Thermo-Calc Software

Thermo-Calc: For All Kinds of Thermodynamic Calculations!

Thermodynamic Calculations for Materials in Corrosive Environments

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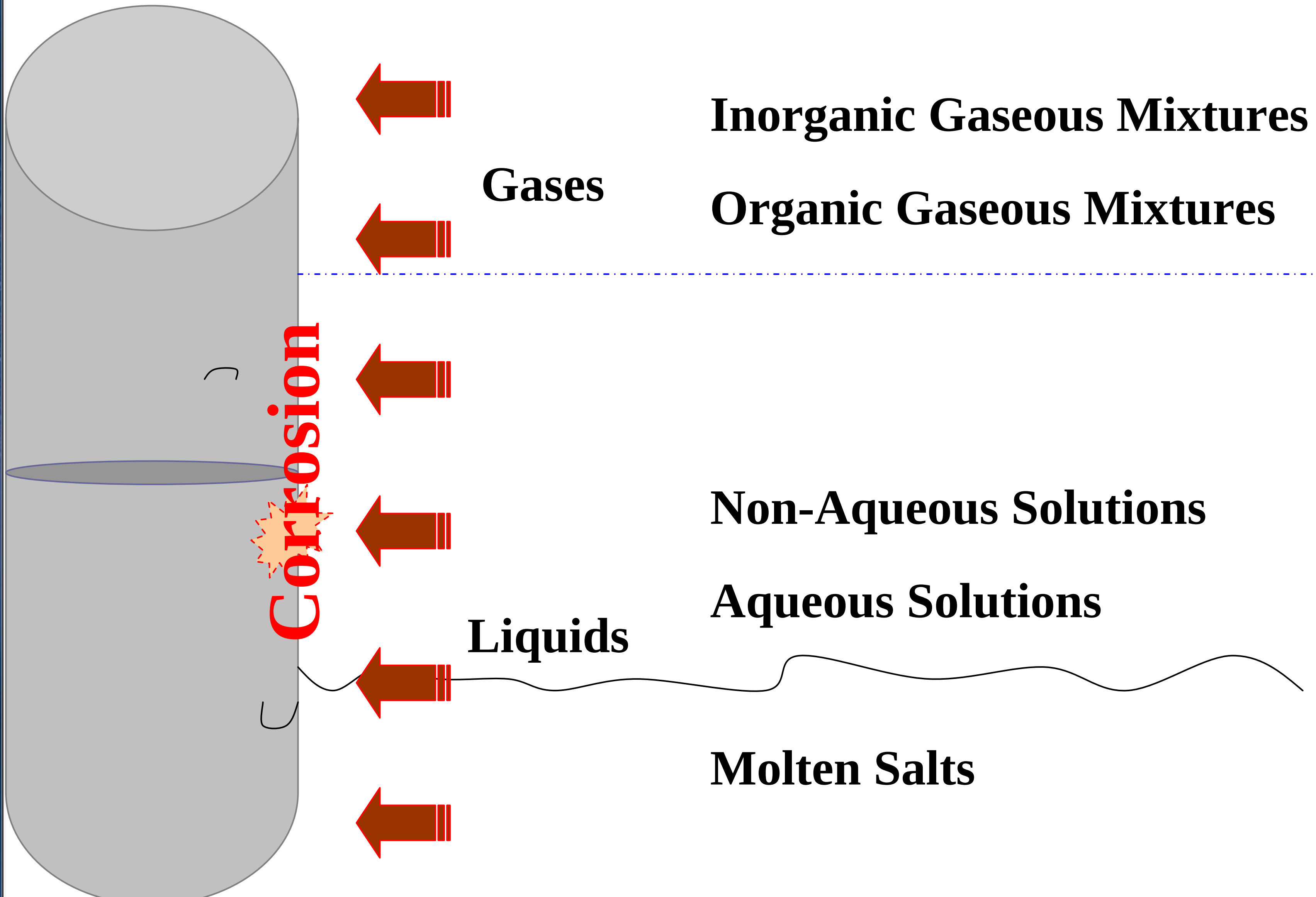
Application Environments



Materials in Applications: Corrosion Types

- Aqueous Corrosion; *Non-Aqueous Corrosion*
- Molten Salt Corrosion
- High-Temperature (Gaseous) Corrosion
- Surface Redox Reactions

Aqueous Solution Models & Databases

Thermo-Calc Software

Thermodynamic models handle EOS & all kinds of thermodynamic properties for various materials.

Following models are now available in Thermo-Calc:

- Component-Energy Model (*interaction on up to ten sublattices):*
  - Redlich-Kister polynomials (Muggianu or Kohler extrapolation)
  - Stoichiometric constraints
  - Interstitial solution
  - Chemical ordering
  - Ionic constituents
- Ionic Two-Sublattice Liquid Model
- Associated Solutions
- Quasi-chemical Model
- Kapoor-Frohberg Cell Model
- Magnetic Ordering
- CVM (Cluster Variation Methods) for chemical ordering
- Birch-Murnagham Model (pressure dependency)
- SUPERFLUID fluid & gaseous mixture
- Aqueous Solution Models (DHLL, SIT, HKF & PITZ) ←-----→ *Databases:* TCAQ2 & AQS2
- Flory-Huggins Model for polymers

Aqueous: Various Applications

MSE R&D:

- Hydro-Metallurgical Processes
- Hydrothermal Formation and Separation Processes
- High-/Low-Temperature Corrosion Processes
- Recycling Processes

Other R&D:

- Aqueous Chemistry
- Chemical Engineering
- Food, Medicine & Energy Production
- Geochemical Systems (Natural Resources)
- Environmental Protections of Water Resources
- Environmental Impact of Nuclear Fuel Waste
- Environmental Assessment of Industrial Pollution
- *... and many more*

Properties in Aqueous-Involving Systems

Thermo-Calc Software

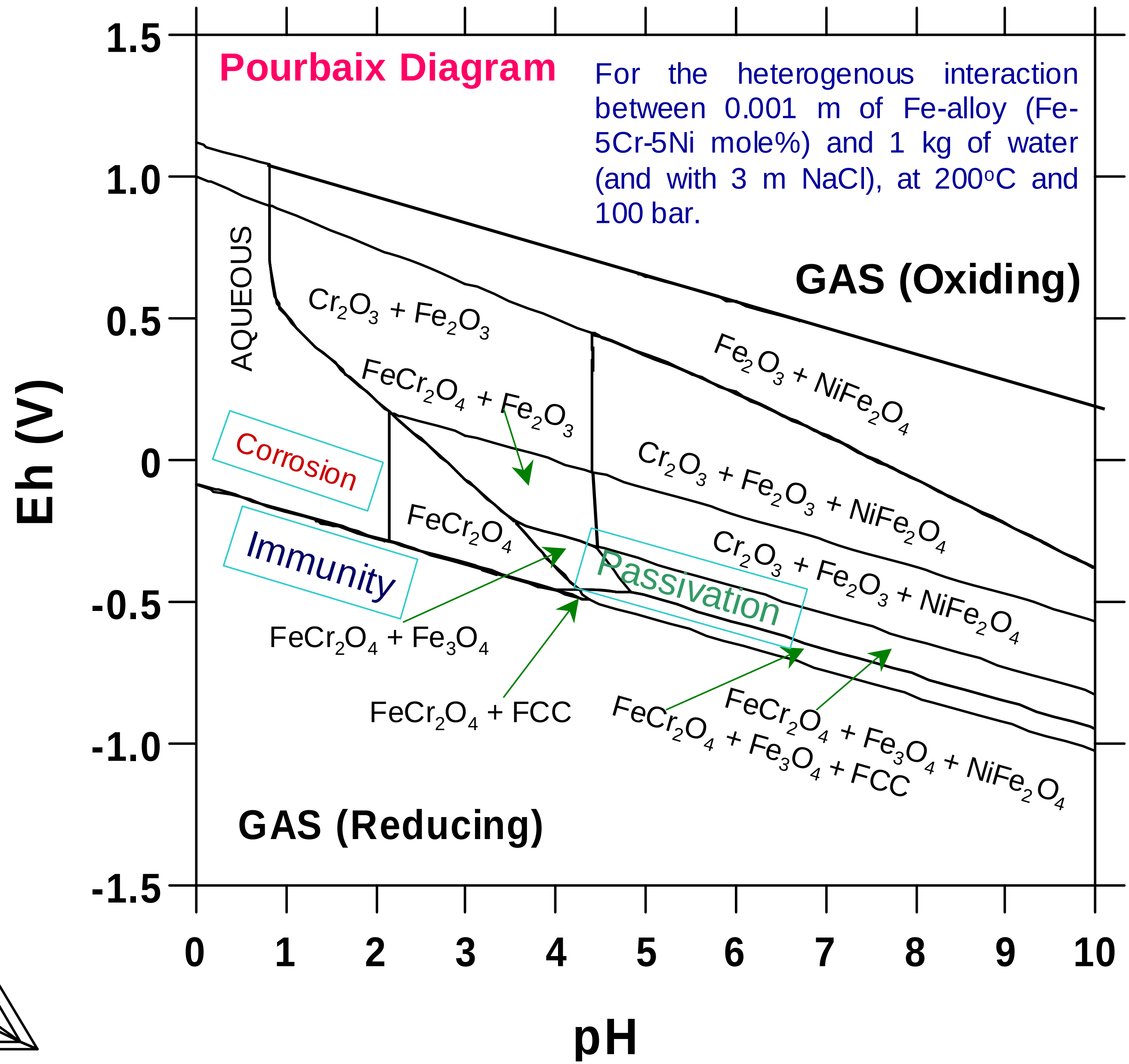
Use Thermo-Calc and Databases to Calculate Heterogeneous Equilibria and Phase/Property Diagrams Involving Aqueous Solutions with following outputs:

T	Temperature (^oC or K)
P	Pressure (Pa)
NP	Stable Phase (mole/kg of water)
BP	Stable Phase (gram/kg of water)
pH	Acidity
Eh	Electronic Potential (V)
Ah	Electronic Affinity (kJ)
pe	Electronic Activity (log10ACRe)
IS	Ionic Strength
TM	Total Concentration (in molality)
Aw	Activity of Water
Oc	Osmotic Coefficient
MF(AQsp)	Mole Fractions of Aqueous Species
ML(AQsp)	Molalities of Aqueous Species
AI(AQsp)	Activities of Aqueous Species
RC(AQsp)	Activity Coefficients of Aqueous Species

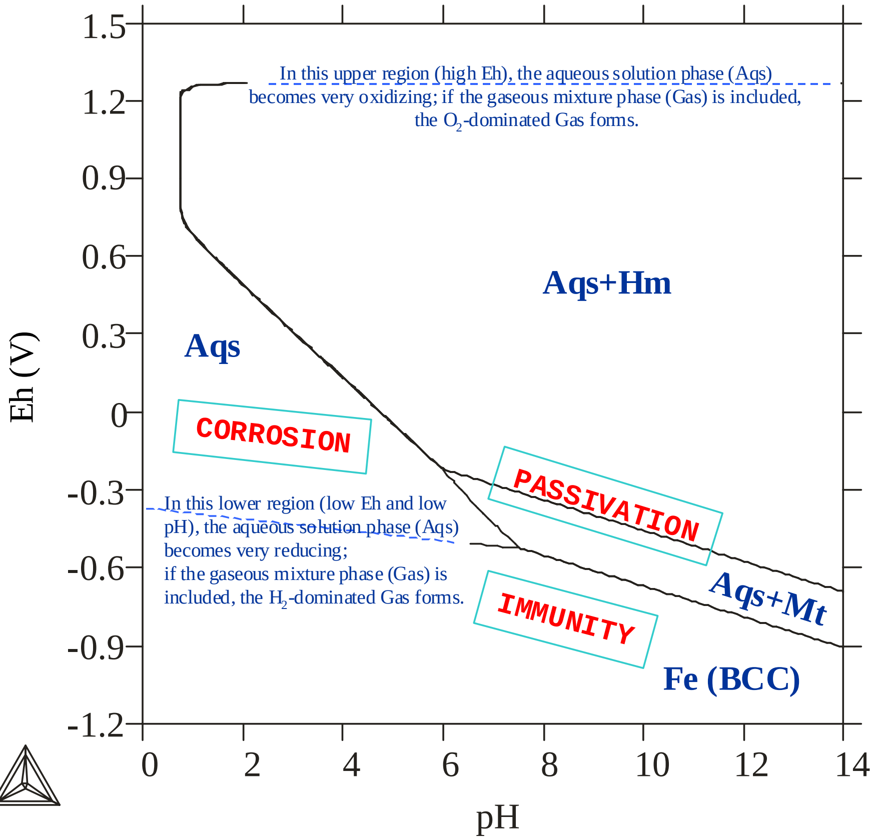
… and many more …

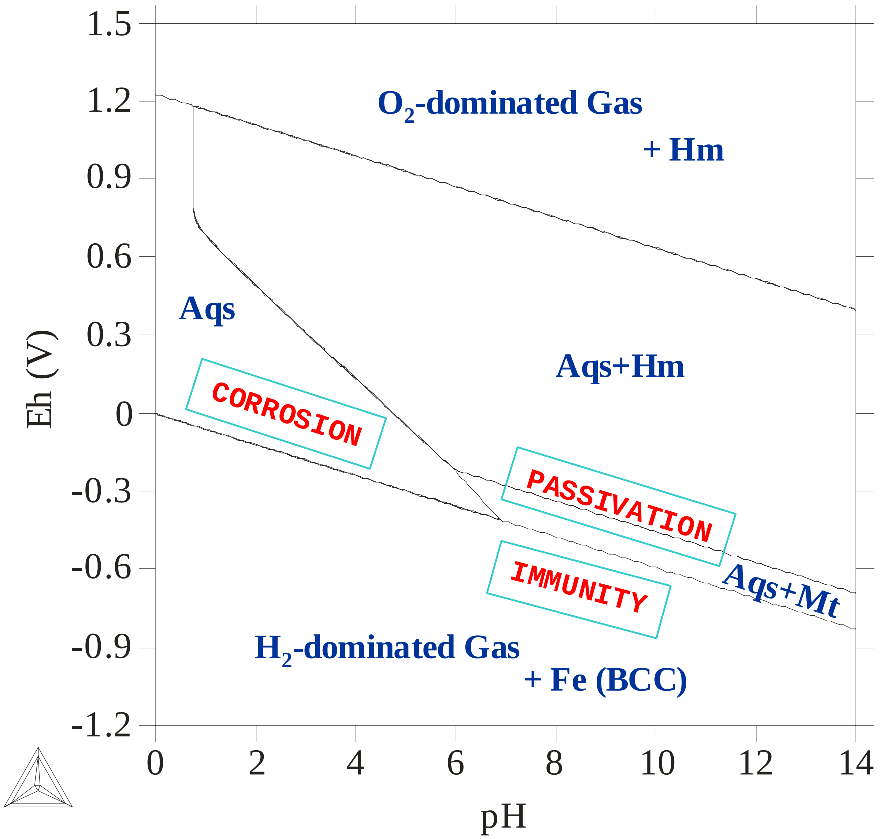
Aqueous Corrosion: Pourbaix Diagrams

Pourbaix Diagrams in Multicomponent Systems



Complete Pourbaix Diagrams !

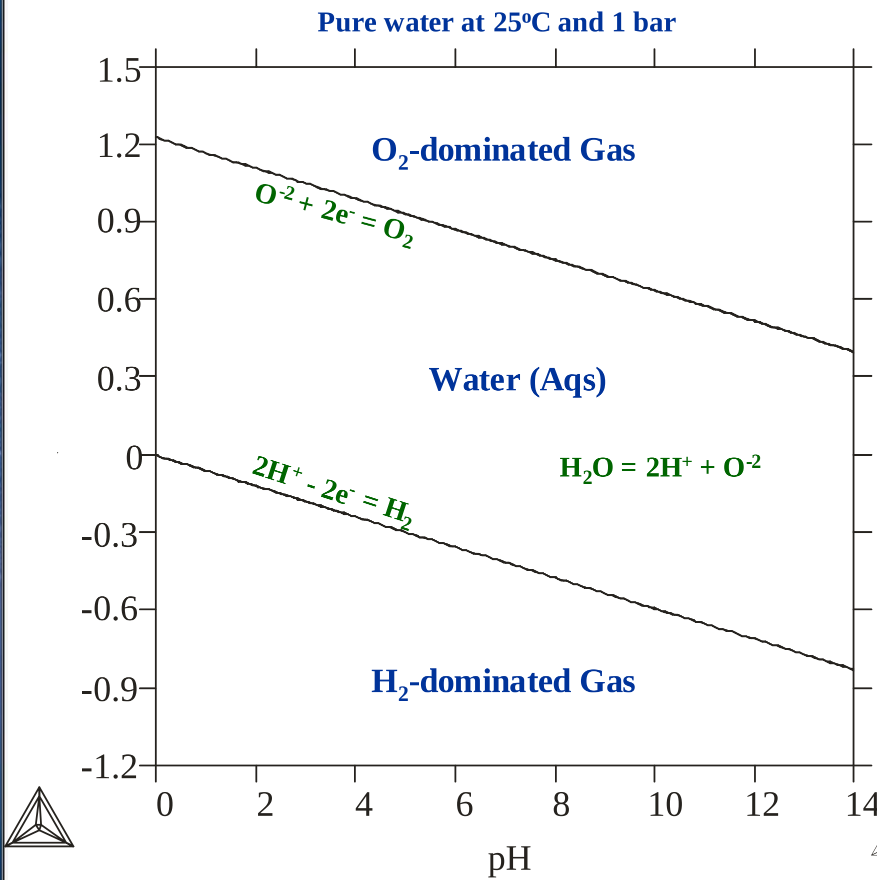


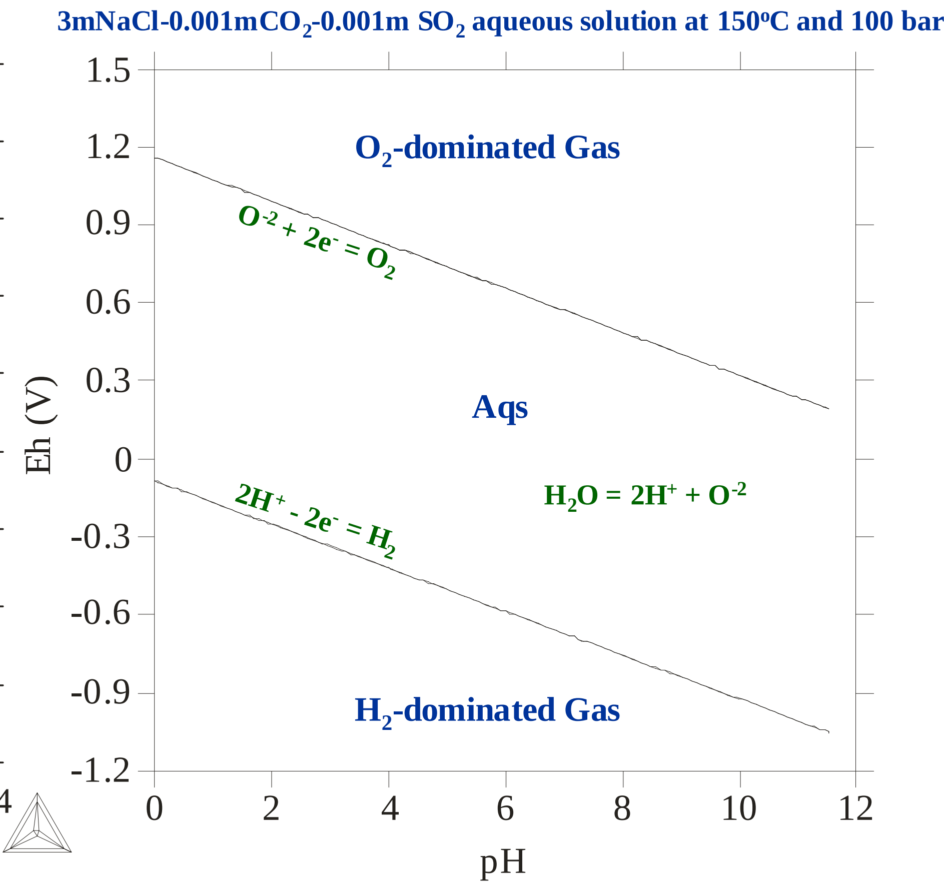


"Pourbaix diagram" of Fe (with 0.001 mole Fe in 1 kg of pure water at 25°C and 1 bar; gas *excluded* in the calculation).

Pourbaix diagram of Fe (with 0.001 mole Fe in 1 kg of pure water at 25°C and 1 bar; gas *included* in the calculation).

Aqueous/Gaseous Phase Boundaries

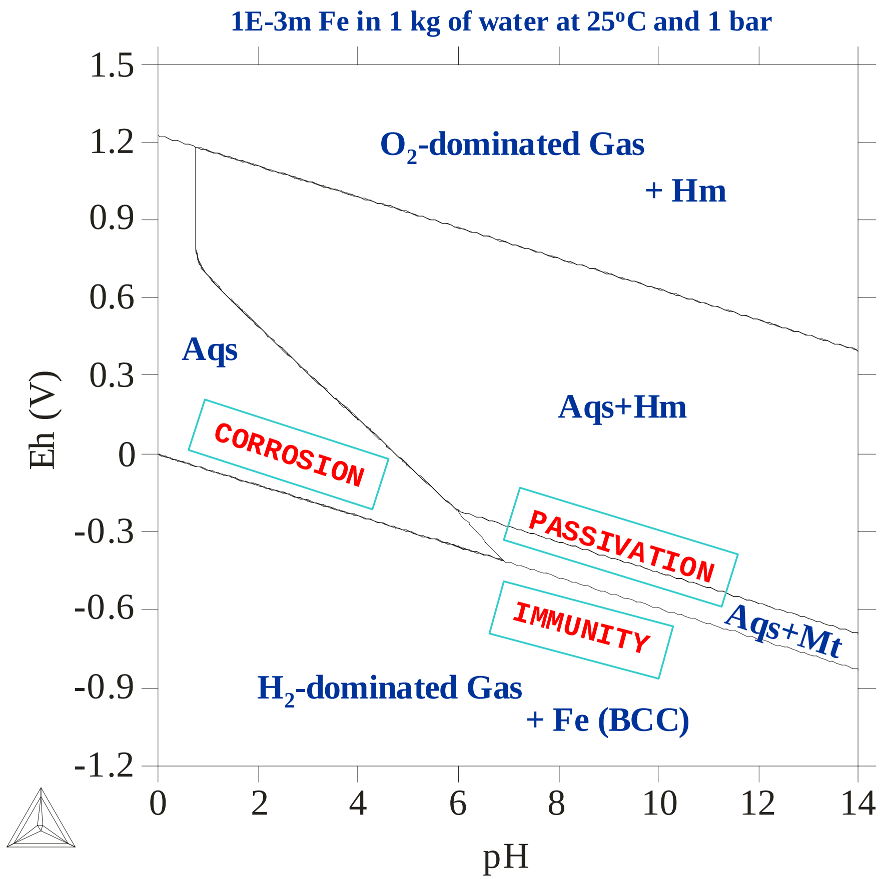




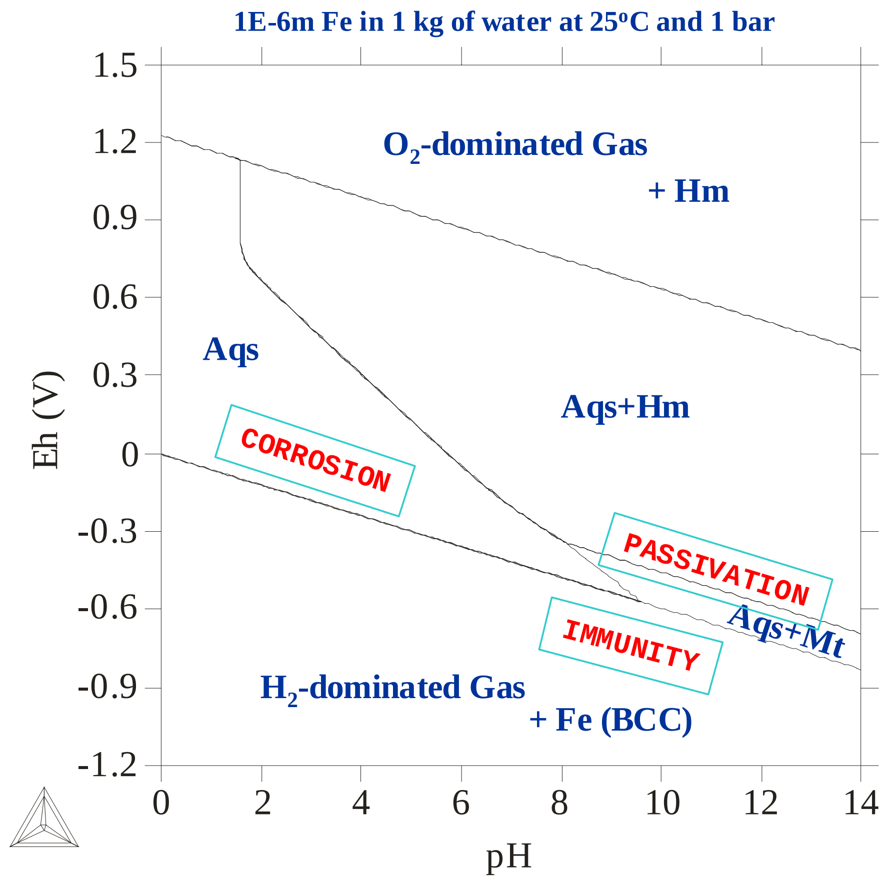
The pH-Eh diagrams for pure water at 25ºC and 1 bar, and for an 3mNaCl-0.001mCO_2-0.001mSO_2 aqueous solution at 150ºC and 100 bar.

