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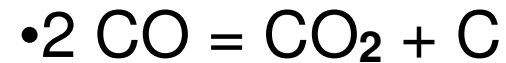
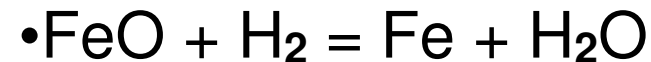
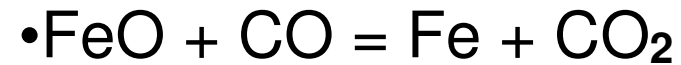
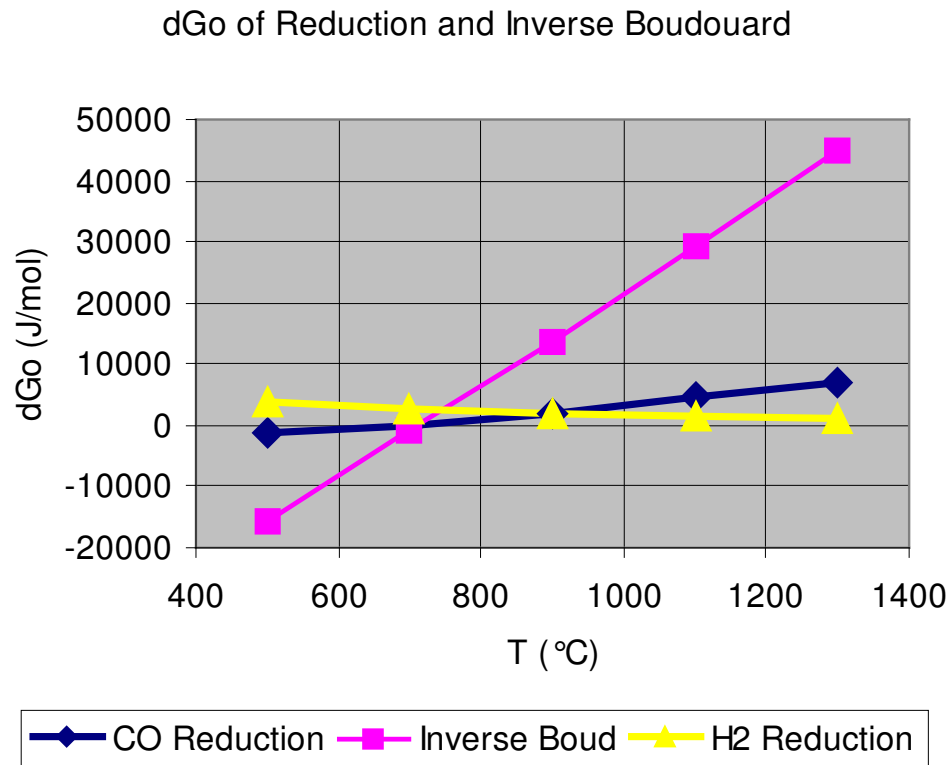
# Gas reduction in Factsage

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influence of reductant and pressure to  
reduction of FeO

**Kees Verweij at GTT Herzogenrath**

# dGo of reduction reactions



CO :

below 700 °C preference for the Boudouard reaction

beyond 700 °C preference for reduction

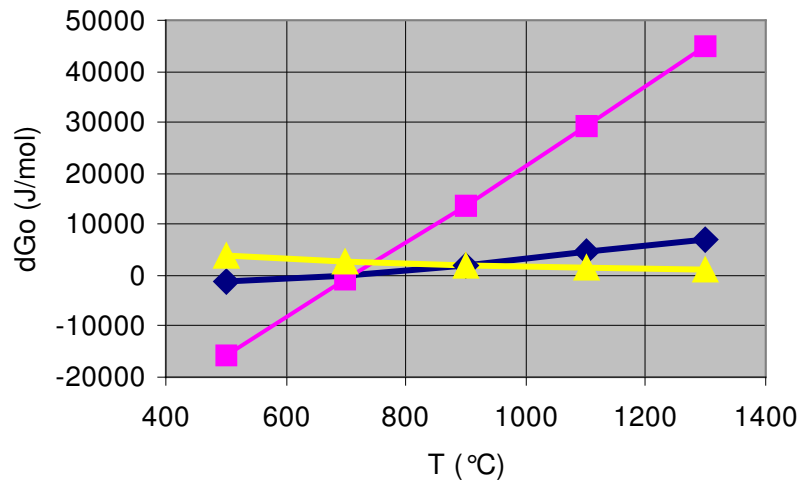
H<sub>2</sub> :

reduction with H<sub>2</sub> at all temperatures, but improves at increasing temperature

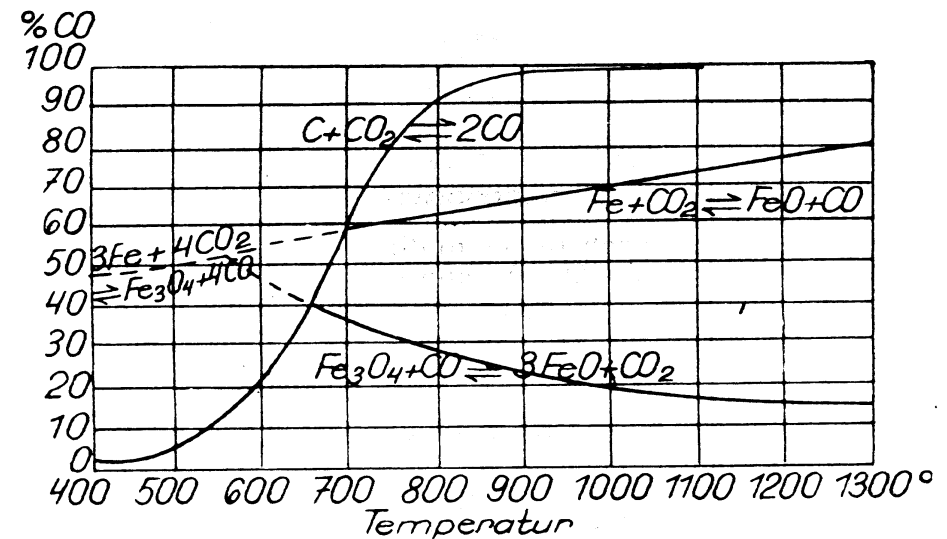
# How does dGo fit to the old presentation ?



