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Influence of Metallic Copper Vapors on the Chemical Composition of a Mixture of Air and Water Vapor Thermal Plasmas in the Temperature Range 1000 K to 20000K

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Abstract: This paper concern the calculation of equilibrium composition of plasma mixture Air-Water vapor and copper vapor in temperatures range 1000K to 20000 K. The plasma is suposed to be in local thermodynamic equilibrium. We used Gibbs free energy minimization method to access the different numerical densities of chemical species as a function of temperature. This data are very important to calculate thermodynamic properties, transport coefficients and modeling electrical arc in circuit breakers. The result shows that the influence of metallic copper vapor is important on equilibrium composition of plasma. In particular the densities of electron in the plasma increase with the percentage of copper vapor for the temperature inferior to 17000K. The increasing of electron densities increase electrical conductivity of plasma and limit the performance of circuit breakers. Also the electrical neutrality is made mainly between electron (e^-) and Cu^+ in low temperature (T < 12000K). We are studying in particular the evolution of the densities of the main chemical species created in this plasma as a function of pressure. We choose four values of pressure (1 atm, 5 atm, 10 atm and 15 atm). The results obtained shows an increasing of chemical densities with the pressure in the mixture in conformity at Dalton's Law. the increasing of the pressure in the plasma retard chemical reactions because it disadvantages the dislocations that constitute dissociation and ionization reactions in the plasma.

Keywords: Plasma, Equilibrium Composition, Gibbs Free Energy, Copper, Electrical Neutrality

1. Introduction

Air and compressed air are used in low and medium voltage circuit breakers for breaking the electrical current through the electric arc. In some regions of high humidity the air contains a certain proportion of water vapor depending on climatic conditions [1, 2]. This water vapor can modify the properties of the plasma created during the interruption of the electric current. In addition, the evaporation of copper contacts in the circuit breaker can also have a significant influence on the chemical composition and the properties of the plasma created in this circuit breaker [3, 4]. Our previous studies have shown the role played by water vapor on the equilibrium composition of an air plasma [2, 5, 6]. The objective of this present study is to show the influence of the metallic copper vapor resulting from the evaporation of the contacts of the copper in circuit breaker on the equilibrium composition of a plasma formed by air and water vapor mixture. In our study, the air is constituted of 80% nitrogen (N_2) and 20% dioxygen (O_2); the other components of the air are neglected. Plasma is a mixture of air, water vapor and copper vapor; so we have plasmas of type $NxOyHzCu_t$; with x, y, z and t are fractional or integer values depending on the initial proportions of the mixture. We used Gibbs free energy minimization method to access the different numerical densities of chemical species in function of temperature [7-13]. These data are important for accessing the transport coefficients and the thermodynamic properties of these types of plasmas. These data are also important for modeling electric arcs and hydrodynamic studies using these same types of plasmas. The study is done in the temperature range from 1000 K to 20000 K and for pressures P = 1 atm, P =5 atm, P = 10 atm and P = 15 atm.

2. Calculation of Equilibrium Composition

The calculation of the equilibrium composition concerns plasma formed of vapor of copper, water vapor and air. The air is constituted of the oxygen atom (O) and nitrogen (N). The water vapor is constituted of the oxygen atom (O) and the hydrogen atom (H) and we are the copper (Cu). This kind of plasmas may be represented by the formula $N_xO_yH_zCu_t$, where x, y, z and t are integer or fractional variables which indicate respectively the number of initial atoms of H, O, N and Cu. These variables are functions of the initial proportions of copper, water vapor and air in the plasma. We tank into account in our calculation fifty five (55) following chemical species:

1. the electrons: e^-;
2. the monatomic species (18): H, H^-, H^+, N, N^-, N^+, N^{++}, N+++, O, O^-, O^+, O^{++}, O+++, Cu, Cu^-, Cu+, Cu++, Cu+++;
3. the diatomic species (20): H_2, H_2^-, $H_2{}^+$, N_2, N_2^-, $N_2{}^+$, NH, NH^-, NH^+, NO, NO^-, NO^+, O_2, O_2^-, $O_2{}^+$, OH, OH^-, OH^+, CuO, Cu_2;
4. the polyatomic species (16): H_2O^+, N_3, O_3, CuO, H_2O, N_2O, NO_2, NH_2, NH_3, N_2O_3, HNO_2, HO_2, N_2O_4, H_2N_2, N_2O_5, HNO_3.