Pourbaix Diagrams: Simple Systems (I)

Pure Fe: under various initial compositions



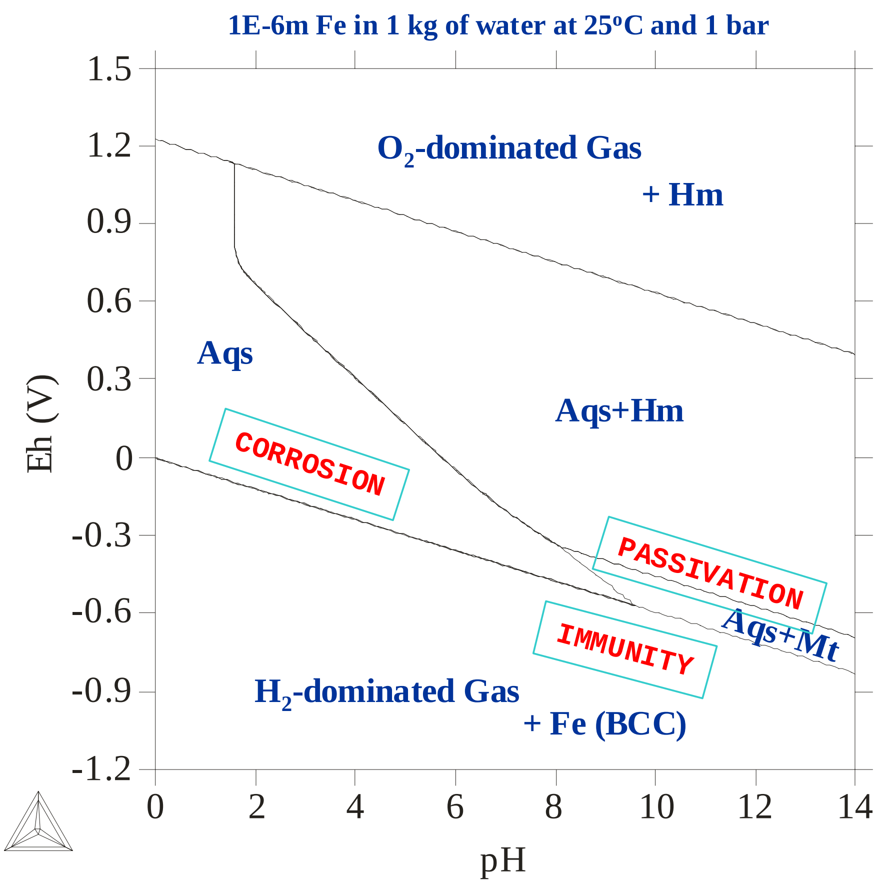
Pourbaix diagram of Fe (with 1E-3 mole Fe in 1 kg of pure water) at 25°C and 1 bar.

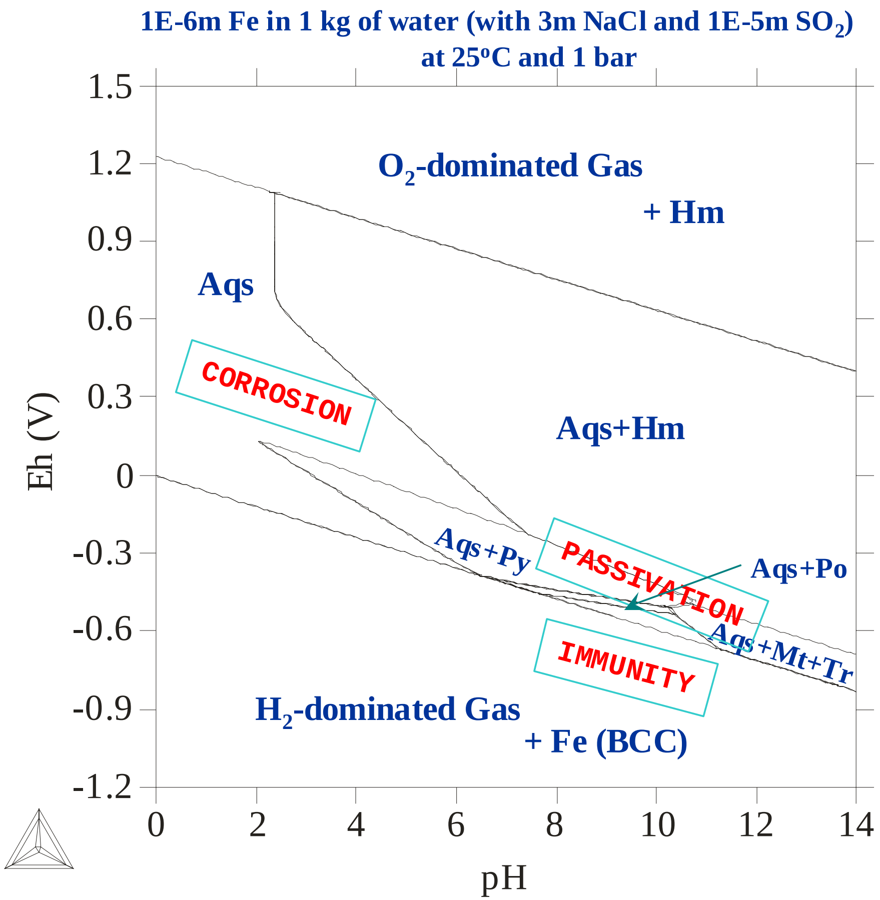


Pourbaix diagram of Fe (with 1E-6 mole Fe in 1 kg of pure water) at 25°C and 1 bar.

Pourbaix Diagrams: Simple Systems (II)

Pure Fe: in different aqueous solutions





Pourbaix diagram of Fe (with 1E-6 mole Fe in 1 kg of pure water) at 25ºC and 1 bar.

Pourbaix diagram of Fe (with 1E-6 mole Fe in 1 kg of water, 3m NaCl and 1E-5 m SO_2) at 25ºC and 1 bar.

Pourbaix Diagrams: Simple Systems (III)

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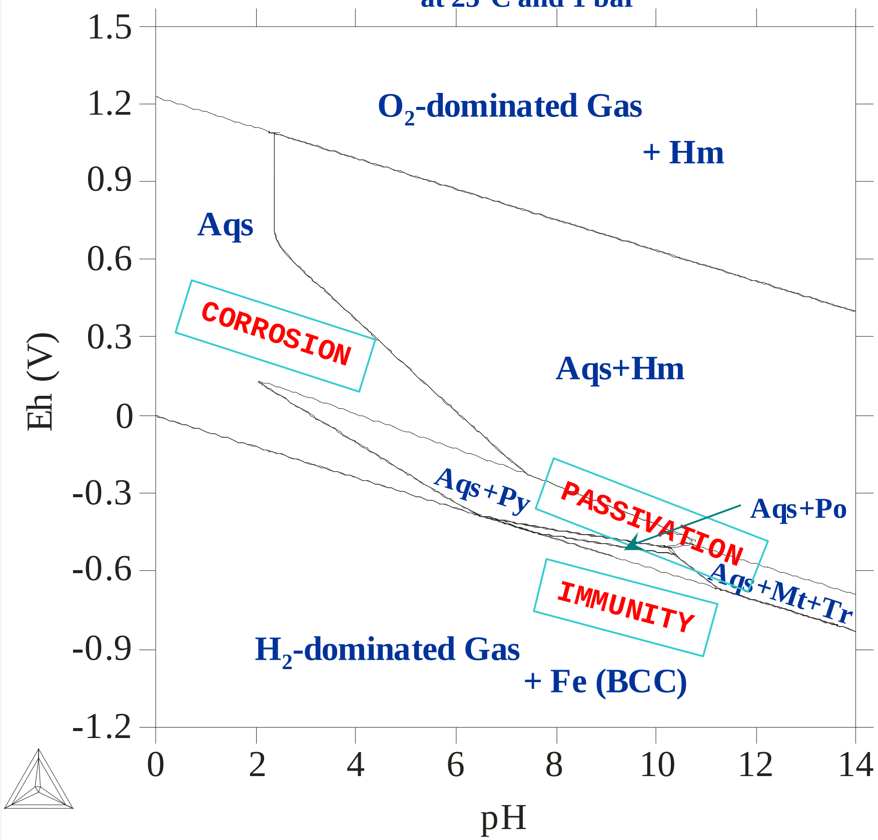
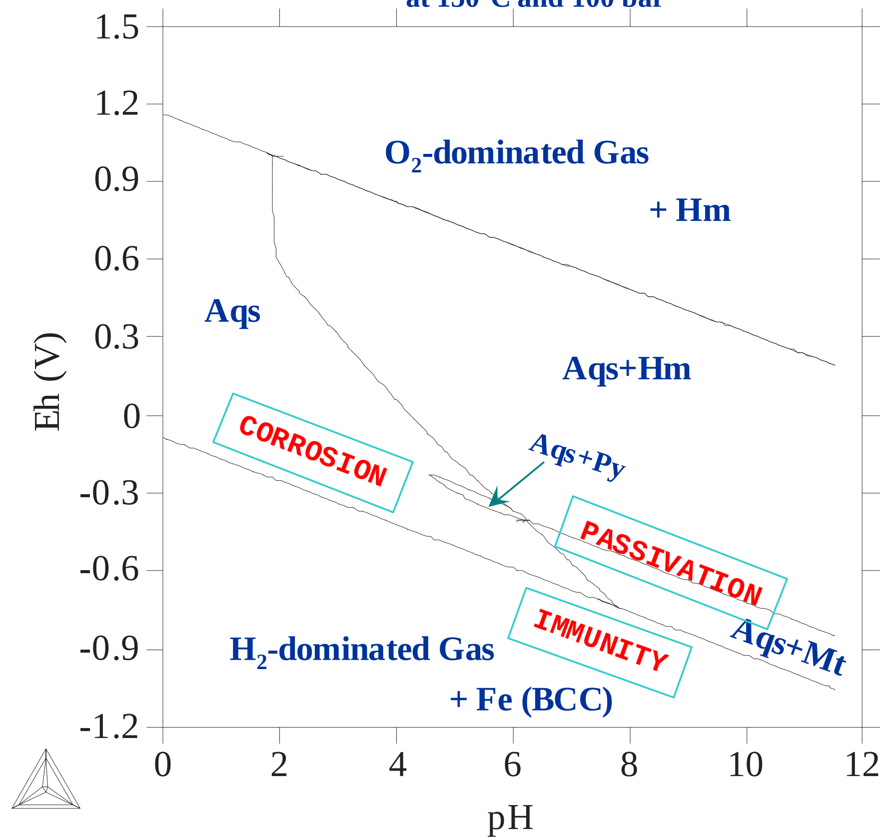
Pure Fe: under different T-P conditions

1E-6m Fe in 1 kg of water (with 3m NaCl and 1E-5m SO_2) at 25°C and 1 bar



1E-6m Fe in 1 kg of water (with 3m NaCl and 1E-5m SO_2) at 150°C and 100 bar



Pourbaix diagram of Fe (with 1E-6 mole Fe in 1 kg of water, 3m NaCl and 1E-5 m SO_2) at 25°C and 1 bar.

Pourbaix diagram of Fe (with 1E-6 mole Fe in 1 kg of water, 3m NaCl and 1E-5 m SO_2) at 150°C and 100 bar.

Complex Heterogeneous Interaction Systems

The shape of a Pourbaix diagram of a complex multi-component alloy and the stability relations of various secondary phases (oxides, hydroxides, sulfides, sulfates, carbonates, nitrates, silicates, halides, or other forms) depend upon the following factors:

- *Initial amount and composition of the alloy/solid materials;*
- *Initial amount and composition of the interacting aqueous solution phase;*
- *Temperature and pressure conditions;*
- *Model treatments on various primary phases and secondary phases: solution or compound*

Complete Pourbaix Diagrams via TC

Thermo-Calc can calculate Pourbaix diagrams and property diagrams, for various multi-component systems with:

- *Complex solution and compound phases (steels/Fe-based alloys, Ni-/Co-based superalloys, Al-/Mg-/Cu-/Ti-/Zr-based alloys, solder alloys, hard materials, ceramics, fuel-cell materials, oxides/hydroxides/sulfides/sulphates/silicates/carbonates/…, etc.), treated by various thermodynamic models;*
- *Complex aqueous solutions, treated by SIT, HKF & PITZ models;*
- *Complex gaseous mixtures, treated by ideal & non-ideal EOS and mixing models;*
- *Wide temperature and pressure ranges.*

Pourbaix Diagrams: Advantages from TC

Complex Phases:	Alloy compound/solution phases; Oxide/Sulfide/Silicate/... solution phases; Aqueous solution phases; Gaseous mixture phases.
Complex Environments:	Very wide P-T ranges; Concentrated aqueous solutions.
Multiple Functionality:	Many types of phase diagrams & property diagrams

Pourbaix Diagrams: TC *vs* Others

Specifications	Thermo-Calc	FACTSage, HSC
Primary phases	Complex alloy solutions (e.g. BCC, FCC, HCP; Sigma, Cementite)	Pure metals (e.g. Fe, Cr)
Secondary phases	Complex *(solution)* oxides/sulfides/silicates/...	Simple *(stoichiometric)* oxides/sulfides/silicates/...
Gaseous mixtures	Ideal/Non-ideal gas mixtures	Ideal gases
Aqueous solutions	Concentrated solutions	Dilute solutions
Applicable P-T	Wide P-T range (up to 5 kbar & 1000^{o}C)	Room P-T conditions
Calculation Tech	Global Minimization + POLY GEM	Normal GEM or EC
Predominance Area	*No*	Y/N
Property Plots	Yes	No
User's Database	Yes	Y/N
Data Assessments	Yes	No
API	*To be implemented* (TQ/TCAPI)	No

Simulations on Corrosions of Steels/Alloys

The following types of calculations can be performed by using the Thermo-Calc software and selective databases, for investigations of corrosion processes of various steels/alloys.

- *Mapping Calculations of Eh-pH diagrams (i.e., the so-called Pourbaix diagrams), and various property diagrams which are relevant to different phase boundaries on a corresponding Eh-pH diagrams;*
- *Mapping or Stepping Calculations of heterogeneous interactions, by changing one or two (or more) controlling variables (temperature, pressure, acidity, electronic potential, salinity, aqueous concentration, alloy composition, etc.)*

A lot of interesting diagrams can be easily calculated and graphically generated, which can be conveniently edited, refined, printed and saved.

Case 1: Corrosion of Stainless Steel

Initial composition of a specific stainless steel (austenite):

Element	*Composition (wt%)*	*Composition (X)*
Fe	68.50	0.687523
Cr	17.00	0.183263
Ni	12.00	0.114608
Mo	2.50	0.014606

Initial composition of interacting aqueous solution:

H_2SO_4 5% (0.537 molality)

Initial temperature and pressure of exposure:

85^oC and 1 bar

Case 1: Corrosion of Stainless Steel

Data Resources:

TCFE5 — **TCS Steels/Fe-Alloys (Solutions) Database**
Steel/Alloy Phases, Oxide/Sulfide Solutions

ION2 — **TCS Oxides/Sulfides (Solutions) Database**
Oxide/Sulfide/Silicate Solutions

SSUB4 — **SGTE Substances (Compounds) Database**
Gaseous mixture,
Oxides, Hydroxides, Sulfides, Sulphates,
Halides, complex salts

TCAQ2 — **TCS Aqueous Solution Database**
Aqueous solution (using SIT model)

AQS2 — **TGG Aqueous Solution Database**
Aqueous solution (using HKF model)

Calculations:

1: Pourbaix diagram and property diagrams
Mapping in pH and Eh

2: Property diagrams
Stepping in Eh

3: Property diagrams
Stepping in temperature

Case 1: Corrosion of Stainless Steel

Thermo-Calc Software

Calculation 1: Pourbaix Diagram Calculation

Bulk composition:

0.1 g stainless steel (i.e., 0.001784 mole austenite)

1 kg H_2O, with $[SO_4^{-2}]$=0.537 molality

T-P conditions:

85^{o}C and 1 bar

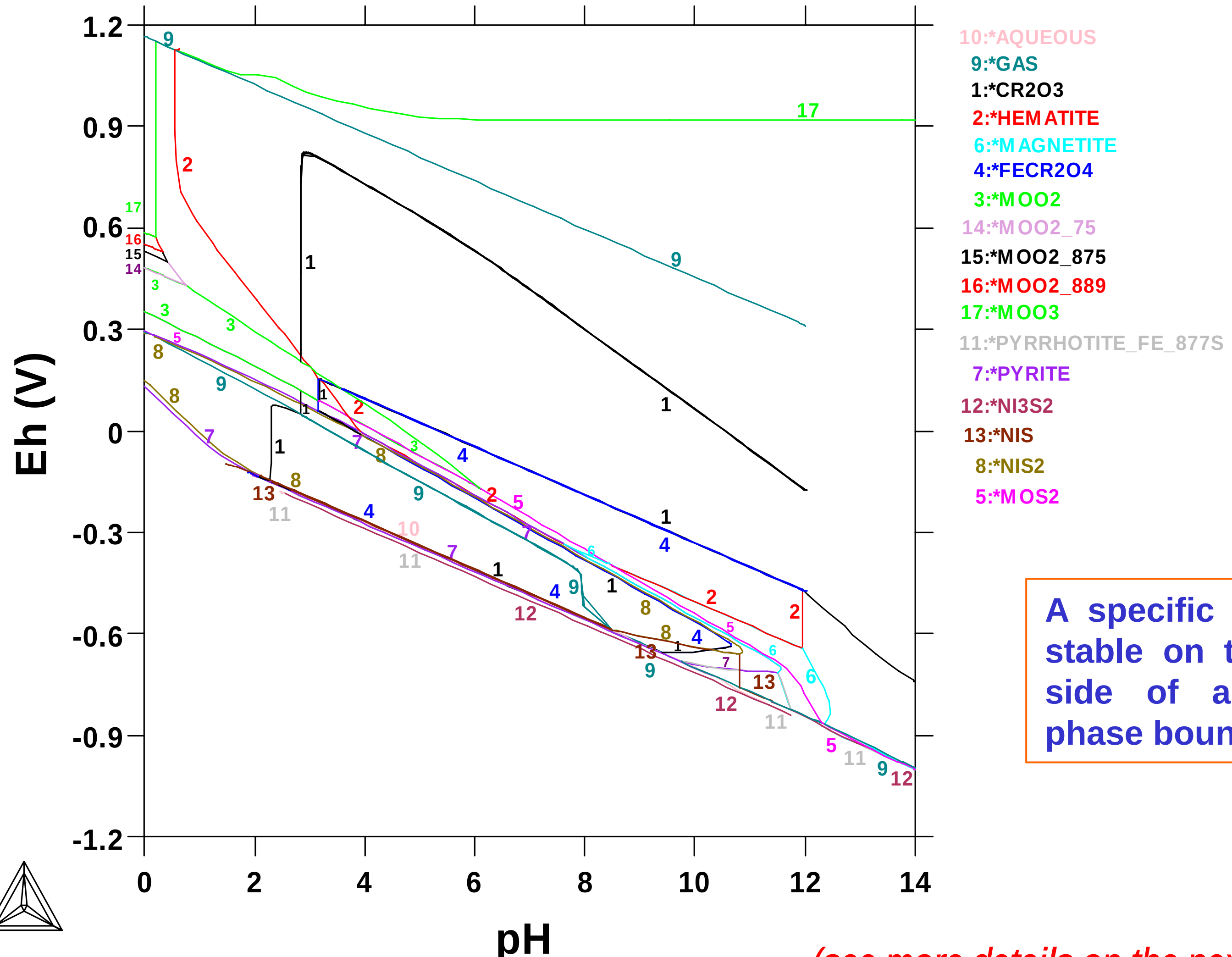
Mapping variables:

pH and Eh

Case 1: Corrosion of Stainless Steel

Calculation 1: Pourbaix Diagram

T=358.15 K, P=1 bar, B(H2O)=1000 g, N(H2SO4)=0.537 m
N(Fe)=1.2266E-3, N(Cr)=3.2695E-4, N(Mo)=2.6058E-5, N(Ni)=2.0446E-4

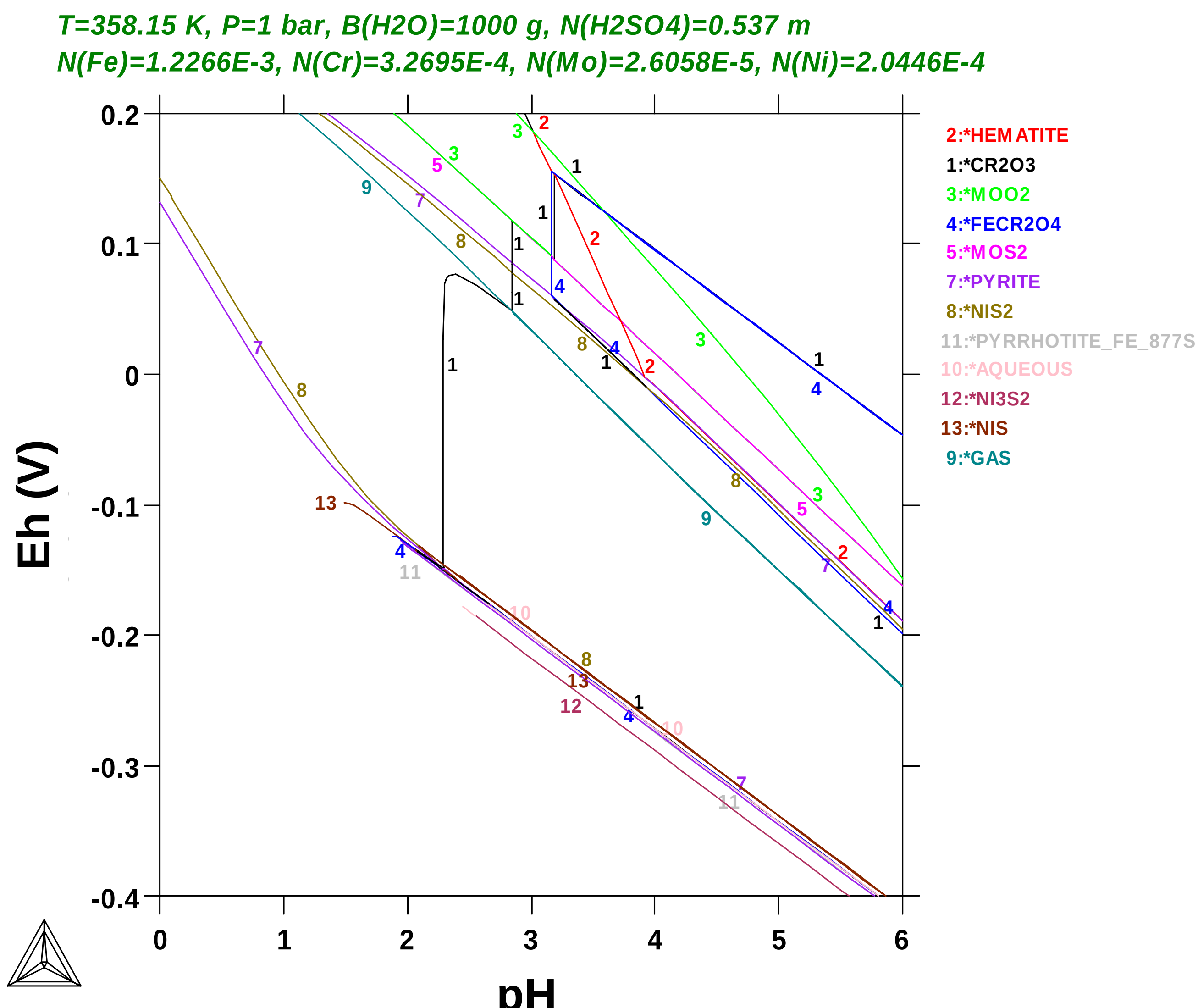


A specific phase is stable on the inner side of a plotted phase boundary.

