CRYOFLUIDS – A Software for Physical Property Data of Cryogenic Fluids

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Thermodynamic and transport properties of process fluids are essential for design of cryogenic equipment. There are several authentic sources of data for thermophysical properties of cryogenic fluids; but many of them do not cover the entire useful range of pressure and temperature. To address to these difficulties, we have developed a user-friendly data bank in our laboratory. The data bank takes data from well-known data sources available in open literature and computes the rest by intelligent extrapolation from available data using standard thermodynamic relations. The paper presents the features of the software and the structure of the program. The program is available in the intranet of the Institute and will be shortly available over Internet.

INTRODUCTION

Thermodynamic and transport properties of process fluids are essential for design of cryogenic equipment. A computerized database can be very helpful to the designer, particularly in a computer aided design environment. There are several authentic sources of data for cryogenic fluids, the well known among them being (a)ALLPROPS from the University of Idaho, USA, (b)MIPPROPS and HELIUM from NIST, and (c)GASPAK and HEPAK from Cryodata, USA. The programs often cover different domains of pressure and temperature and different properties. No single program covers the full range or temperature and pressure that a cryogenic engineer is ordinarily interested in. Further, the cost of the programs also becomes a factor for occasional users, students and researchers in developing countries

To address to these difficulties, we have developed a computerized databank named CRYOFLUIDS, which is currently available over our Institute's intranet and will be served to the cryogenic community over the Internet. The program is not based on any new computational approach or empirical correlation; instead, we have computed and stored property data at selected points on the p-T plane in computer memory and calculate the values at desired points by intelligent interpolation or extrapolation. The software contains a user-friendly interface and facility for addition of new fluids and revision of source data.

THE STRUCTURE OF CRYOFLUIDS

CRYOFLUIDS covers seven thermodynamic and two transport properties of fourteen cryogenic fluids. The thermodynamic properties are pressure, temperature, density, enthalpy, entropy, isobaric specific heat C_p and isochoric specific heat C_v. The two transport properties are viscosity and thermal conductivity. The chemical species included in the software are Nitrogen, Oxygen, Argon, Normal Hydrogen, ParaHydrogen, Helium, Methane, Ethane, Propane, Iso-Butane, Normal Butane, Water and Carbon-Dioxide. Water and Carbon-Dioxide are not cryogenic fluids, but are used frequently in many cryogenic processes. Some of the spcial features of CRYOFLUIDS are the following.

(1) It predicts properties in both tabular and graphical forms. The input conditions may be given in one of the four combinations: (1)pressure and temperature (ii)pressure and vapour fraction (iii)pressure and enthalpy or (iv)pressure and entropy.

(2) The user can examine the source data and make changes as he thinks necessary. The program has the provision of updating fluid source data and of adding new fluids if more reliable data are available.

INPUT OF BASIC DATA

Basic thermodynamic and transport property data has been provided to the software at selected points in the p-T plane. The points have been expressed in terms of reduced temperature and reduced pressure. As the non-ideality of gas behaviour is highest near the critical point and close to the phase boundaries, we have provided a larger concentration of points in this region, and a somewhat sparse distribution away from these points. Reduced pressures have been chosen in geometric progression and reduced temperatures in arithmetic progression. Tables 1 and 2 give the distribution of source data points in the reduced p-T plane.

Table1: Number of source data points over the specified range of reduced pressure

Range of Reduced Pressure	Number of Points
0.0001 to 0.8	15
0.8 to 1.2	15
1.2 to 3	10
3 to 25	5

Table 2: Number of source data points over the specified range of reduced temperature

Range of Reduced Temperature	Increment in Reduced Temperature
Melting Point to 0.5	0.025
0.5 to 0.8	0.030
0.8 to 1.3	0.010
1.3 to 2.0	0.014
>2.0	0.240

Thermodynamic Properties

Basic thermodynamic properties have been taken from the software ALLPROPS 4.2 [1] over the range of temperature and pressure covered by the software. Outside the range, we have used empirical relations and standard thermodynamic relations to compute the values and provide to CRYOFLUIDS as basic data. The isobaric specific heat C_p is a fundamental quantity from which other properties such as enthalpy and entropy can be calculated. We have computed C_p at these points by using the empirical relation (Eq. 1) suggested by Scott and Sontagg [4].

$$Cp = 1/M [A + B \theta + C\theta^2 + D \theta^3 + E/ \theta^2] \quad (1)$$

where C_p is given in kJ/ kg K, θ= T/ 100, the temperature T being expressed in Kelvin. M is the molecular weight (kg/kmol) and A, B, C, D, E are constants taken from Reference [4].

