# DEVELOPMENT OF CALCULATION ROUTINES FOR THERMOPHYSICAL GAS PROPERTIES

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**Abstract.** *The Nuclear Energy Division (ENU) of the Institute for Advanced Studies (IEAv) has started a project called TERRA (Technology for Advanced Fast Reactors). This project aims at establishing the key technologies for allowing the development of nuclear microrreactors for space applications, both for power generation and propulsion. As a part of the TERRA project, a computer program for performing thermodynamic static simulation of a Closed Brayton Cycle Loop (CBCL) was developed, adopting Helium gas as the working fluid. The TERRA project also considers other gases and their mixtures to be simulated, namely Argon, Nitrogen, Hydrogen, Neon, Xenon, $CO_2$ and mixtures such as Air and Helium-Xenon. The CBCL simulation with these gases will allow dimensioning the loop to be able to operate with a variety of working fluids. To allow the simulation of these gases, the development of computational routines to calculate physical and thermodynamic properties of the gases and their mixtures was needed, in a way that the resulting routines could be inserted into the CBCL simulation program. This work presents the developing effort to produce these computational routines, as well as the construction of a computer program that aims to provide the user with data on properties such as thermal conductivity, viscosity, specific heat at constant pressure and volume (Cp, Cv), specific heat ratio and enthalpy as functions of temperature for the mentioned gases and their mixtures.*

***Keywords****: nuclear energy, propriedade de gases, ciclo Brayton, space application.*

## 1. INTRODUCTION

The TERRA project – Technology for Advanced Fast Reactors (Guimarães *et al.*, 2007) is being conducted at the Nuclear Energy Division of the Institute for Advanced Studies. This program aims on a long term at acquiring the capacity and developing the technology of building advanced fast reactors to generate heat and electric energy for supplying space vehicles equipment. It is also possible to use such reactors for a propulsive effect. On a medium term the project aims at establishing the concept of a fast microrreactor to generate electricity at isolated areas and inhospitable situations. These medium and long term objectives draw a general view of the TERRA program. Considering the specific or short term objectives (approximately 4 years), it is considered:

1. To develop and build a gas-based Closed Brayton Cycle Loop (CBCL), in order to analyze the thermal cycles technology for generating electric power, supply of heat from the heat source and rejection of heat from the heat sink;
2. Computational analysis to identify the types of nuclear fuels, enrichment and geometrical forms of fast and small nuclear reactor core;
3. To identify the needs of R&D of an electric energy generation system based on a fast microrreactor;
4. To build heat pipe systems in order to analyze its performance with dependence of the used technology and its geometry, as a system of passive heat conduction and rejection; and
5. To couple the Closed Brayton Cycle Loop with a set of heat pipes.

As a part of the thermal cycles study, it was developed a simulation program for a Closed Brayton Cycle Loop operating with Helium as working fluid and using conventional heat source and heat sink (Camillo *et al.*, 2008). Considering the need to simulate the closed cycle loop with other working fluids, namely $CO_2$, Xenon, Neon, Hydrogen, Argon, Nitrogen and Air, it was necessary to develop computational routines that calculate the thermo-physical properties of these gases and their mixtures. These routines would then be inserted into the existing simulation program.

This work presents the working effort of gathering and analyzing the thermo-physical properties of the gases and their mixtures, aiming at the development of computational routines that can enlarge the focus of the simulator program under development. The coupling of these routines with the simulation program will allow for specifying the closed cycle loop to work with several working fluids.

Along with the development of the routines to be coupled with the simulation program, it was developed a computer program called ProTerraCBF, which presents the user thermo-physical properties of the chosen gases. This software calculates properties such as: thermal conductivity, viscosity, specific heat at constant pressure (Cp) and volume (Cv), specific heat ratio, density and enthalpy. The user can choose which gas to work with, and a temperature range.

