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SIMULATION OF THE DIRECT CARBOTHERMAL REDUCTION OF SiO_2 FOR Si METAL USING MATLAB® AND ASPEN-HYSYS®

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ABSTRACT

Silicon metal is one of the most important metals produced from silica by carbothermic reduction in the electric arc furnace which works at high temperatures between 1000 to 3000 ^oC. The objective of this work is to simulate the direct carbothermal reduction of SiO_2 for Si metal by using a thermodynamic calculation of Gibb's free energy minimization with MATLAB® and Aspen HYSYS®. The comparison of simulation using MATLAB® with reference [10] revealed close results. By increasing the mole ratio up to 10 increases the Si formation and increases the ratio more than 10 mole ratio had very bad results,and not economically viable. Here we did comparison between simulation results using MATLAB® with real assumption and ASPEN HYSYS®.

Keywords: *Silicon Metal; Carbothermic Reduction; Arc Furnace; Simulation; MATLAB®; ASPEN HYSYS®*

1. INTRODUCTION

Silicon metal is one of the most important metals produced from silica for more than 100 years by carbothermic reduction in the electric arc furnace. Electric arc furnaces (EAFs) are used in steel making by recycling steel scrap. The industry consumes 400 kilowatts / ton of steel at1-3h [1]. EAF was considered as energy regulator reactor [2]. EAF's works at high temperatures between 1000 ^oC to 2000 ^oC. To study the dynamic model which contains all features of static model plus it contains the information from reaction kinetics and process dynamic, reactions mechanism and reactions kinetics of such complex system have to be achieved first.

But because the experiments have difficulties at high temperatures more than 1500°C, and also because of the multiplicity of reactions and the relationship between them did not agree on the reactions that occur in the electric arc furnace to produce silicon. There are at least 17 possible reactions. Therefore, SiO_2 + SiC reaction mechanisms and effect of added gases in the temperature range 1270 -1430 ° C were studied [1] and [3]. While kinetics and mechanisms of the liquid Si – C were presented and discussed [4]. Further, the chemistry of carbothermal synthesis of β-SiC has been displayed [5]. Furthermore, a model has been developed for the rapid carbothermal reduction synthesis of fine

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silicon carbide powders [6]. The production of SiO gas in EAF reactor was discussed [7]. Selected reactions mechanisms in carbothermic reduction for Si production are displayed [8]. Finally, carbothermic reactions for reduction of silica to produce silicon were defined and reaction kinetics was determined [9].

In 1978 a computer program named SOLGASMIX for the computation of chemical equilibrium in high temperature systems by using the free energy minimization method has been used [2]. The carbothermal reduction of SiO_2 to Si as a function of mole ratio of SiO_2, SiC and C in the temperature range of 0 – 3000 ^oC by using a thermodynamic calculation of Gibb's free energy minimization were simulated [10]. Main findings of this study is the Si metal formed in the SiO_2-C system at 1250°C and completed its formation at 1500-2000 °C with an excess of C. In addition SiC to SiO_2-C system completes SiO_2 transformation to Si and stimulates the reduction of system temperature and excess carbon. The objective of this work is to use different MATLAB® and ASPEN HYSYS® simulator to simulate the carbothermal reduction of SiO_2 to Si by using the free energy minimization method.

2. Simulation

Thermodynamic equilibrium calculations of Gibb's free energy minimization were performed with ASPEN- HYSYS® simulator, and MATLAB®. For simulation, the following assumptions were used (i) possible reactants and products – SiO_2, SiC, C, Si, SiO, and CO; (ii) feeding materials- SiO_2, C, and/or SiC; (iii) temperature range 0 – 2000 ^oC; (iv) pressure 1 atm; (v) reactor type- fixed bed batch reactor; (vi) ASPEN-HYSYS® simulator were used to calculate the equilibrium composition as a function of temperature and feed mole ratio of SiO_2,C and/or SiC. MATLAB® was used as well with more assumption that gases are ideal or real. The reaction mechanism of carbothermal reduction of SiO_2 by carbon that used in this study were presented by Filsinger and Bourric, 1990 [9] as demonstrated by Equations (1) – (7).

$$SiO_2 + C \rightarrow SiO + CO \quad (1)$$

$$SiO_2 + 3C \rightarrow SiC + 2CO \quad (2)$$

$$2SiO_2 + SiC \rightarrow 3SiO + CO \quad (3)$$

$$SiO + 2C \rightarrow SiC + CO \quad (4)$$

$$SiO + SIC \rightarrow 2Si + CO \quad (5)$$

$$SiO_2 + 2Si \rightarrow 2SO \quad (6)$$

$$3SiO_2 + 2SiC \rightarrow Si + 4SiO + 2CO \quad (7)$$

Thermodynamic equilibrium calculations performed by MATLAB® and ASPEN-HYSYS® (V7.1) to find out the equilibrium products distribution with the effect of reaction temperature in the SiO_2–C and SiO_2-SiC–C system. Janaf Tables [11] have used to get ideal Gibb's free energy (G_i) then used it, but real Gibb's free energy calculated by:

$$G_{1=}G_{if} + RTLny_1 + RTln\acute{\emptyset}_1 \quad (8)$$

For solids and liquids $\acute{\emptyset}$ =1

Where R is gas constant; T is Temperature; y_1 is mole ratio of compound 1; $\acute{\emptyset}$: is fugacity coefficient. When y_1= zero neglected RTLny1. To calculate $\acute{\emptyset}$ for mixture of two gases (SiC, SiO) was used the equations in literature [12]. Table 1 displays physical properties of SiO and SiC.

Table 1 Physical properties of Silicon monoxide and Silicon carbide.

Physical properties	T_C (K)	P_C (bar)	w	T_b (K)	References
SiO	3672.5161	990.5799	1.136101	2150	[13]
SiC	3384.300741	717.51219	0.87625	1908	[13] and [14]

$$Ln\acute{\emptyset}_1 = \frac{P}{RT}\left(B_{11} + y^2{}_2\delta_{12}\right) \qquad (9)$$

$$Ln\acute{\emptyset}_2 = \frac{P}{RT}\left(B_{22} + y^2{}_1\delta_{12}\right) \qquad (10)$$

$$\delta_{12} = 2B_{12} - B_{11} - B_{22} \qquad (11)$$

Where B_{11}, $B_{22:}$ values of pure-species virial coefficients; B_{12}: cross coefficients; y_1, y_2 : mole ratio

To calculate B_{11}, B_{22} and B_{12} [15]:

$$B_{ij} = \frac{RT_{c_{ij}}}{P_{c_{ij}}}\left(B^{\circ} + w_{ij}\,B^{1}\right) \qquad (12)$$

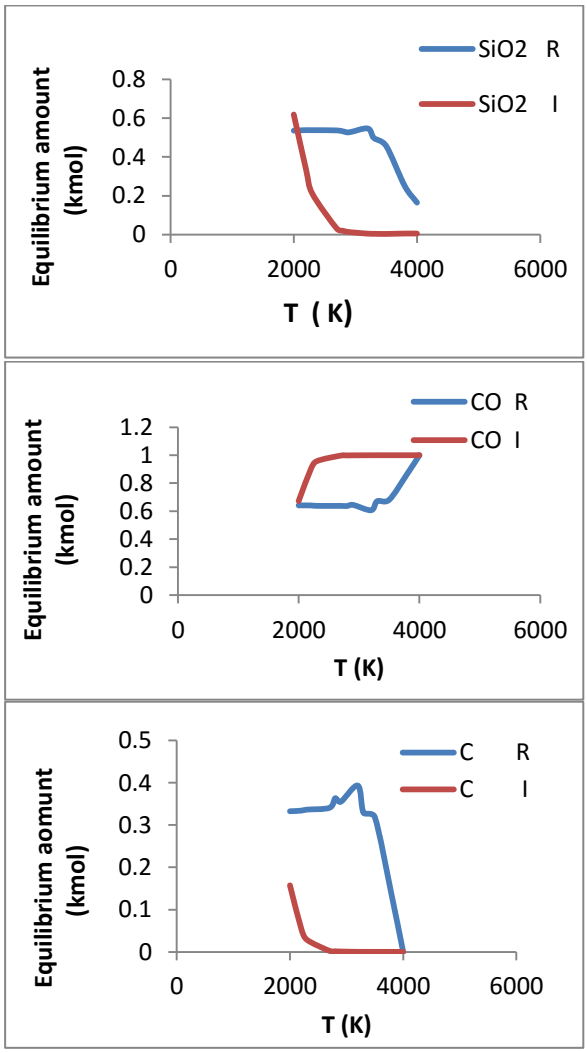
To calculate w_{ij} was used the equations in literature [13] and [16].