(see more details on the next two slides)

Case 1: Corrosion of Stainless Steel

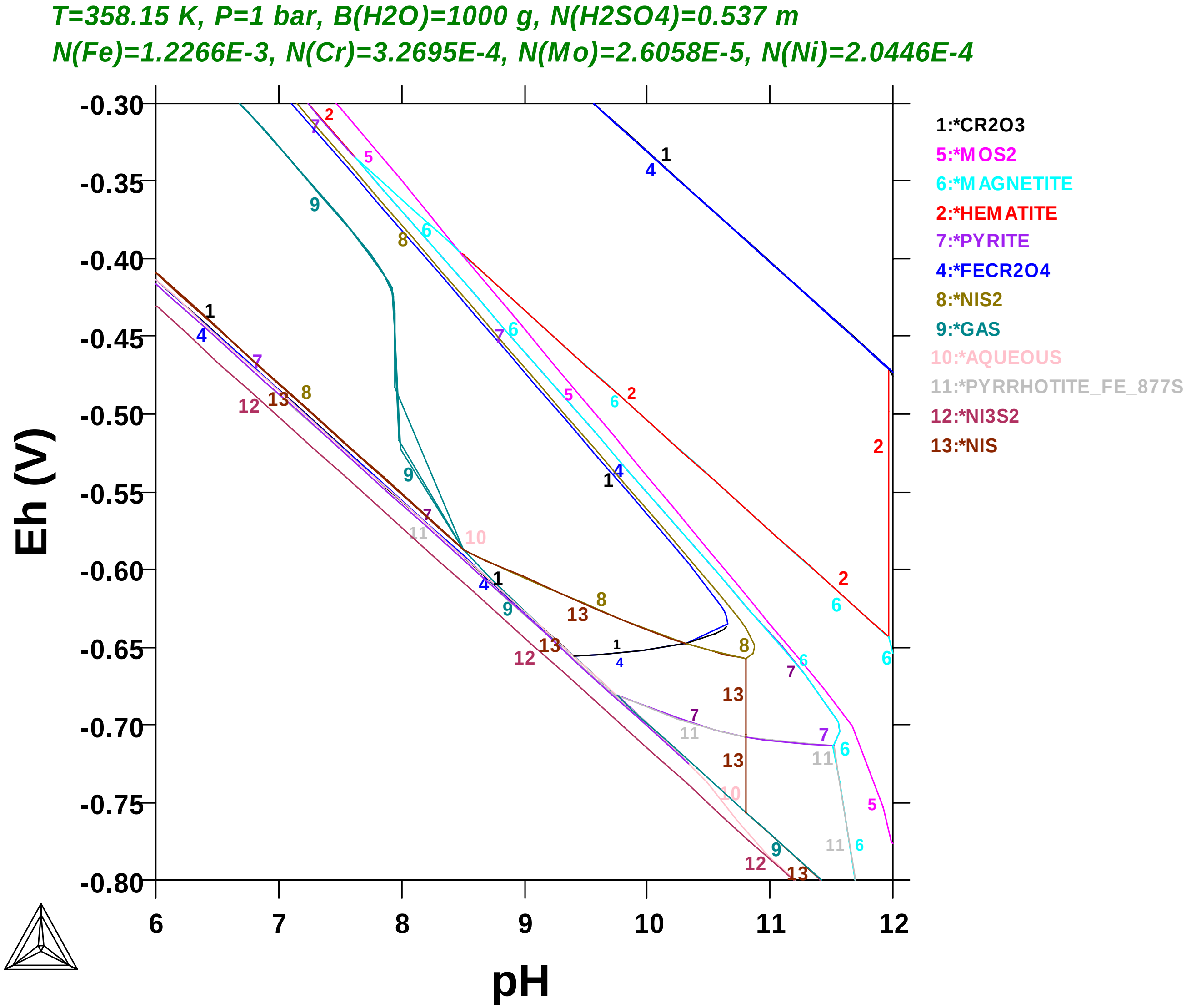
Calculation 1: Pourbaix Diagram (enlarged for the low pH range)



Thermo-Calc Software

Case 1: Corrosion of Stainless Steel

Calculation 1: Pourbaix Diagram (enlarged for the high pH range)



Case 1: Corrosion of Stainless Steel

Calculation 2: Property Diagram Calculation

Bulk composition:

0.1 g stainless steel (i.e., 0.001784 mole austenite)

1 kg H_2O, with $[H_2SO_4]$=0.537 molality (i.e., 5wt%)

T-P conditions:

85^{o}C and 1 bar

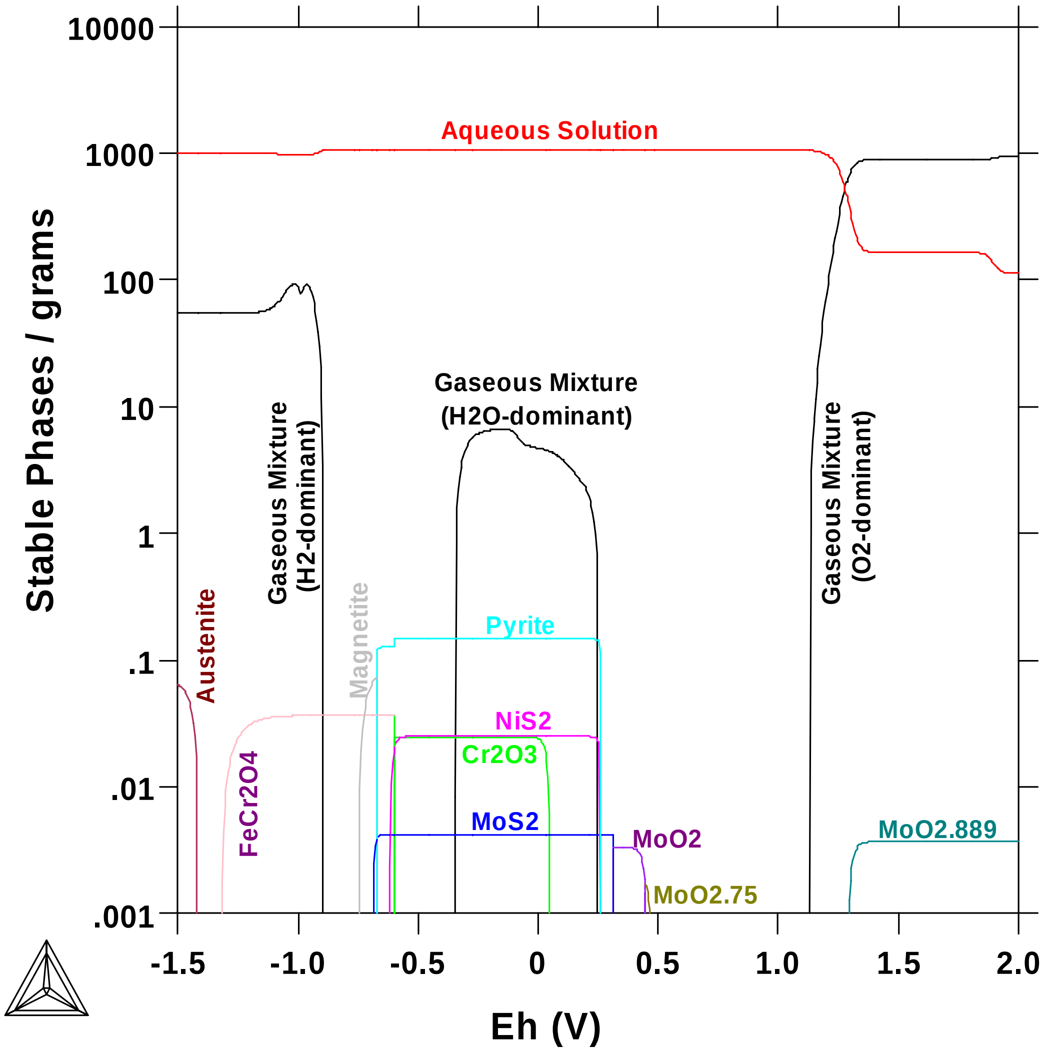
Stepping variable:

Eh (from –1.5 to 2.0 V)

Case 1: Corrosion of Stainless Steel

Calculation 2: Stable Phase Compositions varied with Eh condition

T=358.15 K, P=1 bar, B(H2O)=1000 g, N(H2SO4)=0.537 m
N(Fe)=1.2266E-3, N(Cr)=3.2695E-4, N(Mo)=2.6058E-5, N(Ni)=2.0446E-4



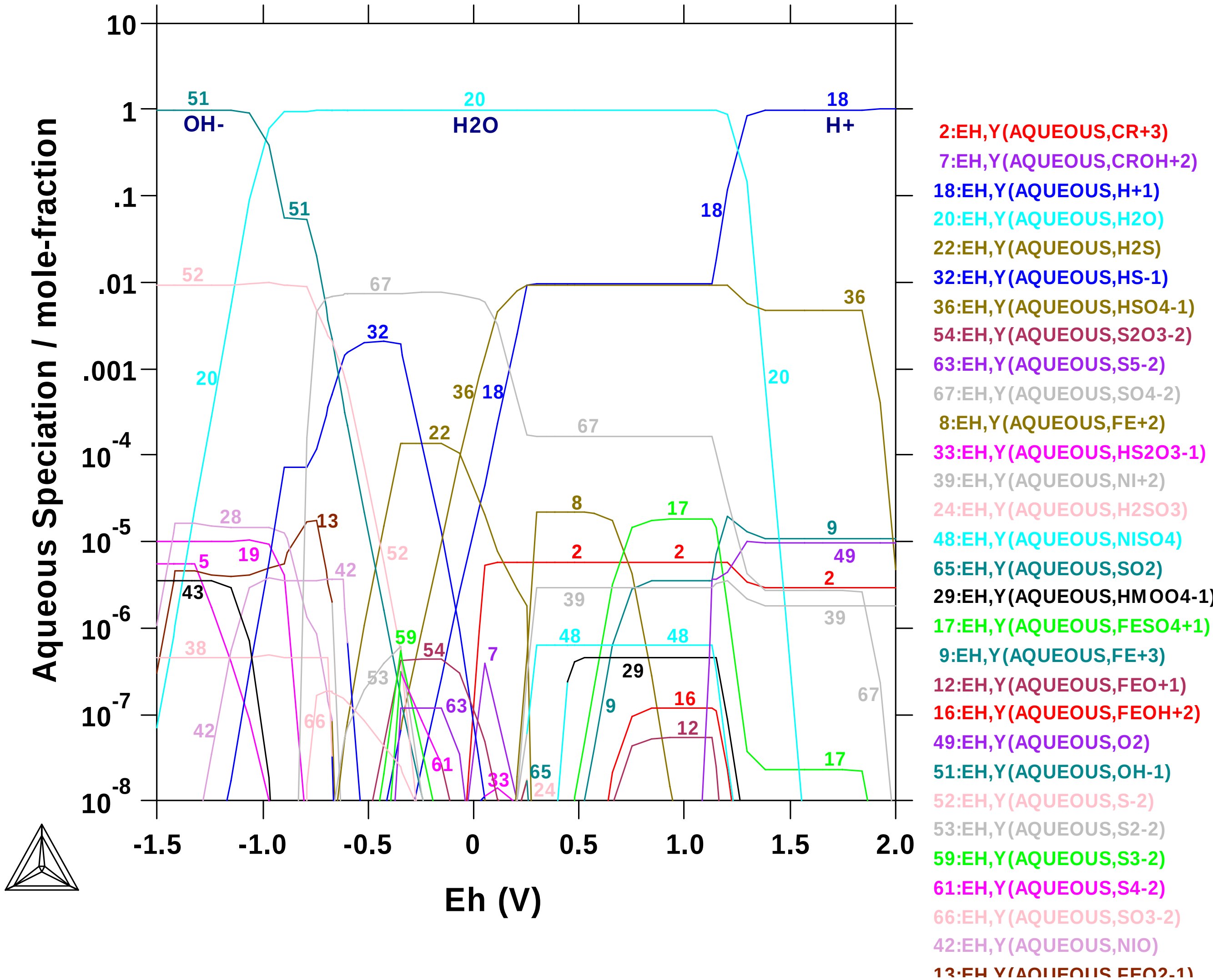
Complex oxide and sulfide solution phases have all been suspended from this testing calculation.

Case 1: Corrosion of Stainless Steel

Thermo-Calc Software

Calculation 2: Major Aqueous Speciation varied with Eh condition:

T=358.15 K, P=1 bar, B(H2O)=1000 g, N(H2SO4)=0.537 m
N(Fe)=1.2266E-3, N(Cr)=3.2695E-4, N(Mo)=2.6058E-5, N(Ni)=2.0446E-4

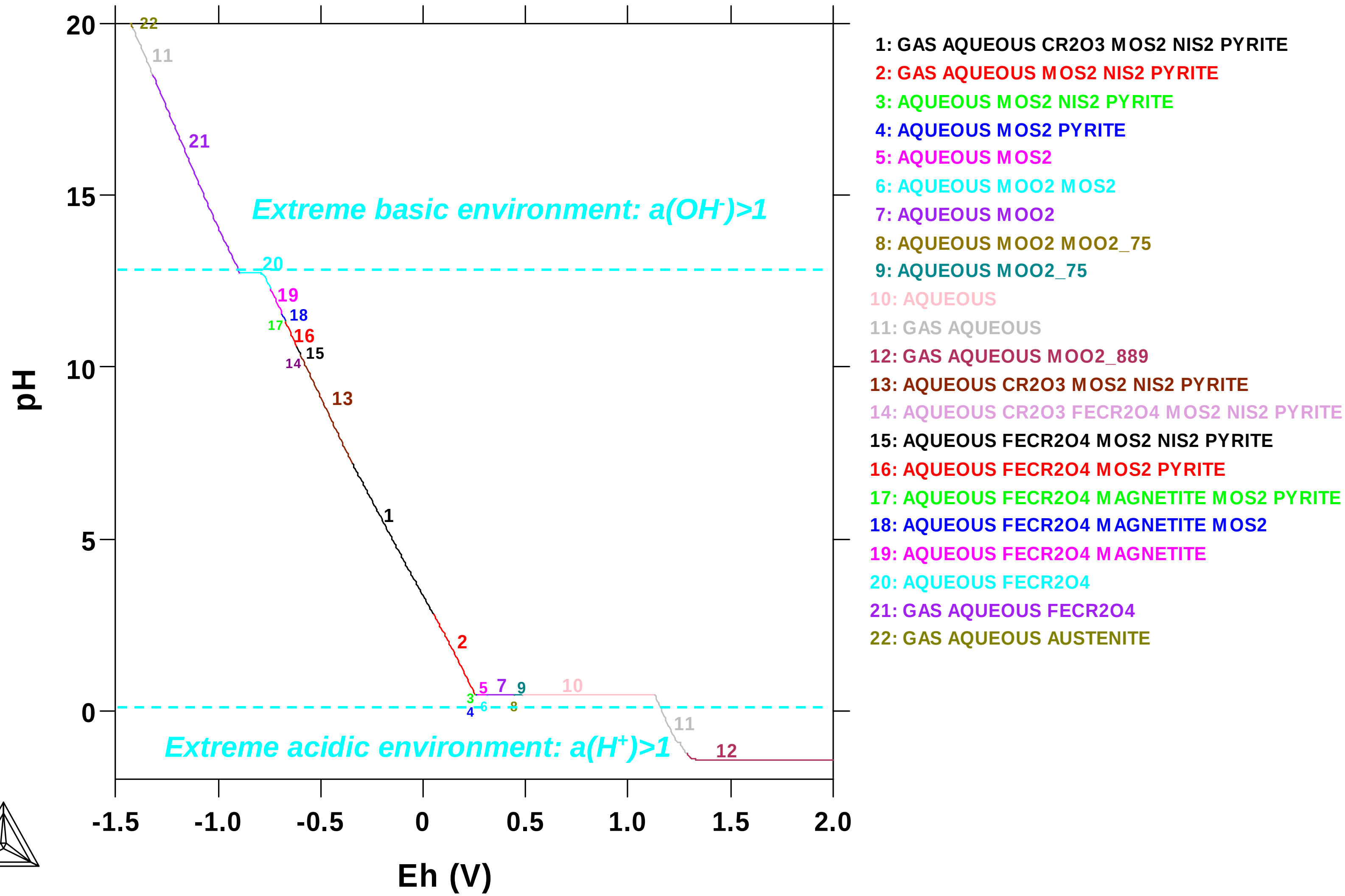


Case 1: Corrosion of Stainless Steel

Thermo-Calc Software

Calculation 2: Ph value varied with Eh condition

T=358.15 K, P=1 bar, B(H2O)=1000 g, N(H2SO4)=0.537 m
N(Fe)=1.2266E-3, N(Cr)=3.2695E-4, N(Mo)=2.6058E-5, N(Ni)=2.0446E-4



Case 1: Corrosion of Stainless Steel

Calculation 3: Property Diagram Calculation

Bulk composition:

0.1 g stainless steel (i.e., 0.001784 mole austenite)

1 kg H_2O, with $[H_2SO_4]$=0.537 molality (i.e., 5wt%)

P condition:

1 bar

Eh condition:

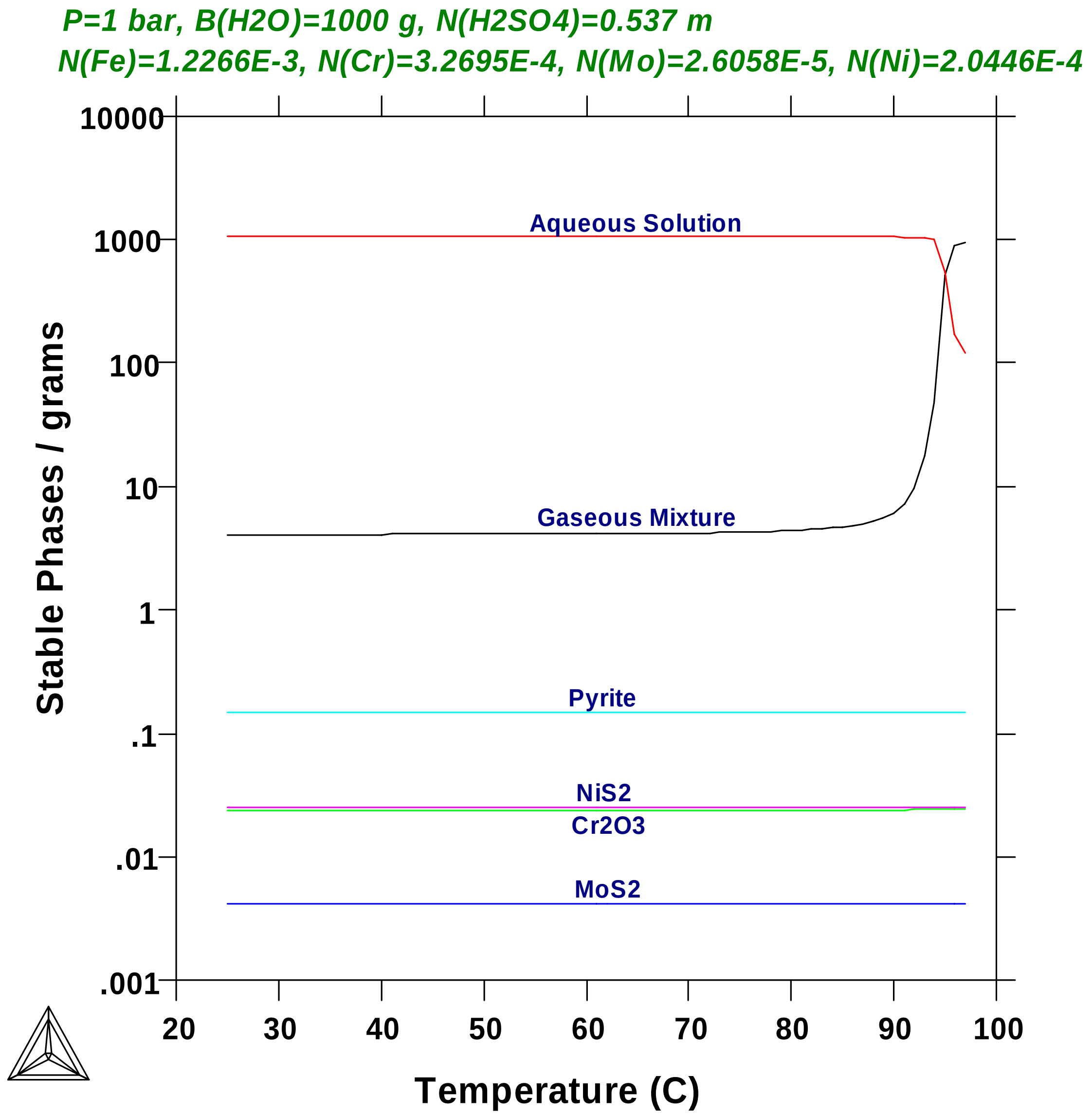
Electronically balanced (Eh=0)

Stepping variable:

Temperature (from 25^{o}C to boiling temperature)

Case 1: Corrosion of Stainless Steel

Calculation 3: Stable Phase Compositions varied with temperature condition



Complex oxide and sulfide solution phases have all been suspended from this testing calculation.

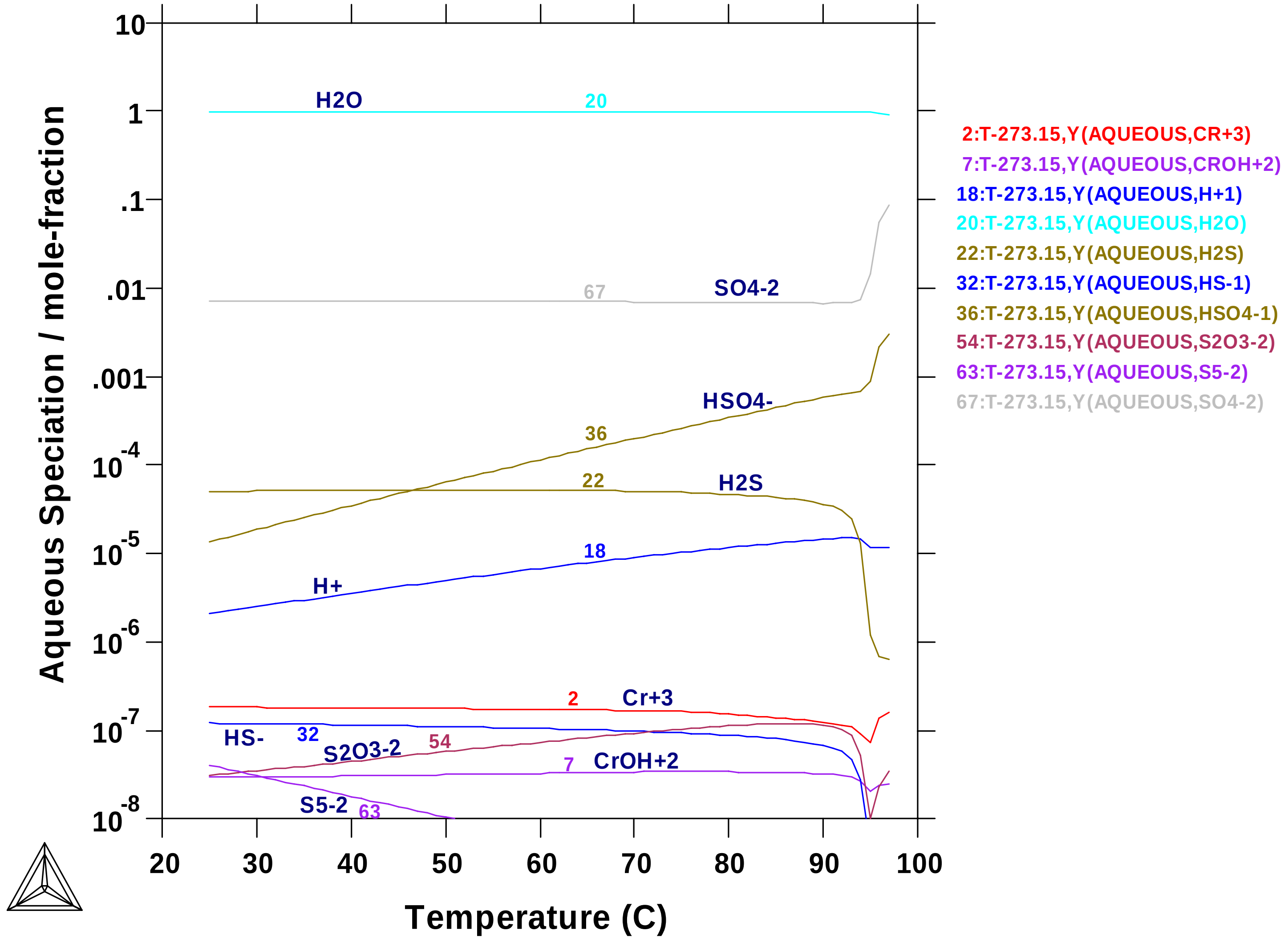
Case 1: Corrosion of Stainless Steel

Thermo-Calc Software

Calculation 3: Aqueous Speciation varied with temperature condition: Part 1

P=1 bar, B(H2O)=1000 g, N(H2SO4)=0.537 m

N(Fe)=1.2266E-3, N(Cr)=3.2695E-4, N(Mo)=2.6058E-5, N(Ni)=2.0446E-4



Case 1: Corrosion of Stainless Steel

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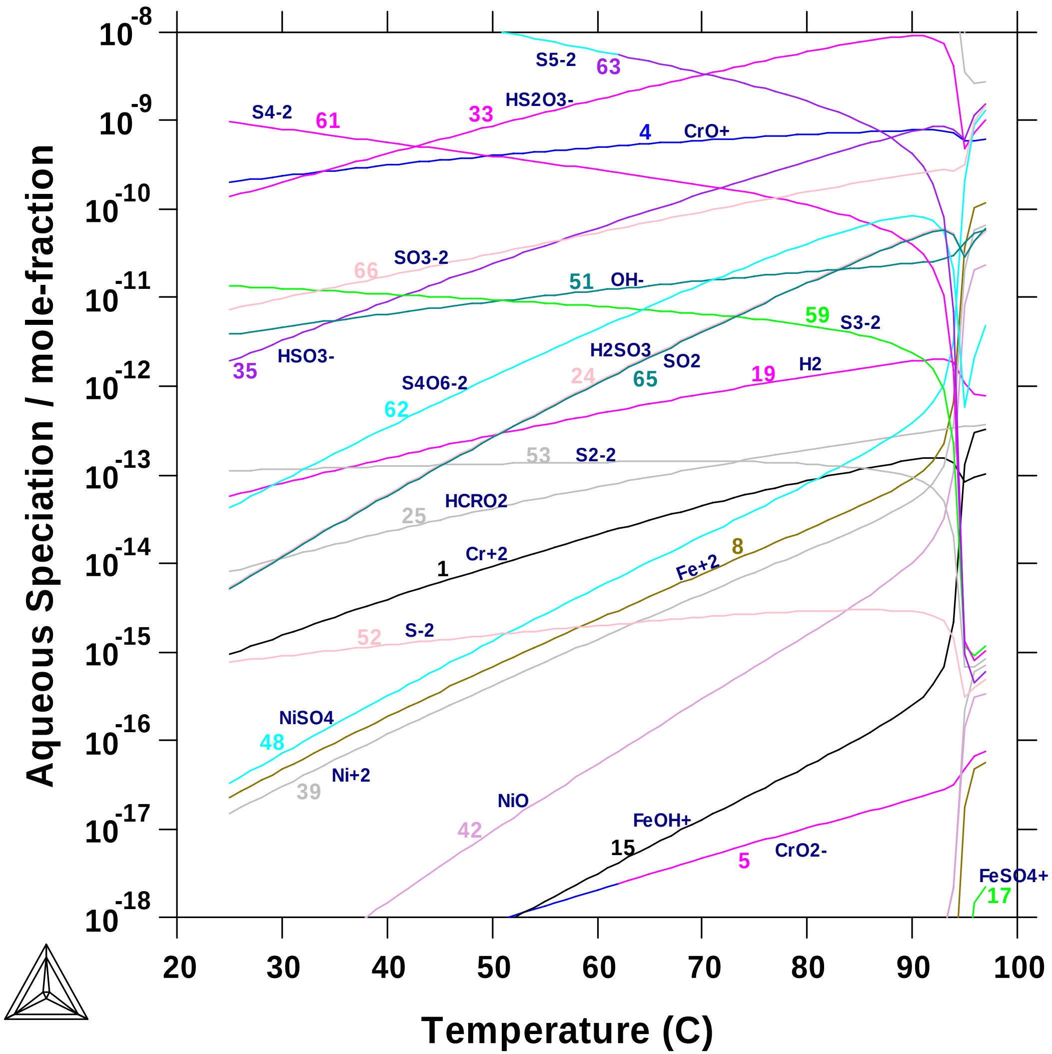
Calculation 3: Aqueous Speciation varied with temperature condition: Part 2