2.1. Determination of Chemical Composition

We use the minimization of Gibbs free energy to determine the composition versus the temperature at atmospheric pressure of the considered plasmas [8-20].

At temperature T and pressure P the Gibbs free energy is written as [8]:

$$G = \sum_{i=1}^{N} n_i \left(\mu_i^0 + RT_i \ln \left(\frac{n_i}{\sum_{j=1}^{N} n_i} \right) + RT_i \ln \left(\frac{P}{P^0} \right) \right) \quad (1)$$

where n_i is the mole number of chemical species, N is the number of different chemical species presented in the plasma and gas, μ_i^0 is the chemical potential of i species at standard pressure P^0 (10^5 P_a), R is the molar gas constant. T_i is the temperature of each chemical species i and is equal to the Temperature T in the considered case since we assume thermal equilibrium.

2.2. Numerical Method

The mole number must be non-negative and satisfy the conservation of nuclei and electrical neutrality, so the different values must satisfy both conditions [8]:

$$\begin{cases} n_i \geq 0 & \forall i \\ \sum_{i=1}^{N} a_{ij} n_i = b_j & j = 0, \cdots, m \end{cases} \quad (2)$$

By introducing the Lagrange multipliers π_k and using a Newton-Raphson numerical method, the following system can be obtained [8-19]:

$$\begin{pmatrix} \frac{RT}{n_1} & \cdots & 0 & a_{1,0} & \cdots & a_{1,4} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \frac{RT}{n_M} & a_{M,0} & \cdots & a_{M,4} \\ a_{1,0} & \cdots & a_{M,0} & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{1,4} & \cdots & a_{M,4} & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} \Delta n_1 \\ \cdot\cdot \\ \Delta n_M \\ \Delta \pi_0 \\ \cdots \\ \Delta \pi_4 \end{pmatrix} = \begin{pmatrix} -\mu_1^0 - RT\ln\frac{n_1}{\sum^M n_i} - RT\ln\frac{P}{P^0} - \sum_{j=0}^{4}\pi_j a_{i,j} \\ \cdots \\ -\mu_M^0 - RT\ln\frac{n_M}{\sum^M n_i} - RT\ln\frac{P}{P^0} - \sum_{j=0}^{4}\pi_j a_{i,j} \\ -\sum_{i=1}^{M}\pi_j a_{i,1} + b_1 \\ \cdots \\ -\sum_{i=1}^{M}\pi_j a_{i,4} + b_4 \end{pmatrix} \quad (3)$$

The dimension of this linear system is N+5. The coefficients b_j depend on the initial volume percentages in the mixture. We calculate the chemical potential of each particle by the data obtained in the works of F. Bendjebbar and al. and using the formula [17]:

$$\mu_i = h_i - T s_i + E_i \quad (4)$$

Where h_i is the specific enthalpy, S_i is the specific entropy and E_i is the formation enthalpy of the chemical species.

For the polyatomic molecules their data are obtained in the JANAF tables [21]. The chemical potential of each particle can be determined by the partition function [22].

Then the values of new molar number and the Lagrangian multipliers are calculated with:

$$\begin{cases} n_i = n_i + \lambda \Delta n_i & \forall i \in [1, N] \\ \pi_j = \pi_j + \lambda \Delta \pi_j & \forall j \in [0, 3] \end{cases} \quad (5)$$

The parameter λ is the highest value included between zero and one that satisfies the following conditions:

$$n_i = n_i + \lambda \Delta n_i \succ 0 \quad \forall i \in [1, N] \quad (6)$$

This step avoids obtaining of negative new mole number that appears when they are far from the solution.

The new values of the molar number and Lagrangian multipliers are used for a new calculation cycle. The convergence is considered to be reached when the values Δn_i satisfy the following relation:

$$\frac{\Delta n_i}{n_i} \prec 10^{-15} \quad \forall i \in [1, N] \quad (7)$$

In the case of our study we take into account 55 chemical species, so N=55.

3. Results and Analyses

We present in this section the results of calculations of equilibrium composition at atmospheric pressure of plasmas formed: 90% air-5% water vapor-5% Cu and 80% air-5% water vapor-10 % Cu, also we show the influence of the percentage of copper on some major chemical species: e^-, H, H^+, N, N^+, O, O^+, NO, NO^+, Cu_2, Cu, Cu^+, H_2O, CuO, CuOH, OH and OH^+.