ASPEN-HYSYS® (V7.1) for the simulation, assumed the conditions as follows: (1) Temperature of feed input same Temperature of product output (This is to observe the change at each temperature). (2) The pressure drop in the reactor equal to zero [17].

3. RESULTS AND DISCUSSION

In this study a simulation of carbothermic reactions Equations (1) – (7) using MATLAB® and Aspen HYSYS® simulator were used to calculate the equilibrium composition as a function of temperature and feed mole ratio of SiO_2, C and/or SiC and the results are compared with similar study using Outokumpu HSC Chemistry software (version 6.1 Outokumpu Research Oy, Pori, Finland) [10].

The results using MATLAB® with ideal assumption were so close to results using HSC software [10]. The comparison between ideal and real cases using MATLAB® is demonstrated in Figure 1 for SiO_2:C equals 1:1. By increasing Si:C up to 10 mol ratio gives good results as displayed in Figure 2, but more than 10 mol ratio does not increase silicon productivity and is not an economical process. Silicon yield in real case is almost half of ideal case, but when adding SiC, the result of adding one mole matches the result of adding 10 mole ratio of carbon. Then in real case, the increase in carbon to 74 mole ratio with the presence of mole from SiC led to bad results for silicon productivity, reaching zero kmol. The following Figures demonstrate the results.



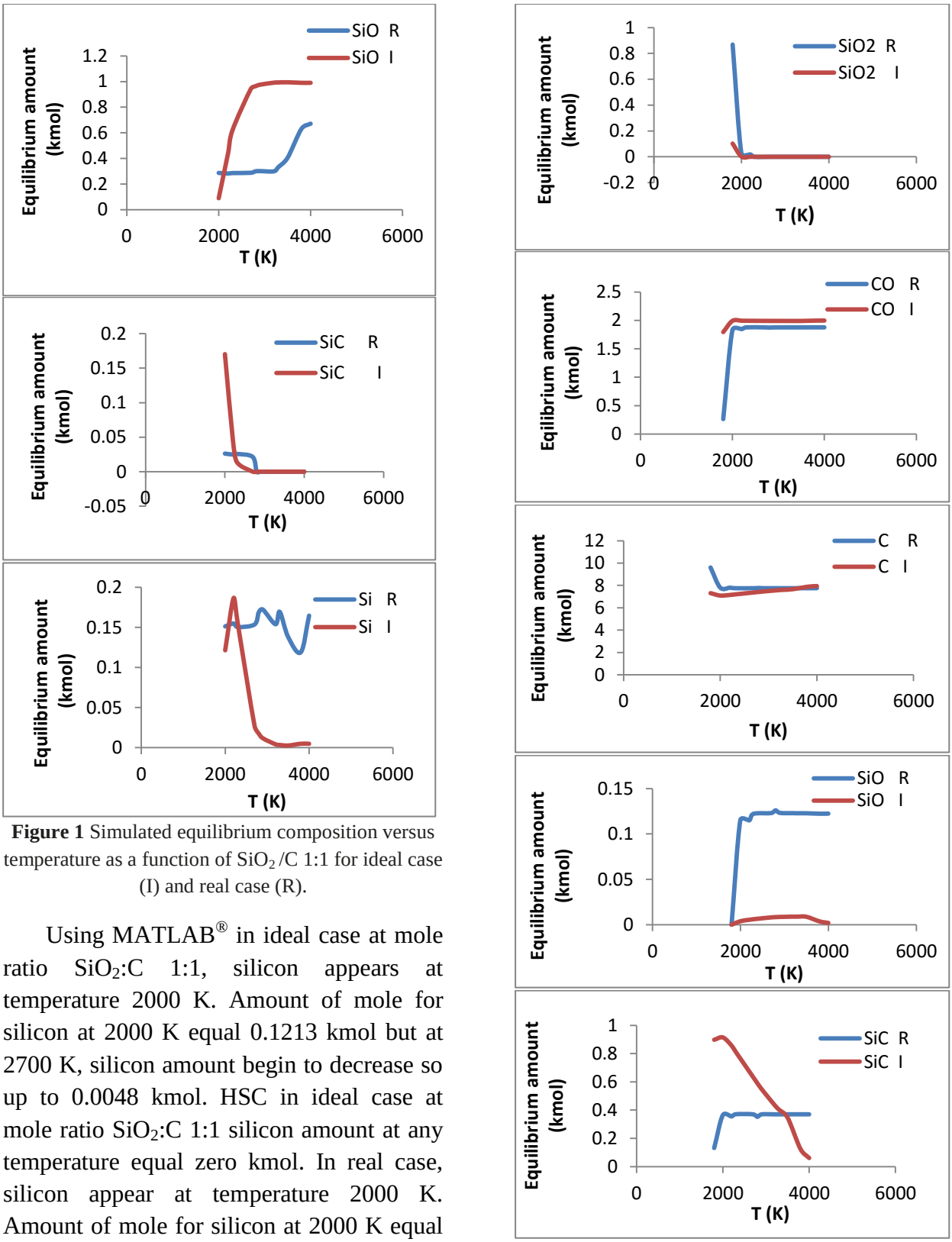


Figure 1 Simulated equilibrium composition versus temperature as a function of SiO_2/C 1:1 for ideal case (I) and real case (R).

Using MATLAB® in ideal case at mole ratio SiO_2:C 1:1, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.1213 kmol but at 2700 K, silicon amount begin to decrease so up to 0.0048 kmol. HSC in ideal case at mole ratio SiO_2:C 1:1 silicon amount at any temperature equal zero kmol. In real case, silicon appear at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.1511 kmol .In real case, silicon at all temperature not decrease or increase a lot. Figure 1 depicts the results.

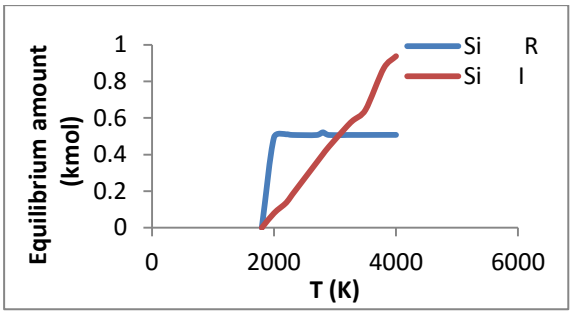
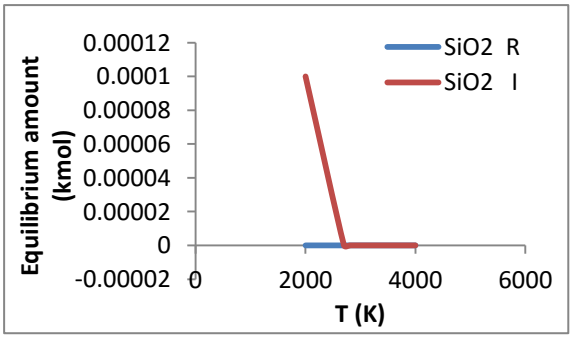
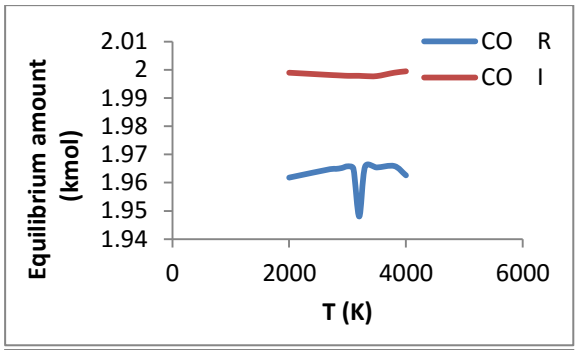
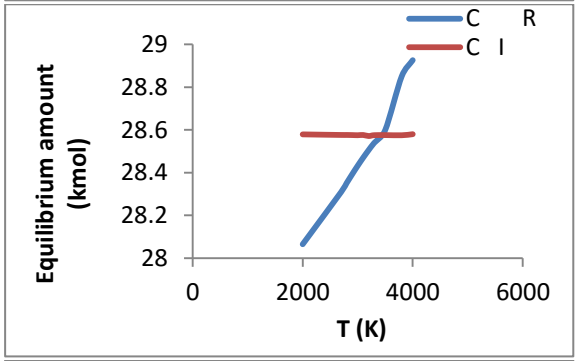


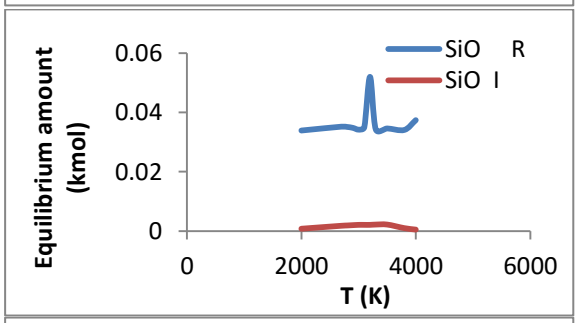
Figure 2 Simulated equilibrium composition versus temperature as a function of SiO_2 /C 1:10 for ideal case (I) and real case (R).