dGo of Reduction and Inverse Boudouard



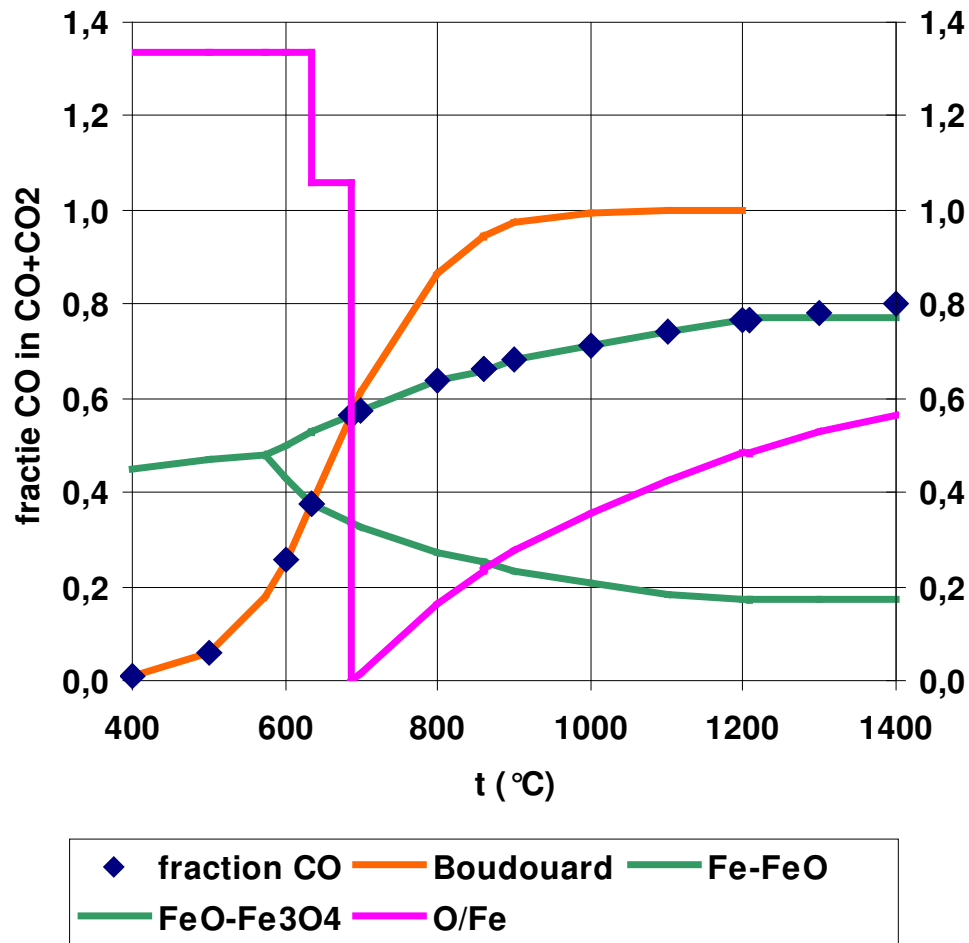
◆ CO Reduction    ■ Inverse Boud    ▲ H2 Reduction



# Bauer Gläserner diagram



65 CO + 28 FeO



base case :

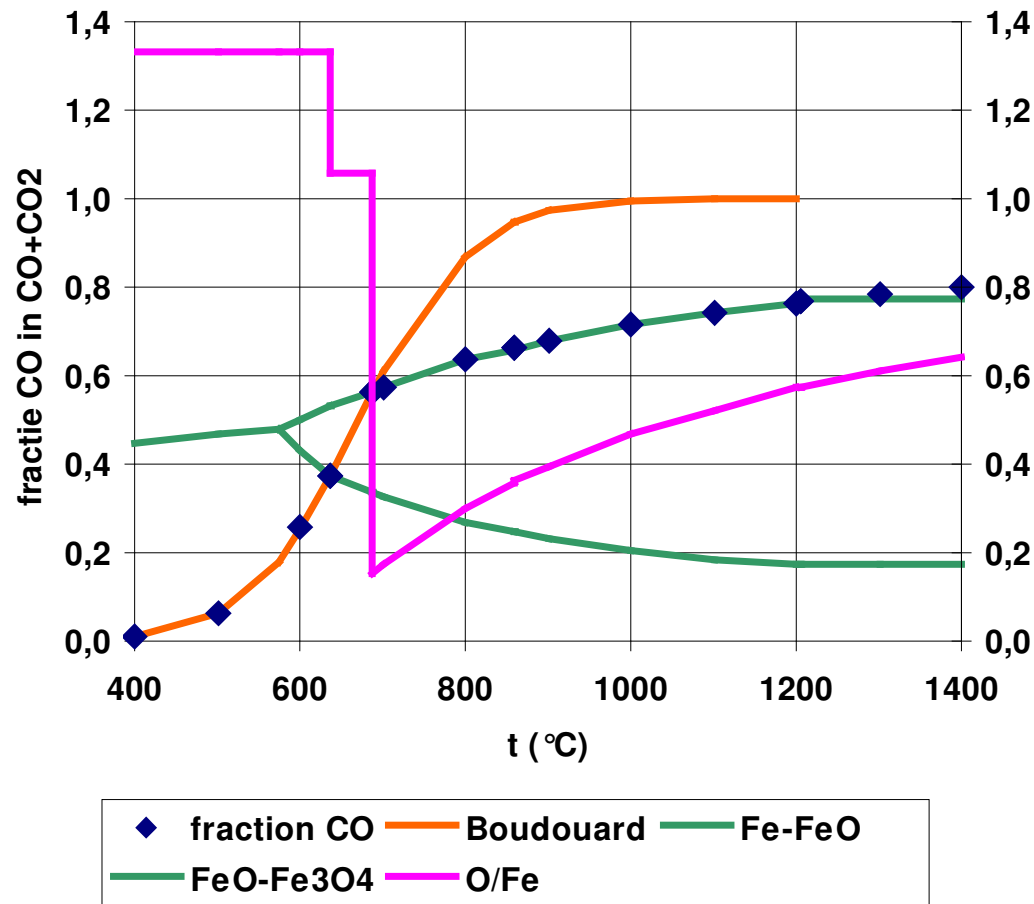
- includes O / Fe line
- Boudouard curve

100 % reduction at  
700 °C

gas equilibria follow  
Boudouard and FeO-  
Fe line

# Shortage of CO

55 CO + 28 FeO



reduction at 700 °C  
below 85 %

O / Fe line increases  
with increase in  
temperature :  
this is due to increase in  
dGo