P=1 bar, B(H2O)=1000 g, N(H2SO4)=0.537 m

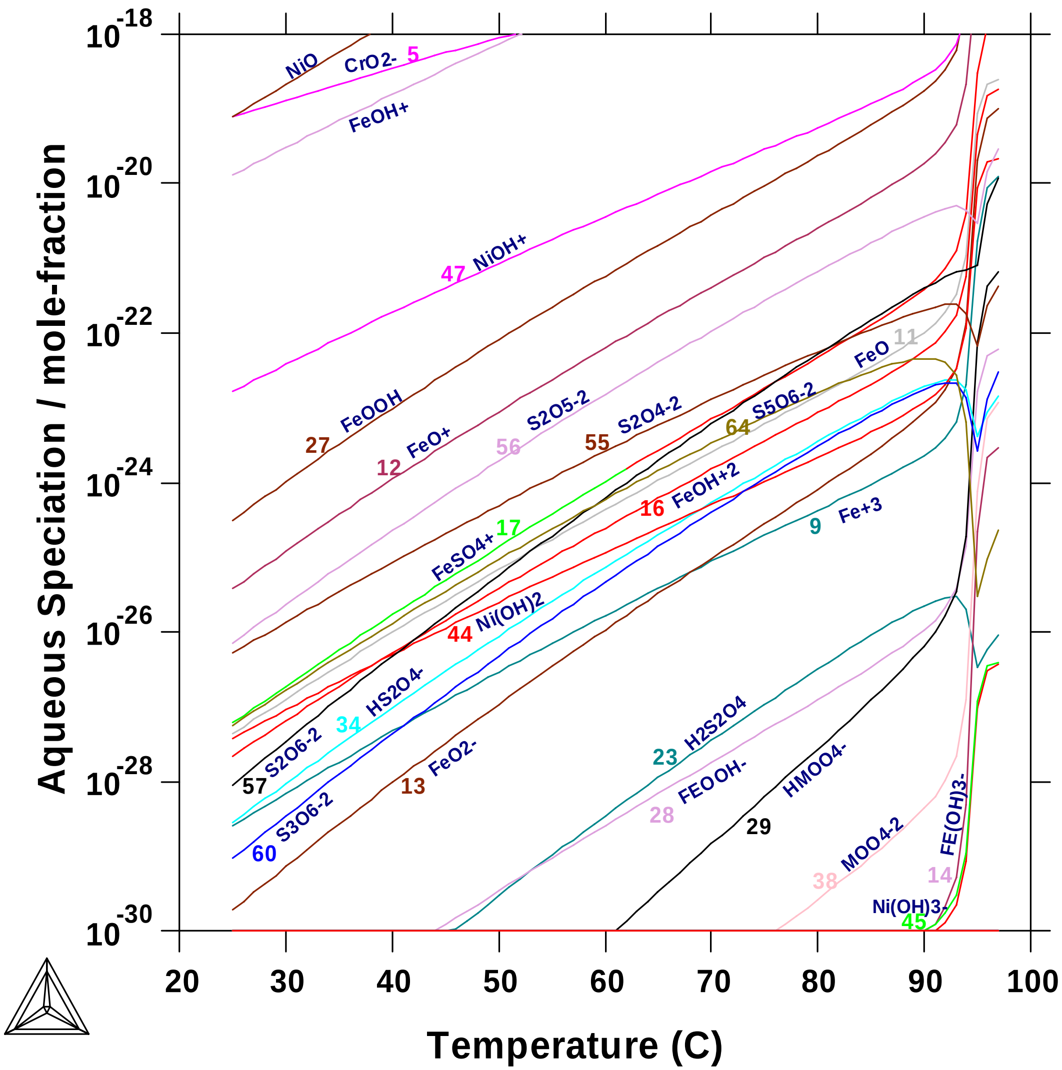
N(Fe)=1.2266E-3, N(Cr)=3.2695E-4, N(Mo)=2.6058E-5, N(Ni)=2.0446E-4



Case 1: Corrosion of Stainless Steel

Calculation 3: Aqueous Speciation varied with temperature condition: Part 3

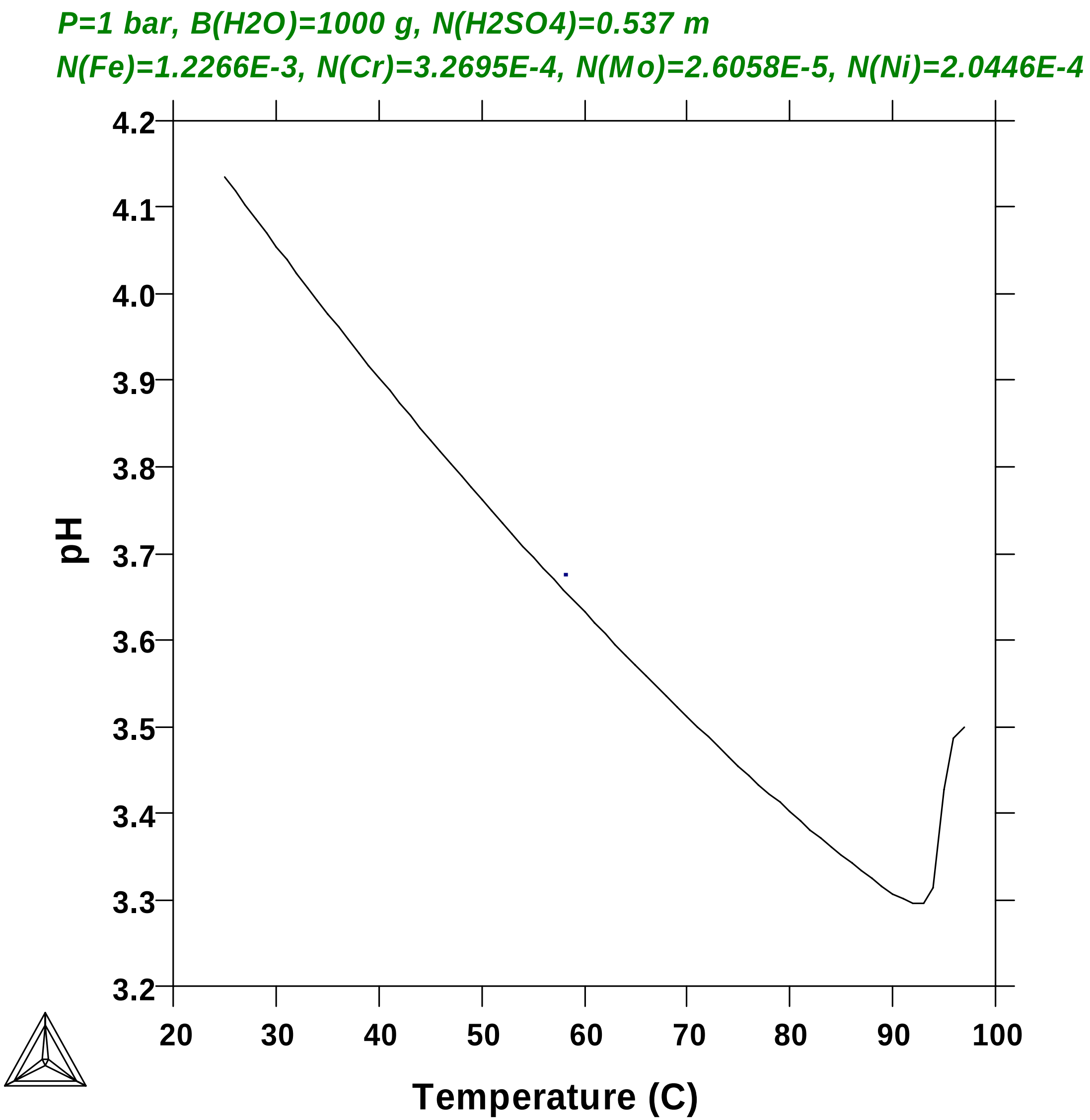
P=1 bar, B(H2O)=1000 g, N(H2SO4)=0.537 m
N(Fe)=1.2266E-3, N(Cr)=3.2695E-4, N(Mo)=2.6058E-5, N(Ni)=2.0446E-4



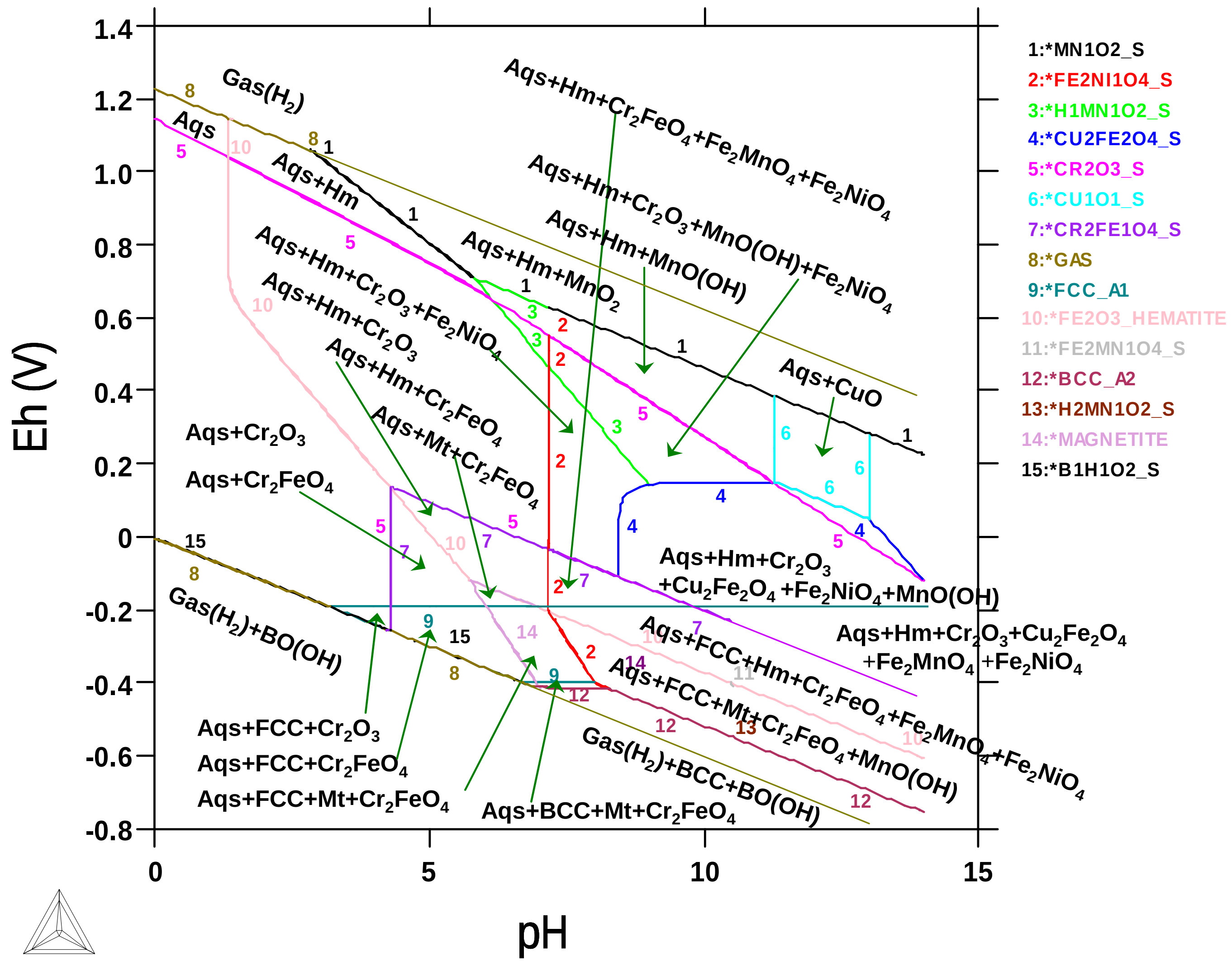
Case 1: Corrosion of Stainless Steel

Thermo-Calc Software

Calculation 3: Ph value varied with temperature condition

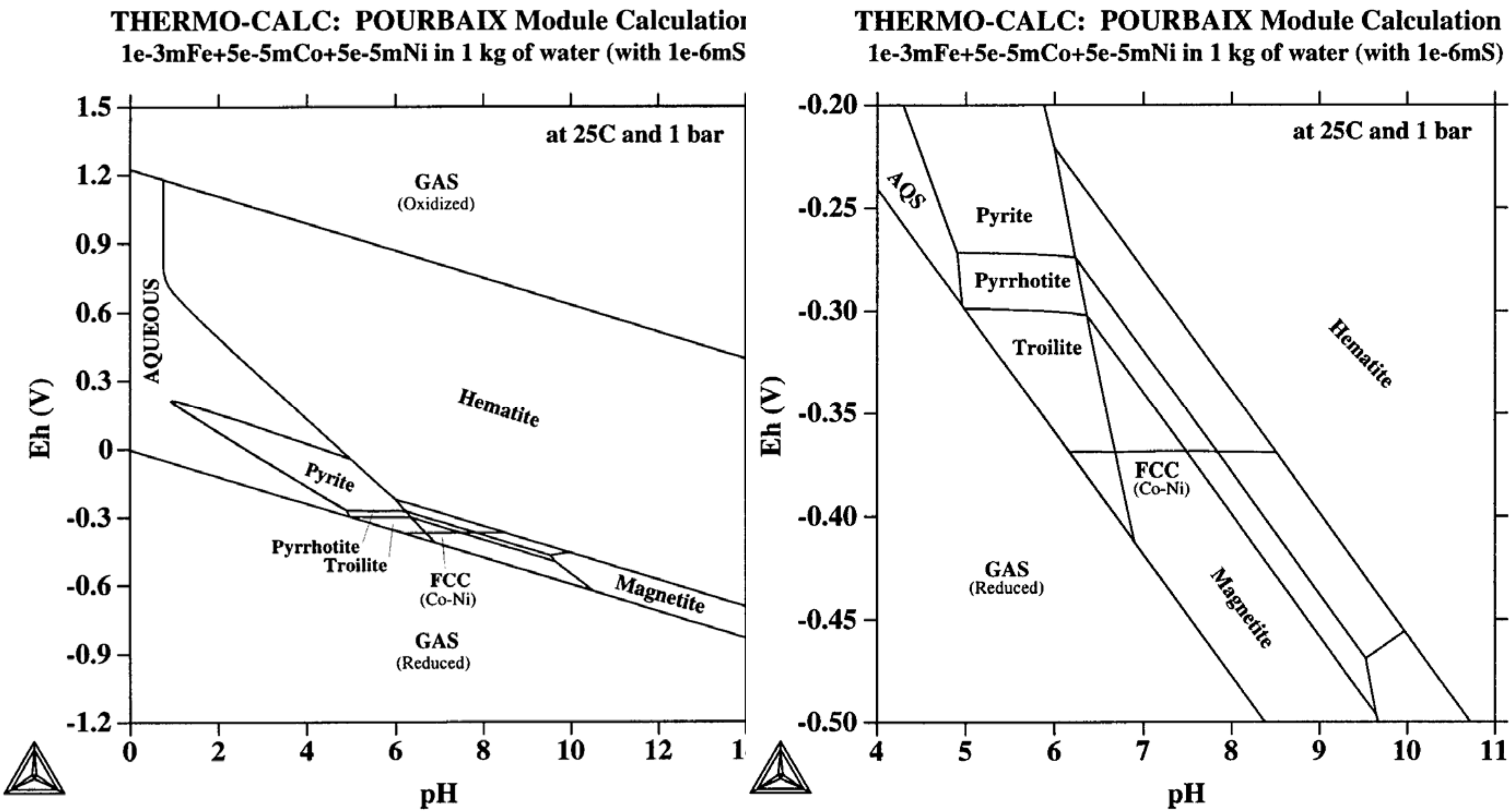


Case 2: Corrosion of Stainless Steel



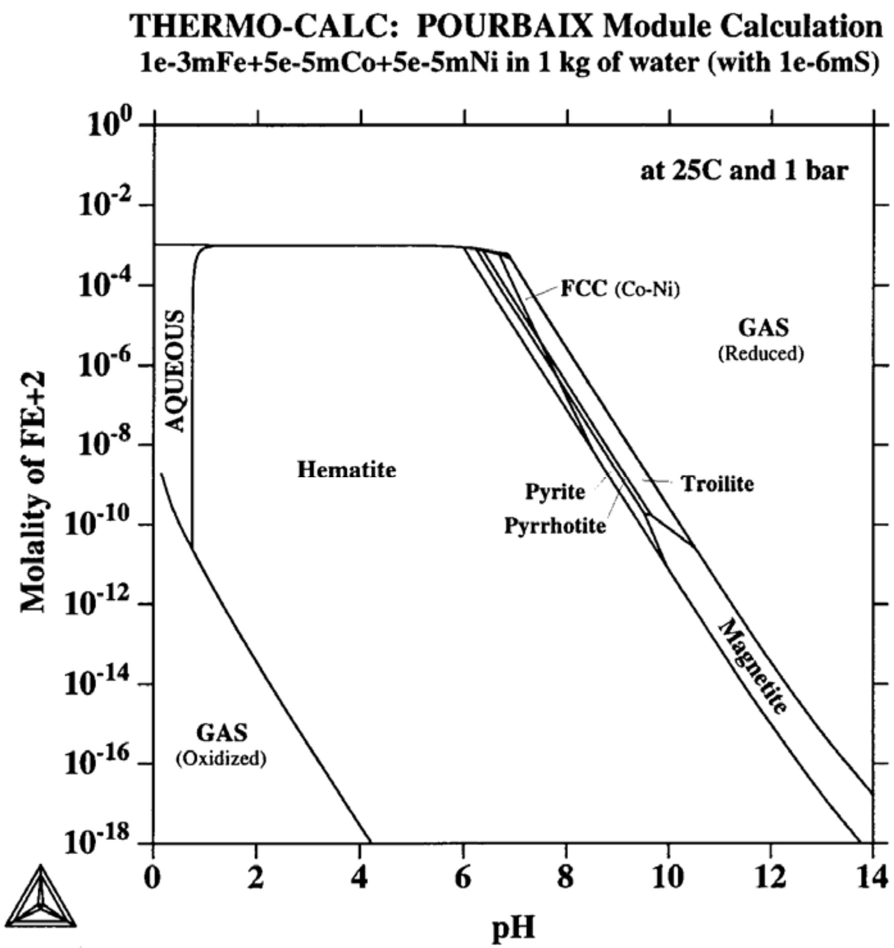
Pourbaix diagrams for the heterogeneous interaction systems between 0.001 m of steel [Fe-7.676Cr-5.0Ni-2.1887Mn-1.0Cu mole%] and 1 kg of water (and with 1.2 m H3BO3, 0.022 m Li and 0.001 m NH3), at 25oC and 1 bar. This application is particular useful for safety assessments of nuclear rectors and nuclear waste repositories.

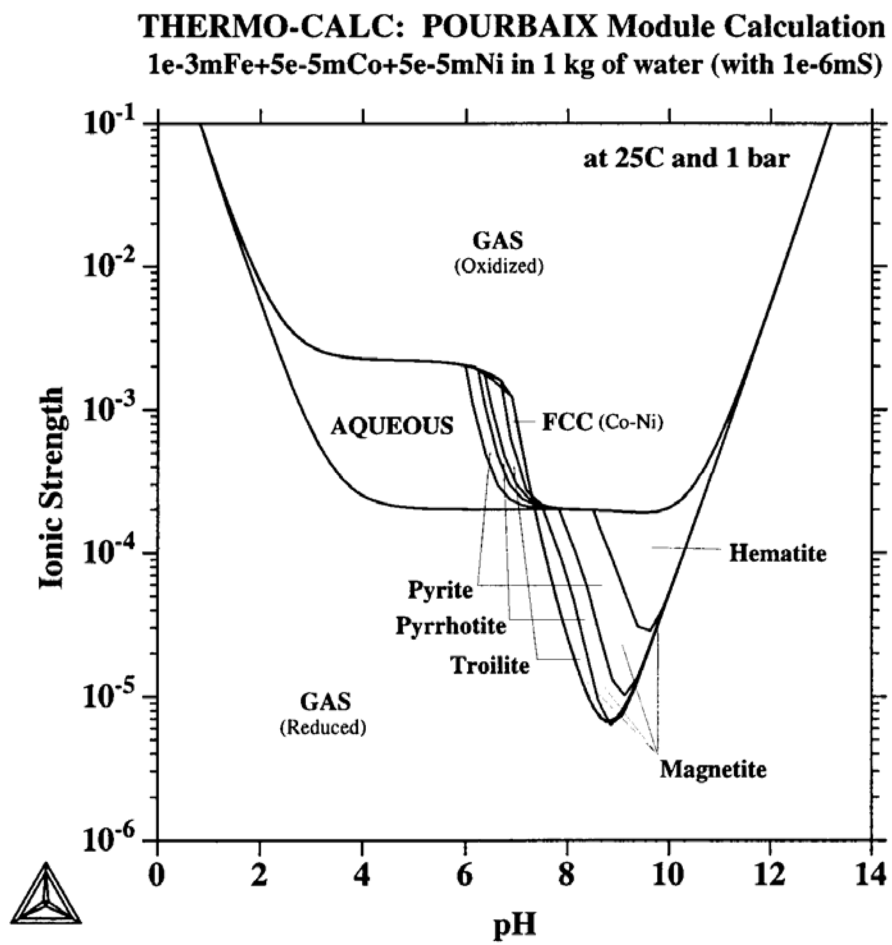
Case 3: Corrosion of Steel



Pourbaix diagram and zoomed part of an Fe-Alloy (consisting of 1E-3 m Fe, 5E-5 m Co and 5E-5 m Ni), interacted with 1 kg of water (with 1E-6 m S) at 25°C and 1 bar.