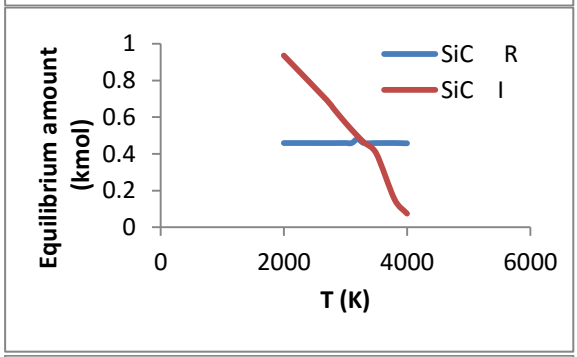
Using MATLAB® in ideal case at mole ratio SiO_2:C 1:10, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.0797 kmol. Then amount of silicon increase so up to 0.9374 kmol at 4000 K. HSC in ideal case at mole ratio SiO_2:C 1:10, silicon appears at temperature 1400 K. Amount of mole for silicon at 1400 K equal 0.05 kmol. Then amount of silicon increases so up to one kmol at 2200 K, but over 2200 K amount of silicon be constant equal one kmol. In real case, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.4939 kmol. In real case, amount of silicon increases so up to 0.5214 kmol at 2800 K. Then amount of silicon at all temperature not decrease or increase a lot. Figure 2 shows it. The results at 2400 K, 2500 K and 2600 K non logic at SiO_2:C 1:10.











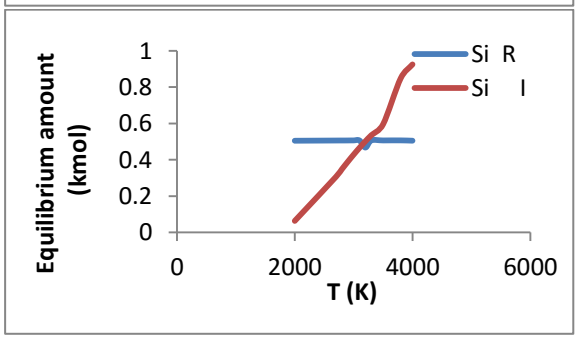
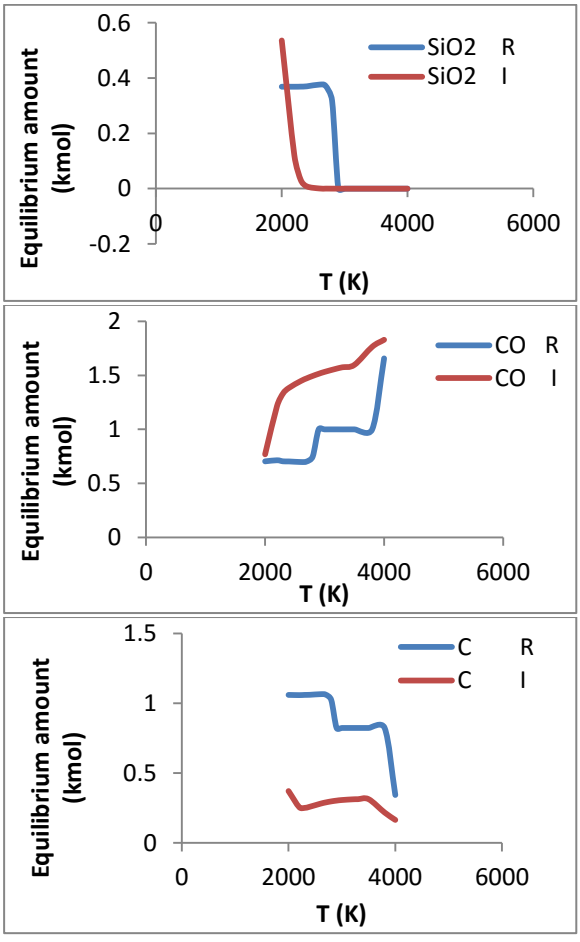


Figure 3 Simulated equilibrium composition versus temperature as a function of SiO_2 /C 1:31 for ideal case (I) and real case (R).

The results at mole ratio SiO_2:C 1:31 similar to results at mole ratio SiO_2:C 1:10.Using MATLAB® in ideal case at mole ratio SiO_2:C 1:31, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.0635 kmol. Then amount of silicon increase so up to 0.9248 kmol at 4000 K. HSC in ideal case at mole ratio SiO_2:C 1:31, silicon appears at temperature 1400 K. Amount of mole for silicon at 1400 K equal 0.05 kmol. Then amount of silicon increase so up to one kmol at 1773 K, but over 1773 K amount of silicon be constant equal one kmol. In real case, silicon appear at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.5047 kmol .In real case, silicon at all temperature not decrease or increase a lot. Figure 3 explains it. The results at 1800 K, 2200 K, 2300K, 2400 K , 2500K and 2600K non logic at SiO_2:C 1:31.



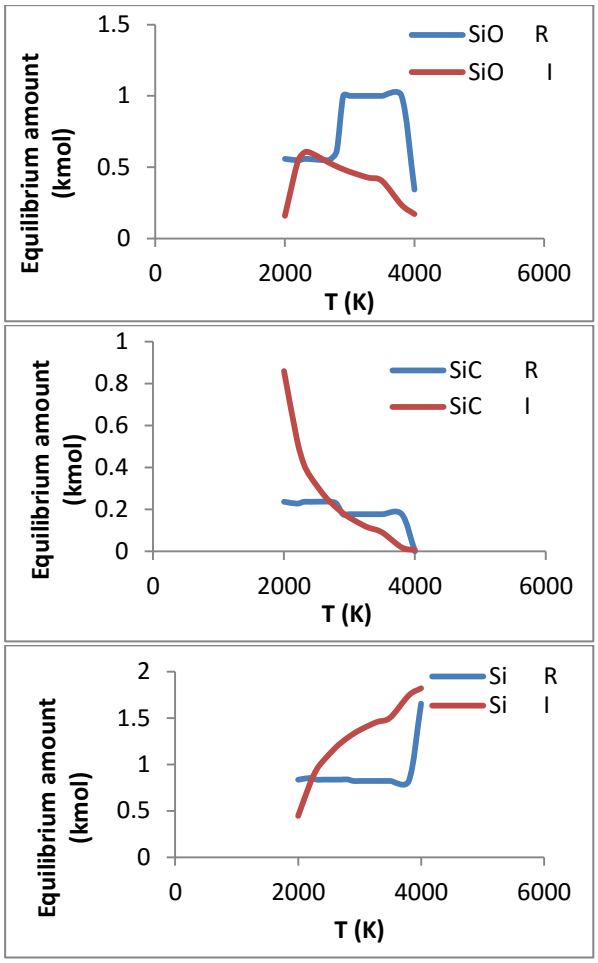
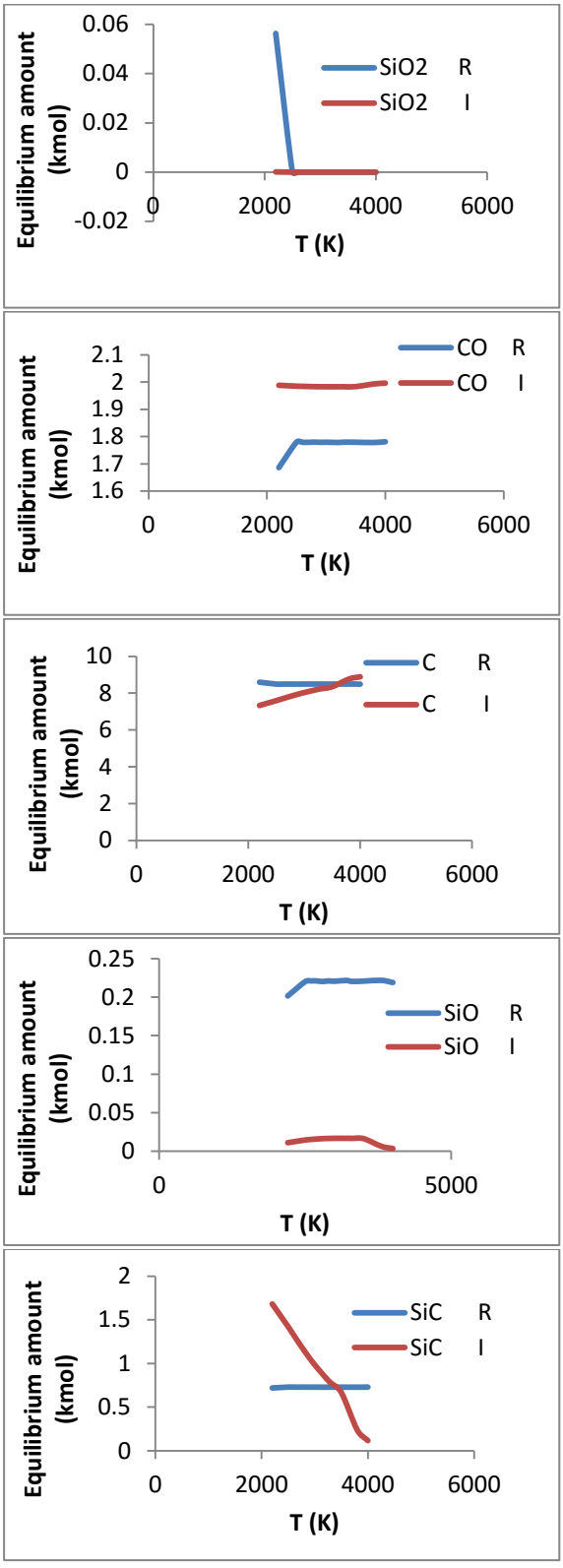