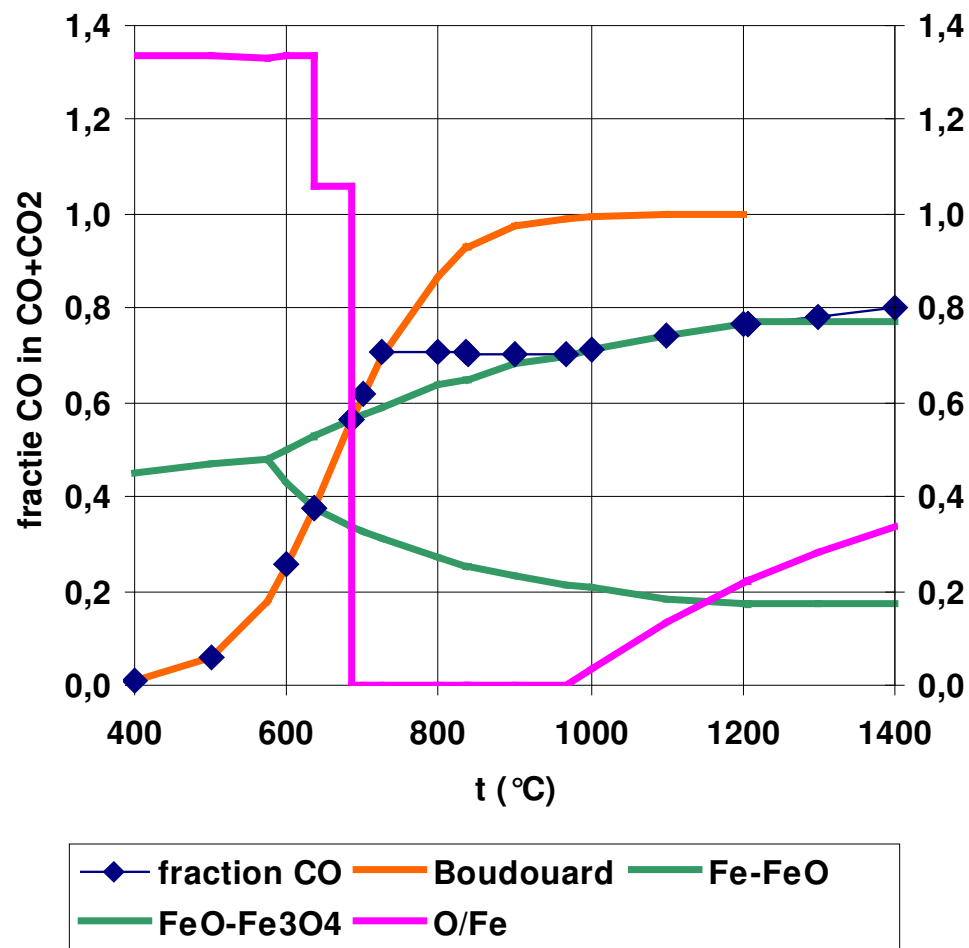
→ equilibrium shifts to  
the left of reaction 1

→ gas usage decreases

# Surplus of CO



95 CO + 28 FeO



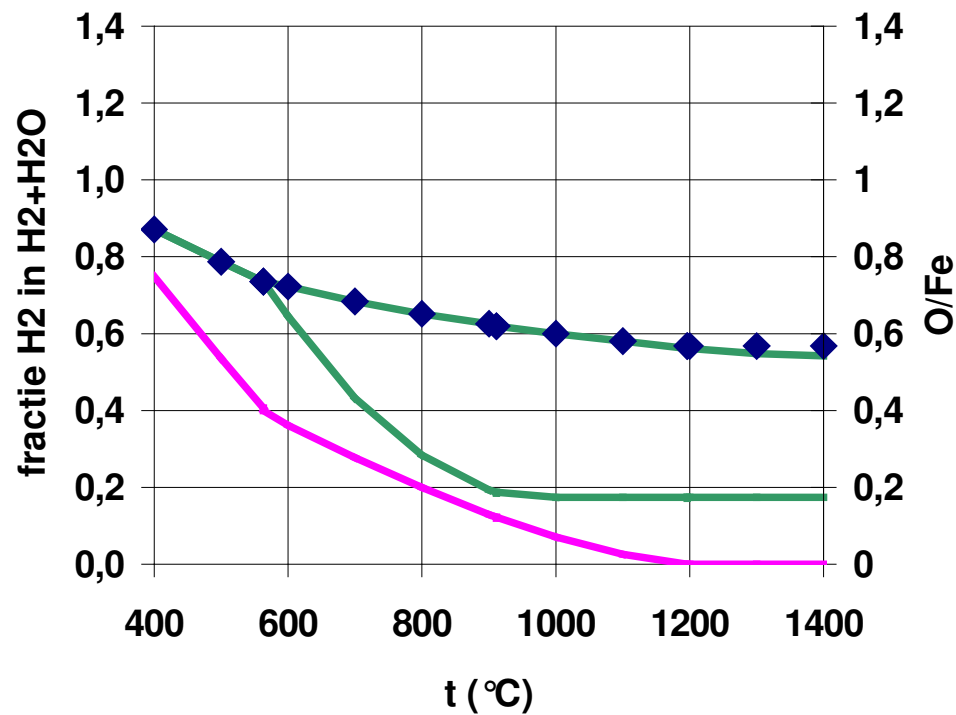
the full reduction is achieved over a broader temperature range

around 700 – 900 °C  
not all CO is used and equilibria deviate from green FeO-Fe line