## 2. THERMO-PHYSICAL PROPERTIES OF THE WORKING FLUIDS

Thermo-physical gases properties data that will be used at the CBCL were researched. The following properties were considered: viscosity, thermal conductivity, specific heat, specific heat ratio, enthalpy and density. It was noticed that for the studied gases these properties present very little dependency on the pressure, considering the pressure range expected for the closed cycle loop (75-300kPa). Figure 1 shows the case of $CO_2$ specific heat, which presented the largest variation of all gases properties with pressure, namely 2.9%, within the pressure range mentioned above. Since the largest variation with respect to pressure is 2.9 %, the pressure dependency of the properties was neglected for all gases.

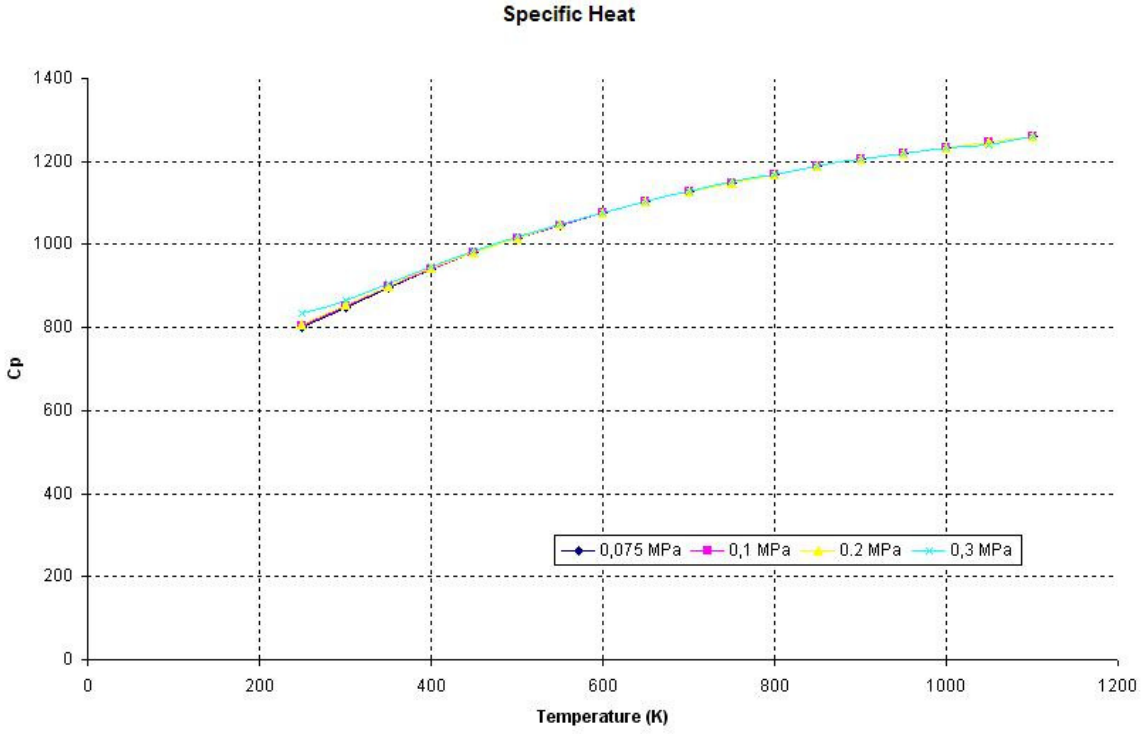


Figure 1. Dependency of specific heat of $CO_2$ with temperature and pressure.

### 2.1. Carbon Dioxide ($CO_2$)

All the following considerations were made for a temperature range from 250 K to 1100 K. The Carbon Dioxide presented a variation between 0.01% and 0.18% in viscosity, between 0.04% and 0.97% in thermal conductivity and between 0.01% and 2.9% in specific heat, considering a pressure range from 75 kPa and 300 kPa (Zucrow and Hoffman, 1976, NIST, 2008). All Carbon Dioxide properties were considered not pressure dependent.

With an isobaric approach, viscosity, thermal conductivity, specific heat, enthalpy and density values were all analyzed with temperature variation and the following equations were obtained through least squared interpolation method.