Other thermodynamic properties are computed by using equations (2), (3), (4) and (5).

Density:

$$\rho = (\rho^* T^*) / T \quad (2)$$

Enthalpy:

$$h = h^* + \int C_p \, dT \quad (3)$$

Entropy:

$$s = s^* + \int C_p \, dT / T \quad (4)$$

Isochoric Specific Heat:

$$C_v = C_p - R/ M \quad (5)$$

The variables with an asterisk refer to known points, e.g. the nearest data point provided by ALLPROPS 4.2 [1]. In equations (3) and (4) the integration is carried over the limits T* to T.

Transport Property Data Source: -

Transport property data such as viscosity and thermal conductivity are not provided by ALLPROPS. We have taken them from the programs MIPROPS and HELIUM by the NIST [2]. Outside the range of MIPROPS, we have used the following empirical relations from Ref [4] to extend the data.

Gas Viscosity: -

Several methods are available to predict gas phase viscosity, the well known among them being the empirical relations suggested by Lucas [3,5,6], Chung et.al. [3], Reichenbug [3]and Brute and Startling [3]. The Lucas and Chung et al's methods employ the same set of relations for both low and high-pressure gas. Lucas method requires T_c, P_c, M, Z_c and μ as input data. However Chung et al's method requires V_c and the acentric factor in addition to those variables. V_c is not readily available for all the fluids and Reichenbug's method cannot be used for inorganic gases. Therefore, we have adopted the Lucas method to compute gas phase viscosity

Liquid Viscosity: -

To predict liquid phase viscosity, we have adopted the method suggested by Van Velzen etal [3,7] and Yaws et.al. [3,8]. This method predicts the saturated liquid viscosity which is modified to incorporate the effect of pressure by the Lucas method [3,6]. This scheme has been employed for all fluids except helium and hydrogen, for which saturated liquid viscosity was determined using the relation from DIPPR databank [9]. The effect of pressure has not been included becasue the negative value of the Pitzer acentric factor for these fluids resulted in negative values of viscosity at many points.

Gas Thermal Conductivity: -

There are several method are available to predict pure gas thermal conductivity and all of them use a dimensionless factor known as the Eucken Factor defined as:

$$\text{Eucken Factor} = (\lambda M^1)/(\eta Cv)$$

where

λ = Thermal Conductivity (W/mK)

M^1= M/100

M = Molecular weight (kg/ kmol)

η = Viscosity (Pa.s)

Cv = Isochoric specific heat (kJ/ kg K)

We have adopted the method of Ely and Hanley [10, 11] because it was found to predict the correct trend in variation of Eucken factor with temperature.

Liquid Thermal Conductivity: -

We have employed different methods for computing thermal conductivity of different liquids in saturated state at a given temperature. Variation due to pressure is incorporated by the Missenard Method [12]. We have used the method of Miller, McGinely and Yaws [13] for nitrogen, oxygen, argon, water, carbon dioxide, methane, ethane, and propane, Latini's method [14,15,16] for isobutene and normal butane, and the empirical relation from the DIPPR databank [9] for helium and hydrogen.

Rules for interpolation and extrapolation

For computing values of the properties from the stored data, we need to use interpolation and extrapolation routines. Best results are obtained if appropriate physical relationships are employed to linearise the interpolation or extrapolation process. Table 3 gives a summary of those relationships.

Table 3: Interpolation relationships employed to interpolate or extrapolate thermophysical property data

Property	Liquid Phase (temperature)	Gas Phase	
		Temperature	Pressure
Density	$\rho=\alpha+\beta T$	$\rho=\alpha+\beta/T$	$\rho=\rho+\beta P$
Enthalpy	$h=\alpha+\beta T$	$h=\alpha+\beta T$	$h=\alpha+\beta P$
Entropy	$s=\alpha+\beta T$	$s=\alpha+\beta \ln(T)$	$s=\alpha+\beta \ln(P)$
Isochoric Specific Heat	$Cv=\alpha+\beta T$	$Cv=\alpha+\beta T$	$C\ Cv=\alpha+\beta P$
Isobaric Specific Heat	$Cp=\alpha+\beta T$	$Cp=\alpha+\beta T$	$Cp=\alpha+\beta P$
Viscosity	$\eta=\alpha+\beta\sqrt{T}$	$\eta=\alpha+\beta\sqrt{T}$	$\eta=\alpha+\beta\sqrt{P}$
Thermal Conductivity	$\lambda=\alpha+\beta T$	$\lambda=\alpha+B\sqrt{T}$	$\lambda=\alpha+\beta P$