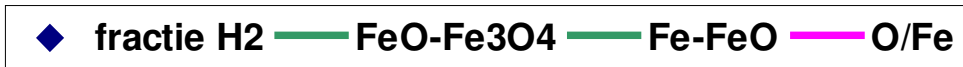
# Reduction with H<sub>2</sub>



65 H<sub>2</sub> + 28 FeO



100 % reduction is achieved beyond 1150 °C

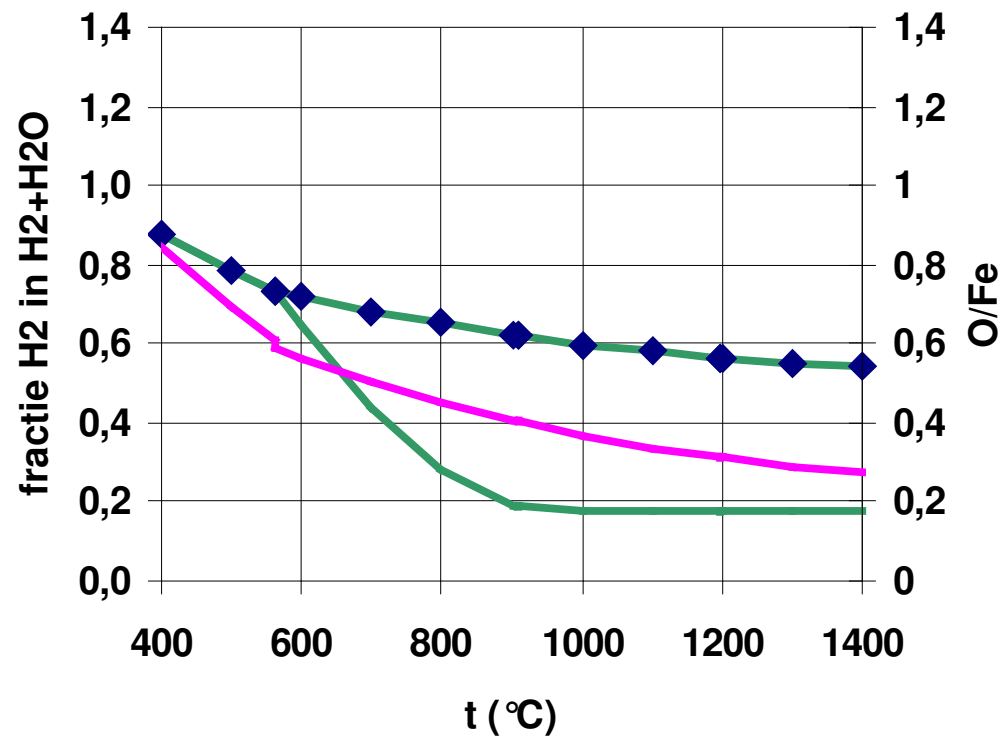


# Shortage of H<sub>2</sub>



45 H<sub>2</sub> + 28 FeO

reduction is worse than 70 %

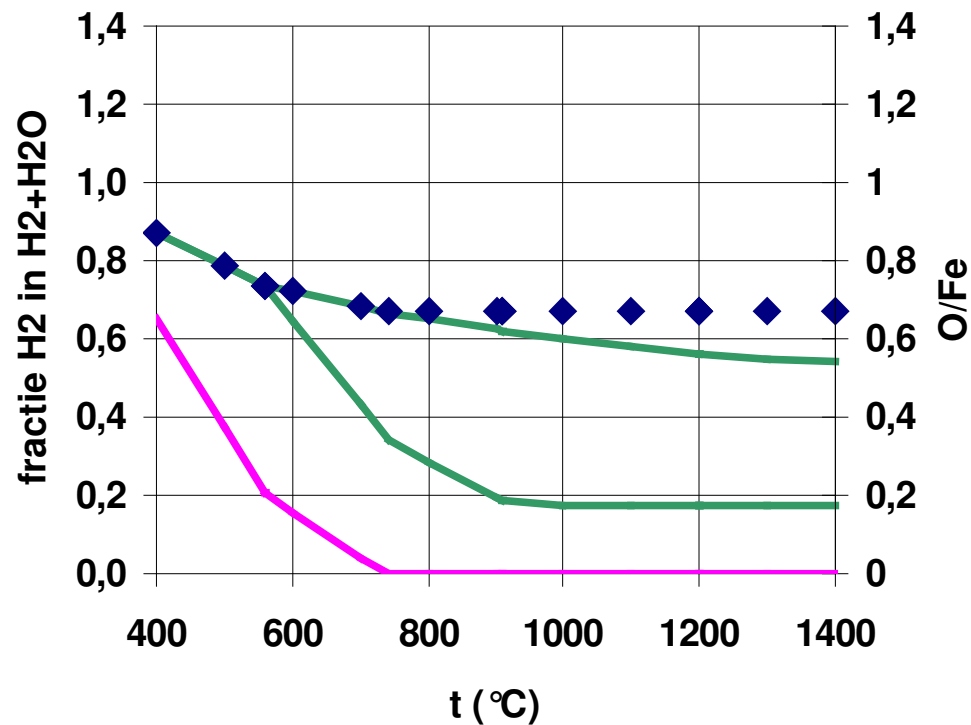




# Surplus of H<sub>2</sub>



85 H<sub>2</sub> + 28 FeO



reduction achieves 100 %  
beyond 750 °C

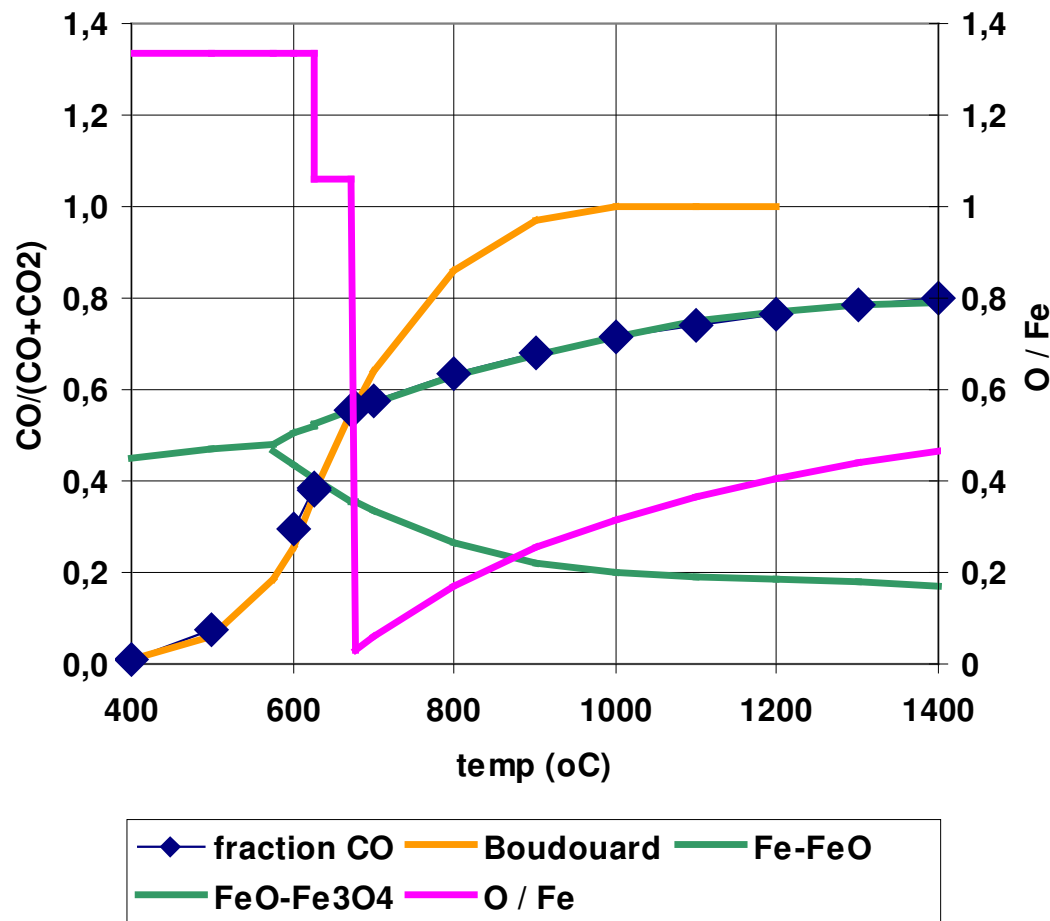
beyond 750 °C there is  
surplus of H<sub>2</sub> available