Thermal conductivity:

$$k = -10^{-9} \times t^2 + 9 \times 10^{-5} \times t - 0.01. \tag{1}$$

Viscosity:

$$\mu = -1 \times 10^{-11} \times t^2 + 6 \times 10^{-8} \times t - 3 \times 10^{-7}. \tag{2}$$

Specific Heat:

$$Cp = 3\times10^{-7}\times t^3 - 0.001\times t^2 + 1.492\times \mathrm{t} + 491.17 . \quad (3)$$

Enthalpy:

$$h = 0.2546\times t^2 + 753.17\times t + 257475 . \quad (4)$$

Density:

$$\rho = 2\times10^{-17}\times \mathrm{t}^6 - 10^{-13}\times \mathrm{t}^5 + 2\times10^{-10}\times t^4 - 2\times10^{-7}\times t^3 + 0.0001\times t^2 - 0.0426\times \mathrm{t} + 7.501 . \quad (5)$$

**2.2. Xenon (Xe)**

All the following considerations were made for a temperature range from 250 K to 750 K. The Xenon presented a variation between 0.1% and 0.5% in viscosity, between 0.2% and 1.8% in thermal conductivity and between 0.2% and 0.4% in specific heat, considering a pressure range of 75 kPa and 300 kPa (Zucrow and Hoffman, 1976, NIST, 2008). All Xenon properties were considered not pressure dependent.

With an isobaric approach, the values of specific heat and specific heat ratio did not present significant variation. Viscosity, thermal conductivity, enthalpy and density values were all analyzed with temperature variation and the following equations were obtained through least squared interpolation method.

Thermal Conductivity:

$$k = -5\times10^{-9}\times t^2 + 2\times10^{-5}\times t + 4\times10^{-5} . \quad (6)$$

Viscosity:

$$\mu = -2\times10^{-11}\times t^2 + 8\times10^{-8}\times t + 2^{-7} . \quad (7)$$

Specific Heat:

$$Cp = 159.1168 \text{ (constant).} \quad (8)$$

Enthalpy:

$$h = -1.8\times10^{-3}\times t^2 + 160.68\times t + 69635 . \quad (9)$$

Density:

$$\rho = -4\times10^{-16}\times t^6 + 10^{-12}\times t^5 - 10^{-9}\times t^4 + 9\times10^{-7}\times t^3 - 0.0003\times t^2 + 0.0368\times t - 0.462 . \quad (10)$$

**2.3. Helium (He)**

All the following considerations were made for a temperature range of 250 K to 1500 K. The Helium presented a variation between 0.001% and 0.04% on its viscosity, between 0.02% and 0.08% on its thermal conductivity and practically no variation on its specific heat, and specific heat ratio considering a pressure range of 75 kPa and 300 kPa (Zucrow and Hoffman, 1976, NIST, 2008). All Helium properties were considered not pressure dependent.

With an isobaric approach, the specific heat presented no significant variation. The viscosity, thermal conductivity, enthalpy and density values were all analyzed with temperature variation and the following equations were obtained through least squared interpolation method.

Thermal Conductivity:

$$k = -5\times10^{-8}\times t^2 + 4\times10^{-3}\times t + 0.0537 . \quad (11)$$

Viscosity:

$$\mu = -6\times10^{-12}\times t^2 + 5\times10^{-8}\times t + 7\times10^{-6}\,. \tag{12}$$

Specific Heat:

$$Cp = 5193 \text{ (constant).} \tag{13}$$

Enthalpy:

$$h = -9.6\times10^{-3}\times t^2 + 5211.2\times t - 220.88\,. \tag{14}$$

Density:

$$\rho = 5\times10^{-19}\times \mathrm{t}^6 - 3\times10^{-15}\times \mathrm{t}^5 + 7\times10^{-12}\times t^4 - 9\times10^{-9}\times t^3 + 7\times10^{-6} t^2 - 0.0027\times \mathrm{t} + 0.5739\,. \tag{15}$$

**2.4. Neon (Ne)**

All the following considerations were made for a temperature range of 250 K to 700 K. The Neon presented a variation between 0.01% and 0.05% on its viscosity, between 0.02% and 0.1% on its thermal conductivity and a maximum of 0.07% on its specific heat, considering a pressure range of 75 kPa and 300 kPa (Zucrow and Hoffman, 1976, NIST, 2008). All Neon properties were considered not pressure dependent.