Figure 4 Simulated equilibrium composition versus temperature as a function of SiO_2 /C/SiC 1:1:1 for ideal case (I) and real case (R).

Mole ratio SiO_2:C:SiC 1:1:1, in ideal case using MATLAB® silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.4456 kmol. Then amount of silicon increases so up to 0.9453 kmol at 2300 K. Final amount of silicon increases one more time so up to 1.8222 kmol at 4000 K. HSC in ideal case, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.01 kmol. Then amount of silicon increases so up to 1 kmol at 2273 K. Final amount of silicon increases one more time so up to 1.7 kmol at 3273 K. In real case, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.836 kmol. In real case, silicon at all temperature not decreases or increases a lot. Just at 4000 K, amount of

mole for silicon equal 1.6567 kmol. Figure 4 explains it.



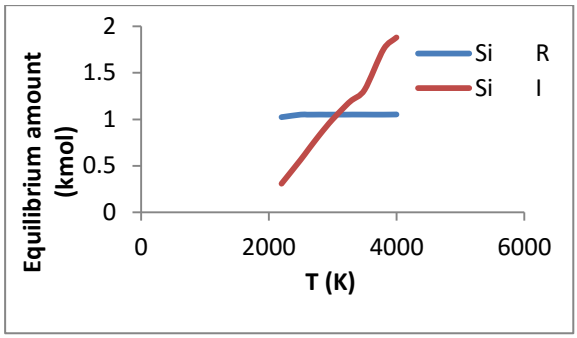
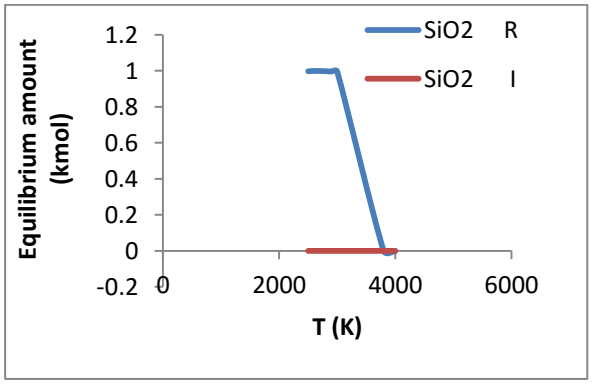


Figure 5 Simulated equilibrium composition versus temperature as a function of SiO_2 /C/SiC 1:10:1 for ideal case (I) and real case (R).

Using MATLAB® in ideal case at mole ratio SiO_2:C:SiC 1:10:1, silicon appears at temperature 2200 K. Amount of mole for silicon at 2200 K equal 0.3079 kmol. Then amount of silicon increase so up to 1.8809 kmol at 4000 K. HSC in ideal case at mole ratio SiO_2:C:SiC 1:10:1, silicon appears at temperature 1273 K. Amount of mole for silicon at 1273 K equal 0.1kmol.Then amount of silicon increase so up to two kmol at 2273 K, but over 2273 K amount of silicon be constant equal two kmol. In real case, silicon appears at temperature 2200 K. Amount of mole for silicon at 2200 K equal 1.0236 kmol. Then amount of silicon at all temperature not decreases or increases a lot. Figure 5 explains it. The results at 1800 K, 2000 K, 2300 K and 2400 K non logic at SiO_2:C:SiC 1:10:1.



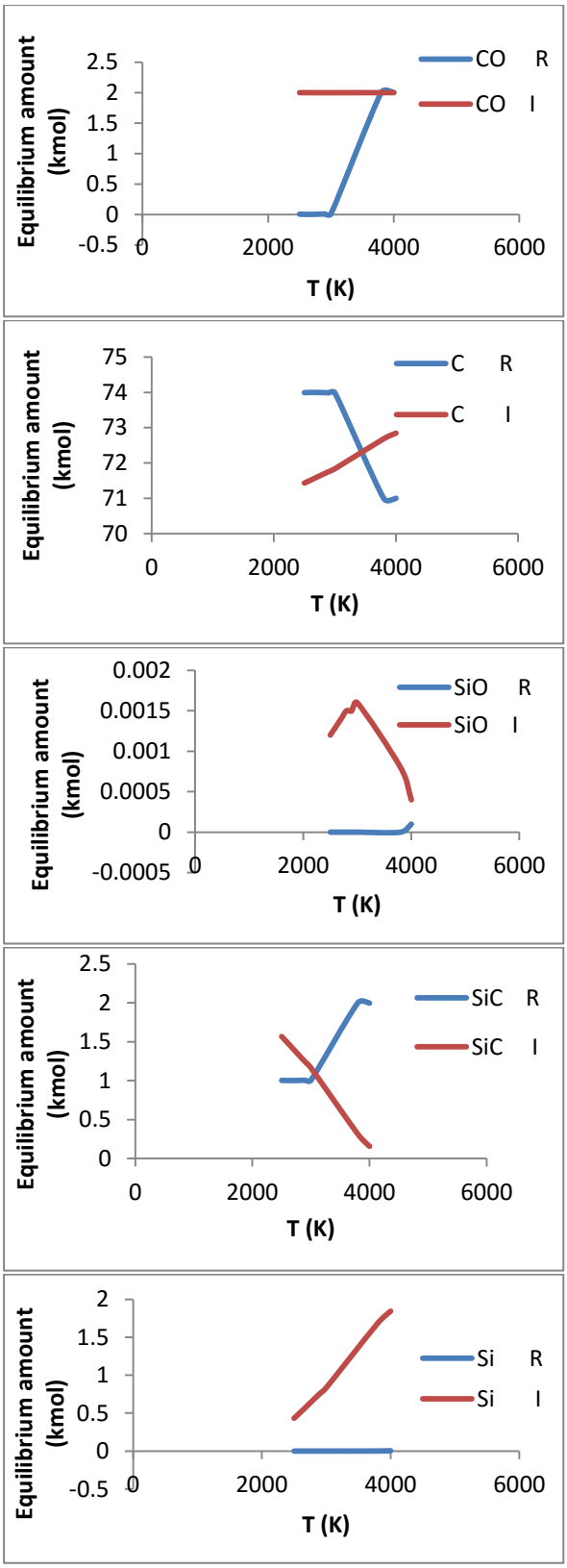


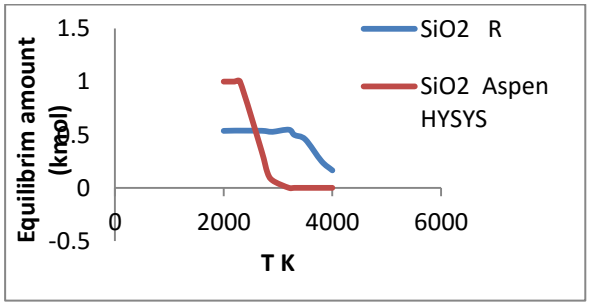
Figure 6 Simulated equilibrium composition versus temperature as a function of SiO_2 /C/SiC 1:74:1 for ideal case (I) and real case (R).

