ETUDE DE L'EQUILIBRE N2 + 3H2 -> 2NH3 AVEC MAPLE

EXPRESSIONS LITTERALES DES QUANTITES DE MATIERE DES ACTIVITES ET DE G(x)

```
> restart;
> with(plots):
> remR:=8.314:remT:=450:remPO:=1:remPT:=2.0:
> remGOA:=0*10^3:remGOB:=0*10^3:remGOC:=-1.6*10^3:
> remNOA:=1:remNOB:=1:NOC:=0:NUA:=-1:NUB:=-3:NUC:=2:
> NA:=NOA+NUA*x;NB:=NOB+NUB*x;NC:=NOC+NUC*x;NT:=NA+NB+NC;

NA := NOA-x
NB := NOB-3*x
NC := 2*x
NT := NOA-2*x+NOB

> actA:=(NA/NT)*(PT/PO);actB:=(NB/NT)*(PT/PO);actC:=(NC/NT)*(PT/PO);

actA := (NOA-x)/(NOA-2*x+NOB)*PT/PO
actB := (NOB-3*x)/(NOA-2*x+NOB)*PT/PO
actC := 2*x/(NOA-2*x+NOB)*PT/PO
```

EXPRESSIONS LITTERALES DE L'ENTHALPIE LIBRE G(x)

```
> GA:=GOA+R*T*ln(actA);GB:=GOB+R*T*ln(actB);GC:=GOC+R*T*ln(actC);
GA := GOA+R*T*ln((NOA-x)/(NOA-2*x+NOB)*PT/PO)
GB := GOB+R*T*ln((NOB-3*x)/(NOA-2*x+NOB)*PT/PO)
GC := GOC+R*T*ln(2*x/(NOA-2*x+NOB)*PT/PO)

> G(x):=NA*GA+NB*GB+NC*GC;
G(x) := (NOA-x)*(GOA+R*T*ln((NOA-x)/(NOA-2*x+NOB)*PT/PO))+(NOB-
3*x)*(GOB+R*T*ln((NOB-3*x)/(NOA-
2*x+NOB)*PT/PO))+2*x*(GOC+R*T*ln(2*x/(NOA-2*x+NOB)*PT/PO))
```

EXPRESSION DE L' AFFINITE -dG/dx à T,P ctes

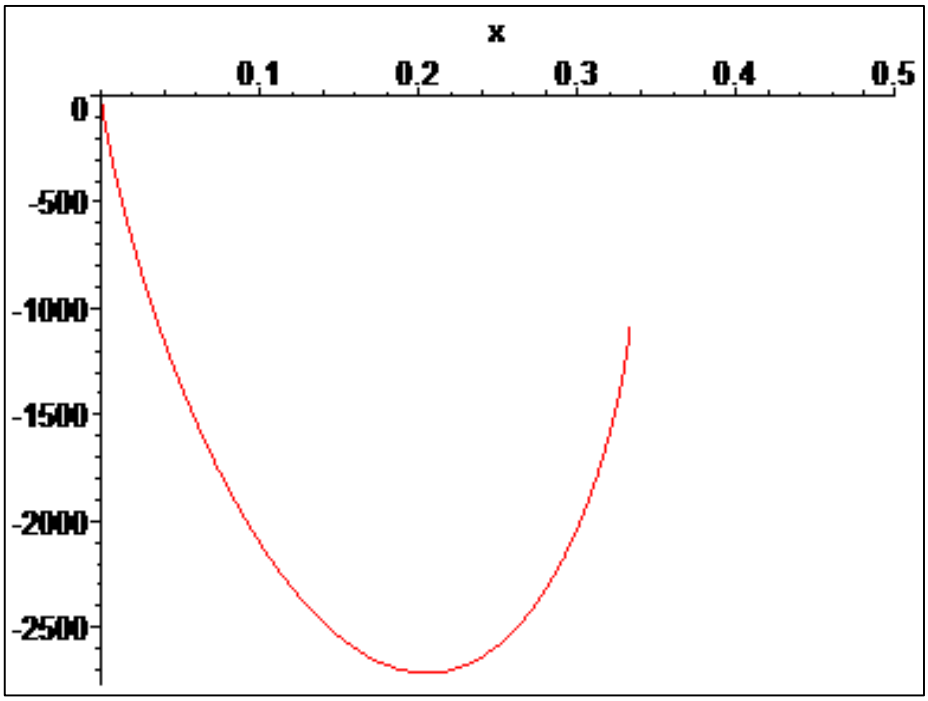
```
> aff:=diff(-G(x),x);
aff := GOA+R*T*ln((NOA-x)/(NOA-2*x+NOB)*PT/PO)-R*T*(-1/(NOA-
2*x+NOB)*PT/PO+2*(NOA-x)/(NOA-2*x+NOB)^2*PT/PO)*(NOA-
2*x+NOB)/PT*PO+3*GOB+3*R*T*ln((NOB-3*x)/(NOA-2*x+NOB)*PT/PO)-R*T*(-
3/(NOA-2*x+NOB)*PT/PO+2*(NOB-3*x)/(NOA-2*x+NOB)^2*PT/PO)*(NOA-
2*x+NOB)/PT*PO-2*GOC-2*R*T*ln(2*x/(NOA-2*x+NOB)*PT/PO)-R*T*(2/(NOA-
2*x+NOB)*PT/PO+4*x/(NOA-2*x+NOB)^2*PT/PO)*(NOA-2*x+NOB)/PT*PO
```