With an isobaric approach, the specific heat did not show significant variation. The viscosity, thermal conductivity, enthalpy and density values were all analyzed with temperature variation and the following equations were obtained through least squared interpolation method.

Thermal Conductivity:

$$k = -4\times10^{-8}\times t^2 + 10^{-3}\times t + 0.0142\,. \tag{16}$$

Viscosity:

$$\mu = -2\times10^{-11}\times t^2 + 8\times10^{-8}\times t + 9\times10^{-6}\,. \tag{17}$$

Specific Heat:

$$Cp = 1030.2 \text{ (constant).} \tag{18}$$

Enthalpy:

$$h = -2\times10^{-3}\times t^2 + 1030.4\times t + 59578\,. \tag{19}$$

Density:

$$\rho = -4\times10^{-16}\times \mathrm{t}^6 + 10^{-12}\times \mathrm{t}^5 + 10^{-9}\times t^4 + 9\times10^{-7}\times t^3 - 3\times10^{-4} t^2 + 0.0368\times \mathrm{t} - 0.462\,. \tag{20}$$

**2.5. Hydrogen ($H_2$)**

All the following considerations were made for a temperature range of 250 K to 1000 K. The Hydrogen presented a variation between 0.09% and 0.6% on its viscosity, between 0.7% and 1.6% on its thermal conductivity and between 0.5% and 1.4% on its specific heat, considering a pressure range of 75 kPa and 300 kPa (Zucrow and Hoffman, 1976, NIST, 2008). All Hydrogen properties were considered not pressure dependent.

With an isobaric approach, the viscosity, thermal conductivity, specific heat, enthalpy and density values were all analyzed with temperature variation and the following equations were obtained through least squared interpolation method.

Thermal Conductivity:

$$k = 2\times10^{-8}\times t^2 + 5\times10^{-3}\times t + 0.0461. \quad (21)$$

Viscosity:

$$\mu = -5\times10^{-12}\times t^2 + 2\times10^{-8}\times t + 3\times10^{-6}. \quad (22)$$

Specific Heat:

$$Cp = -9\times10^{-14}\times t^6 + 4\times10^{-10}\times t^5 - 6\times10^{-7}\times t^4 + 6\times10^{-4}\times t^3 - 0.2993\times t^2 + 79.557\times t + 5826.8. \quad (23)$$

Enthalpy:

$$h = 0.3823\times t^2 + 14114\times t - 306361. \quad (24)$$

Density:

$$\rho = 2\times10^{-18}\times t^6 - 7\times10^{-15}\times t^5 - 10^{-11}\times t^4 - 10^{-8}\times t^3 + 6\times10^{-6} t^2 - 0.002\times t + 0.3473. \quad (25)$$

**2.6. Argon (Ar)**

All the following considerations were made for a temperature range of 250 K to 700 K. The Argon presented a variation between 0.1% and 0.46% on its viscosity, between 0.5% and 1.3% on its thermal conductivity and between 0.4% and 1.32% on its specific heat, considering a pressure range of 75 kPa and 300 kPa (Zucrow and Hoffman, 1976, NIST, 2008). All Argon properties were considered not pressure dependent.

With an isobaric approach, the viscosity, thermal conductivity, specific heat, enthalpy and density values were all analyzed with temperature variation and the following equations were obtained through least squared interpolation method.

Thermal Conductivity:

$$k = -2\times10^{-8}\times t^2 + 5\times10^{-5}\times t + 0.0015. \quad (26)$$

Viscosity:

$$\mu = -2\times10^{-11}\times t^2 + 8\times10^{-8}\times t + 2\times10^{-6}. \quad (27)$$

Specific Heat:

$$Cp = 9\times10^{-19}\times t^6 - 3\times10^{-15}\times t^5 + 4\times10^{-12}\times t^4 - 3\times10^{-9}\times t^3 + 10^{-6}\times t^2 - 0.0003\times t + 0.5479. \quad (28)$$