Using MATLAB® in ideal case at mole ratio SiO_2:C:SiC 1:74:1, silicon appears at temperature 2500 K. Amount of mole for silicon at 2500 K equal 0.4322 kmol. Then amount of silicon increases so up to 1.8439 kmol at 4000 K. HSC in ideal case at mole ratio SiO_2:C:SiC 1:74:1, silicon appears at temperature 973 K. Amount of mole for silicon at 973 K equal 0.2 kmol. Then amount of silicon increases so up to two kmol at 1773 K, but over 1773 K amount of silicon be constant equal two kmol. In real case, silicon appears at temperature 2200 K. Amount of mole for silicon at 2200 K equal 1.0236 kmol. In real case, silicon did not appear at all temperature, just at 3800 k and 4000 k amount of silicon equal 0.0012, 0.0041 respectively. Figure 6 explains it. The results at 1800 K, 2000 K, 2200 K, 2300 K and 2400 K non logic at mole ratio SiO_2:C:SiC 1:74:1.

MTLAB® real case and Aspen HYSYS®

Aspen HYSYS® is almost the same as real case results, but if carbon reaches 74 mole ratio, the silicon is producing then fade when temperatures increase.

Some elements and compounds appear in the Aspen HYSYS® had values zero and this do not mean fading, but mean evaporate at high temperatures and this only shows HYSYS® [9]. The following figures explain results.



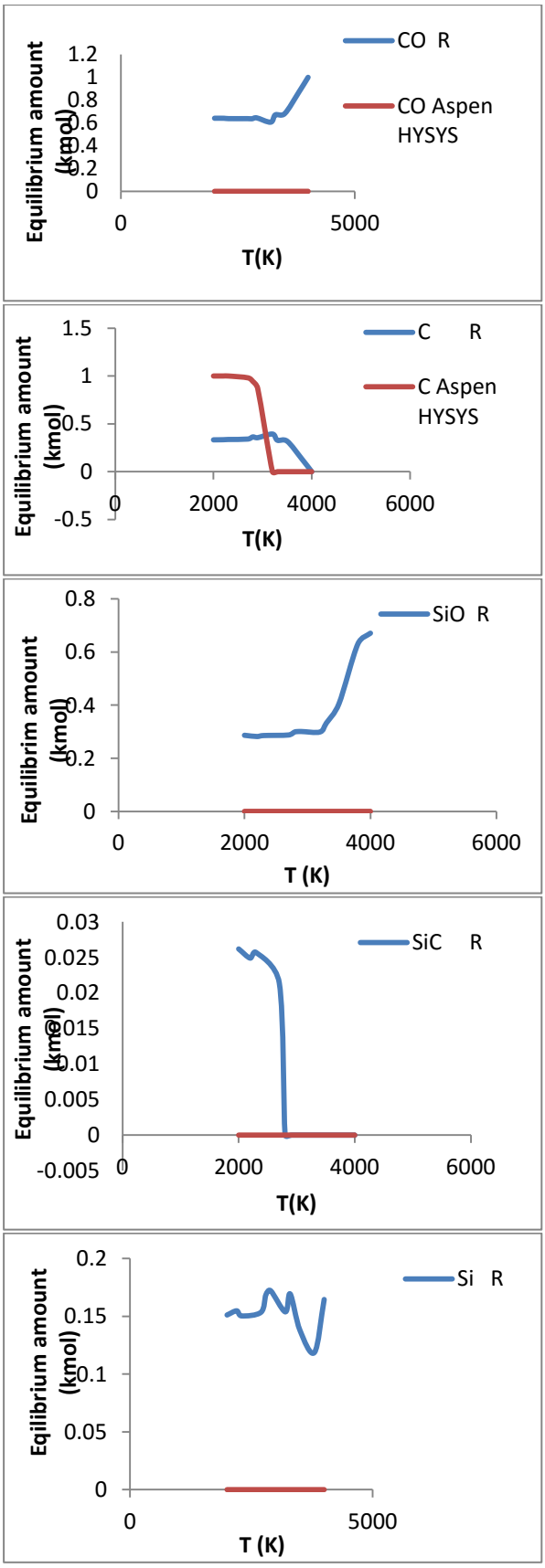
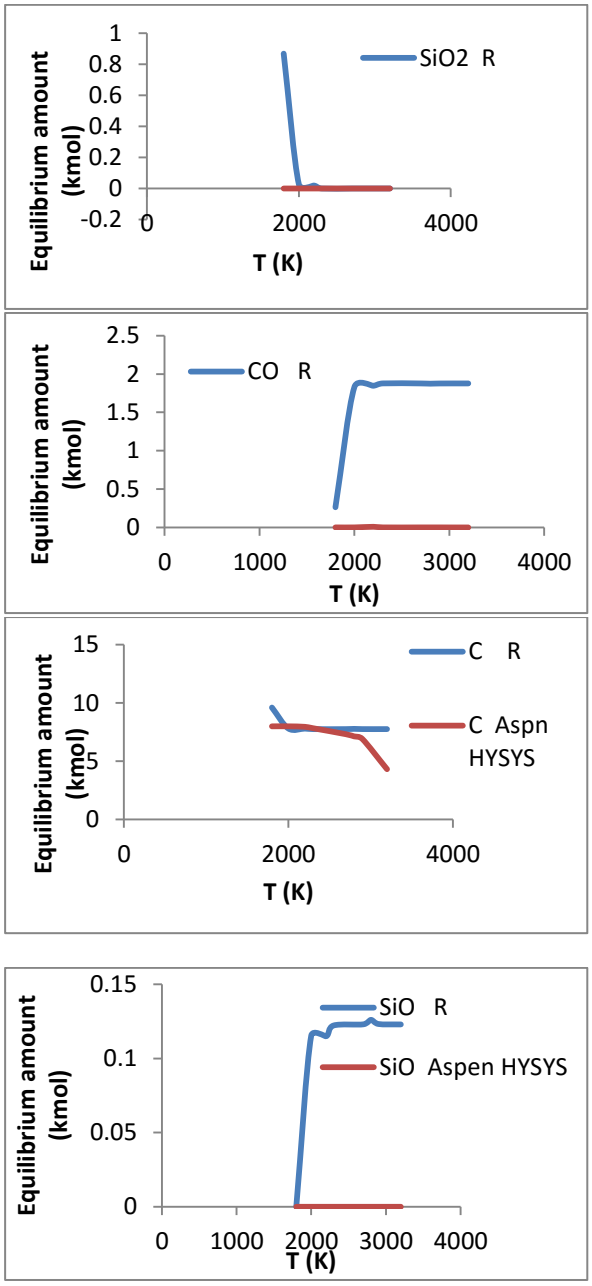


Figure 7 Simulated equilibrium composition versus temperature as a function of SiO_2 /C 1:1 for MTLAB® real case (R) and Aspen HYSYS®.

In SiO_2:C 1:1, CO and SiO evaporate at high temperature in Aspen HYSYS®. The amount of silicon in Aspen HYSYS® at SiO_2:C 1:1, at all temperature equal zero. Also in real case using MATLAB® had very little amount appears at 2000 K equal 0.1511 kmol and amount of silicon at all temperature not decreases or increases a lot. Figure 7 explains it.