3.1. Composition of Mixtures Plasmas of Air, Water Vapor and Cooper

In the figures 1 and 2, we represent respectively the concentration of chemical species versus temperature at atmospheric pressure and local thermodynamic equilibrium (LTE) of the plasmas formed of 90% air-5% water vapor -5% copper and of 80% air-5% water vapor -10% Copper. On these figures, we can see three (3) phases. The first phase concerns temperature less than 2000 K (T < 2000 K). In this domain, the main chemical species are molecules: N_2, O_2, H_2O, Cu_2 and CuOH. The second phase concerns the temperature range of 2000 K to 10000 K (2000 K < T < 10000 K). In this interval, the main chemical species are: N_2, O_2, Cu, NO, OH, H_2, N, O, H Cu^+ and e^-. The third phase concerns temperature above 10000 K (T > 10000 K). In this range, the main chemical species are: N, O, H, H^+, O^+, N^+ and e^-. The analyses of the curves show that the numerical density of the neutral particles H, O, N and Cu depend of the percentage of the initial mixture. The electrical conductivity is directly linked to the electronic density of the medium. In low temperatures (T < 12000 K) the electrical neutrality is made mainly between e^- and Cu^+ because the ionization energy of the particle Cu is low than those of N, H and O. We can therefore note that the numerical densities of the copper atoms will have a considerable influence on the properties of the plasma formed for temperatures below 10000K.

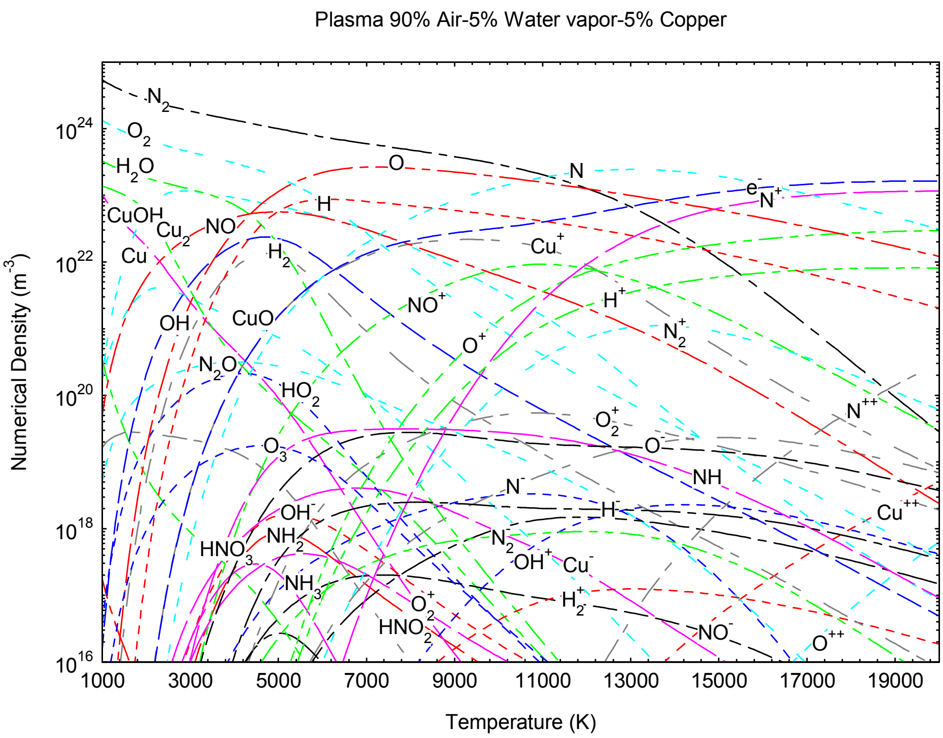

Figure 1. *Evolution of numerical densities versus temperature of plasma formed of mixture 90%Air-5%Water vapor-5%Copper.*