Enthalpy:

$$h = -10^{-6}\times t^2 + 0.5222\times t - 0.6309. \quad (29)$$

Density:

$$\rho = 10^{-16}\times t^6 - 5\times10^{-13}\times t^5 + 7\times10^{-10}\times t^4 - 5\times10^{-7}\times t^3 + 0.0002\times t^2 - 0.0581\times t + 801823. \quad (30)$$

### 2.7. Nitrogen ($N_2$)

The Nitrogen properties are calculated according to equations using tabulated constants. According to Zucrow and Hoffman (1977), the values of properties for Nitrogen are calculated by Eq. (31) and Eq (32). The $A_n$ values are listed in Tab. 1 and, the *a*, *b*, *c*, *d* and *e* values are listed in Tab. 2. They have accuracies of within 0.25% for temperatures from 270 to 600 K, within 1% from 610 to 1600 K and within 2% from 1610 to 2200 K.

Zucrow and Hoffman (1977) also state that this model of properties is for pressures at or below atmospheric, but the calculated values are still accurate to within 1% at pressures up to 1.2 MPa at 300 K and 2.2 MPa at 500 K, and further increases in temperature have the effect of reducing the pressure dependence of Nitrogen properties.

To calculate viscosity, the following equation is used:

$$\mu = \frac{\sqrt{t}}{A_0 + \frac{A_1}{t} + \frac{A_2}{t^2} + \frac{A_3}{t^3} + \frac{A_4}{t^4}} \; N \cdot s / m^2 \cdot 10^{-6}. \tag{31}$$

Table 1. Constants for property calculation of gases.

| Gas / 270 to 1000K | $A_0$ | $A_1$ | $A_2$ | $A_3$ | $A_4$ |
|---|---|---|---|---|---|
| Air | 0.552795 | $2.81\times10^{2}$ | $-1.35\times10^{5}$ | $3.94\times10^{7}$ | $-4.14\times10^{9}$ |
| N2 | 0.579561 | $2.85\times10^{2}$ | $-1.32\times10^{5}$ | $3.71\times10^{7}$ | $-3.75\times10^{9}$ |
| $CO_2$ | 0.624736 | $1.40\times10^{2}$ | $5.53\times10^{5}$ | 0 | 0 |
| H2 | 1.074552 | $6.57\times10^{2}$ | $-1.96\times10^{5}$ | $2.29\times10^{7}$ | 0 |

To calculate the specific heat, the following equation is used:

$$\overline{C}_p = \left(a + bt + ct^2 + dt^3 + et^4\right)R \,. \tag{32}$$

Table 2. Constants for calculation of specific heat of Air.

| GAS | a | b | c | d | e |
|---|---|---|---|---|---|
| O2 | 3.6256 | -1.87822 | 7.05545 | -6.76351 | 2.1556 |
| N2 | 3.67483 | -1.20815 | 2.32401 | -0.63218 | -0.225773 |
| Ar | 2.5 | 0 | 0 | 0 | 0 |

To calculate the specific heat at constant volume (*Cv*), the following equation was used, where R is the gas constant:

$$\overline{C}_v = \overline{C}_p - R \,. \tag{33}$$

The thermal conductivity was calculated using the following equation (Granet, 1974):

$$k = \frac{\overline{C}_p \times \mu \times (9\times\gamma - 5)}{4\times\gamma}. \tag{34}$$

Density:

$$\rho = 1\times10^{-11}\times t^4 - 2\times10^{-8}\times t^3 + 2\times10^{-5}\times t^2 - 0.012\times t + 3.324 \,. \tag{35}$$

Enthalpy:

$$h = -2.14\times10^{-8}\times t^2 + 1.52\times10^{-4}\times t^2 + 0.896\times t + 19.71 \,. \tag{36}$$

### 2.8. Air (78.11% $N_2$, 20.96% $O_2$, 0.93 % Ar)

All the following properties were calculated assuming no pressure dependency. Due to the fact that Air is a mixture of gases, to calculate some of its properties one has to take into account the fractions that its composing gases. For the calculation of the Air viscosity, the following equation is used (Zucrow and Hoffman, 1977):

$$\mu = \frac{\sqrt{t}}{A_0 + \frac{A_1}{t} + \frac{A_2}{t^2} + \frac{A_3}{t^3} + \frac{A_4}{t^4}} \quad N \cdot s / m^2 \cdot 10^{-6}. \tag{37}$$