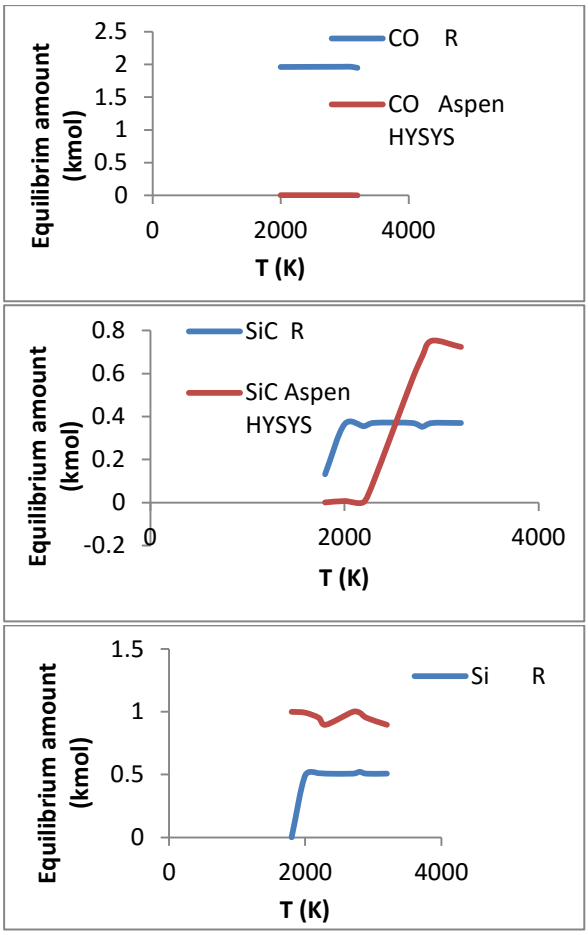


Figure 8 Simulated equilibrium composition versus temperature as a function of SiO_2 /C 1:10 for MTLAB® real case (R) and Aspen HYSYS®.

Using Aspen HYSYS® at mole ratio SiO_2:C1:10, silicon appears at temperature 1800 K. Amount of mole for silicon at 1800 K equal 0.999 kmol. Then amount of silicon did not increase or decrease a lot. In MATLAB® in real case, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.4939 kmol. Then amount of silicon at all temperature did not decrease or increase a lot. Figure 8 explains it. Also in mole ratio SiO_2: C 1:10 when we tried to raise the temperature above 3200 K, all elements and compounds appeared in the state of evaporation.

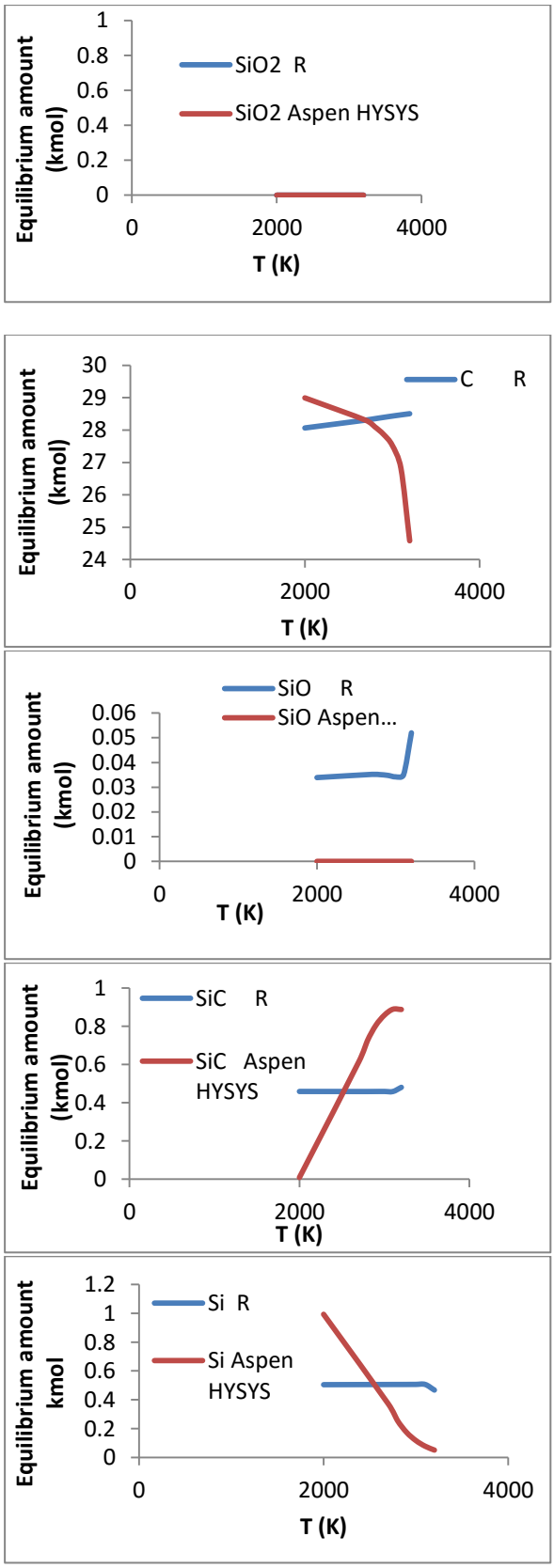
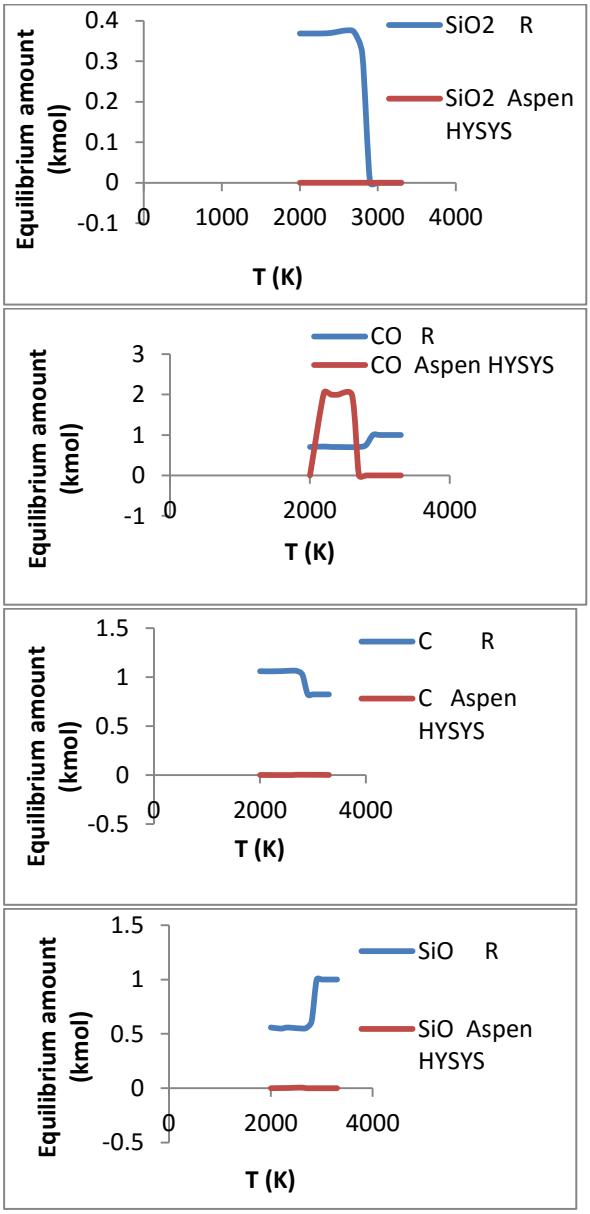


Figure 9 Simulated equilibrium composition versus temperature as a function of SiO_2 /C 1:31 for MTLAB® real case (R) and Aspen HYSYS®.

In SiO_2:C 1:31, figure 9 SiO_2 (R) line same SiO_2 Aspen HYSYS® line. Using

Aspen HYSYS® at mole ratio SiO_2:C1:31, silicon appears at temperature 1800 K. Amount of mole for silicon at 2000 K equal 0.993 kmol. Then amount of silicon decreases a lot up to 0.05104 kmol at 3200 K. In MATLAB in real case, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.5047 kmol. Then amount of silicon at all temperature did not decrease or increase a lot. Figure 9 explains it.