ORGANIZATION OF THE PROGRAM

The software CRYOFLUIDS consists of two important parts: data retrieval and data updating. Seven C++ classes, namely: *DataRetrieval*, *Interpolation, TempSec*, *EnthalpySec*, *EntropySec*, *QualitySec* and *Enter* have been written and linked together to form the data retrieval part. The basic architecture is based on hybrid inheritance. A schematic representation of class hierarchy is shown in Fig 1. *DataRetrieval* is the main base class from which the class *Interpolation* has been derived. Four classes *TempSec, EnthalpySec, EntropySec* and *QualitySec* have been derived from *Interpolation* by declaring the later as a virtual base class. Finally, *Enter* is derived from the last four classes. These classes have been developed by using fairly standard procedures Object Oriented Programming.

Updating of existing fluid data tables and adding new fluids to the data bank is the second most important feature of CRYOFLUIDS. *Intialisation* is the main basic class from which the class store is derived. Five classes: *GasViscosity, GasThend, LiqViscosity, LiqThend* and *PropGen* are derived from this class. Finally, *Mgenet* is derived from the last five classes. A Schematic representation of the class hierarchy is shown in Fig 2.

ERROR IN ESTIMATION OF PROPERTY VAUES

Table 2 shows the error in thermodynamic and transport properties computed by CRYOFLUIDS for Nitrogen at different pressure and temperature combinations. It can be taken as an example of performance of the software. Errors in density, C_p, C_v are calculated on percent basis by using following formula.

$$\% \text{ Error in Property}=(P_{CRYOFLUIDS} - P_{ALLPROPS4.2})*100/\ P_{ALLPROPS4.2}$$

The error in Viscosity and Thermal Conductivity is calculated by using following formula.

$$\% \text{ Error in Property}==(P_{CRYOFLUIDS} - P_{MIPPROPS})*100/\ P_{MIPPROPS}$$

The error in Enthalpy and Entropy is not computed on percent basis but is expressed as a difference in temperature given by two sources for the same value of enthalpy or entropy. It is computed by the relation:

$$\text{Difference in Temperature } \Delta T\ (K)= T_{CRYOFLUIDS} - T_{ALLPROPS4.2}$$