The $A_n$ coefficient values are found in Tab. 1 (Zucrow and Hoffman, 1977). For specific heat calculation:

$$\overline{C}_p = \left(a + bt + ct^2 + dt^3 + et^4\right)R. \tag{38}$$

The *a*, *b*, *c*, *d* and *e* values are found in Tab. 2 (Zucrow and Hoffman, 1977). Considering that Air is a mixture, its specific heat will be the sum of each specific heat gas component, considering their respective volumetric concentration.

$$\overline{C}_p = \sum_{i=1}^{3} X_i \overline{C}_{pi} = X_{N_2} \overline{C}_{p,N_2} + X_{O_2} \overline{C}_{p,O_2} + X_{Ar} \overline{C}_{p,Ar}. \tag{39}$$

To calculate the specific heat at constant volume (*Cv*), the following equation is used:

$$\overline{C}_v = \overline{C}_p - R. \tag{40}$$

To calculate the thermal conductivity, the following equation is used (Granet, 1974):

$$k = \frac{\overline{C}_p \times \mu \times (9 \times \gamma - 5)}{4 \times \gamma}. \tag{41}$$

Density:

$$\rho = 1.17 \times 10^{-11} \times t^4 - 2.08 \times 10^{-8} \times t^3 + 2.07 \times 10^{-5} \times t^2 - 1.14 \times 10^{-2} \times t + 3.14. \tag{42}$$

Enthalpy:

$$h = -7.31 \times 10^{-5} \times t^3 + 0,347 \times t^2 + 872 \times t + 17211. \tag{43}$$

## 3. ProTerraCBF

The ProTerraCBF program, on its independent operation, can give the user a library of information on thermo-physical properties of the following gases: Air, Argon, Carbon Dioxide, Helium, Hydrogen, Nitrogen, Neon and Xenon. The user can choose to visualize single gas properties or any mixture of noble gases. For the latter case, the user must inform the volumetric fraction each gas will occupy at the final mixture. The user may also choose to specify a temperature to produce the specific property values. Figure 2 shows the ProTerraCBF graphical interface.