→ equilibria deviate from  
FeO – Fe line

# Replacement of CO by H<sub>2</sub>



28 FeO + 55 CO + 10 H<sub>2</sub> 1 atm

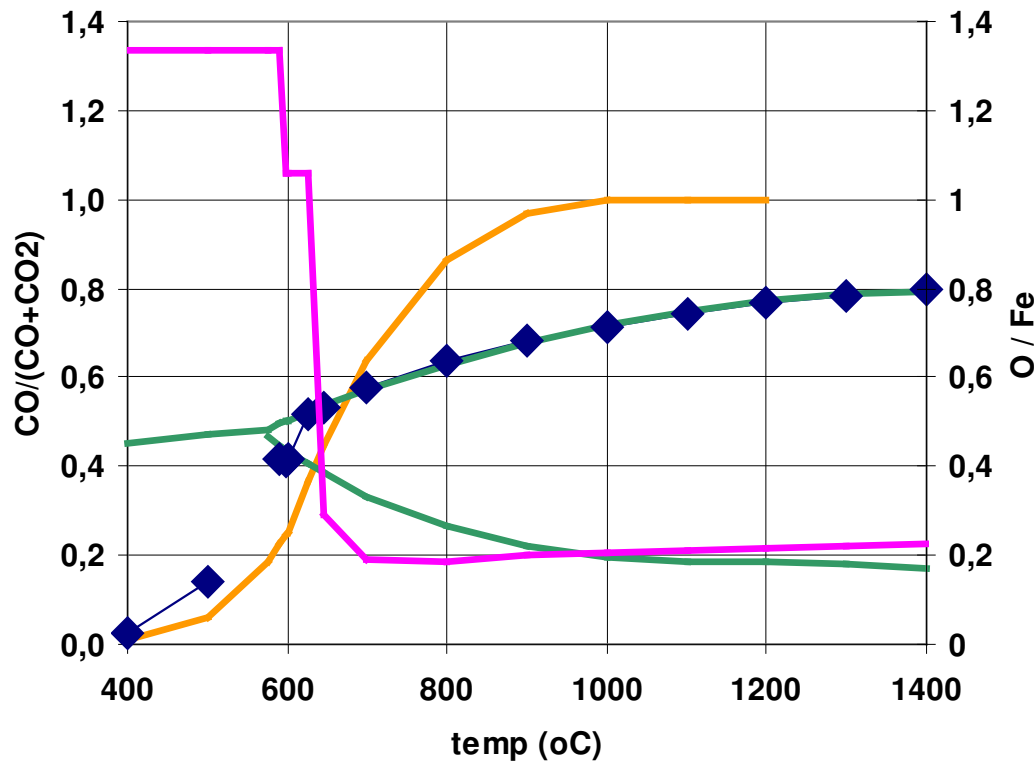


maximum reduction  
at 700 °C is 95 %

# Replacement of CO by H<sub>2</sub>



28 FeO + 30 CO + 35 H<sub>2</sub> 1 atm

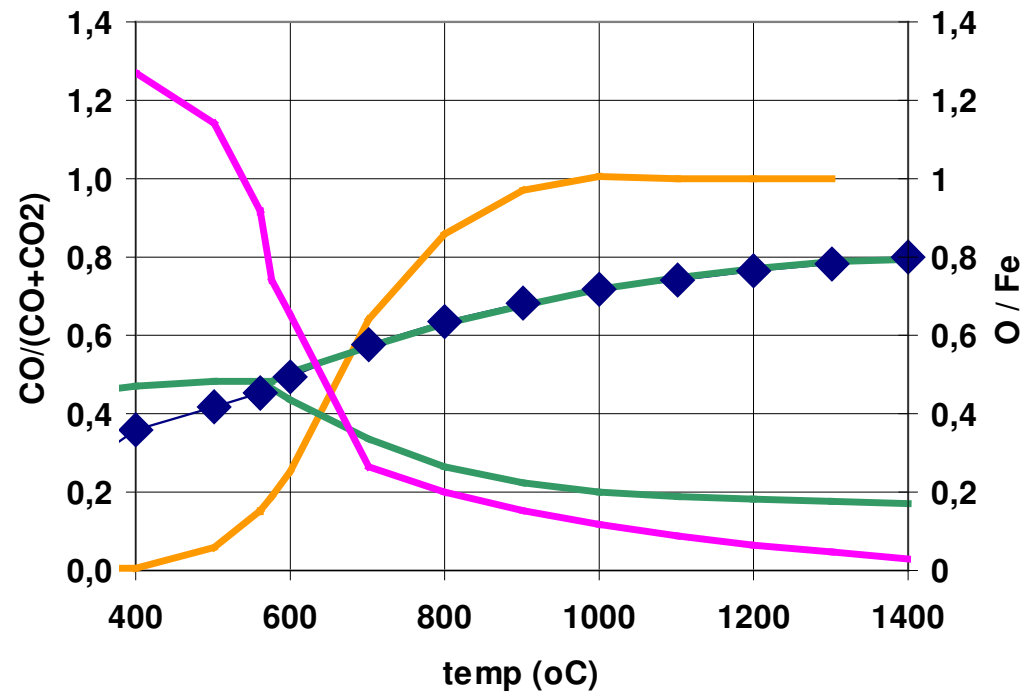


maximum reduction of 80 % over the temperature range is possible

# Replacement of CO by H<sub>2</sub>

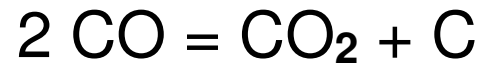


28 FeO + 10 CO + 55 H<sub>2</sub> 1 atm



O / Fe starts to resemble that of pure H<sub>2</sub>

# Boudouard 1 : influence of p

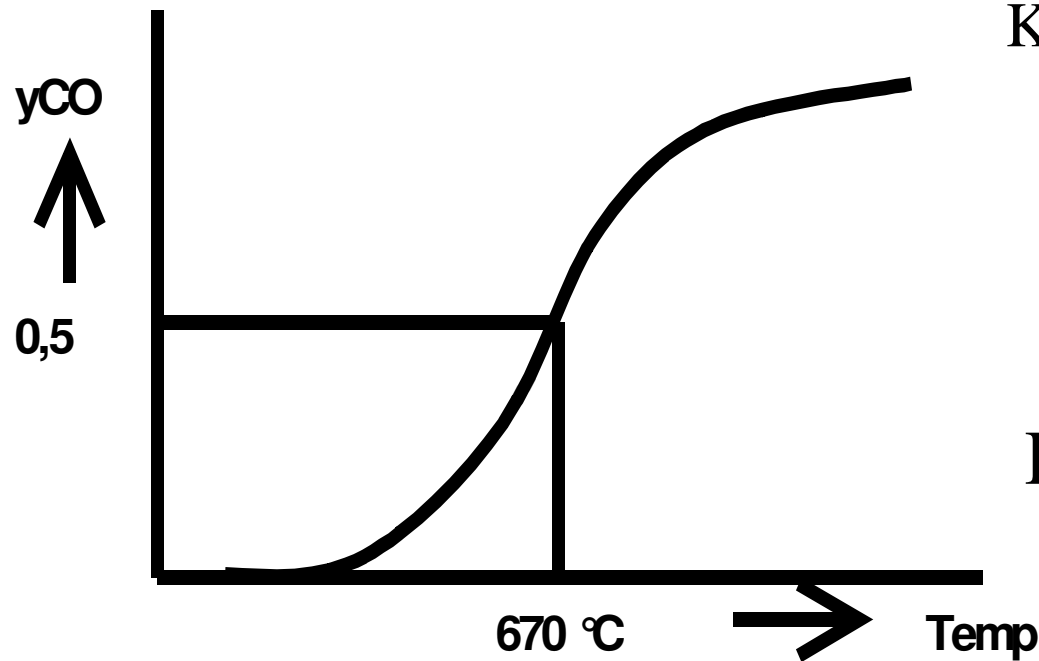


$$\Delta G_{\text{reaction}} = \Delta G^0 + RT * \ln K$$

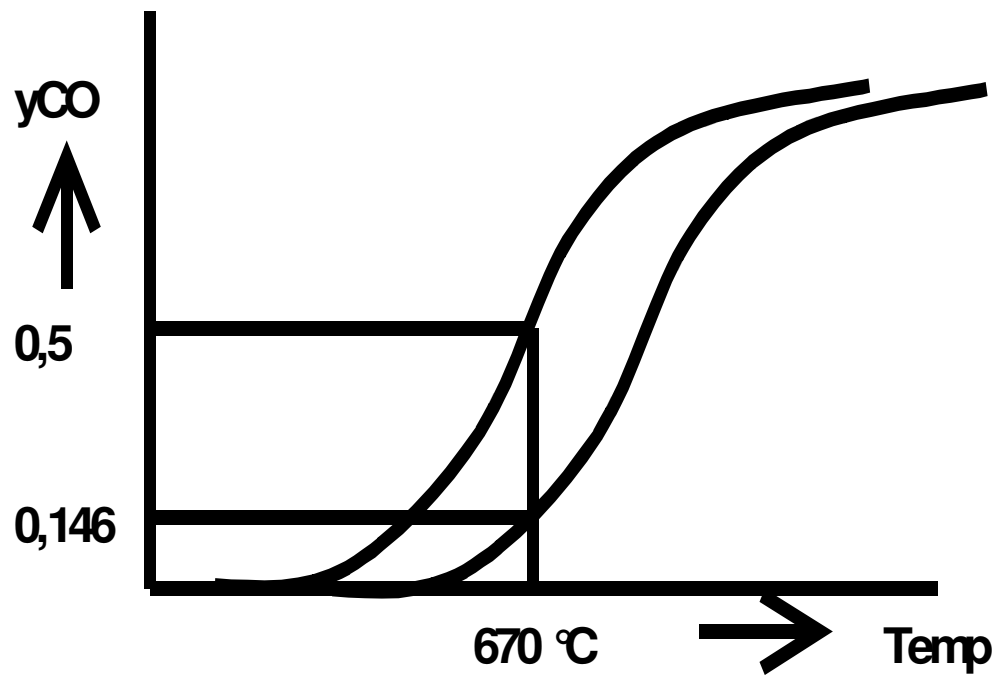