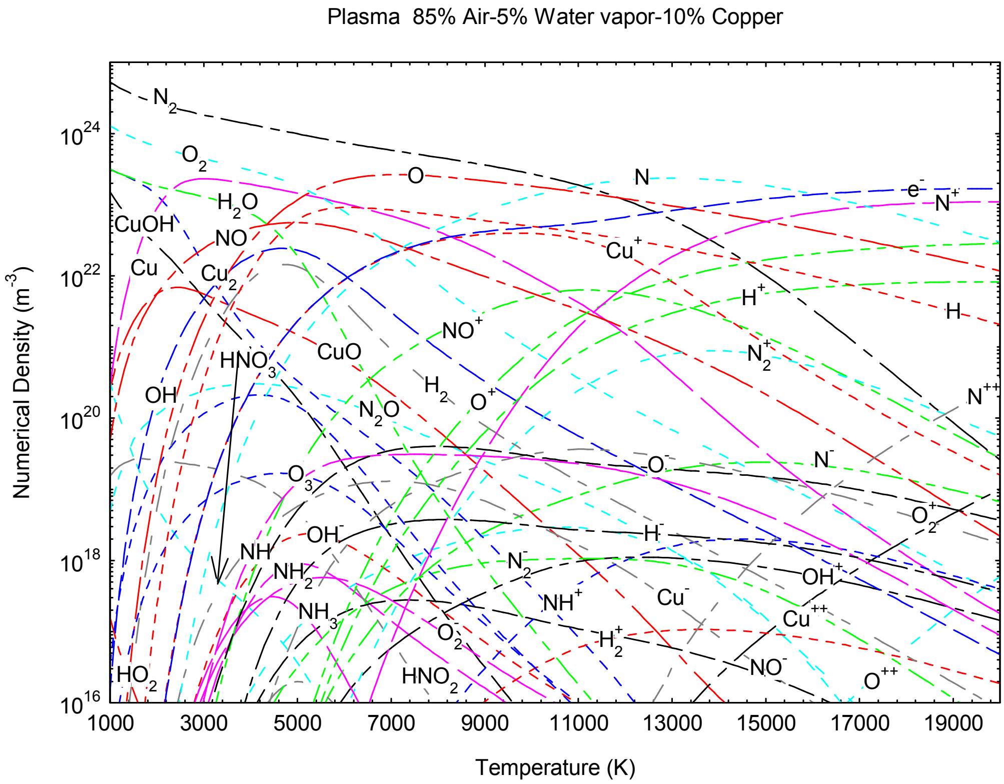

Figure 2. *Evolution of numerical densities versus temperature of plasma formed of mixture 85%Air-5%Water vapor-10%Copper.*

For high temperature (T > 12000 K), the ionization of the atoms H, O and N take place to the production of electrons and the electrical neutrality is made mainly between e^-, N^+, O^+ and H^+. We remark that in this range of temperature ionization of N to N^+ contributes most to electrons production. The copper molecule Cu_2 dissociates around 1500 K. The water molecule H_2O dissociates around 3800 K, O_2, H_2, NO and OH molecules dissociate around 5000 K. The diazote molecule N_2 dissociate around 9000 K. On these figures, we note that the polyatomic species: O_3, H_2O, CuO, N_2O, NH_3, N_2O_3, HNO_2, HO_2, N_2O_4, H_2N_2, N_2O_5 and HNO_3 appear only in very low temperature and their concentrations are often very low These particles are low energies of dissociation. These particles disappear rapidly with temperature because their dissociation energies are low. The electronegative chemical species namely: H^-, Cu^-, O^-, OH^-, NO^-, O_2^-, N_2^- and H_2^- species appear with low concentration. However, these particles could have a significant influence on the electrical conductivity of the plasma, because they capture electrons and decrease their mobility in the plasma.