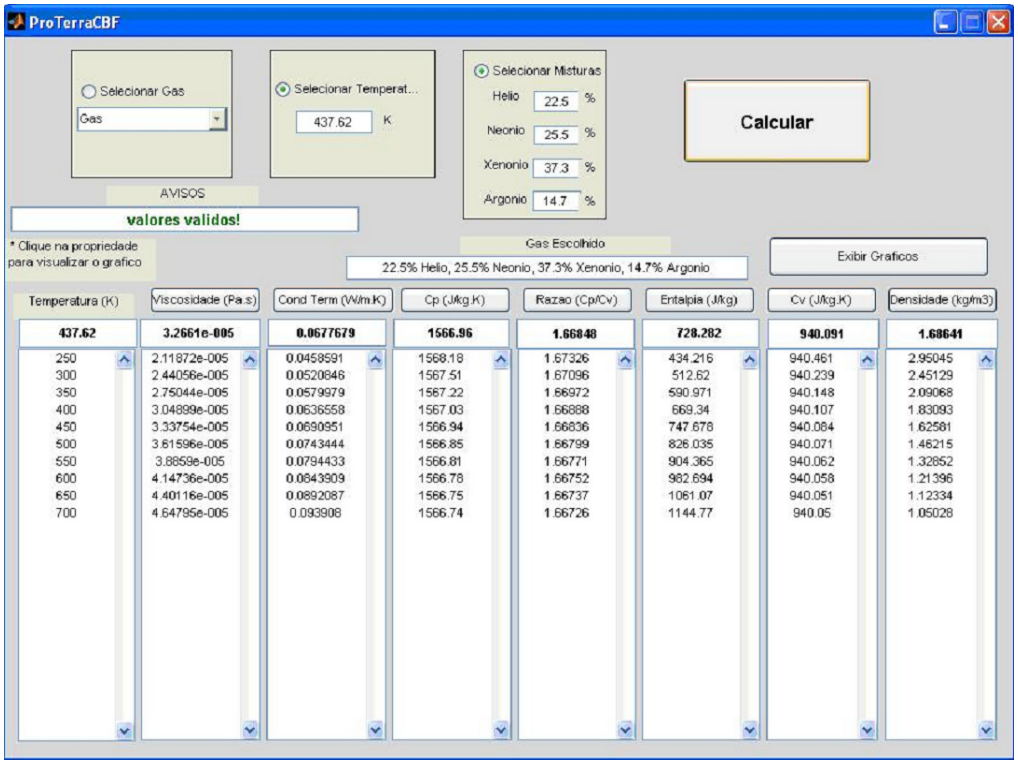


Figure 2. ProTerraCBF

When clicking on the button “Calcular”, the user can visualize a table of properties on screen. The ProTerraCBF can also show isolated or grouped graphics containing the temperature dependency of the properties, as it can be seen in Figure 3 and 4.

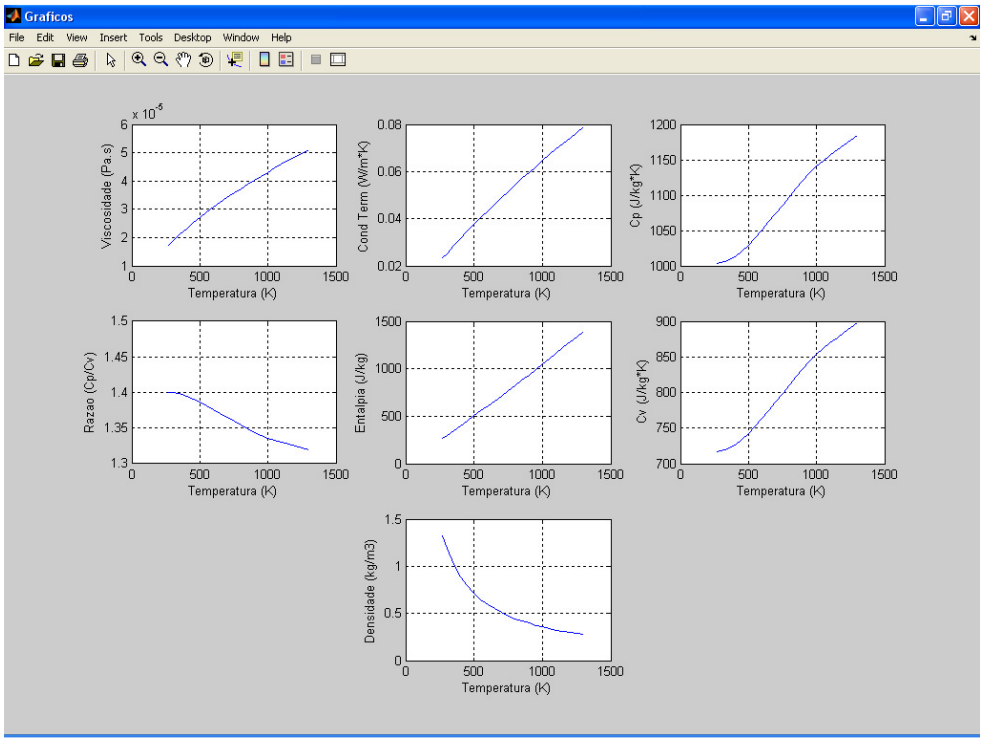


Figure 3. Grouped graphics supplied by the ProTerraCBF.