TRACE DES COURBES

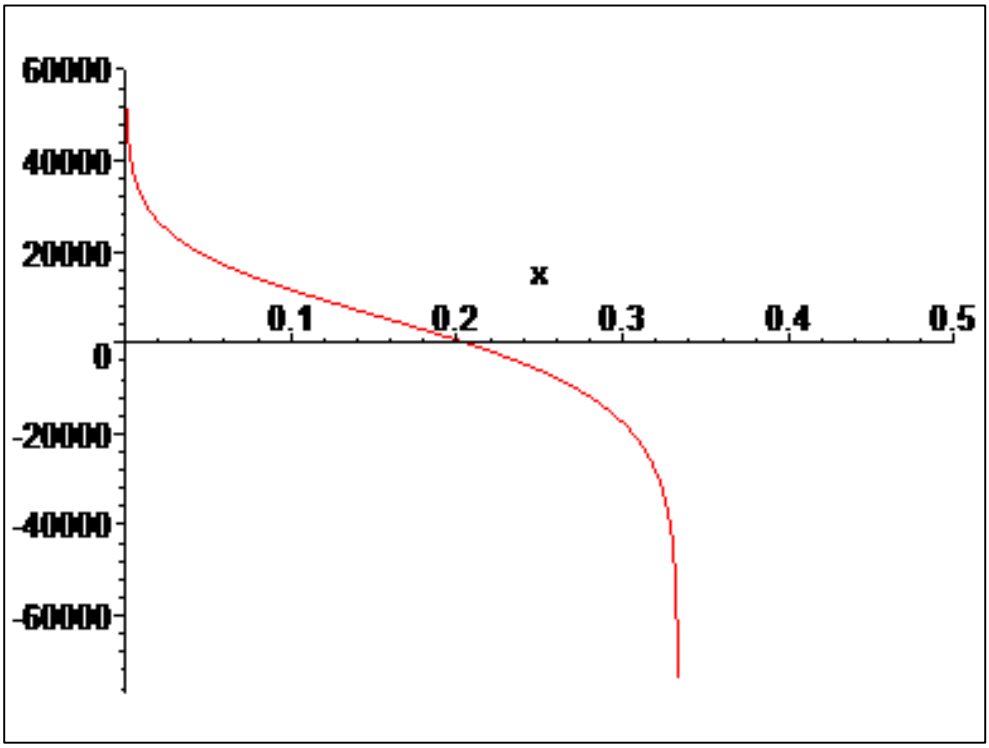
```
> plot(G(x),x=0..0.5);
> plot(aff(x),x=0..0.5);
```