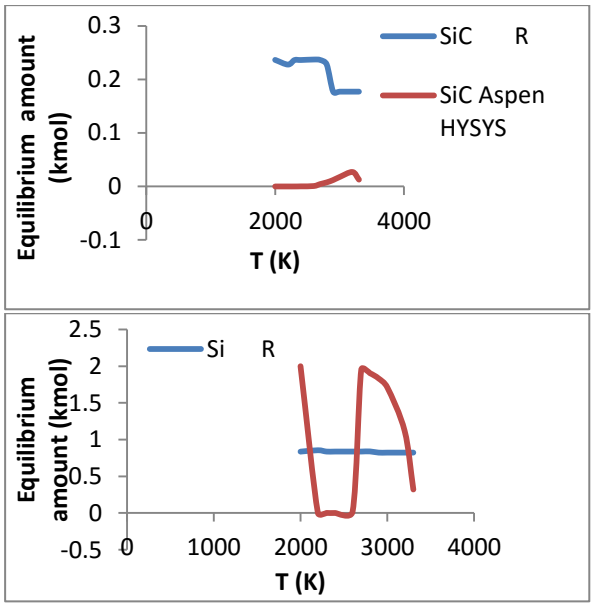
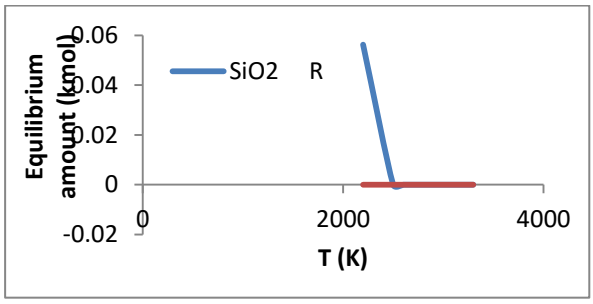


Figure 10 Simulated equilibrium composition versus temperature as a function of SiO_2 /C/SiC 1:1:1 for MTLAB® real case (R) and Aspen HYSYS®.

Using Aspen HYSYS® at mole ratio SiO_2:C:SiC 1:1:1, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 1.999 kmol. Then amount of silicon decreases a lot up to 0.00084 kmol at 2200 K to 2600 K. Then amount of silicon increases at 2700 K equal 1.954 kmol. Final at 3300 K, amount of silicon decreases equal 0.32048 kmol. In MATLAB in real case, silicon appears at temperature 2000 K. Amount of mole for silicon at 2000 K equal 0.836 kmol. Then amount of silicon at all temperature not decrease or increase a lot. Figure 10 explains it.



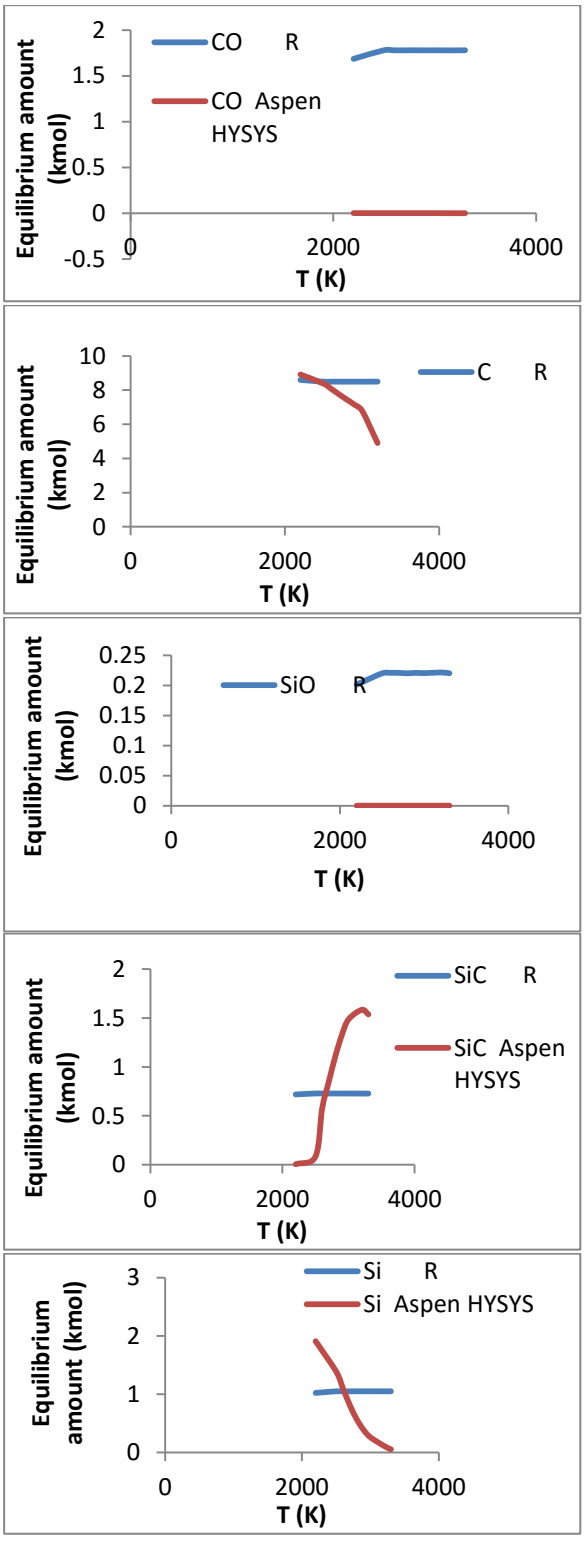
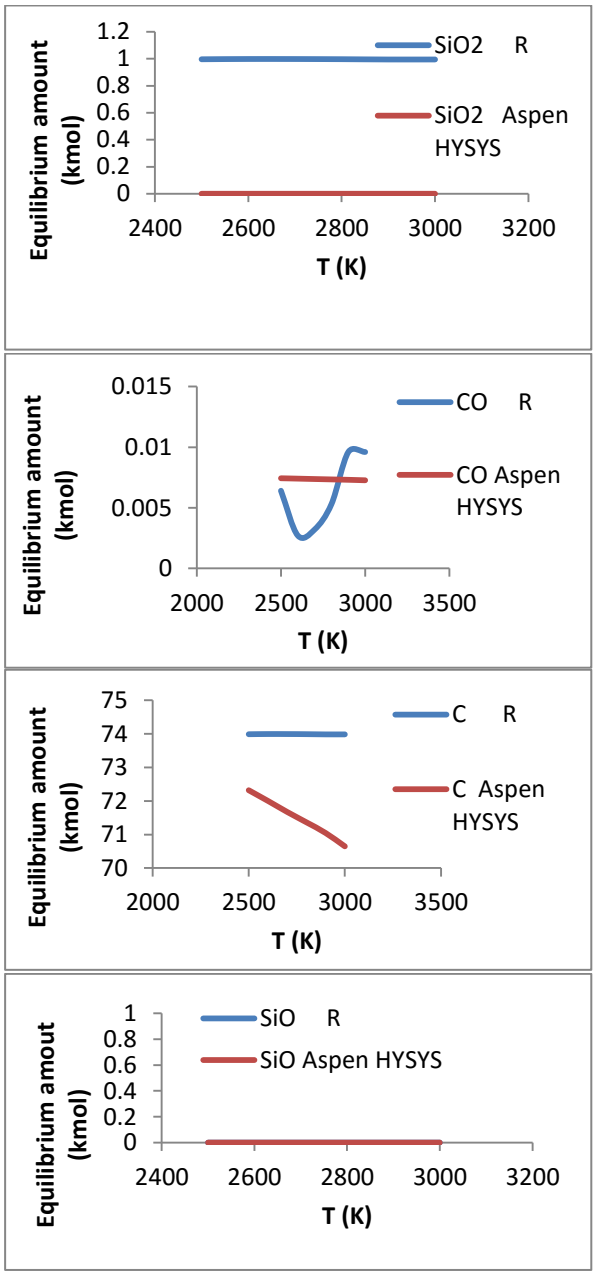


Figure 11 Simulated equilibrium composition versus temperature as a function of SiO_2 /C/SiC 1:10:1 for MTLAB® real case (R) and Aspen HYSYS®.

In mole ratio SiO_2:C:SiC 1:10:1, when we tried to raise the temperature above 3200 K, all elements and compounds appeared in the state of evaporation. CO evaporates at high temperature in Aspen HYSYS®. Using Aspen HYSYS® at mole ratio SiO_2:C:SiC 1:10:1, silicon appears at temperature 2200 K. Amount of mole for silicon at 2200 K equal 1.910341 kmol. Then amount of silicon decreases with high temperature so up to 0.0563 kmol at 3300 K. In MATLAB® in real case, silicon appears at temperature 2200 K. Amount of mole for silicon at 2200 K equal 1.0236 kmol. Then amount of silicon at all temperature did not decrease or increase a lot. Figure 11 explains it.



