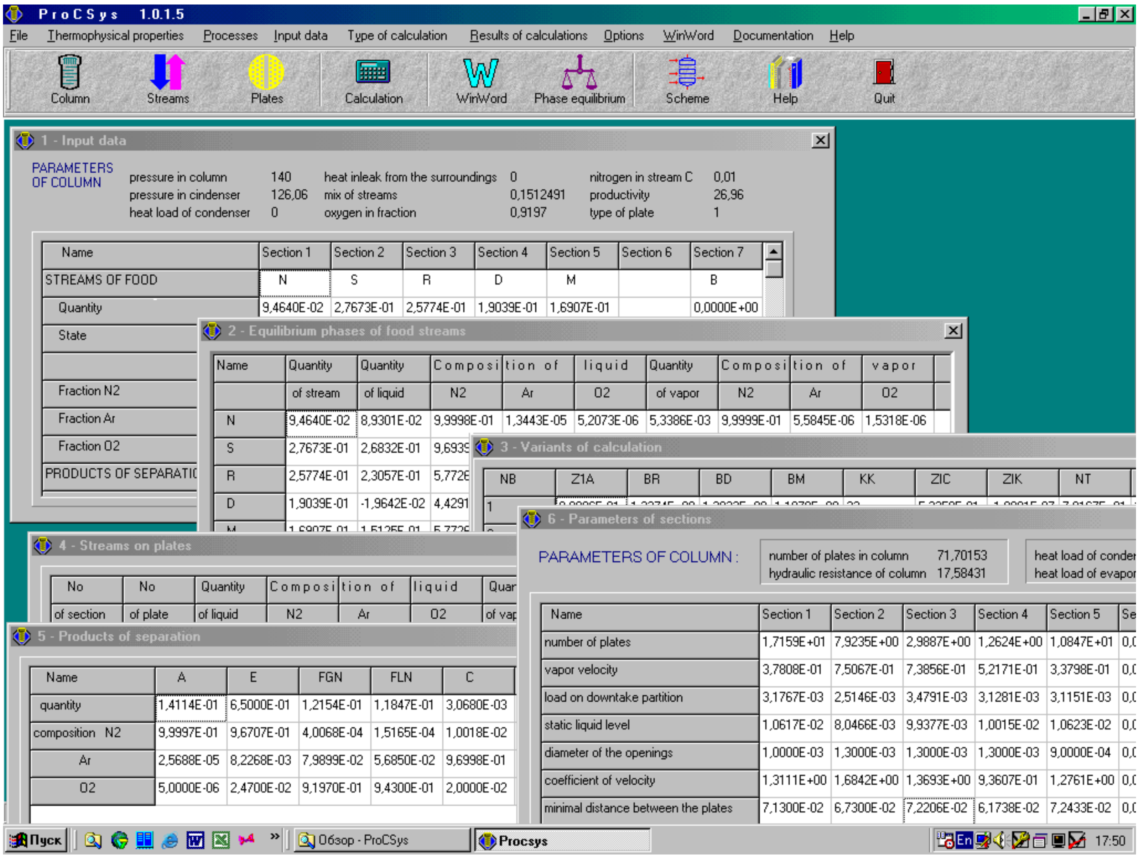
ProCSys 1.0.1.5
File Thermophysical properties Processes Input data Type of calculation Results of calculations Options WinWord Documentation Help
Column Streams Plates Calculation WinWord Phase equilibrium Scheme Help Quit
1 - Input data
PARAMETERS OF COLUMN
pressure in column 140
pressure in cindenser 126,06
heat load of condenser 0
heat inleak from the surroundings 0
mix of streams 0,1512491
oxygen in fraction 0,9197
nitrogen in stream C 0,01
productivity 26,96
type of plate 1
Name Section 1 Section 2 Section 3 Section 4 Section 5 Section 6 Section 7
STREAMS OF FOOD N S R D M B
Quantity 9,4640E-02 2,7673E-01 2,5774E-01 1,9039E-01 1,6907E-01 0,0000E+00
State
Fraction N2
Fraction Ar
Fraction O2
2 - Equilibrium phases of food streams
4 - Streams on plates
5 - Products of separation
Name A E FGN FLN C
quantity 1,4114E-01 6,5000E-01 1,2154E-01 1,1847E-01 3,0680E-03
composition N2 9,9997E-01 9,6707E-01 4,0068E-04 1,5165E-04 1,0018E-02
Ar 2,5688E-05 8,2268E-03 7,9899E-02 5,6850E-02 9,6998E-01
O2 5,0000E-06 2,4700E-02 9,1970E-01 9,4300E-01 2,0000E-02
3 - Variants of calculation
6 - Parameters of sections
PARAMETERS OF COLUMN :
number of plates in column 71,70153
hydraulic resistance of column 17,58431
Name Section 1 Section 2 Section 3 Section 4 Section 5
number of plates 1,7159E+01 7,9235E+00 2,9887E+00 1,2624E+00 1,0847E+01
vapor velocity 3,7808E-01 7,5067E-01 7,3856E-01 5,2171E-01 3,3798E-01
load on downtake partition 3,1767E-03 2,5146E-03 3,4791E-03 3,1281E-03 3,1151E-03
static liquid level 1,0617E-02 8,0466E-03 9,9377E-03 1,0015E-02 1,0623E-02
diameter of the openings 1,0000E-03 1,3000E-03 1,3000E-03 1,3000E-03 9,0000E-04
coefficient of velocity 1,3111E+00 1,6842E+00 1,3693E+00 9,3607E-01 1,2761E+00
minimal distance between the plates 7,1300E-02 6,7300E-02 7,2206E-02 6,1738E-02 7,2433E-02
Пуск Обзор - ProCSys Procsys 17:50

Fig. 3