VALEURS NUMERIQUES ET CALCUL

```
> restart;
> with(plots):

> R:=8.314:T:=450:PO:=1:PT:=2.0:
> GOA:=0*10^3:GOB:=0*10^3:GOC:=-1.6*10^3:
> NOA:=1:NOB:=1:NOC:=0:NUA:=-1:NUB:=-3:NUC:=2:
> NA:=NOA+NUA*x;NB:=NOB+NUB*x;NC:=NOC+NUC*x;NT:=NA+NB+NC;
NA := 1-x
NB := 1-3*x
NC := 2*x
NT := 2-2*x
>
actA:=(NA/NT)*(PT/PO);actB:=(NB/NT)*(PT/PO);actC:=(NC/NT)*(PT/PO)
;
actA := 2.0*(1-x)/(2-2*x)
actB := 2.0*(1-3*x)/(2-2*x)
actC := 4.0*x/(2-2*x)

> GA:=GOA+R*T*ln(actA);GB:=GOB+R*T*ln(actB);GC:=GOC+R*T*ln(actC);
GA := 3741.300*ln(2.0*(1-x)/(2-2*x))
GB := 3741.300*ln(2.0*(1-3*x)/(2-2*x))
GC := -1600.0+3741.300*ln(4.0*x/(2-2*x))

> G(x):=NA*GA+NB*GB+NC*GC;
G(x) := 3741.300*(1-x)*ln(2.0*(1-x)/(2-2*x))+3741.300*(1-
3*x)*ln(2.0*(1-3*x)/(2-2*x))+2*x*(-1600.0+3741.300*ln(4.0*x/(2-
2*x)))

> aff:=diff(-G(x),x);
aff := 3741.300*ln(2.0*(1-x)/(2-2*x))-1870.650000*(-2.0/(2-
2*x)+4.0*(1-x)/(2-2*x)^2)*(2-2*x)+11223.900*ln(2.0*(1-3*x)/(2-
2*x))-1870.650000*(-6.0/(2-2*x)+4.0*(1-3*x)/(2-2*x)^2)*(2-
2*x)+3200.0-7482.600*ln(4.0*x/(2-2*x))-1870.650000*(4.0/(2-
2*x)+8.0*x/(2-2*x)^2)*(2-2*x)

> plot(G(x),x=0..0.5);
> plot(aff(x),x=0..0.5);
```



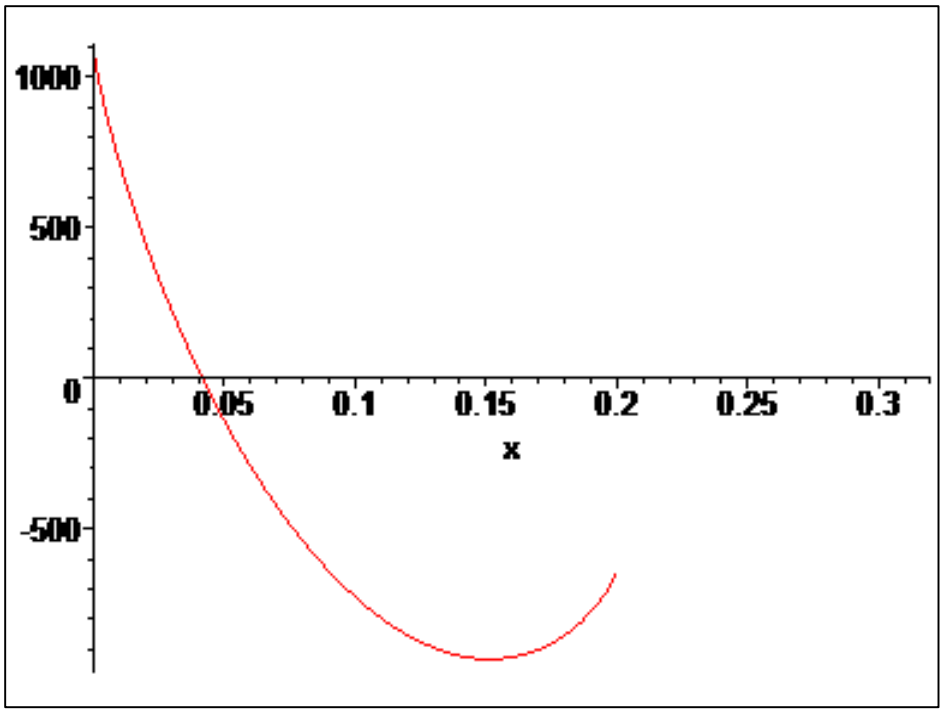
G(x) présente un minimum pour x = 0,2 mol.