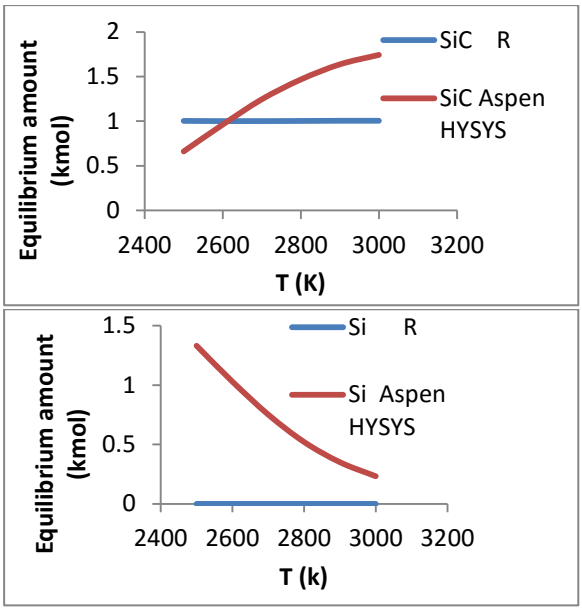


Figure 12 Simulated equilibrium composition versus temperature as a function of SiO_2 /C/SiC 1:74:1 for MTLAB® real case (R) and Aspen HYSYS®.

In mole ratio SiO_2: C : SiC 1:74:1, when we tried to raise the temperature above 3000 K, all elements and compounds appeared in the state of evaporation. Carbon up to 74 moles in SiO_2 to C to SiC 1:74:1 it causes very bad results of silicon production. Figure 12 SiO (R) line same SiO Aspen HYSYS® line. Using Aspen HYSYS® at mole ratio SiO_2:C: SiC 1:74:1, silicon appears at temperature 2500 K. Amount of mole for silicon at 2500 K equal 1.330 kmol. Then amount of silicon decreases with high temperature so up to 0.232416 kmol at 3000 K. In MATLAB® in real case, silicon did not appear at all temperature. Amount of mole for silicon equal zero. Figure explains it.

4. CONCLUSION

Carbon and silicon carbide are major species which effect of silicon production. One mole of silicon carbide had the same effect of 10 moles of carbon in process without silicon carbide. Also addition of more carbon gives bad results, but addition of silicon carbide has improved the interaction. Best mole ratio SiO_2/C/SiC 1:10:1.

Upon comparing of the MATLAB® and Aspen HYSYS® with results from Outokumpu, observed that in ideal Gibb's free energy the results so close to results from Outokumpu, but in real Gibb's free energy the results half the equilibrium amount of silicon.

When used Aspen HYSYS®, we saved time that need to give the optimum results, and getting a lot information about all element in the process. Some elements and compounds appear in the Aspen HYSYS® had values zero and this do not mean fading, but mean evaporate at high temperatures.
In some temperature give non logic results because they form a transition phase in silicon production and vary according to the concentration of moles.

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APPENDIX

Suppose we want to solve numerically two polynomial equations $f_1(y_1,y_2)=0$; $f_2(y_1,y_2)=0$ where it is difficult to choose the proper initial condition. The method of continuation is used [18]. Instead, solve

$$h_1(y_1,y_2,t)=(1-t)g_1(y_1,y_2)+tf_1(y_1,y_2)=0$$

$$h_2(y_1,y_2,t)=(1-t)g_2(y_1,y_2)+tf_2(y_1,y_2)=0$$

Where we choose the initial condition which solves g_1 and g_2. The procedure is as follows: start with t=0 the solution is $g_1 = g_2=0$. Then increment t to t=t+DT and solve the two equations with the initial conditions obtained from the previous iteration until t=1 at which $h_1=f_1$ and $h_2=f_2$; we usually work with complex numbers to avoid singularity. The following is the MATLAB® code:

```
 N=50  ;dt=1/N;nc=10;
   n0=[1+i;nc+i;i];  % initial
condition

   for j=1:N+1
       t=(j-1)*dt;
      n1 = fsolve(@(n1)
chimequSiOfun(n1,t,nc) ,n0);
      n0=n1;
   end
   A=[1 0 1 0 1 1;2 0 0  1 1 0;0
1 1 1 0 0];b=[1 2 nc]';
   A1=A(:,1:3);A2=A(:,4:6);
   n2=inv(A2)*(b-A1*n1);
   n=[n1; n2]
J=-inv(A2)*A1

function f=chimequ1fun(y1,t)
  G1=4610;G2=-46030; G3=-47940;
G4=-94610;
  G5=0; T=1000; R=1.987;

g1=G1/(R*T);g2=G2/(R*T);g3=G3/(R
*T);g4=G4/(R*T);g5=G5/(R*T);
   A=[1 0 1 1 0;0 1 1 2 0;4 2 0
0 2];b=[2 3 14]';
   A1=A(:,1:2);A2=A(:,3:5);

   y2d=-inv(A2)* A1;           %
derivative of y2 with respect to
y1
   k=[g1  g2]+[g3 g4 g5]*y2d;
   c=exp(-k);
   y2=inv(A2)*(b-A1*y1);
   y=[y1; y2];
```

```
    yt=y(1)+y(2)+y(3)+y(4)+y(5);

    f1=y(1)*y(4)*yt^2-
c(1)*y(3)^2*y(5)^2;% f1 and f2
are now polynomials
    f2=y(2)*y(3)-c(2)*y(4)*y(5);
     g1h=(y(1)-2-i);
     g2h=(y(2)-3-i);
     f1=(1-t)*g1h+t*f1;
     f2=(1-t)*g2h+t*f2;
     f=[f1,f2];

end
```

محاكاة لإختزال ثاني أكسيد السيليكون بالحرارة والكربون لمعدن السيليكون بإستخدام MATLAB® و Aspen HYSYS®

الملخص:

عنصر السيليكون من أهم العناصر التي تدخل في الكثير من الصناعات، لذلك كان الهدف من هذا العمل هو محاكاة لدراسة محاكاة حول التخفيض المباشر للكربون للحرارة لثاني أكسيد السيليكون لمعدن السيليكون ، حيث استخدامنا لهذة المحاكاة تقنيات حسابية تعرف بال MATLAB® وAspen HYSYS® . وذلك من خلال دراسة درجات الحرارة والعلاقة بينها وبين التفاعلات داخل فرن القوس الكهربائي وعدد المولات المنتجة لكل منتج وخاصة السيليكون وذلك باستخدام طريقة خفض الطاقة الحرة.

لقد قمنا بعمل هذة الدراسة على الحالة المثالية للطاقة الحرة وايضا الحالة الحقيقية للطاقة الحرة ولوحظ أن الكربون وكربيد السيليكون هي الأنواع الرئيسية التي تؤثر على إنتاج السيليكون. وان واحد مول من كربيد السيليكون له نفس تأثير ١٠ مول من الكربون عندما تكون مولات التشغيل خالية من كربيد السيليكون. وايضا لوحظ ان اضافة المزيد من الكربون تعطي نتائج سيئة. لذلك ان اردنا اختيار افضل نتائج تكون عندما يكون ١٠ مولات من الكربون مقابل مول واحد من ثاني اكسيد السيليكون وايضا مول واحد من كربيد السيليكون.

عند مقارنة MATLAB® وAspen HYSYS® بنتائج Outokumpu الاساسية في المقال الذي تم محاكاتة وجدنا انه في الحالة المثالية للطاقة الحرة كانت النتائج قريبة جدا من نتائج ال Outokumpu. على خلاف الحالة الحقيقية للطاقة الحرة كان انتاج السيليكون تقريبا يصل الى نصف انتاج السيليكون في الحالة المثالية.

عند استخدام Aspen HYSYS®، قمنا بتوفير الوقت الذي نحتاجة لتحديد النتائج المثالية وايضا يوفر هذا البرنامج المعلومات الكثير حول جميع العناصر . ولكن كان الهدف من استخدام اكثر من برنامج انه في حالة عدم توفر احدهما يمكن الاستعانة بالآخر.قد تظهر بعض العناصر والمركبات في Aspen HYSYS® بقيم صفرية ، وهذا لا يعني عدم وجودها ، ولكن تتبخر في درجات الحرارة العالية.

في بعض درجات الحرارة تعطي نتائج غير منطقية لأنها تشكل مرحلة انتقالية في إنتاج السيليكون وتختلف باختلاف تركيز المولات.