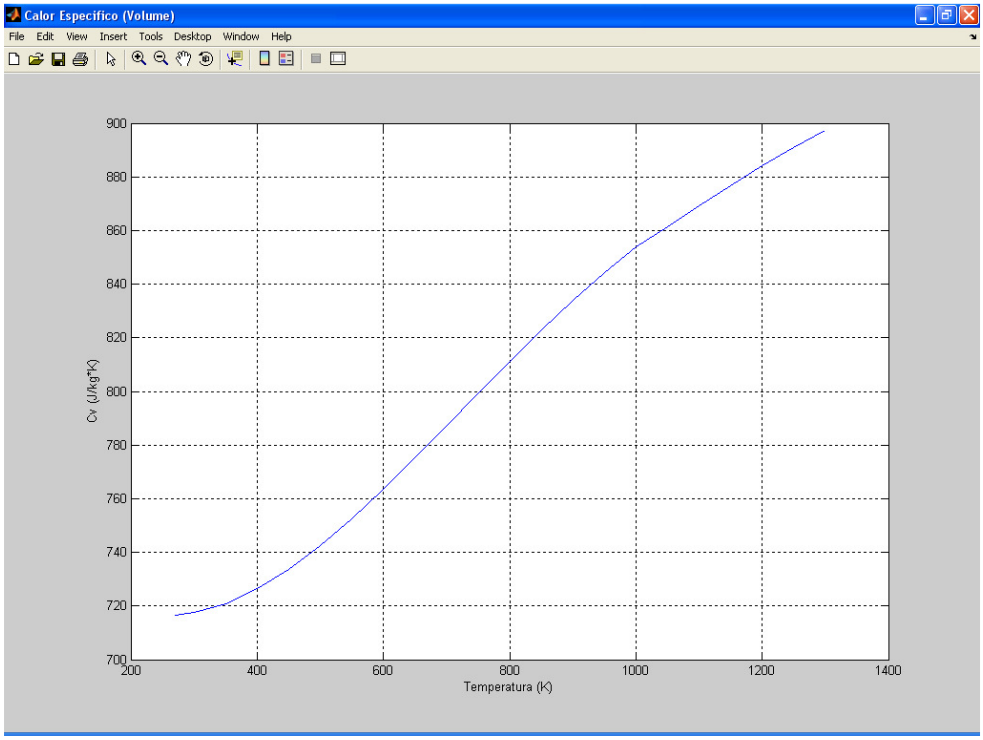


Figure 4. Isolated Graphic supplied by the ProTerraCBF.

## 4. CONCLUSIONS AND OBSERVATIONS

There is a negligible error for the results obtained by the TerraProCBF. This error is due to the operation of the interpolation method adopted. This kind of error can be noticed by the user when selecting a temperature value displayed on the proper table. For instance, when selecting Helium and 250 K, the density shown at the temperature specification box presents a deviation of 1.32% when compared to the one provided by the table below. This occurs because the value of the temperature specification boxes is calculated by an equation obtained by interpolation of the values displayed at the table.

It is expected that the data and interpolation uncertainties will propagate onto the CBCL design. At this moment there is no way to specify consistently the size of the final error. These estimates will be measured with the construction of the device. Obviously, corrections will be feedback at that time.

## 5. REFERENCES

Camillo, G.P., Guimarães, L.N.F., Placco, G.M. and Borges, E.M., 2008, "A Preliminary Design For a Simplified Closed Brayton Cycle Modeling For a Space Reactor Application", Proceedings of ENCIT 2008, Belo Horizonte, MG, Brasil, 8 p.

Granet, I., 1974, "Thermodynamics and Heat Power", Reston Publishing Company, INC., New York, USA, pp. 367 – 376.

Guimarães, L.N.F., Nascimento, J.A., Borges, E.M., Caldeira, A.D. and Dias, A.F., 2007, "Atividades da ENU na área de tecnologia nuclear avançada: previsão de recursos necessários para a primeira fase do programa TERRA", Institutional Report, IEAv-ENU/012/2007, São José dos Campos, SP, Brazil.

NIST, National Institute of Standards and Technology. 1 Dec. 2008, < http://webbook.nist.gov/chemistry/>.

Zucrow, M.J., Hoffman, J.D., 1976, "Gas Dynamics", John Wiley & Sons, Vol.I, West Lafayette, Indiana, pp. 20-57.

Zucrow, M.J., Hoffman, J.D., 1977, "Gas Dynamics - Multidimensional flow", John Wiley & Sons, Vol.II, West Lafayette, Indiana, pp. 459-471.

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