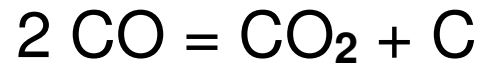
$$K = \frac{a_c * y_{\text{CO}_2} * P_{\text{total}}}{y_{\text{CO}}^2 * P_{\text{total}}^2} = \frac{y_{\text{CO}_2}}{y_{\text{CO}}^2 * P_{\text{total}}}$$

$$y_{\text{CO}} = 0,5$$

$$K = \frac{y_{\text{CO}_2}}{y_{\text{CO}}^2 * 1} = \frac{0,5}{0,25 * 1} = 2$$



# Boudouard 2 : influence of p



$$y_{\text{CO}} = 0,5$$

$$K = \frac{y_{\text{CO}_2}}{y_{\text{CO}}^2 * 1} = \frac{0,5}{0,25 * 1} = 2$$

$$\Delta G^0 (1 \text{ atm}) = \Delta G^0 (20 \text{ atm}) \rightarrow$$

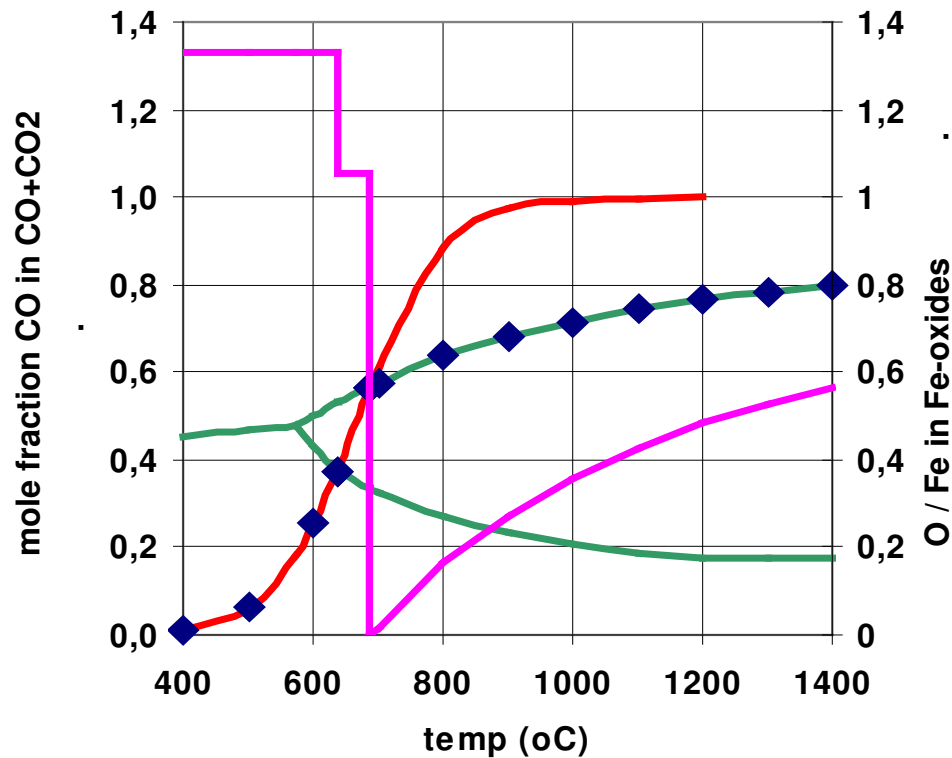
$$RT * \ln K (1 \text{ atm}) = RT * \ln K (20 \text{ atm})$$

$$K = \frac{y_{\text{CO}_2}}{y_{\text{CO}}^2 * 20} = \frac{1 - y_{\text{CO}}}{y_{\text{CO}}^2 * 20} = 2$$

