1. From vapor pressure data at 1550 C the following data has been found for the Ni − Fe solution (data adapted from Gaskell). Complete the table.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| item | data | | | | | | | | | | |
| X\_Ni | 1.0000 | 0.9000 | 0.8000 | 0.7000 | 0.6000 | 0.5000 | 0.4000 | 0.3000 | 0.2000 | 0.1000 | 0.0000 |
| X\_Fe |  |  |  |  |  |  |  |  |  |  |  |
| a\_Ni w.r.t. pure l | 1.0000 | 0.8900 | 0.7660 | 0.6200 | 0.4850 | 0.3740 | 0.2830 | 0.2070 | 0.1360 | 0.0670 | 0.0000 |
| γ\_Ni |  |  |  |  |  |  |  |  |  |  |  |
| ln(γ\_Ni) |  |  |  |  |  |  |  |  |  |  |  |
| αNi |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |

2. Using Gibbs −Duhem equation find γFe at XFe = 0.40. Use the trapezoidal rule for integration. Use both the [–(X2/X1).d ln γ; Eq.1 below] and [α.dX2; Eq.2] integrations, and compare.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| item | data | | | | | | | | | | |  |
| X\_Ni | 1.0000 | 0.9000 | 0.8000 | 0.7000 | 0.6000 | 0.5000 | 0.4000 | 0.3000 | 0.2000 | 0.1000 | 0.0000 |  |
| X\_Fe | 0.0000 | 0.1000 | 0.2000 | 0.3000 | 0.4000 | 0.5000 | 0.6000 | 0.7000 | 0.8000 | 0.9000 | 1.0000 |  |
| a\_Ni w.r.t. pure l | 1.0000 | 0.8900 | 0.7660 | 0.6200 | 0.4850 | 0.3740 | 0.2830 | 0.2070 | 0.1360 | 0.0670 | 0.0000 |  |
| γ\_Ni | 1.0000 | 0.9889 | 0.9575 | 0.8857 | 0.8083 | 0.7480 | 0.7075 | 0.6900 | 0.6800 | 0.6700 | 0.6700 |  |
| ln(γ\_Ni) | 0.0000 | -0.0112 | -0.0434 | -0.1214 | -0.2128 | -0.2904 | -0.3460 | -0.3711 | -0.3857 | -0.4005 | -0.4005 |  |
| αNi | -1.1700 | -1.1173 | -1.0857 | -1.3485 | -1.3299 | -1.1614 | -0.9612 | -0.7573 | -0.6026 | -0.4944 | -0.4005 |  |
| X\_Ni/X\_Fe | inf | 9.0000 | 4.0000 | 2.3333 | 1.5000 | 1.0000 | 0.6667 | 0.4286 | 0.2500 | 0.1111 | 0.0000 |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| diff area gamma# | − | -0.2097 | -0.2468 | -0.1752 | -0.0970 | -0.0464 | -0.0137 | -0.0050 | -0.0027 | 0.0000 | 0.0000 | For Eq.1 |
| int area gamma## | − | -0.7964 | -0.5867 | -0.3399 | -0.1647 | -0.0677 | -0.0213 | -0.0076 | -0.0027 | 0.0000 | 0.0000 | For Eq.1 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| diff area alpha# | -0.1144 | -0.1102 | -0.1217 | -0.1339 | -0.1246 | -0.1061 | -0.0859 | -0.0680 | -0.0549 | -0.0447 | 0.0000 | For Eq.2 |
| int area alpha## | -0.9643 | -0.8500 | -0.7398 | -0.6181 | -0.4842 | -0.3596 | -0.2535 | -0.1676 | -0.0996 | -0.0447 | 0.0000 | For Eq.2 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| γ\_Fe from γ\_Ni | − | 0.4510 | 0.5562 | 0.7118 | 0.8482 | 0.9345 | 0.9789 | 0.9924 | 0.9973 | 1.0000 | 1.0000 |  |
| a\_Fe from γ\_Ni | − | 0.0451 | 0.1112 | 0.2135 | 0.3393 | 0.4673 | 0.5873 | 0.6947 | 0.7979 | 0.9000 | 1.0000 |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| γ\_Fe from αNi | 0.3812 | 0.4726 | 0.5677 | 0.7154 | 0.8479 | 0.9331 | 0.9774 | 0.9915 | 0.9968 | 0.9998 | 1.0000 |  |
| a\_Fe from αNi | 0.0000 | 0.0473 | 0.1135 | 0.2146 | 0.3391 | 0.4665 | 0.5865 | 0.6940 | 0.7975 | 0.8998 | 1.0000 |  |

{ Calculations done by spreadsheet. Verify}

ln γFe|XFe = 0.4= − (1)

ln γFe|XFe = 0.4= −αNi XNiXFe − = −αNi XNiXFe + (2)

# diff(erential) area is for area under the curve between two points. ## int(egral) area is the total area from X1=1 to X1 =X1.

The difference in the activity calculated by the two different equations is due to the approximation in the trapezoidal rule.

3. Since we assume the FeO-MnO to be solid, write the following equation taking FeO(s) and MnO(s) as standard states:

MnO(s) + Fe(l) = FeO(s) + Mn(l); K1873 = (a­FeO XMn . γoMn ) / (aMnO . X­Fe) = (X­FeO XMn . γoMn ) / (XMnO . X­Fe). Calculate XFeO/XMnO and then XFeO and XMnO ,

since X­FeO + XMnO = 1. From phase diagram verify whether the solution is indeed solid. Else liquid.