3.2. Influence of the Percentage of Copper on the Equilibrium Composition

To estimate the effect of the percentage of metallic vapor of copper on the equilibrium composition, we have shown in Figures 3 and 4 the numerical densities of the majority chemical species. We have varied the percentage of metallic copper vapor as 1%, 2%, 3%, 4%, 5% and 10% in the mixture. The direction of the arrows indicates the increasing direction of the percentages of copper. The evolution of the curves shows that the numerical density of the chemical species N_2, O_2, H_2O, NO, H_2, O, N and H vary very little when the percentage of copper increases in the mixture. We note that on the others hand the numerical densities of the chemical species NO^+, CuO, Cu_2, OH^+, CuOH, Cu, e- and Cu^+ increase when the percentage of copper increases in the medium. The chemical species containing the copper atom increase more with the percentage of metallic copper vapor. We also note that the numerical densities of the N^+, O^+ and H^+ particles decrease when the percentage of copper increases in the plasma. In particular, the electron density increases with the percentage of copper. This is due to the fact that electroneutrality is mainly made between the electrons and the Cu^+ ion for temperatures below 12,000K. At high temperatures (T> 17,000K) the electron density is independent of the copper vapor rate. This is explained by the fact that the plasma tends to be fully ionized, so it does not depend on the type of plasma. The electrical conductivity is directly linked to the electronic density, the shape of the electronic density shows that the electrical conductivity will increase with the copper content, especially for temperatures below 12000K. As the minimization of the electrical conductivity is desired in the circuit breakers for breaking the electric arc, significant evaporation of the copper contacts will reduce the performance of the circuit breaker for breaking the electric arc.

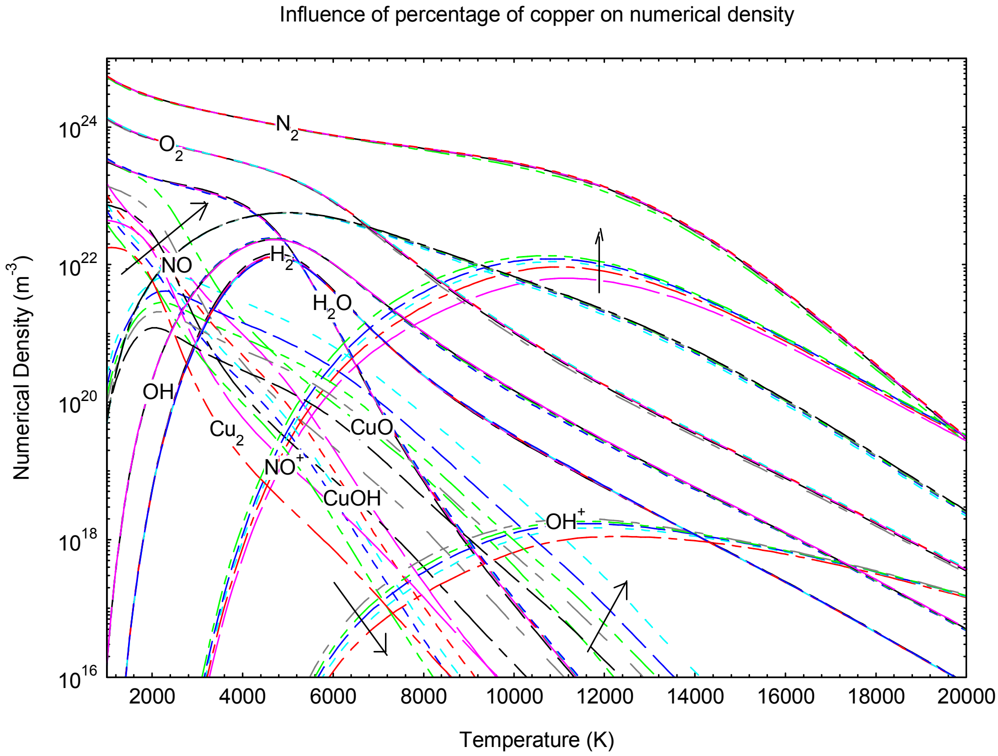

Figure 3. *Influence of the percentage of metallic copper vapor on numerical densities versus temperature of majority chemical species in the plasma.*