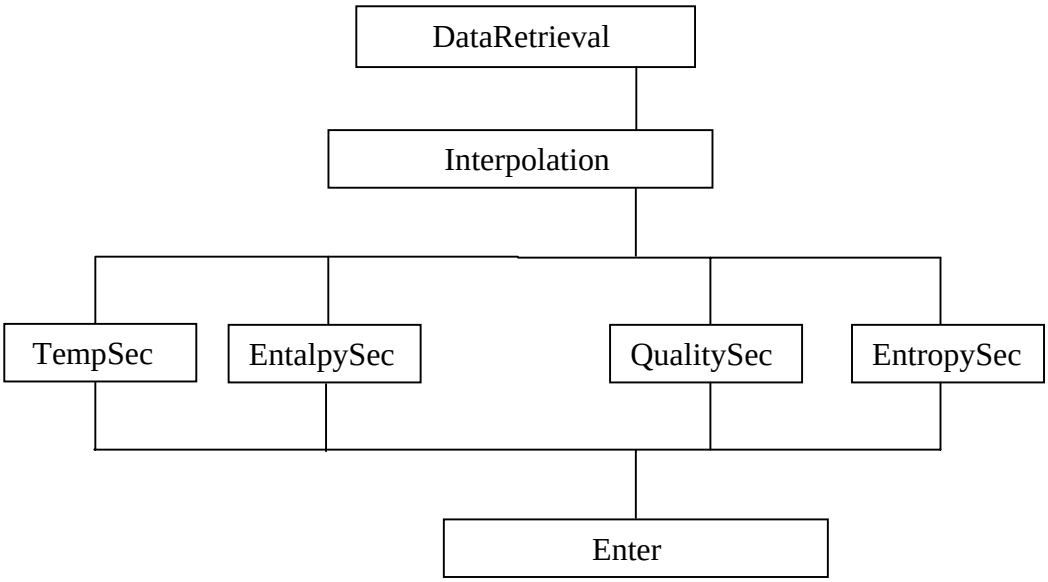

Figure 1: Class Hierarchy for Data Retrieval routines

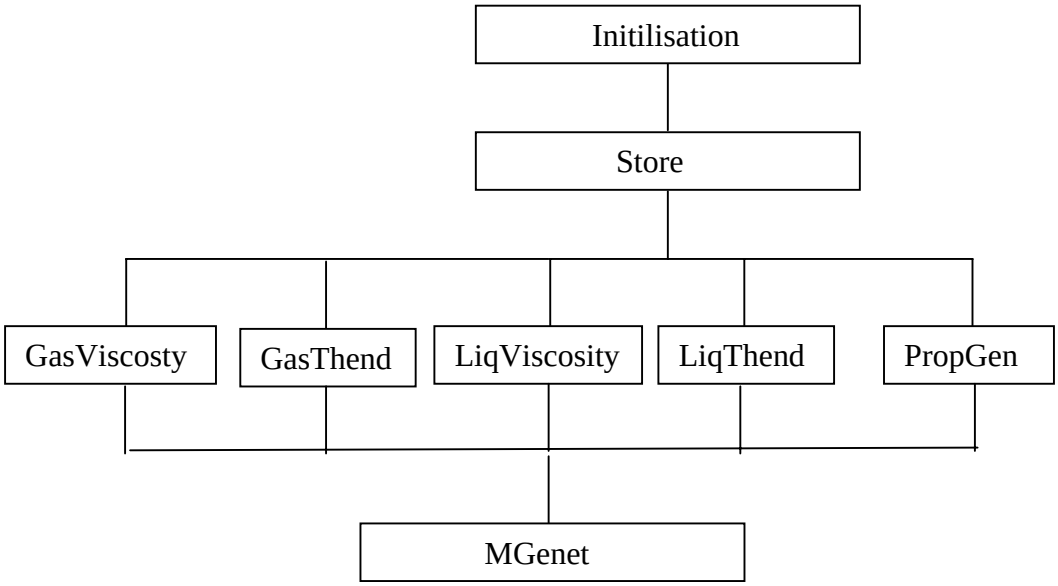

Fig 2: Class Hierarchy of routines for Updating data or Adding New Fluid

CONCLUSION

CRYOFLUIDS is a user-friendly software which can be employed for design and analysis of cryogenic equipment and processes. It should serve as a useful to the cryogenic community, particularly to the students and researchers without access to expensive data banks.

Table 4: Error in prediction of thermophysical data of Nitrogen

P (bar)	T (K)	Density (%)	Enthalpy ΔT (K)	Entropy ΔT (K)	Cp (%)	Cv (%)	Viscosity (%)	Thermal Conductivity (%)
1	70	-0.00345	-0.001	0.016	0.02978	0	0.302109	-0.0181185
1	77.2	-0.0009	-0.003	0.001	0	0	0.030164	0.18596
1	77.4	0.026352	0.008	0.01	0.233662	0.282799	0.377358	-1.21053
1	126.2	0.022252	0	0	0	0.001342	0.011765	0.35
1	300	-0.02671	0	0.02	0.009603	0.00942	-0.5	0.05814
15	100	-0.02799	-0.02	0	0.127004	0.021174	0.175202	-0.08342
15	110.3	-0.00969	0	0	0.07595	0.017286	0.08365	1.03102
15	110.4	0.043637	0.01	0.01	0.213134	0.068688	-0.64706	-1.39189
15	126.2	0.381274	0.03	0.09	0.426591	0.075608	0.391304	0.32
15	300	0.02369	0.02	0.04	0.037594	0.013394	0.076923	0.31203
30	110	-0.00031	0	0	0.023964	0.004133	-0.04895	-0.02817
30	123.5	-0.26083	-0.03	-0.03	4.450659	0.429261	-0.46512	1.75537
30	123.7	0.373689	0.02	0.02	3.84973	0.311833	0.118644	-9.84416
30	126.2	0.247355	0.03	0.03	1.489074	0.146628	-0.07143	0.121457
30	300	0.041409	0.04	0.04	0.06432	0.018663	-0.25946	-0.1449275
34	120	-0.01687	0	0	0.137907	0.015334	-0.05432	-0.027818
34	126.2	0.98518	0	0	14.69403	1.134175	N/P	N/P
34	300	0.04697	0.05	0.05	0.063993	0.014645	0.281081	0.1474820
100	120	-0.0087	-0.01	-0.01	0.040486	0.003189	-0.01066	-0.039953
100	126.2	-0.01545	-0.01	0	0.068599	0.007548	0.593429	0.5019455
100	300	0.111897	0.13	0.15	0.192469	0.041848	-0.06965	0.2163
500	120	-0.03999	-0.02	0.04	0.068142	-0.01974	-0.04794	-0.117331
500	126.2	-0.04591	-0.03	0.02	0.075166	-0.01	-0.06042	0.14091
500	300	-0.23435	0	0.12	0.021882	0.039424	0.255814	0.277487

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