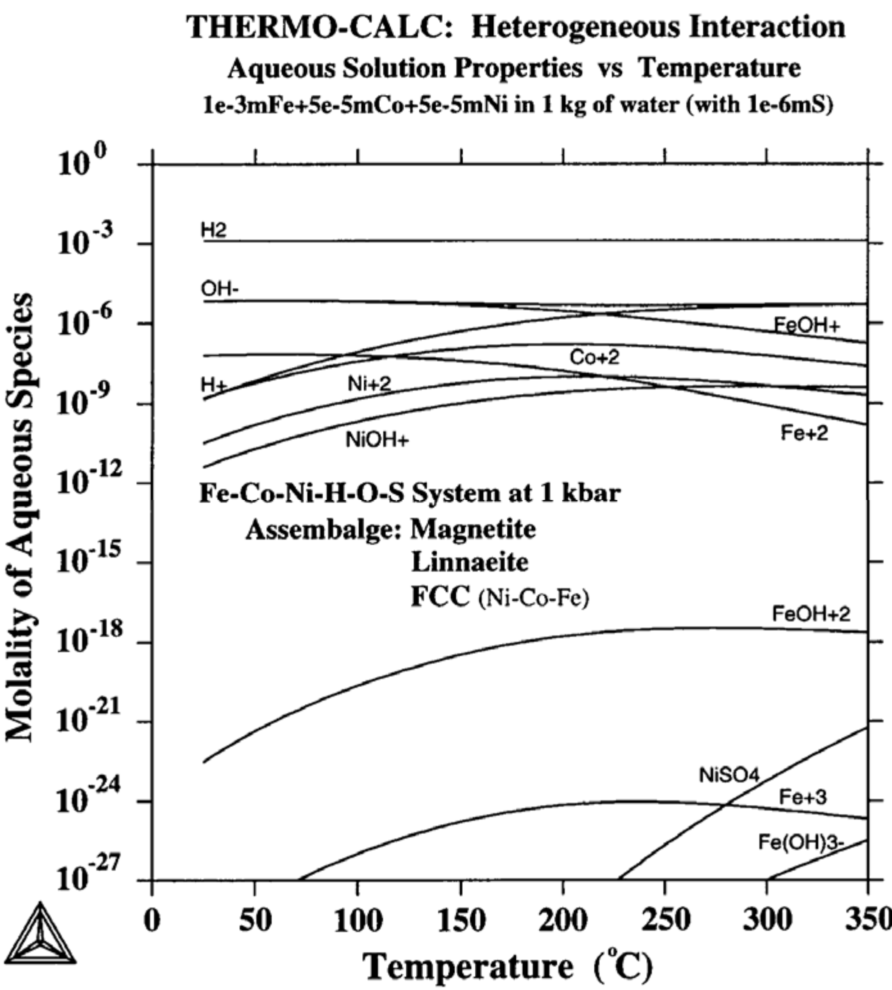
Case 3: Corrosion of Steel

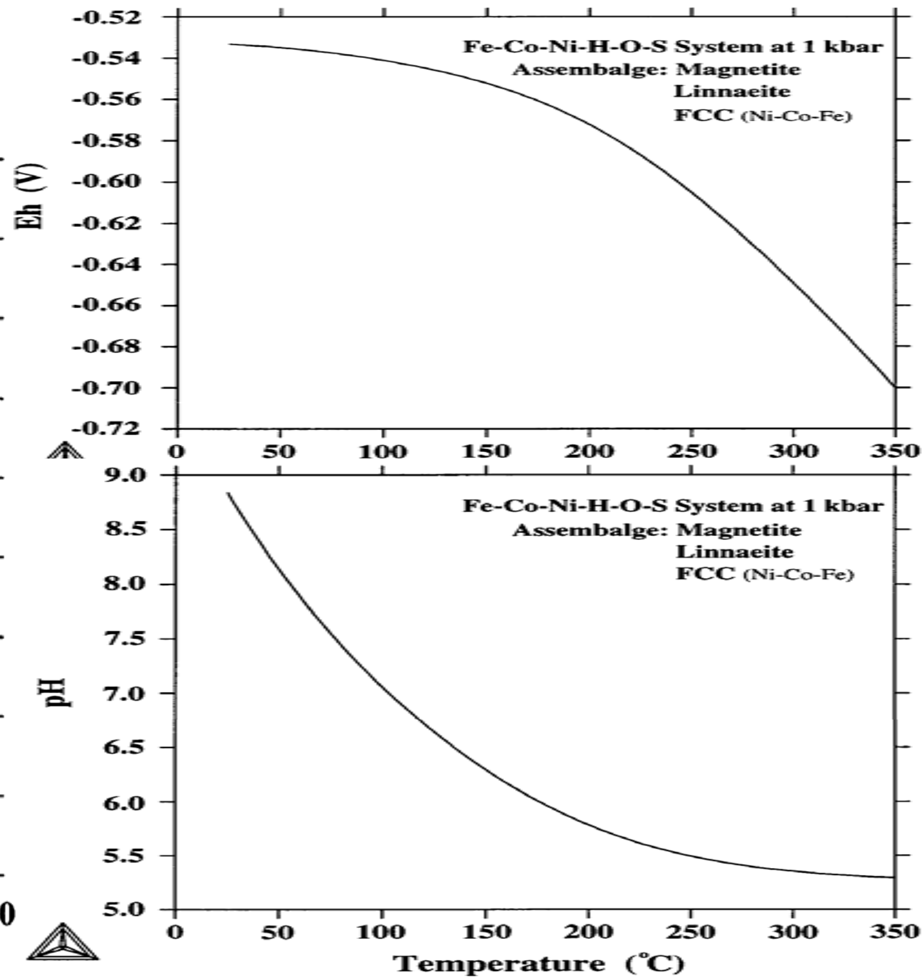




Fe^{+2} molality *vs.* pH and Ionic strength *vs.* pH diagrams for the heterogeneous interaction between an Fe-Alloy (consisting of 1E-3 m Fe, 5E-5 m Co and 5E-5 m Ni) and 1 kg of water (with 1E-6 m S) at 25°C and 1 bar.

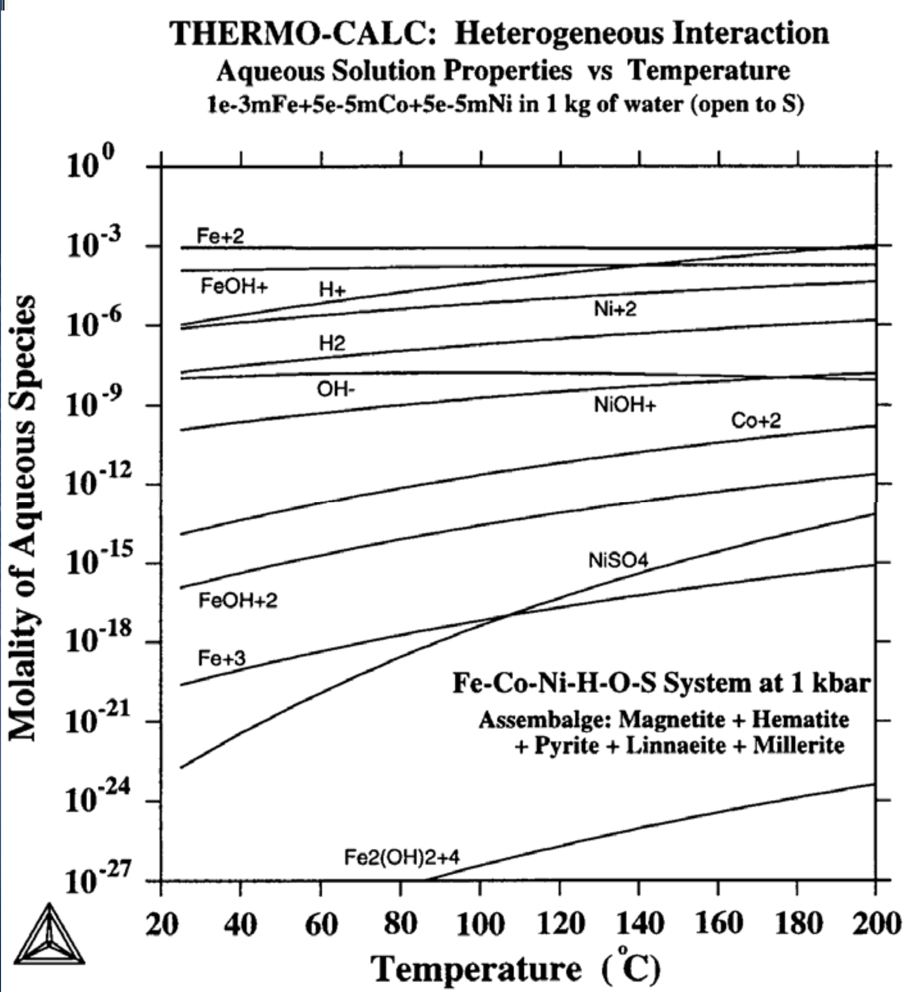
Case 3: Corrosion of Steel

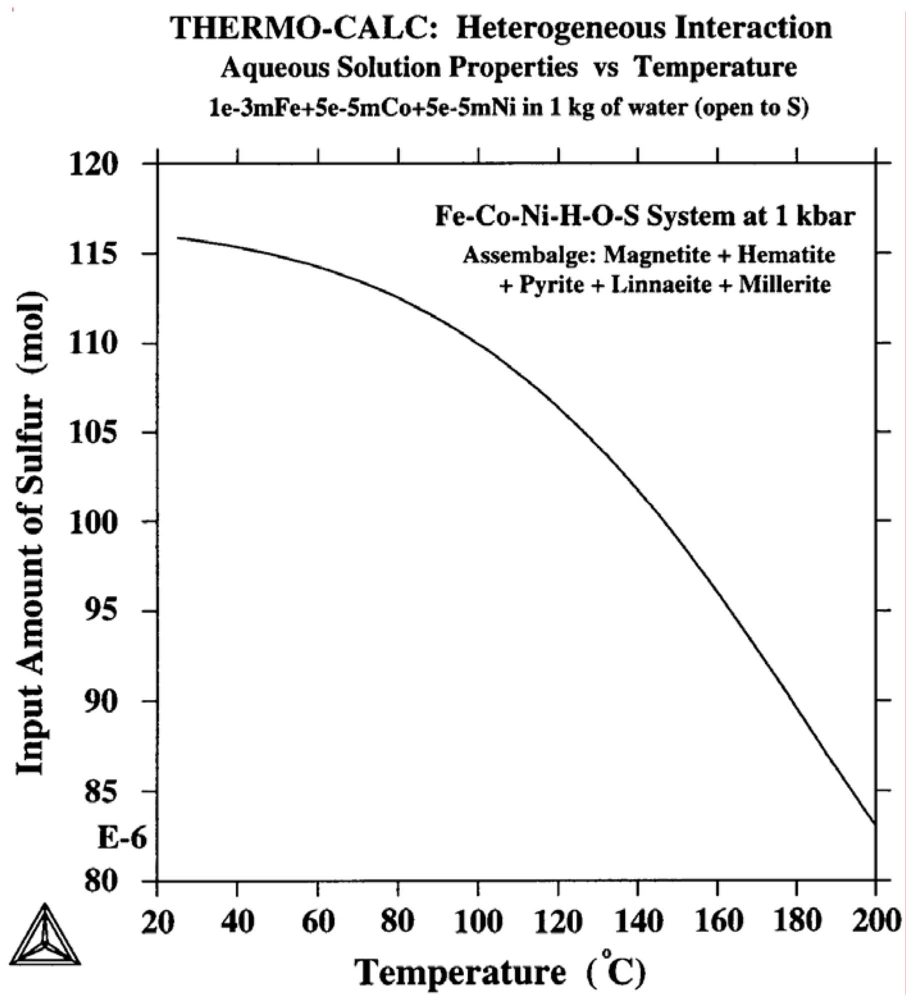




Dependencies of aqueous concentration, Eh and pH on temperature for the equilibrium assemblage Magnetite-Linnaeite-FCC(Ni-Co-Fe) in the heterogeneous interaction between an Fe-Alloy (consisting of 1E-3 m Fe, 5E-5 m Co and 5E-5 m Ni) and 1 kg of water (with 1E-6 m S) at 1 kbar.

Case 3: Corrosion of Steel





Variations of aqueous concentration, and of input amount of sulfur, with temperature for the equilibrium assemblage Magnetite-Hematite-Pyrite-Linnaeite-Millerite in the heterogeneous interaction between an Fe-Alloy (consisting of 1E-3 m Fe, 5E-5 m Co and 5E-5 m Ni) and 1 kg of water (open to S) at 1 kbar.

Case 3: Corrosion of Steel

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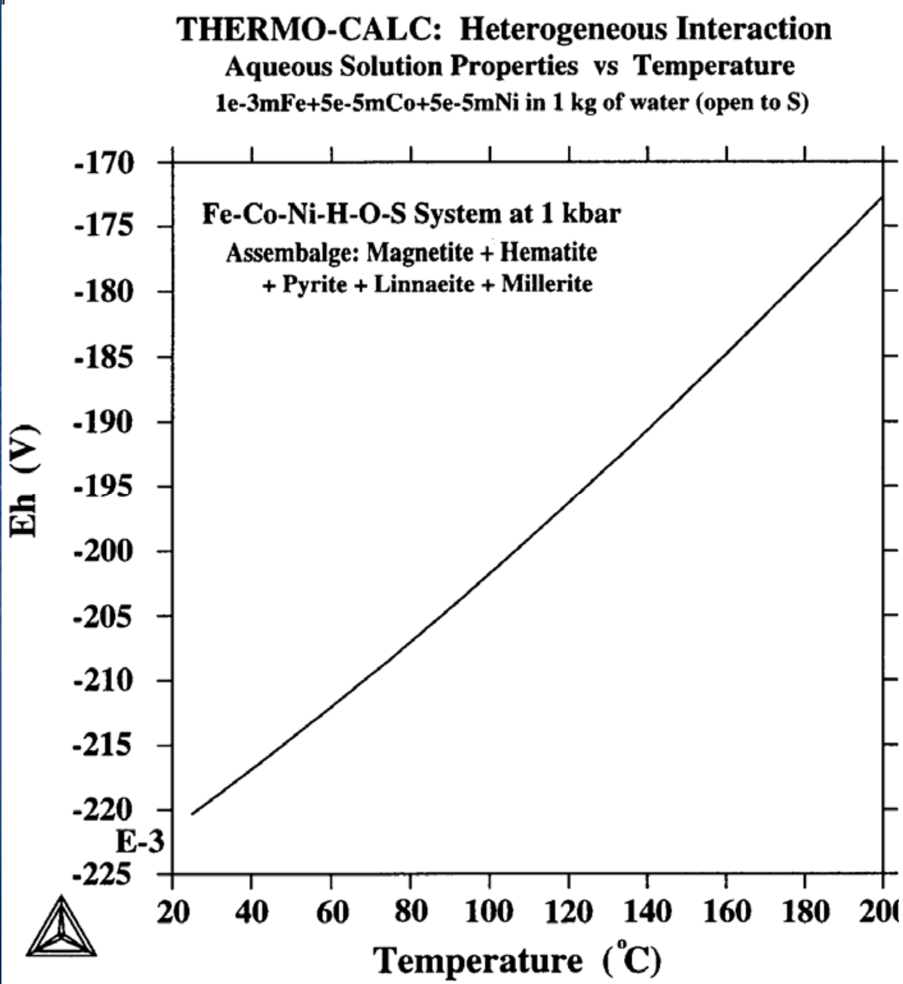
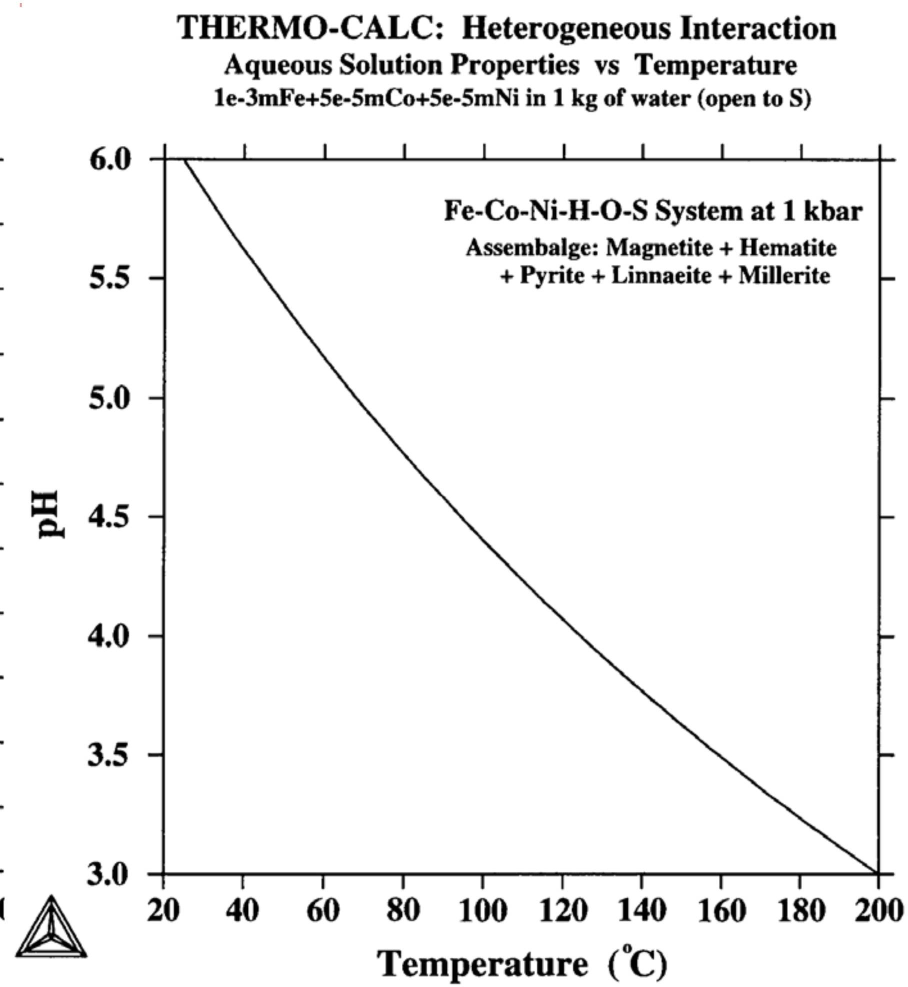
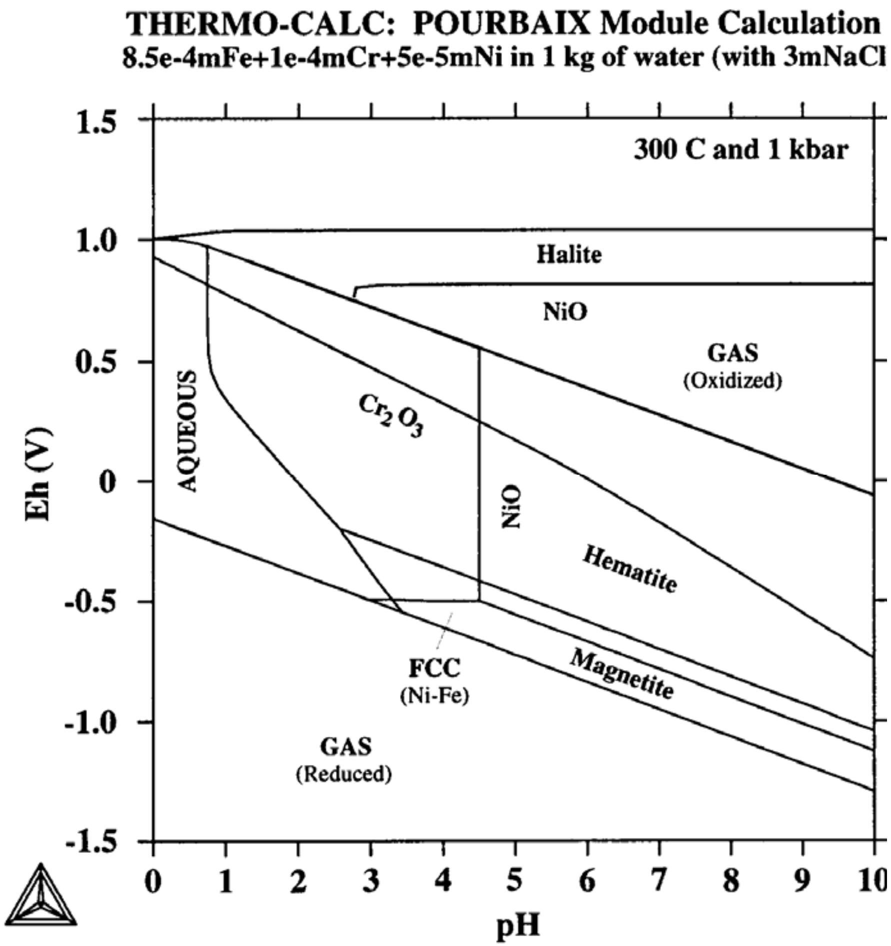
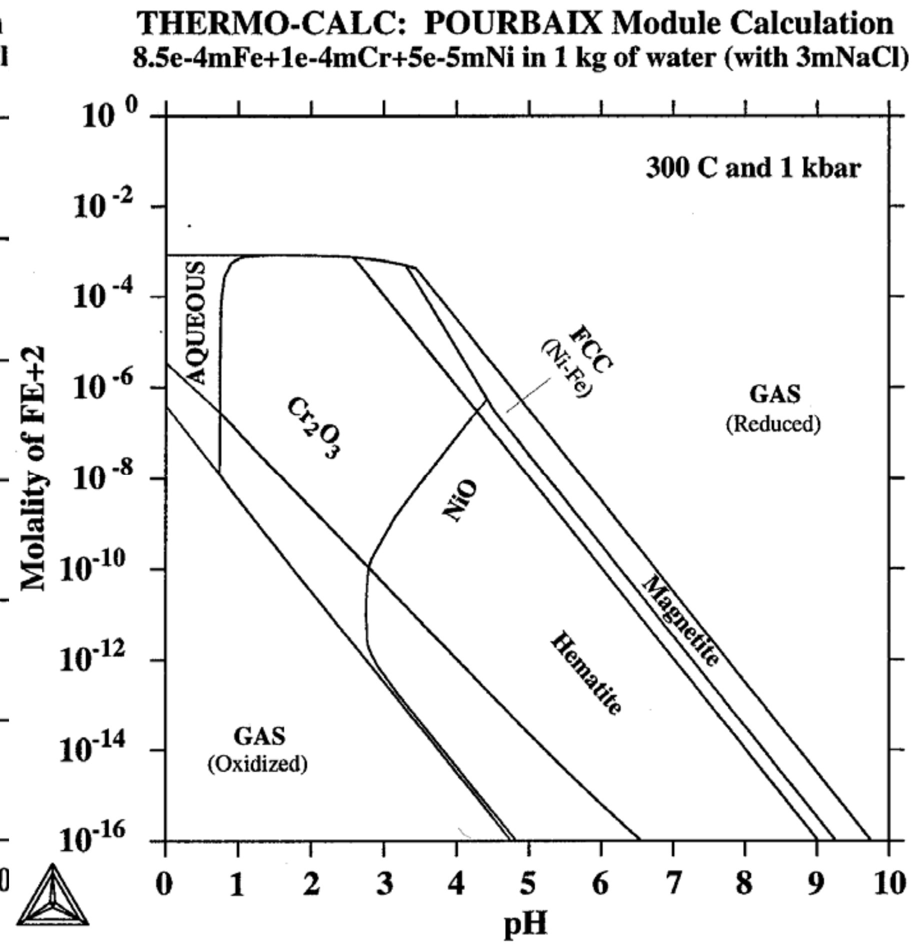




Variations of Eh and pH with temperature for the equilibrium assemblage Magnetite-Hematite-Pyrite-Linnaeite-Millerite in the heterogeneous interaction between an Fe-Alloy (consisting of 1E-3 m Fe, 5E-5 m Co and 5E-5 m Ni) and 1 kg of water (open to S) at 1 kbar.

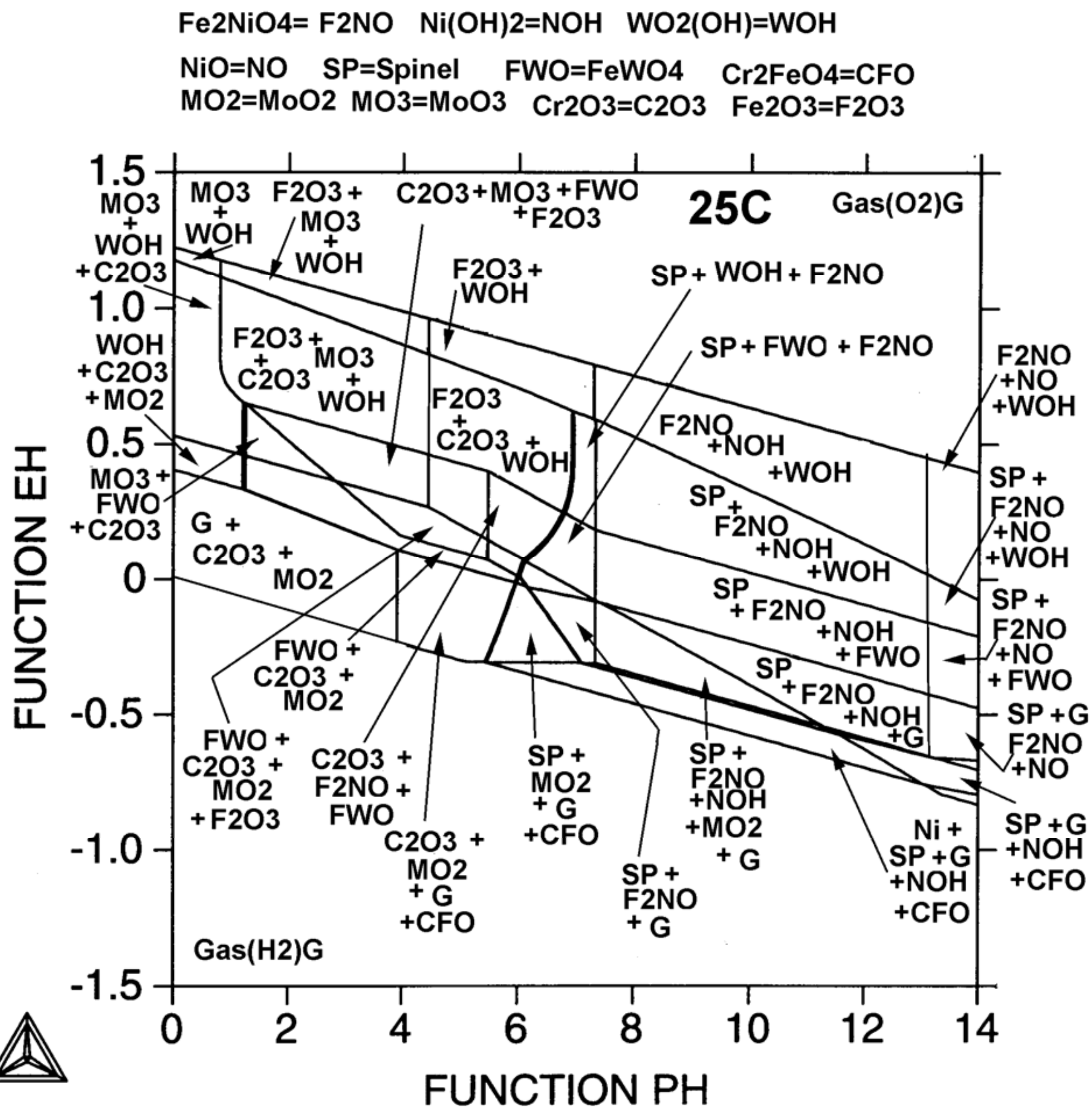
Case 3b Corrosion of Steel





Pourbaix diagram, and Fe^{+2} molality *vs.* pH diagram, for the heterogeneous interaction between an Fe-Alloy (consisting of 8.5E-4 m Fe, 1E-4 m Cr and 5E-5 m Ni) and 1 kg of water (with 3 m NaCl) at 300°C and 1 kbar.