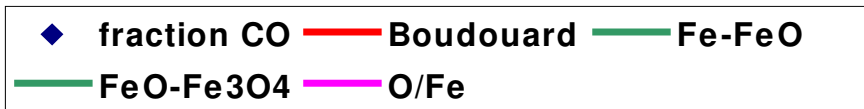
$$\rightarrow y_{\text{CO}} = 0,146$$

# Base case at 1 atm

65 CO + 28 FeO 1 atm



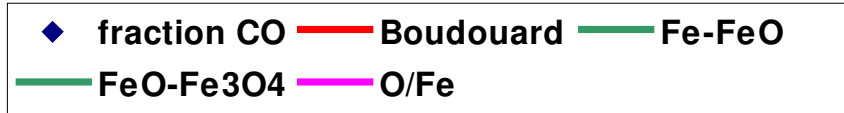
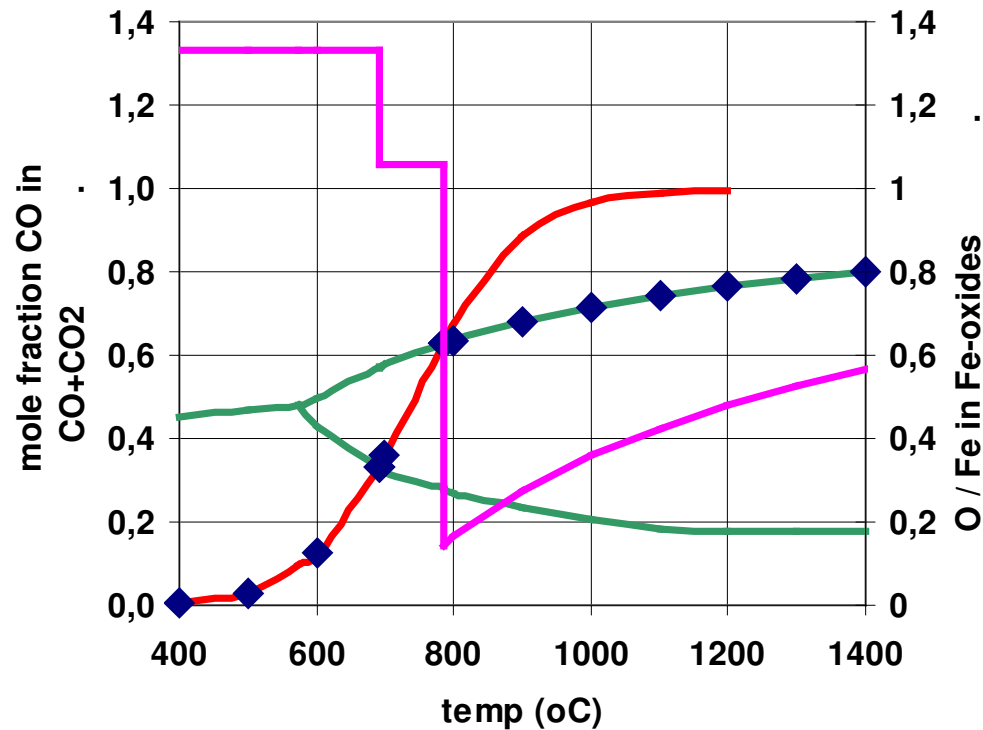
100 % reduction at 700 °C