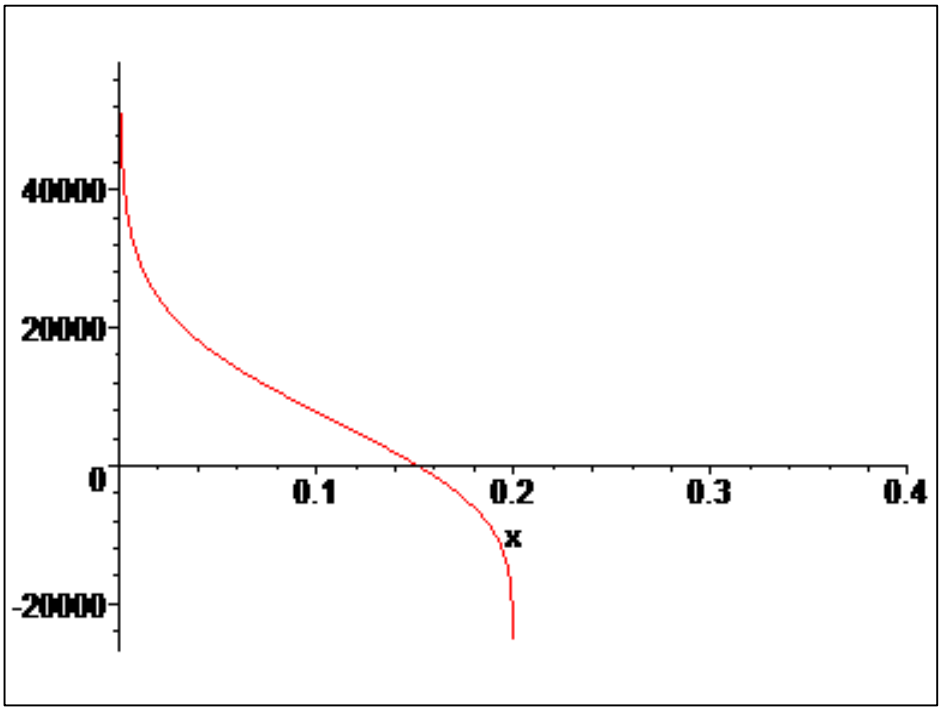
cela correspond à une valeur nulle pour l'affinité $A = -(dG/dx)_{T,P}$

VALEURS NUMERIQUES 2ème cas

```
> restart;
> with(plots):

> R:=8.314:T:=450:PO:=1:PT:=2.0:
> GOA:=0*10^3:GOB:=0*10^3:GOC:=-1.6*10^3:
> NOA:=0.2:NOB:=1:NOC:=0:NUA:=-1:NUB:=-3:NUC:=2:
> NA:=NOA+NUA*x;NB:=NOB+NUB*x;NC:=NOC+NUC*x;NT:=NA+NB+NC;
NA := .2-x
NB := 1-3*x
NC := 2*x
NT := 1.2-2*x
>
actA:=(NA/NT)*(PT/PO);actB:=(NB/NT)*(PT/PO);actC:=(NC/NT)*(PT/PO)
;
actA := 2.0*(.2-x)/(1.2-2*x)
actB := 2.0*(1-3*x)/(1.2-2*x)
actC := 4.0*x/(1.2-2*x)

> GA:=GOA+R*T*ln(actA);GB:=GOB+R*T*ln(actB);GC:=GOC+R*T*ln(actC);
GA := 3741.300*ln(2.0*(.2-x)/(1.2-2*x))
GB := 3741.300*ln(2.0*(1-3*x)/(1.2-2*x))
GC := -1600.0+3741.300*ln(4.0*x/(1.2-2*x))

> G(x):=NA*GA+NB*GB+NC*GC;
G(x) := 3741.300*(.2-x)*ln(2.0*(.2-x)/(1.2-2*x))+3741.300*(1-
3*x)*ln(2.0*(1-3*x)/(1.2-2*x))+2*x*(-
1600.0+3741.300*ln(4.0*x/(1.2-2*x)))

> aff:=diff(-G(x),x);
aff := 3741.300*ln(2.0*(.2-x)/(1.2-2*x))-1870.650000*(-2.0/(1.2-
2*x)+4.0*(.2-x)/(1.2-2*x)^2)*(1.2-2*x)+11223.900*ln(2.0*(1-
3*x)/(1.2-2*x))-1870.650000*(-6.0/(1.2-2*x)+4.0*(1-3*x)/(1.2-
2*x)^2)*(1.2-2*x)+3200.0-7482.600*ln(4.0*x/(1.2-2*x))-
1870.650000*(4.0/(1.2-2*x)+8.0*x/(1.2-2*x)^2)*(1.2-2*x)

> plot(G(x),x=0..0.32);
> plot(aff(x),x=0..0.4);
```



cette fois, G(x) présente un minimum pour x = 0,15 mol.



>

qui correspond à une valeur nulle pour l'affinité $A = -(dG/dx)_{T,P}$