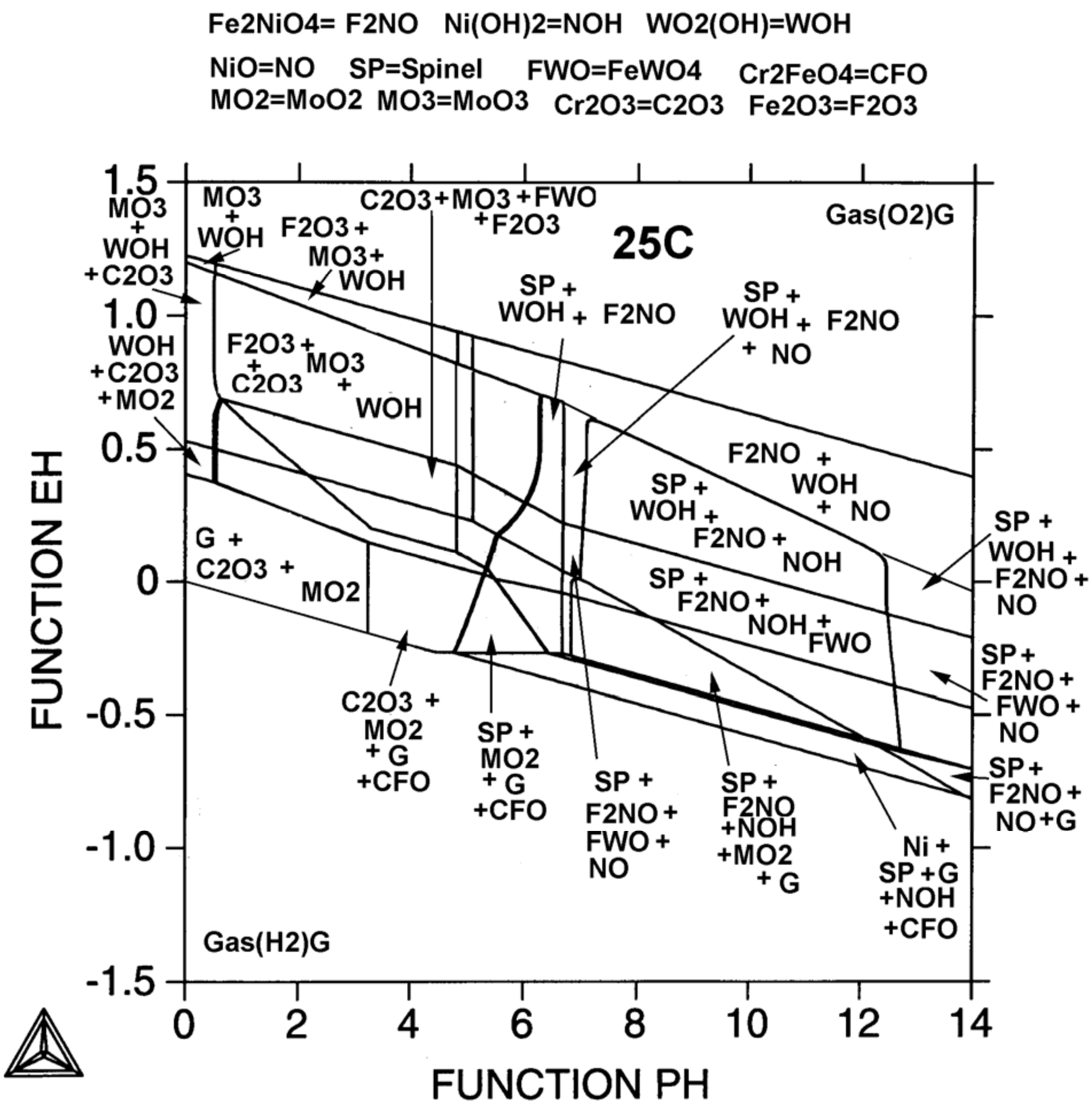
Case 4: Corrosion of C22 Superalloys



Calculated Pourbaix diagram for 58.1Ni-21.3Cr-13.6Mo-4.0Fe-3.0W (1 gm total) in 1 kg of water at 25°C.

Larry Kaufman, 2002: DOE-UCRL-JC-150606

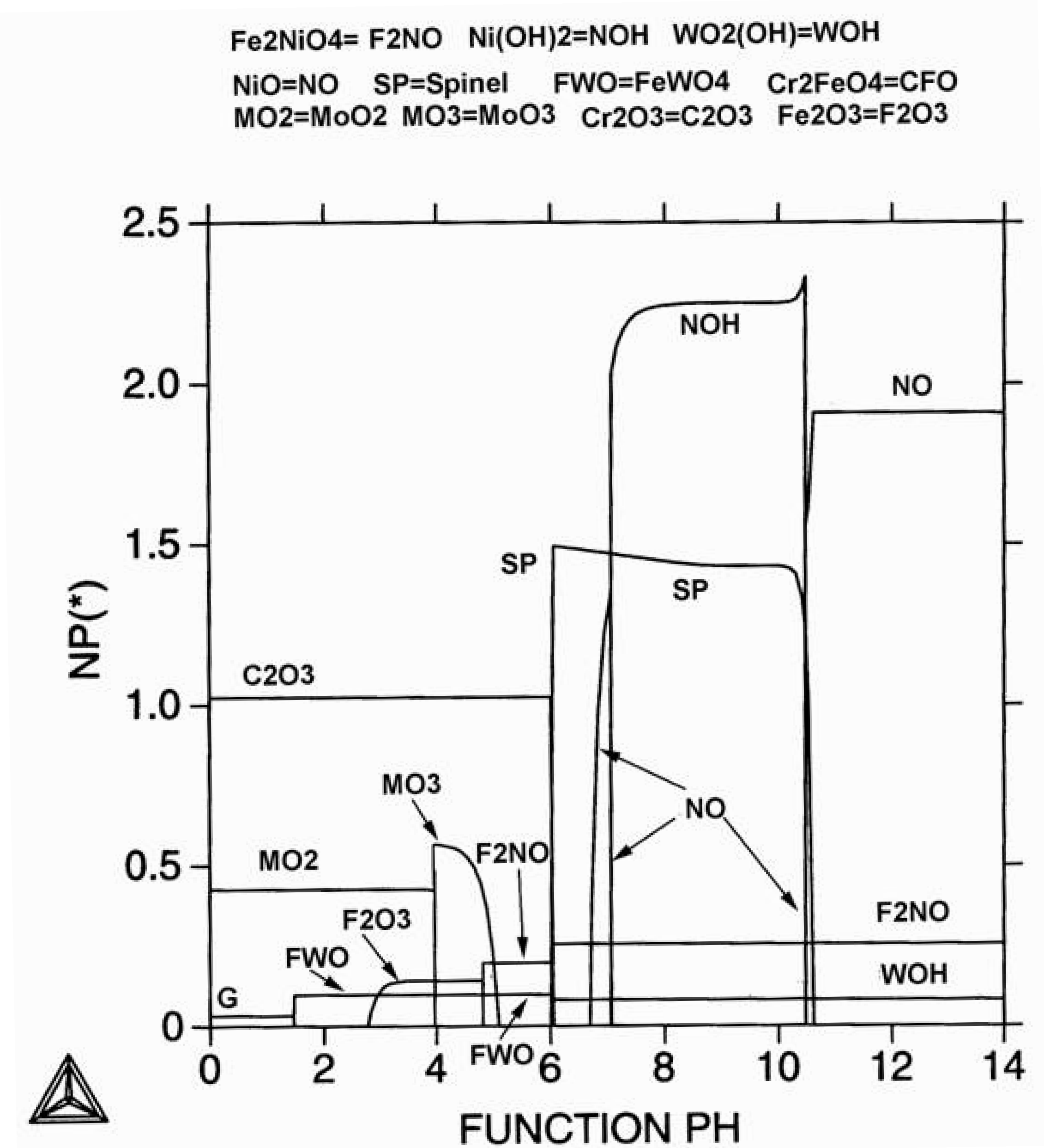
Case 4: Corrosion of C22 Superalloys



Calculated Pourbaix diagram for 58.1Ni-21.3Cr-13.6Mo-4.0Fe-3.0W (100 gm total) in 1 kg of water at 25°C.

Larry Kaufman, 2002: DOE-UCRL-JC-150606

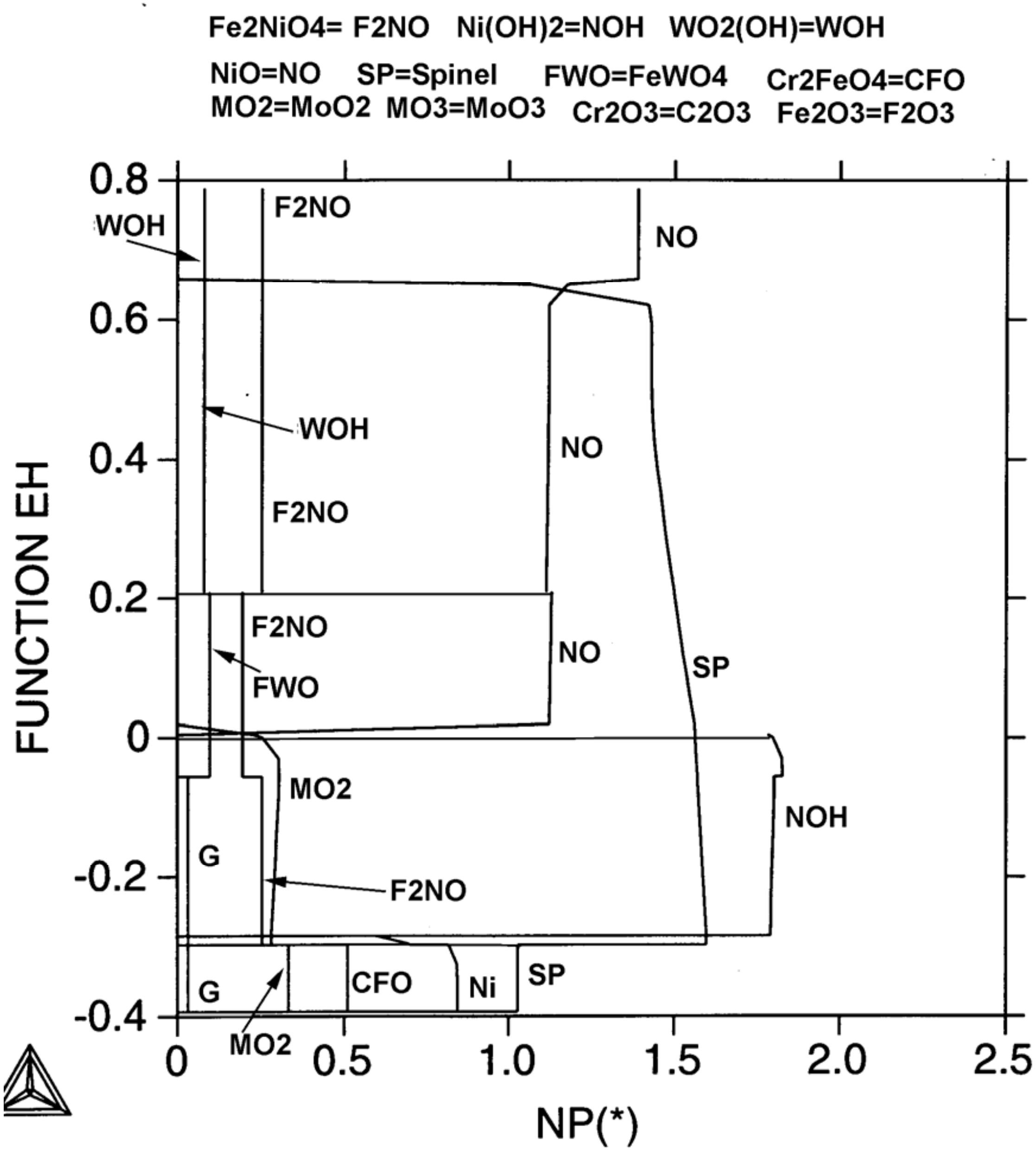
Case 4: Corrosion of C22 Superalloys



Calculated Pourbaix diagram for 58.1Ni-21.3Cr-13.6Mo-4.0Fe-3.0W (100 gm total) in 1 kg of water at 25°C.

Larry Kaufman, 2002: DOE-UCRL-JC-150606

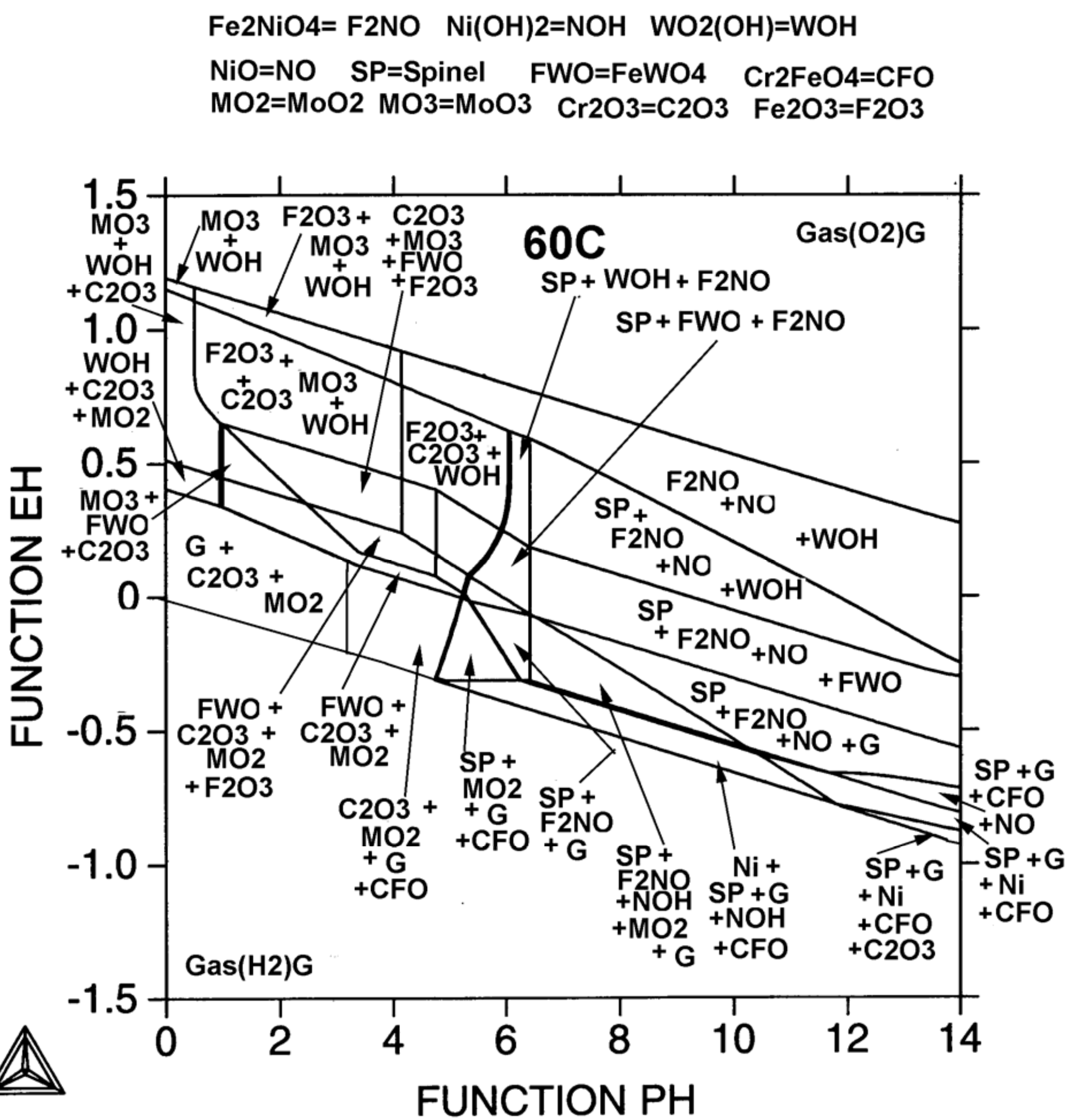
Case 4: Corrosion of C22 Superalloys



Calculated Pourbaix diagram for 58.1Ni-21.3Cr-13.6Mo-4.0Fe-3.0W (100 gm total) in 1 kg of water at 25^{o}C.

Larry Kaufman, 2002: DOE-UCRL-JC-150606

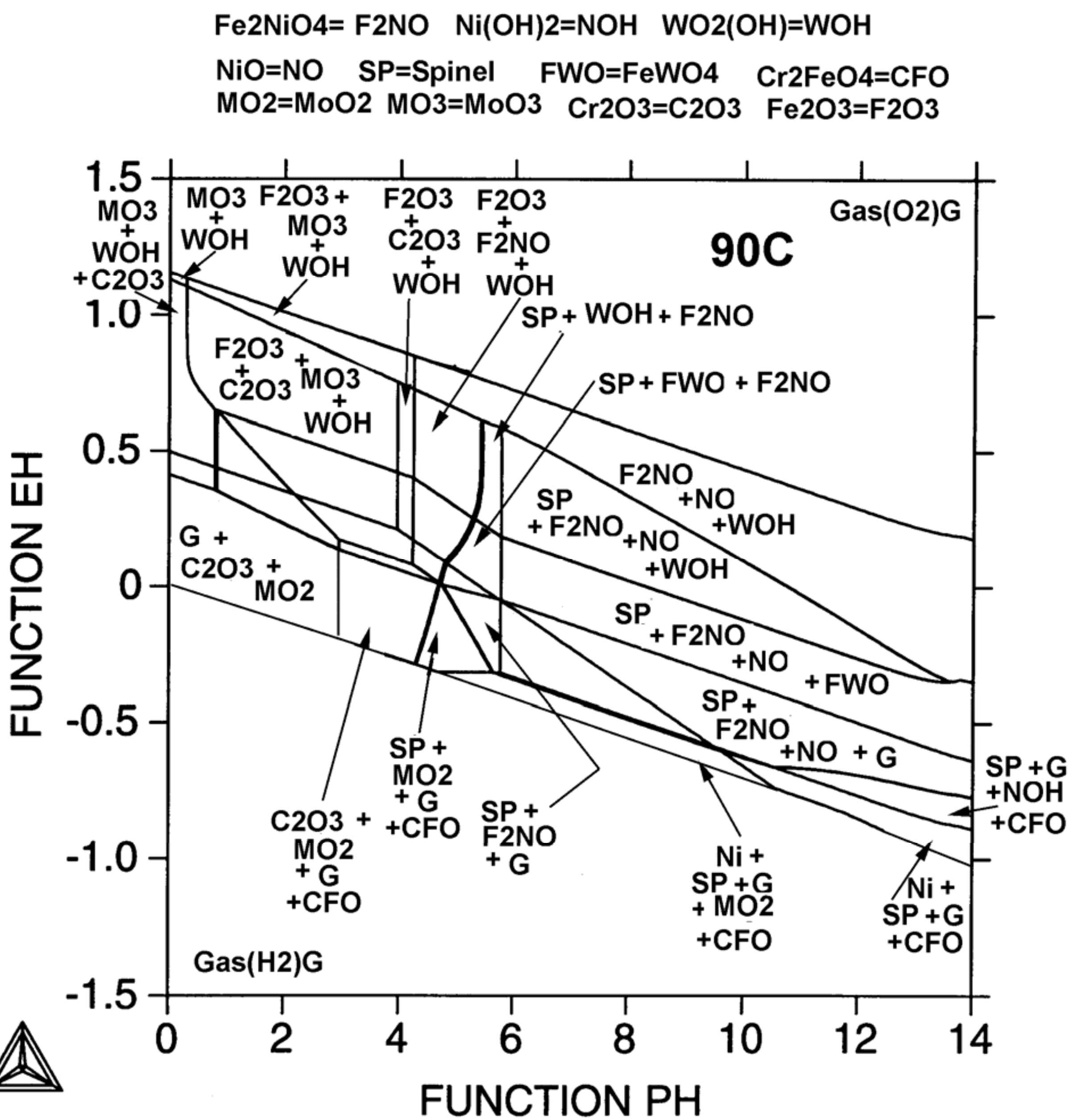
Case 4: Corrosion of C22 Superalloys



Calculated Pourbaix diagram for 58.1Ni-21.3Cr-13.6Mo-4.0Fe-3.0W (1 gm total) in 1 kg of water at 60^{o}C.

Larry Kaufman, 2002: DOE-UCRL-JC-150606

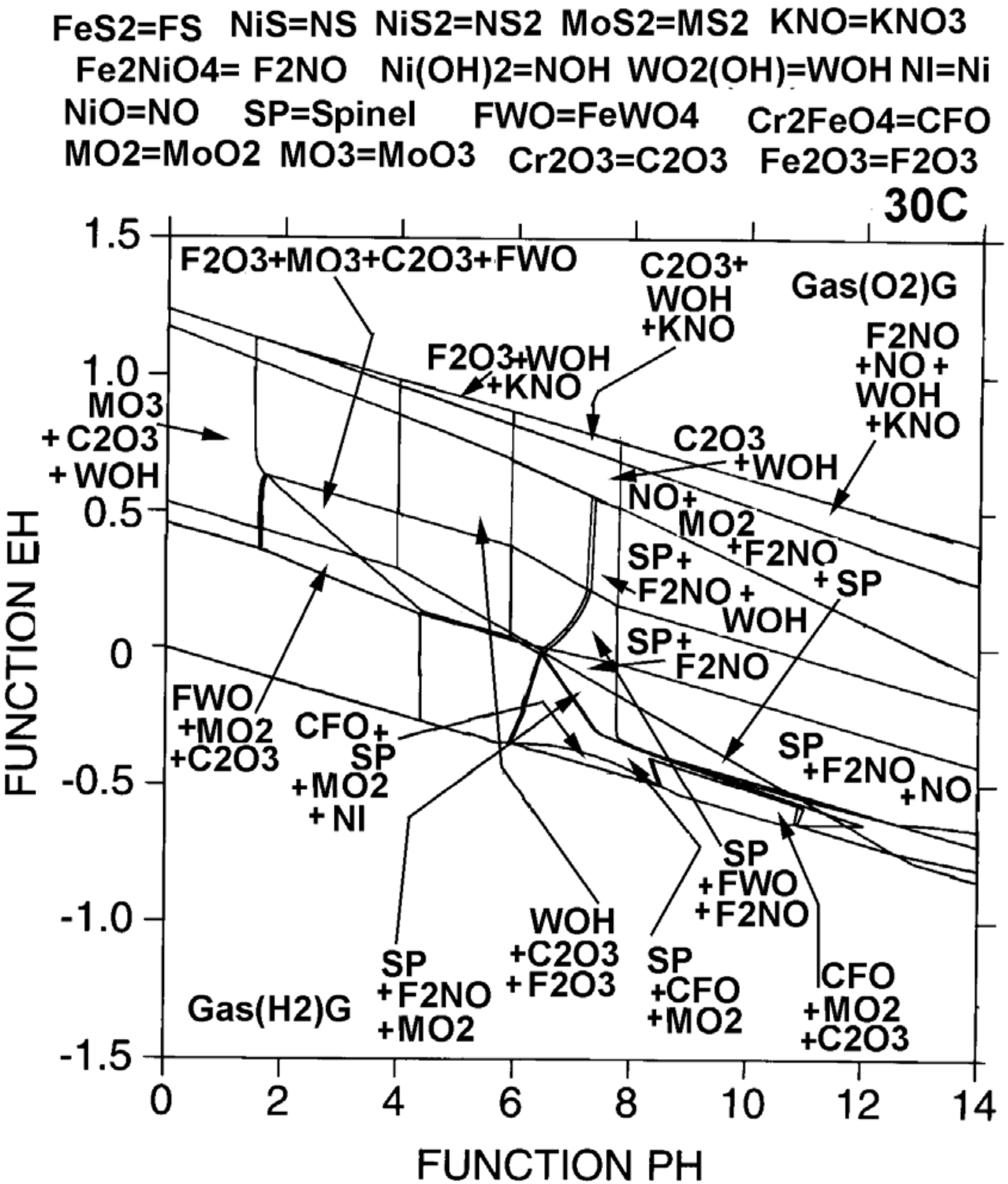
Case 4: Corrosion of C22 Superalloys



Calculated Pourbaix diagram for 58.1Ni-21.3Cr-13.6Mo-4.0Fe-3.0W (1 gm total) in 1 kg of water at 90°C.