# CO at 5 atm



65 CO + 28 FeO 5 atm



reduction of FeO reduces from 100 % at 700 °C to 85 % at 780 °C

due to shift of Boudouard curve

reduction equimolecular in gas

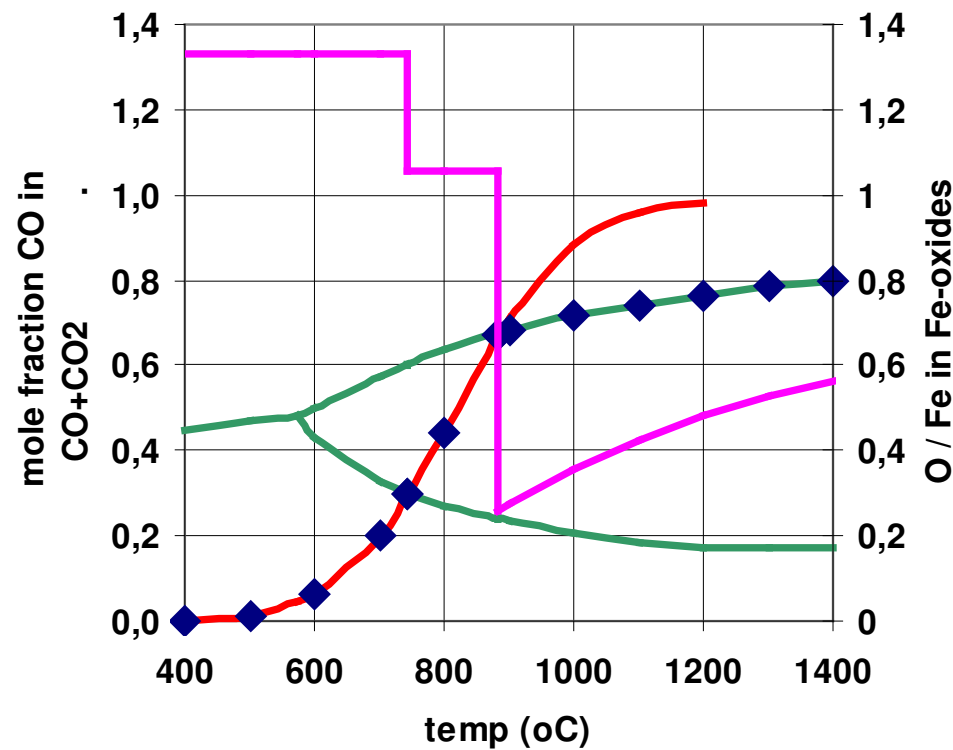
→ no shift in FeO-Fe line



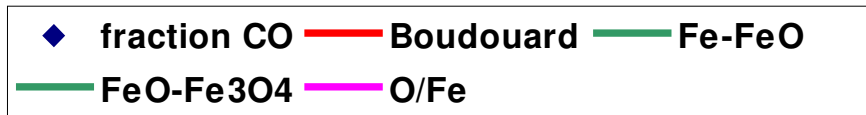
# CO at 20 atm



65 CO + 28 FeO 20 atm

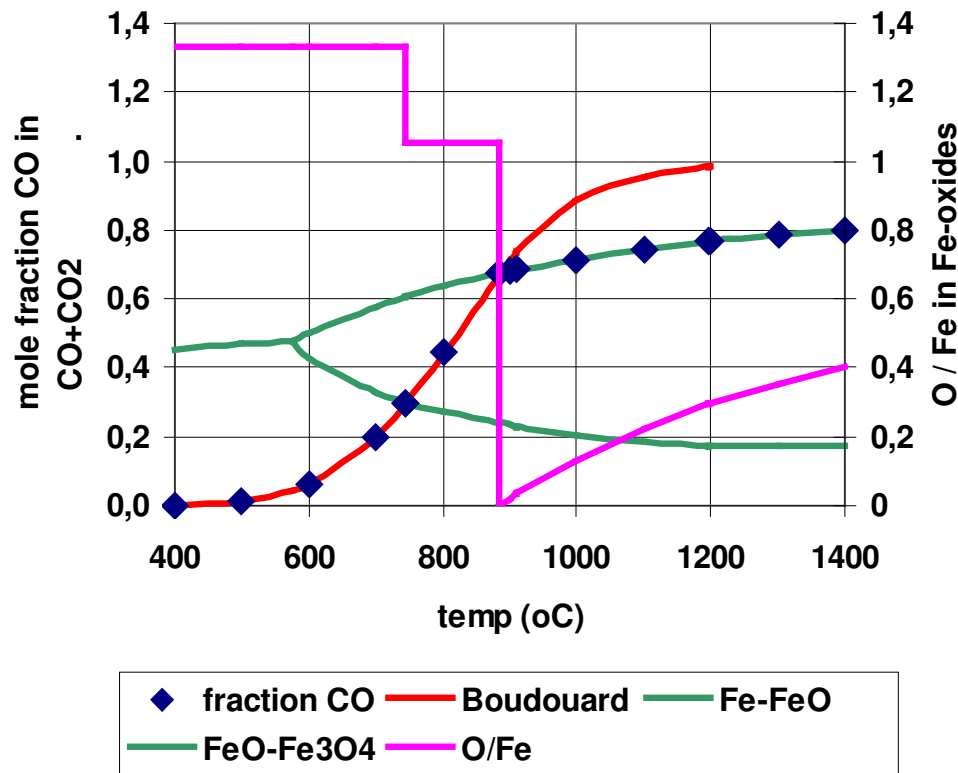


reduction less than 80 %



# Reduction back to 100 %

86 CO + 28 FeO 20 atm



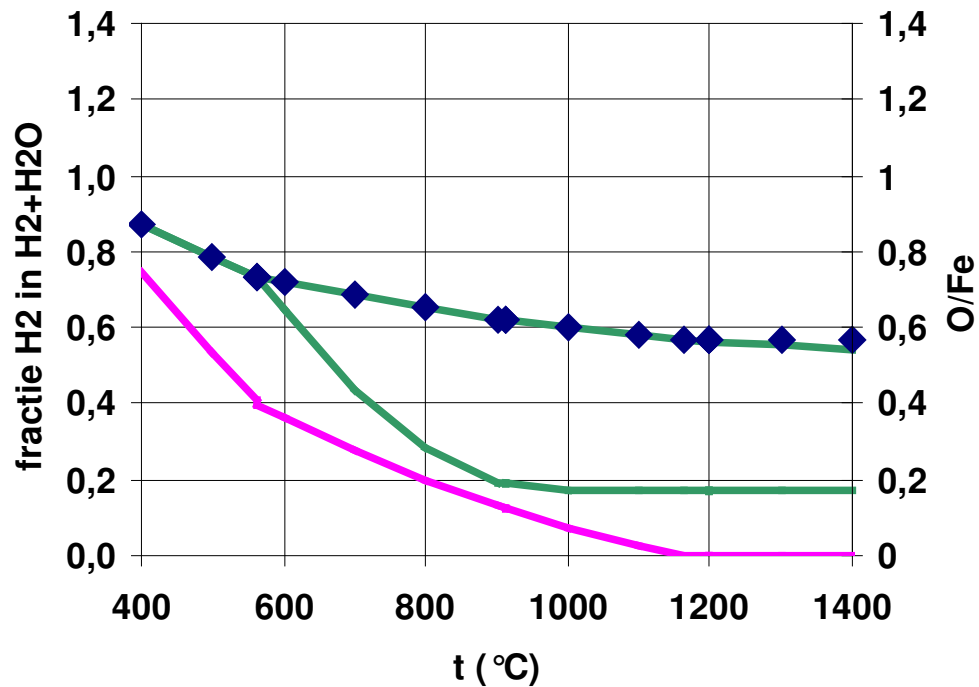
reduction back to 100 %  
due to surplus of CO

(86 instead of 65 moles  
of CO)

# H<sub>2</sub> at 20 atm



65 H<sub>2</sub> + 28 FeO at 20 atm



◆ fractie H<sub>2</sub> — FeO-Fe<sub>3</sub>O<sub>4</sub> — Fe-FeO — O/Fe

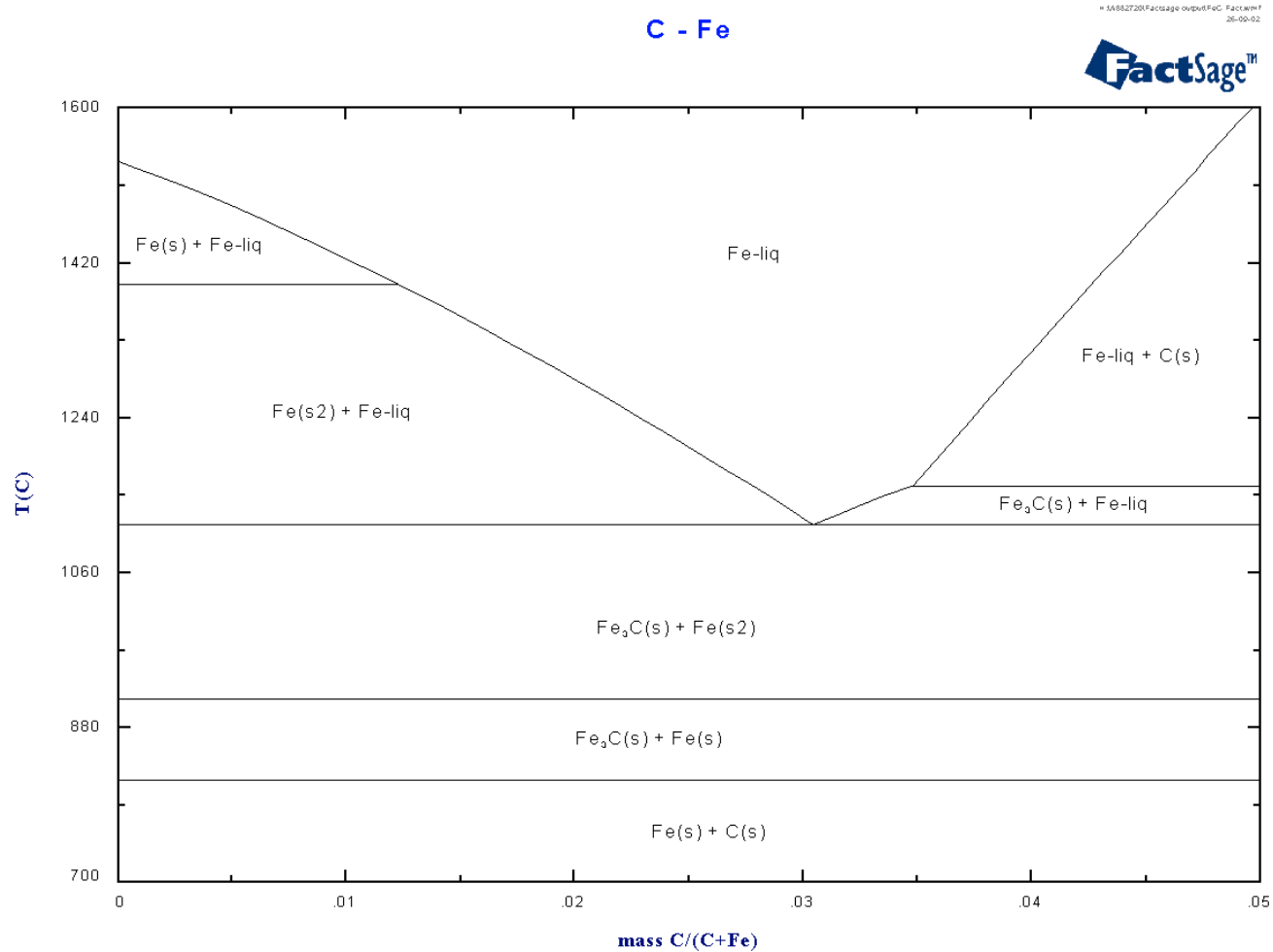
no Boudouard

equimolecular reaction

→ no  $P_{\text{total}}$  in K

no change in K due to change in pressure

# Fe C diagram FS50 data



# Fe C diagram 9148C10G data