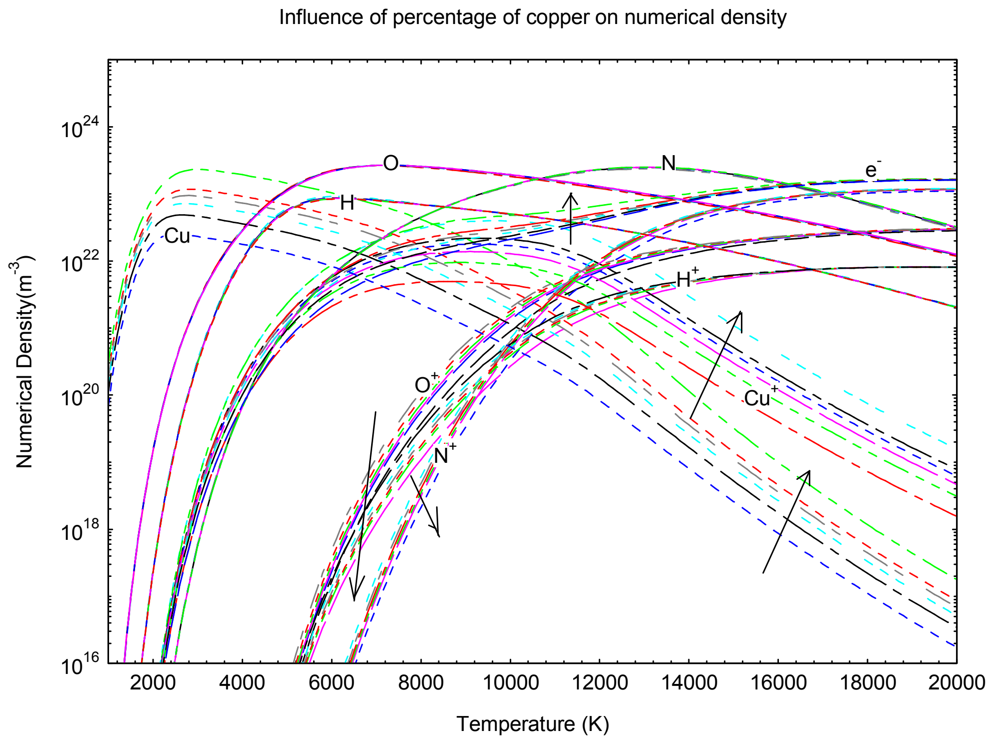

Figure 4. *Influence of the percentage of metallic copper vapor on numerical densities versus temperature of majority chemical species in the plasma.*

3.3. Influence of the Pressure on the Equilibrium Composition

To appreciate the influence of pressure on the plasma equilibrium composition of the mixture, we have presented in figures 6 and 7, the evolution in function of temperature the numerical densities of the main chemical species in the plasma formed by 90% Air-5% Water vapor and 5% copper vapor. We have retained four (4) values of pressure: P = 1 atm, P = 5 atm, P = 10 atm and P = 15 atm. In each figure, the arrows indicate the increasing direction of the pressure.

The numerical densities of all chemical species increases if the pressure increases in the plasma. This is explained by Dalton's Law or the Law of perfect gases (P = nkT). The average energy per particle will therefore decreases. As the dissociation and ionization reactions are endothermic, chemical reactions occur hardly in the plasma. Indeed, at a fixed temperature, when the pressure increases, chemical density must be increases to verify the law of Dalton.

Generally, the increasing of the pressure retard chemical reactions because it disadvantages the dislocations that constitute dissociation and ionization reactions in the plasma. It can therefore be said that dissociation and ionization reactions occur at high temperature if the pressure increases in the plasma.