Larry Kaufman, 2002: DOE-UCRL-JC-150606

Case 4: Corrosion of C22 Superalloys

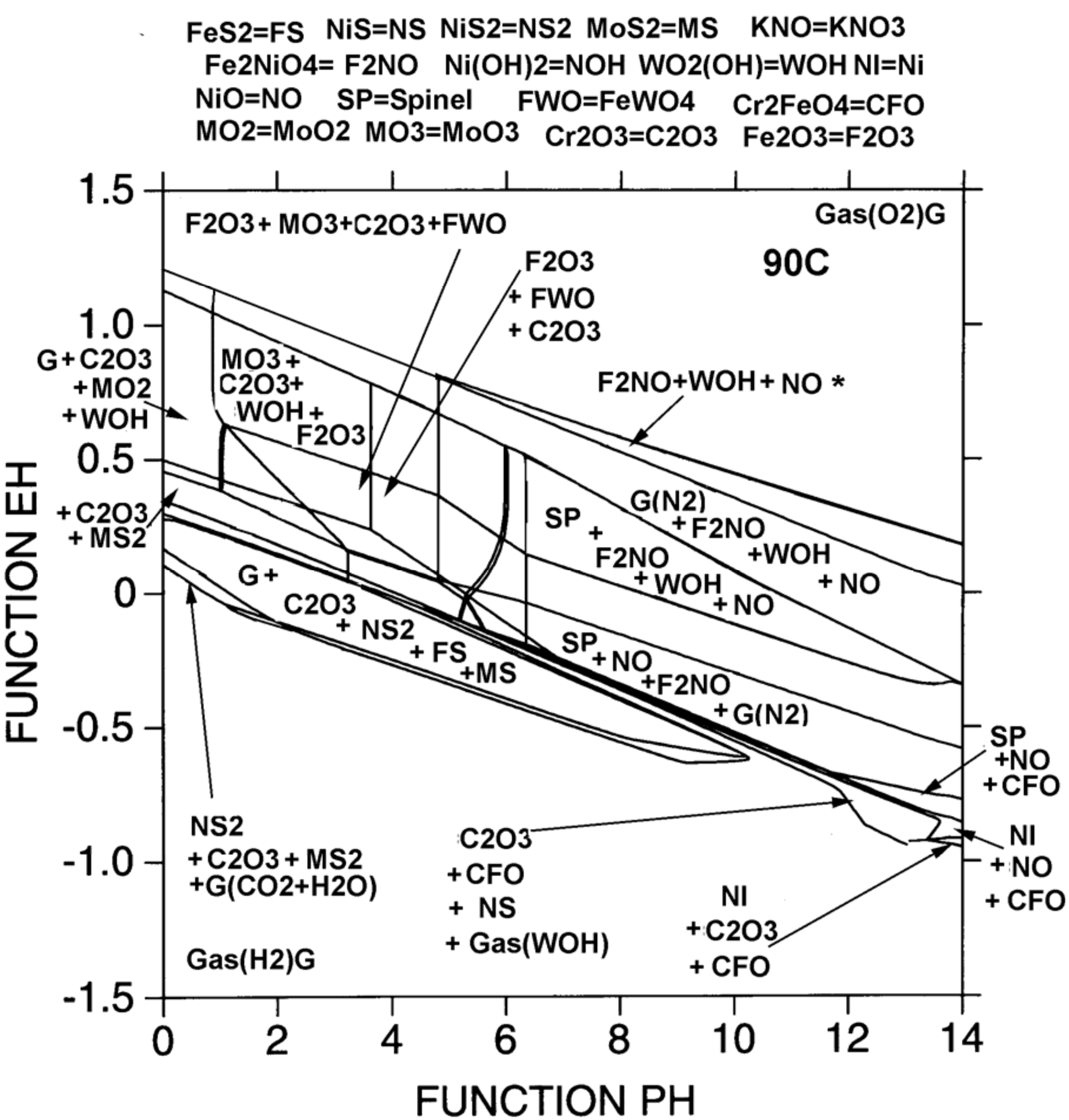


Calculated Pourbaix diagram for 58.1Ni-21.3Cr-13.6Mo-4.0Fe-3.0W (1 gm total) in Basic Simulated Water (BSW) at 30°C.

The BSW contains 1000 gms of H_2O, 141.7 gms of NO_3^{-1}, 186.6 gms of Na^{+1}, 166.0 gms of Cl^{-1} and 70.1 gms of K^{+1}. The following components of BSW were not included: 6.1 gms of SiO_2, 1.51 gms of F^{-1}, 64.2 gms of CO_3^{-2} and 15.8 gms of SO_4^{-2}. The entire stable Aqueous Solution Range also contains N_2 GAS except for the small sliver near the O_2 GAS boundary that contains solid KNO_3 .

Larry Kaufman, 2002: DOE-UCRL-JC-150606

Case 4: Corrosion of C22 Superalloys



Calculated Pourbaix diagram for 58.1Ni-21.3Cr-13.6Mo-4.0Fe-3.0W (1 gm total) in Basic Acidic Water (BAW) at 90ºC.

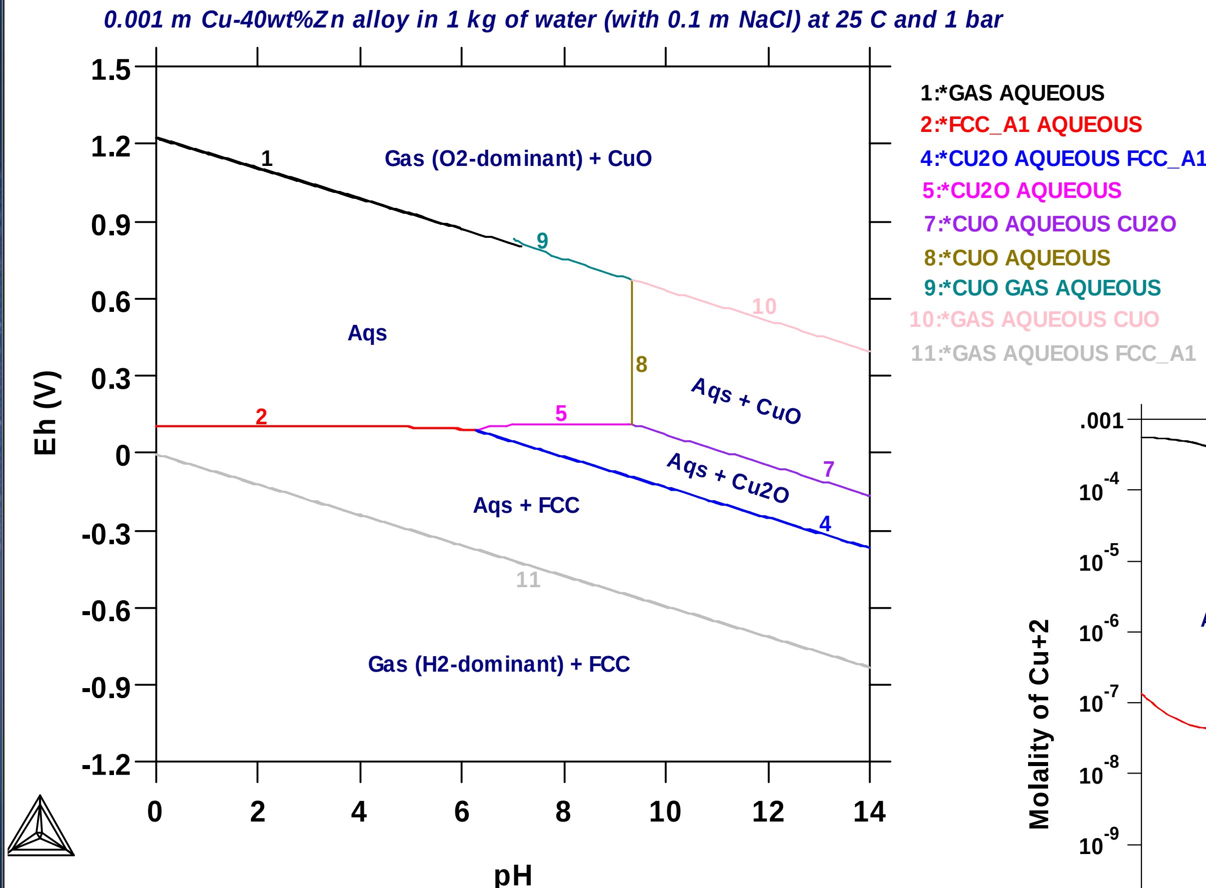
The BAW contains 1000 gms of H_2O, 23.0 gms of NO_3^{-1}, 1,37.6 gms of Na^{+1}, 24.25 gms of Cl^{-1} and 38.6 gms of SO_4^{-2}. The following components of SAW were not included: 1.0 gms. of Ca^{+2}, 3.4 gms of K^{+1}, 0.058 gms of SiO_2, and 1.0 gms of Mg^{+2} . The entire space is covered by an aqueous solution and a gas phase whose composition varies except for the regions noted with asterisks(*) in which there is no gas phase.

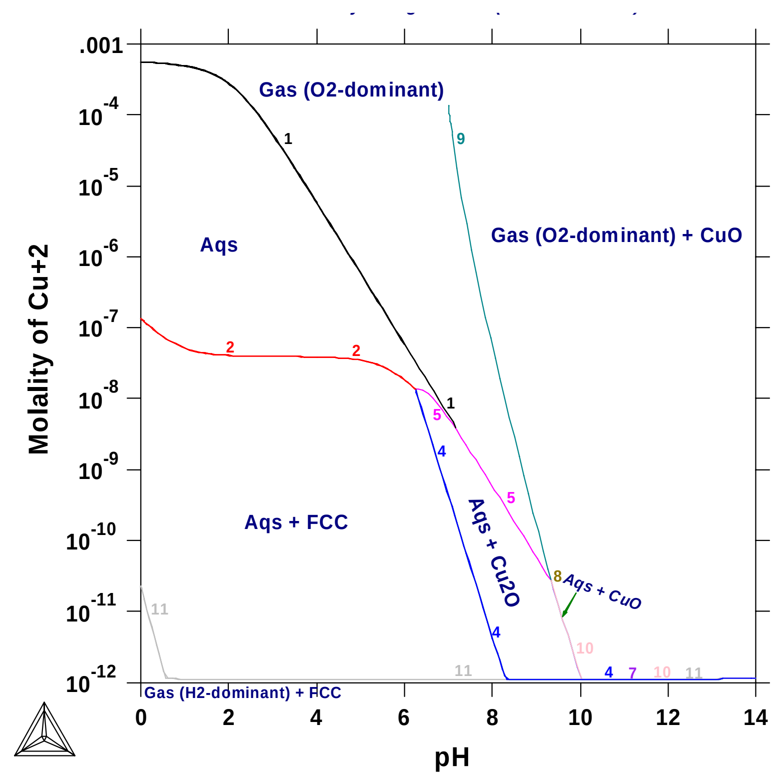
Larry Kaufman, 2002: DOE-UCRL-JC-150606

Case 5: Corrosion of Cu-40Zn Alloy

THERMO-CALC (2004.03.23): Pourbaix Diagram

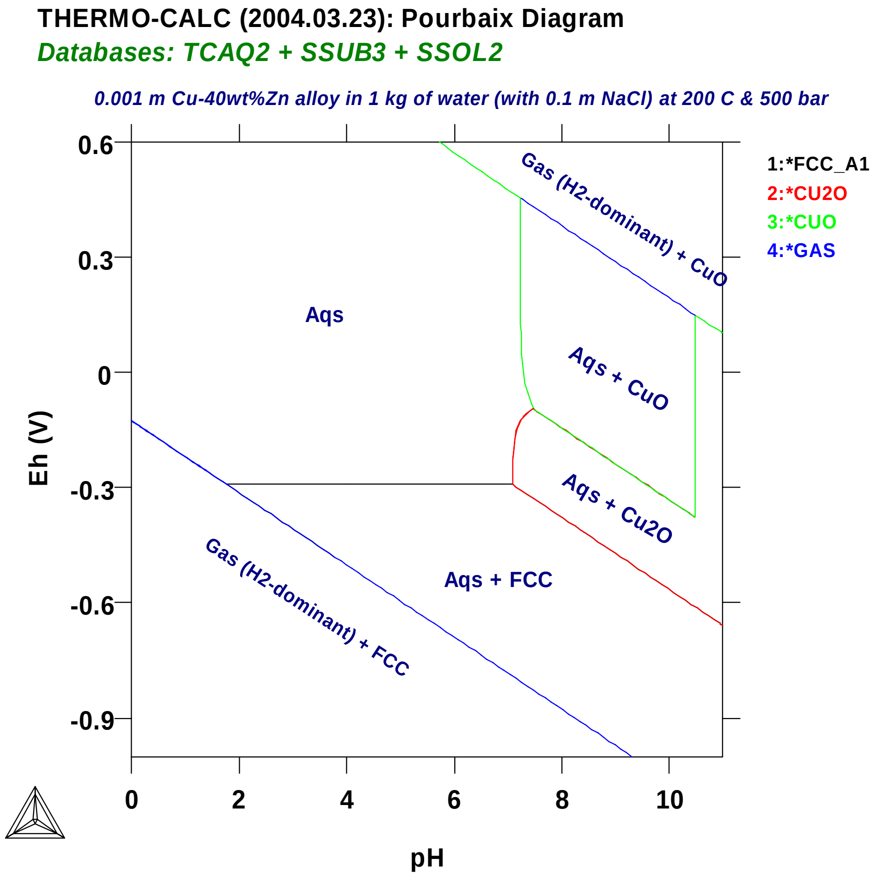
Databases: TCAQ2 + SSUB3 + SSOL2



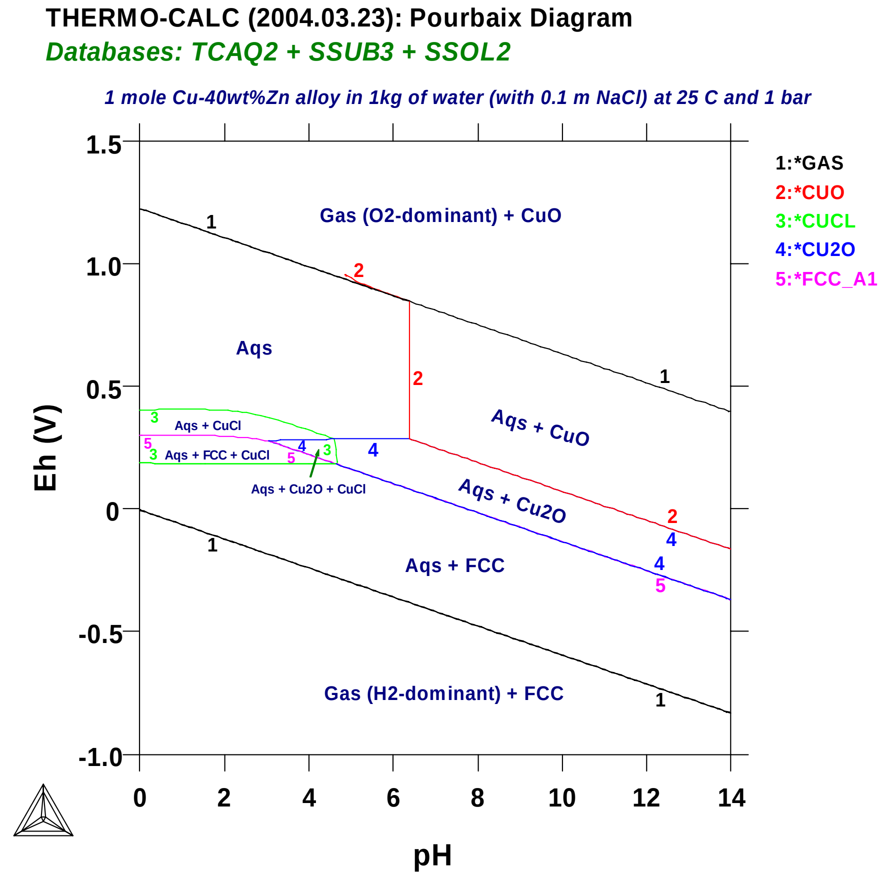


Calculated Pourbaix Diagram and related variation of m(Cu^{+2}) property for 0.001 mole Cu-40wt%Zn Alloy in 1 kg of Water (with 0.1 m NaCl) at 25°C and 1 bar.

Case 5: Corrosion of Cu-40Zn Alloy



Calculated Pourbaix Diagram for 0.001 mole Cu-40wt%Zn Alloy in 1 kg of Water (with 0.1 m NaCl) at 200^{o}C and 100 bar.

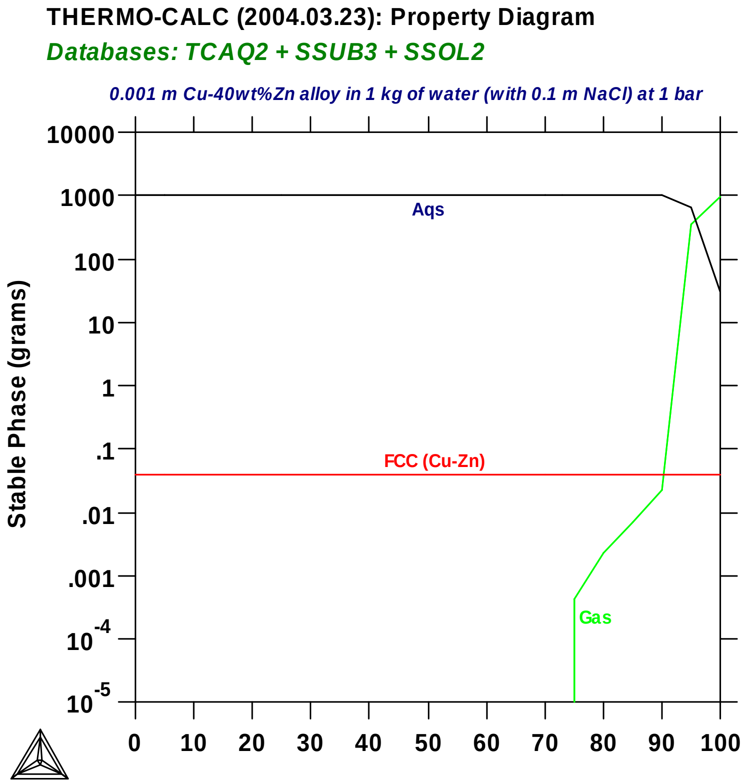


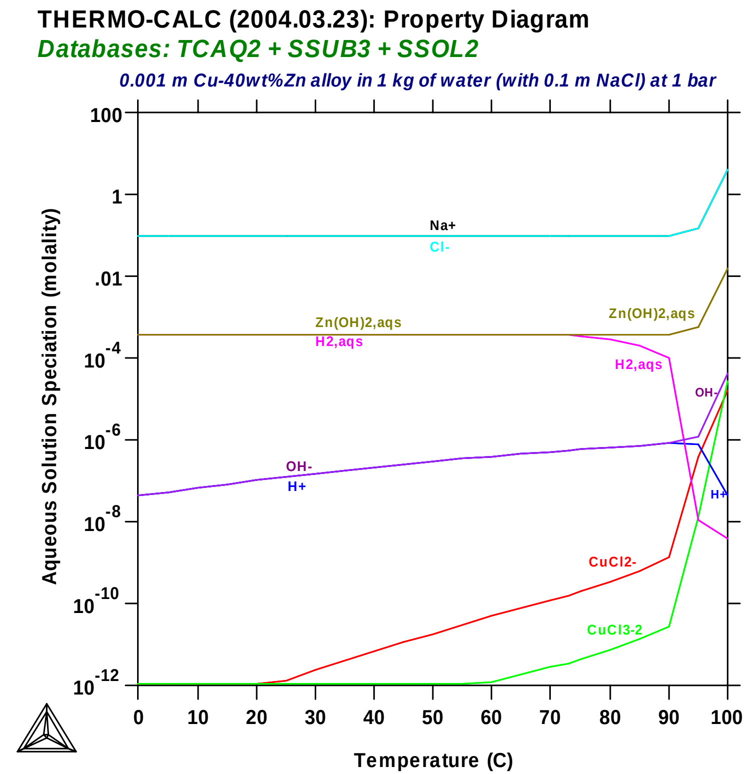
Calculated Pourbaix Diagram for 1 mole Cu-40wt%Zn Alloy in 1 kg of Water (with 0.1 m NaCl) at 25^{o}C and 1 bar.

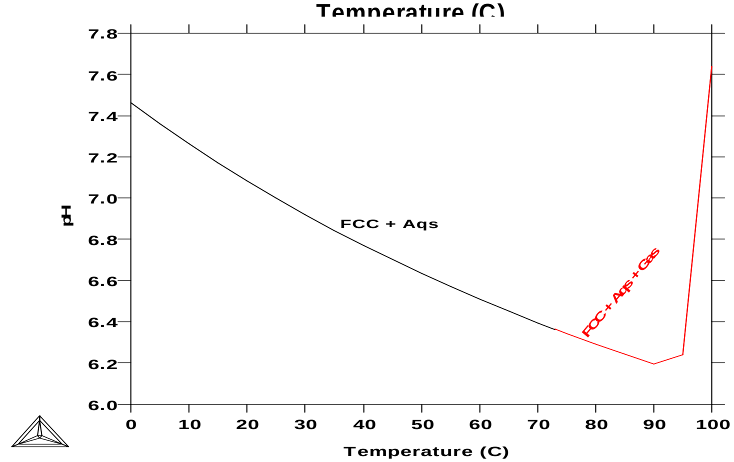
Case 5: Corrosion of Cu-40Zn Alloy

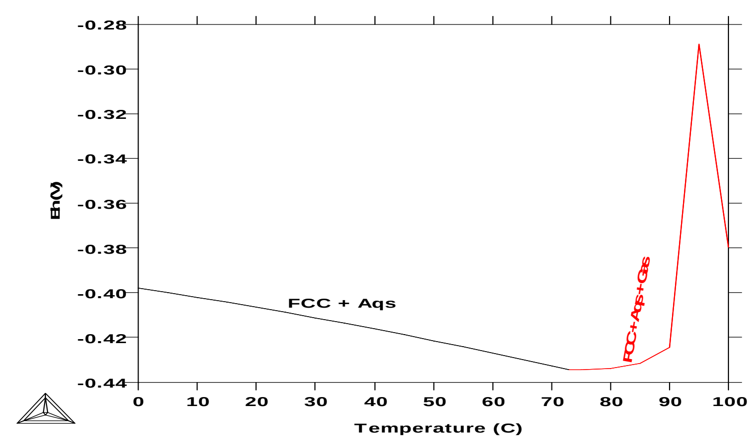
Thermo-Calc Software

Calculated Property Diagrams for 0.001 mole Cu-40wt%Zn Alloy in 1 kg of Water (with 0.1 m NaCl) at 1 bar and varied temperatures.