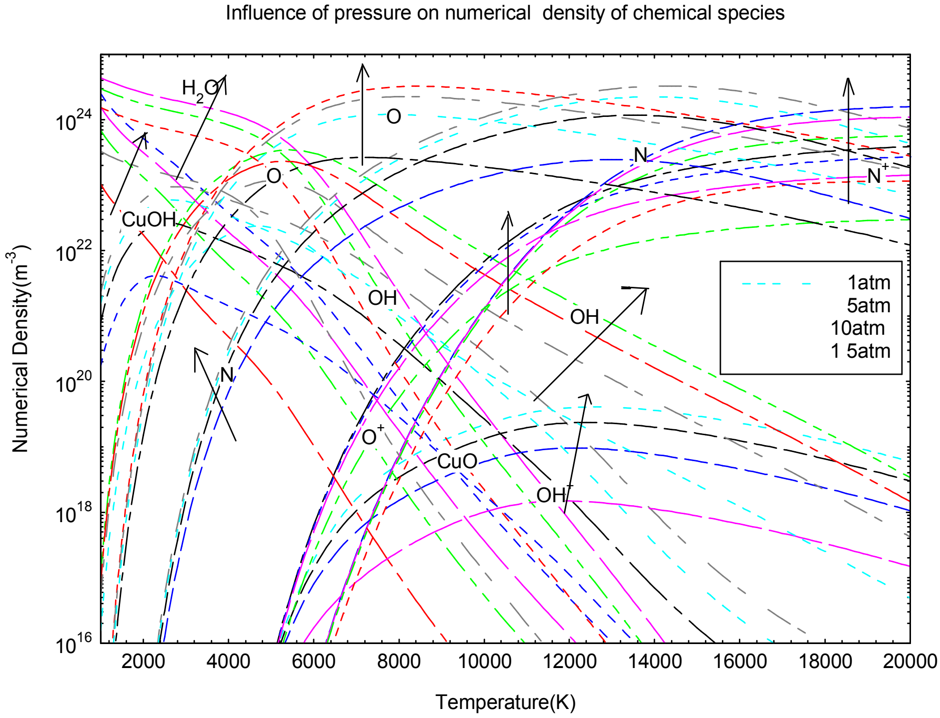

Figure 5. *Influence of the pressure on numerical densities versus temperature of majority chemical species in the plasma (H_2O; CuOH; O; CuO; OH; O^+; N^+; N).*

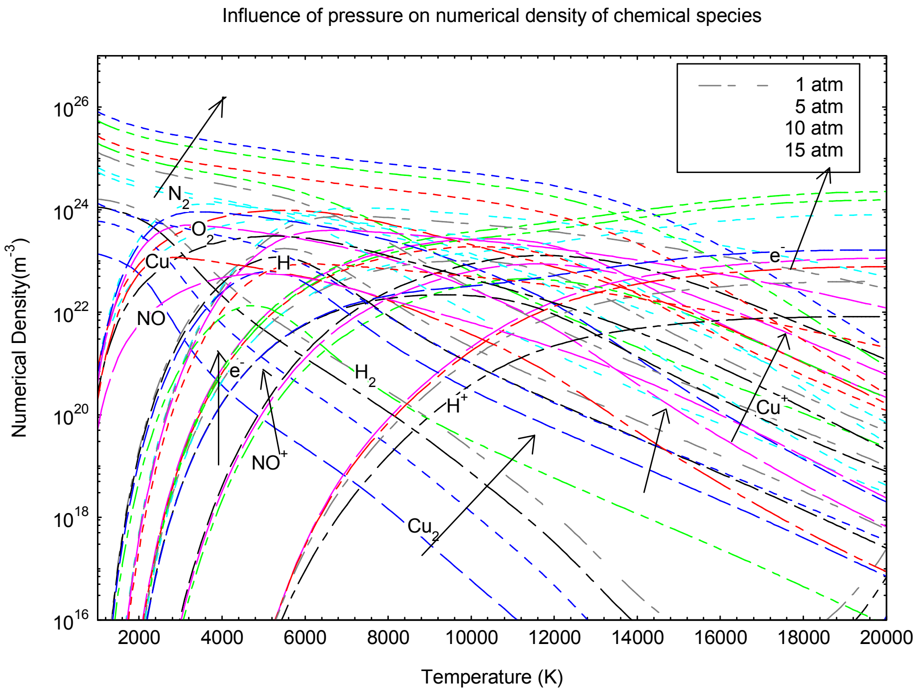

Figure 6. *Influence of the pressure on numerical densities versus temperature of majority chemical species in the plasma (e^-; O_2; Cu; H^+; Cu^+; H_2; Cu_2; NO; N_2; H; NO^+).*

4. Conclusion

The calculation of the numerical densities versus temperature have shown the influence of the copper vapors coming from the contacts of the circuit breakers on the chemical composition of the plasma of mixture of air and water vapor. The study showed that in general the numerical densities of chemical species containing the copper atom increase with the addition of copper to the medium. Electroneutrality is mainly made between the electrons and the Cu^+ copper ion for temperatures below 12000K. The electron density increases with the percentage of copper for temperatures below 17000K. The result are also shown that the increasing of pressure on the plasma induce the increasing of the chimical density and retard the chemical reactions. The electrical conductivity is directly linked to the electronic density, the behavior of the electronic density shows that the electrical conductivity will increase with the copper content in the plasma, especially for temperatures below 17000K. As a minimum electrical conductivity is desired in the circuit breakers for breaking the electric arc, significant evaporation of the copper contacts could reduce the performance of the circuit breaker for breaking the electric current. However, the equilibrium composition calculations alone do not make it possible to highlight the role of copper vapor on the interruption of the electric current. The calculations of the transport coefficients, and more particularly the thermal conductivity could highlight it. There is also the dynamic viscosity of the plasma that you need to get an idea of the speed of movement of the electric arc.

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