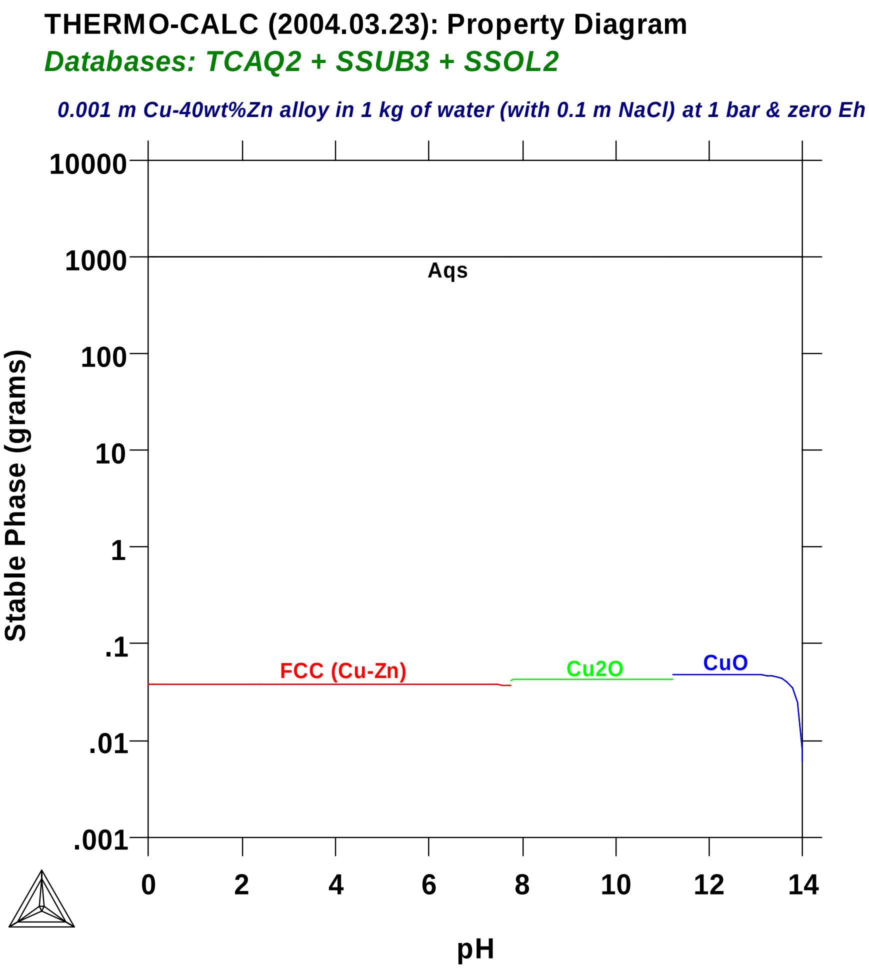


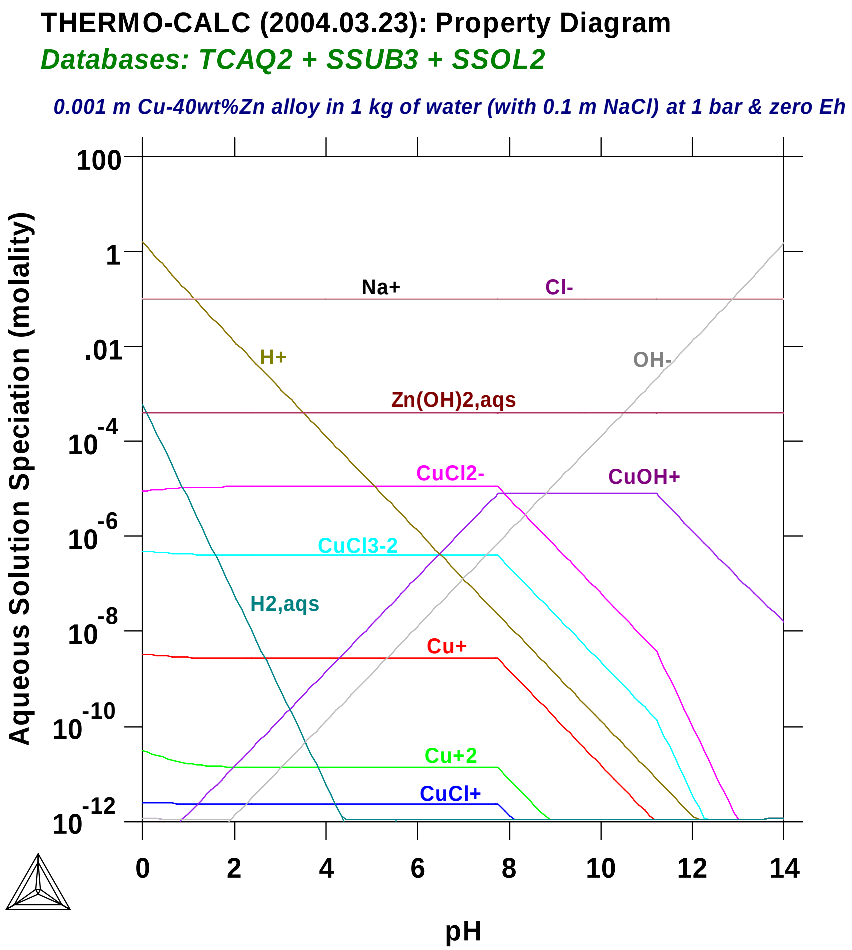






Case 5: Corrosion of Cu-40Zn Alloy



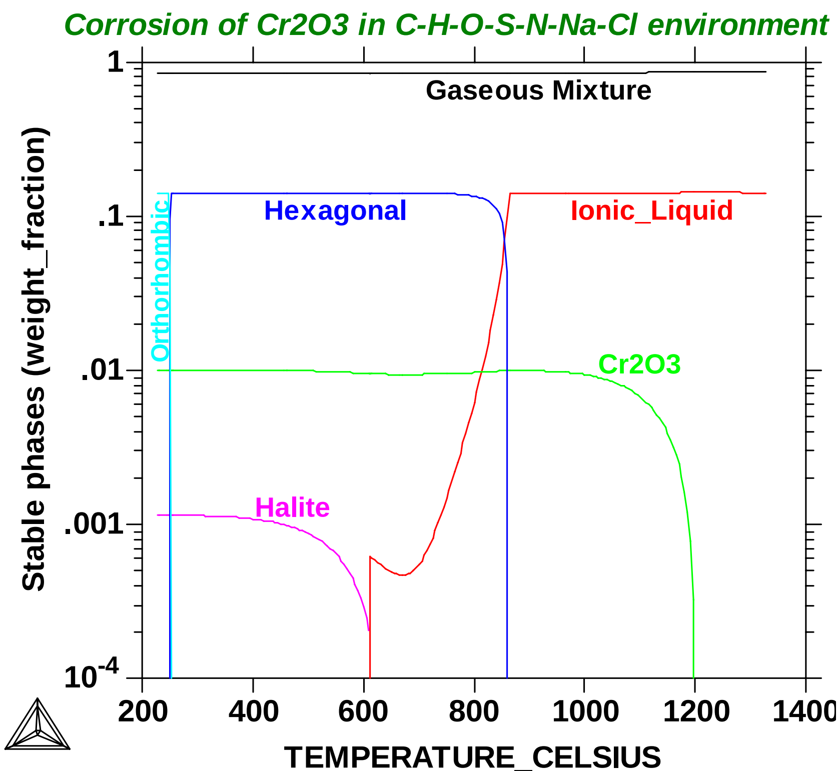


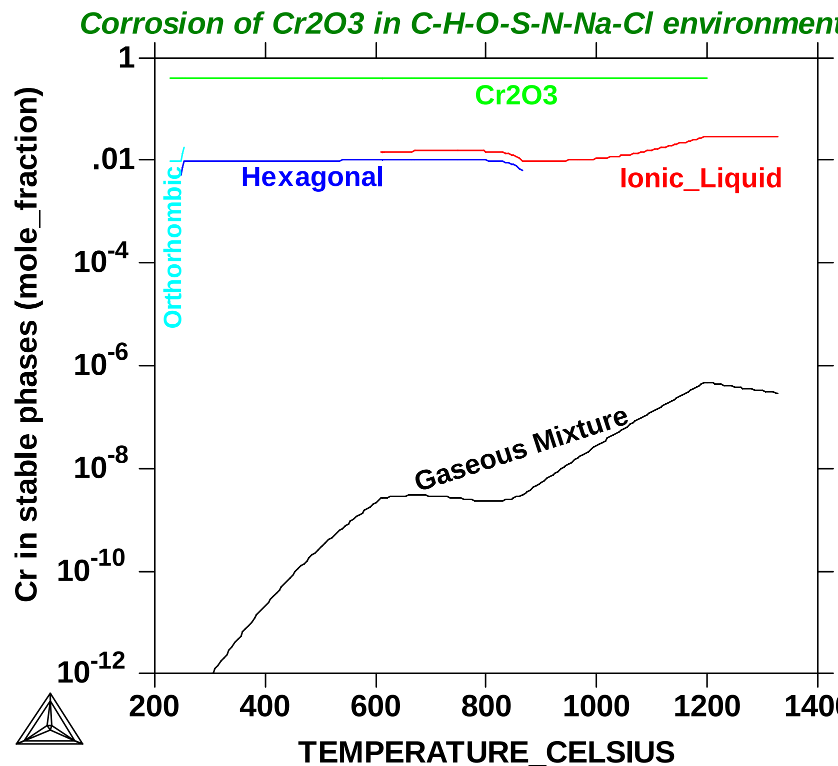
Calculated Property Diagrams for 0.001 mole Cu-40wt%Zn Alloy in 1 kg of Water (with 0.1 m NaCl) at 25oC, 1 bar, zero Eh and varied acidity.

Salt Corrosion

Example: Salt Corrosion of Alloy Surface

Using the SALT database (and/or in a combination with other databases), one can calculate various types of phase diagrams and property diagrams for heterogeneous interaction systems/processes involving molten salts.





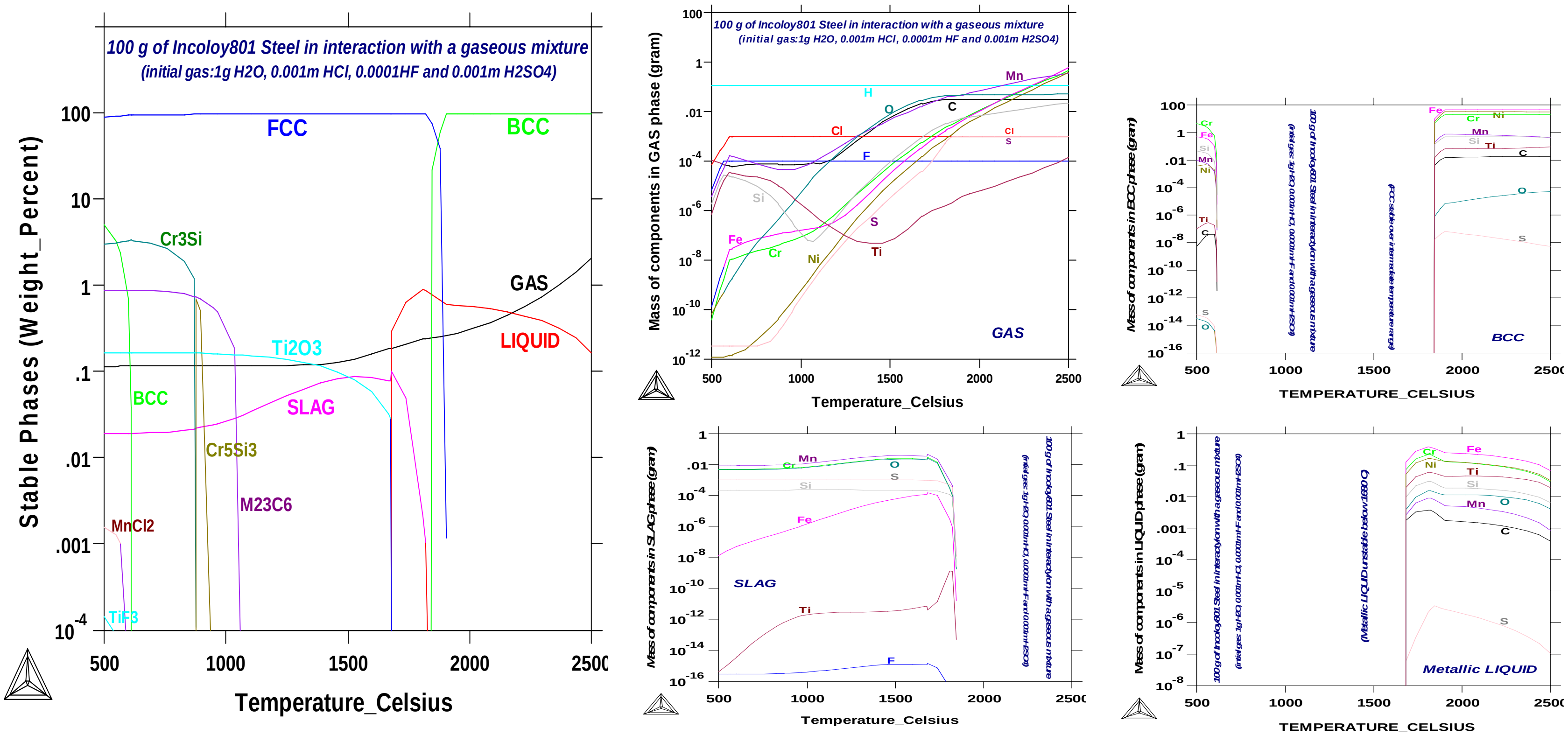
As a typical form in the oxide layer on the surface of stainless steels, Ni-based superalloys, etc, Cr_2O_3 provides a protection from corrosion attacks by hot or molten salts, high-temperature gases, or aqueous solutions. This calculation illustrates that under certain aggressive conditions, the Cr_2O_3 layer may be dissolved by the attacking salts, and thus the applied alloy may be exposed to further corrosion attacks from oxidizing and sulphidising environments.

Gaseous Corrosion

Thermo-Calc Software

Example: High-Temperature (Gaseous) Corrosion of Alloys

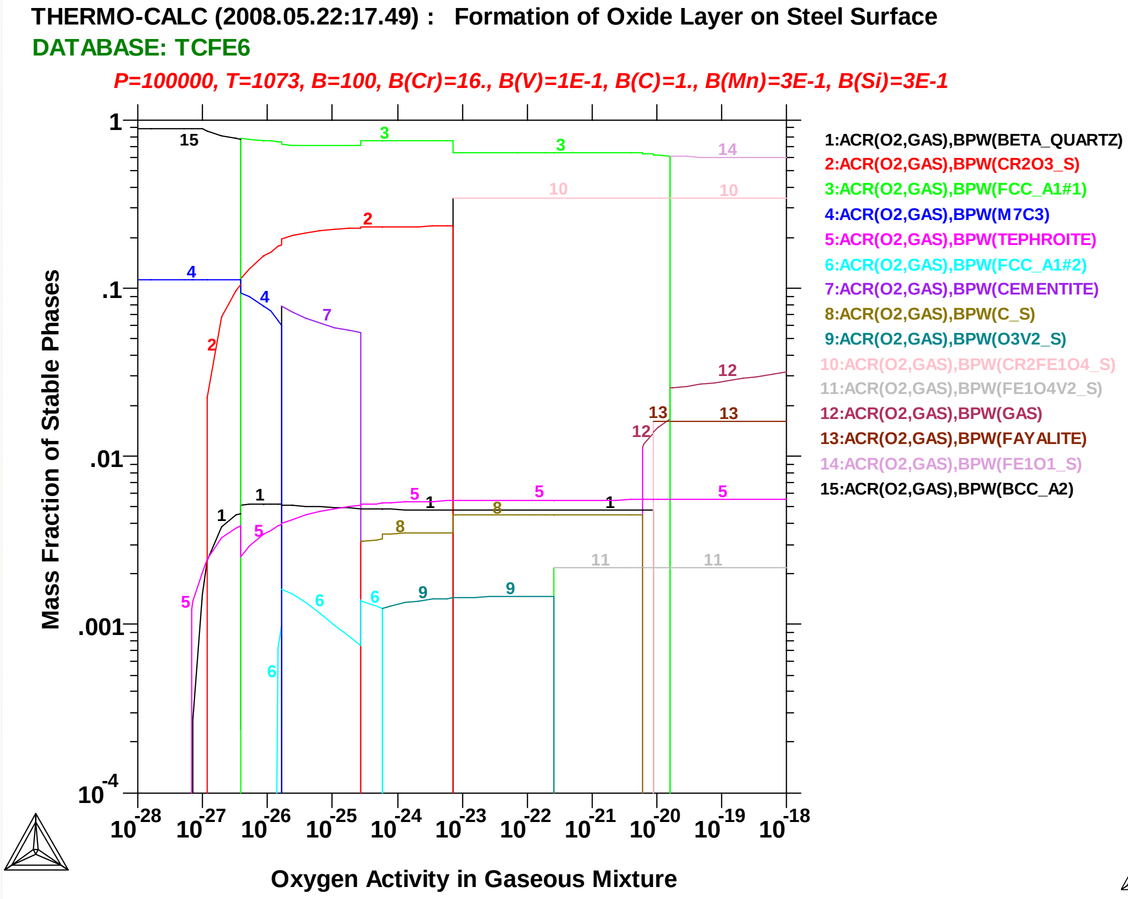
Using the TCMP2 or SSUB3 database (and/or in a combination with other alloy databases), one can calculate various types of phase diagrams and property diagrams for heterogeneous interaction systems/processes involving gaseous mixtures.

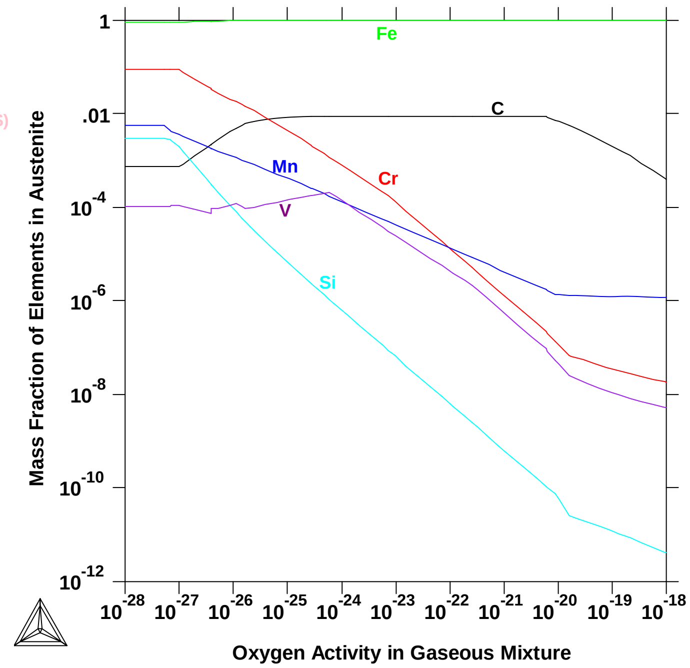


Calculated property diagrams of the heterogeneous interaction between 100 g of Incoloy 801 steel (wrought Fe-based superalloy with a composition of Fe44.5-Ni32-Cr20.5-Ti1.1-Mn0.8-Si0.5-C0.05 wt%) and a gas mixture (of 1 g H2O, 0.001 m HCl, 0.0001 m HF and 0.001 m H_2SO_4). The calculation shows that the gas mixture will dissolve the steel components (especially with increasing temperatures), meanwhile LIQUID phase or SLAG+Ti_2O_3 phases may form during the interaction over certain temperature ranges.

Surface Redox Reactions (I)

Example: Formation of Oxide Layer on Steel Surface: Protection against corrosion



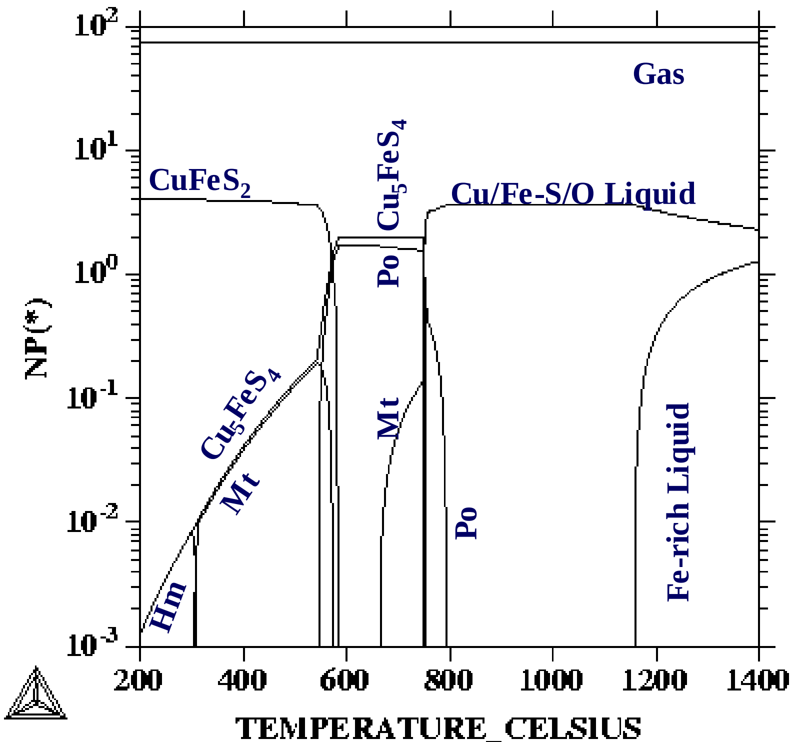


Stable phases and element distribution of remaining austenite during the surface oxidation of the Fe-16Cr-0.3Mn-0.3Si-.01V-1C (wt%) steel at 800°C, as a function of oxygen activity in the atmosphere.

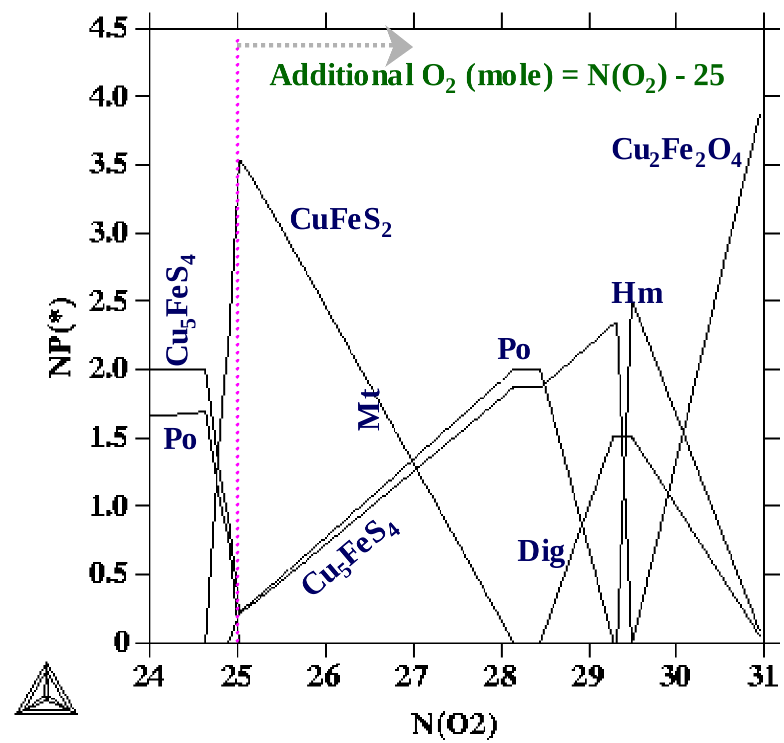
Surface Redox Reactions (II)

Example: Oxidation of Sulfides ($CuFeS_2$)

Using the ION database, one can calculate various types of phase diagrams and property diagrams for oxidation processes of multiple-metal sulfides (e.g., $CuFeS_2$, FeS_2) or mixtures (e.g., $CuFeS_2$-FeS_2), to find optimal temperatures and initial bulk compositions (especially the additional oxygen input).



Stable phases during oxidation of $CuFeS_2$, as a function of the temperature condition. The calculation is made for an interaction system of 2 moles $CuFeS_2$ and 50 moles of vapour, at 1 bar and various temperatures (200 to 1400°C).



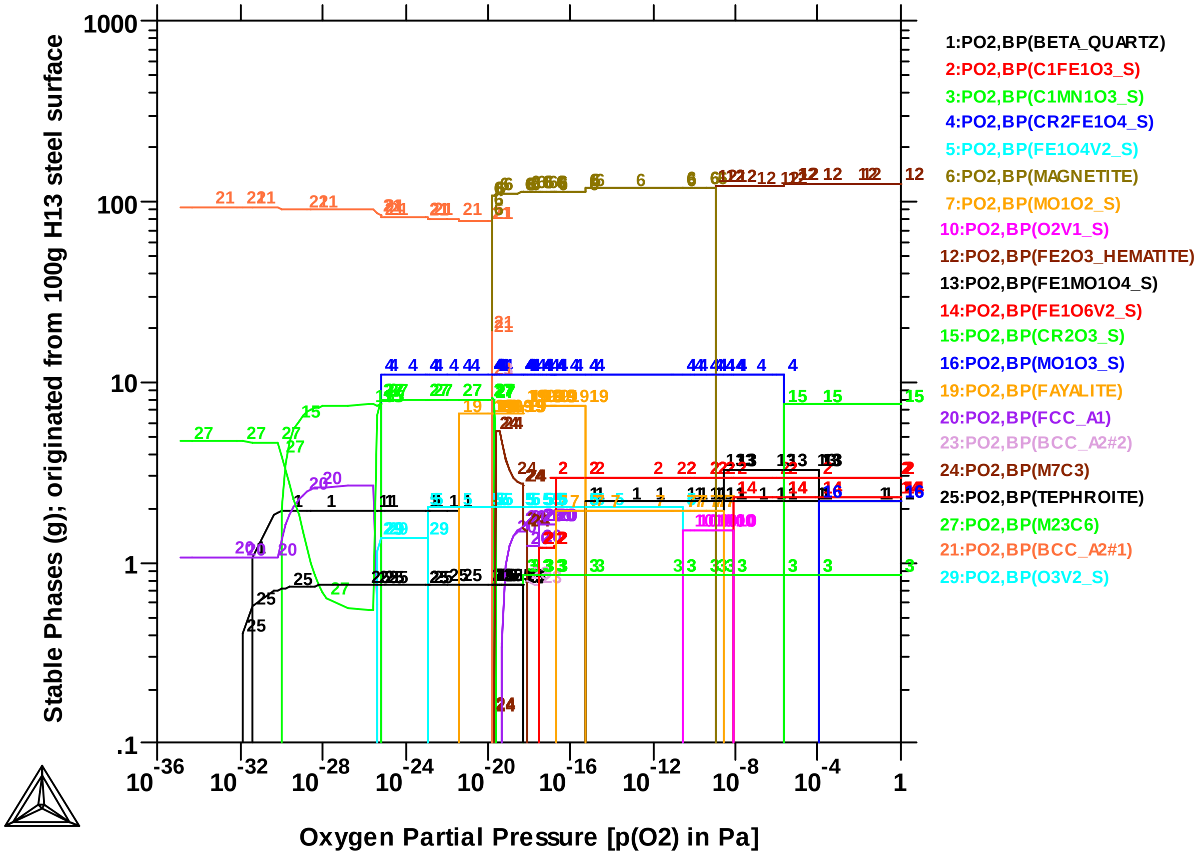
Stable phases during oxidation of $CuFeS_2$, varied with the additional oxygen amount. The calculation is made for an interaction system of 2 moles $CuFeS_2$ and 50 moles of vapour, at 550°C, 1 bar and various additional amounts of O_2.

Thermo-Calc Software

Surface Redox Reactions (III)

Example: Oxidation of H13 Hot Work Steel

THERMO-CALC (2008.02.29:16.47) :
DATABASE:SSOL4
P=1E5, T=873.15, B(FE)=90.63, B(CR)=5.14, B(MN)=0.41, B(SI)=1.02, B(C)=0.4, B(V)=0.93, B(MO)=1.46, B(S)=1E-3, B(P)=9E-3;

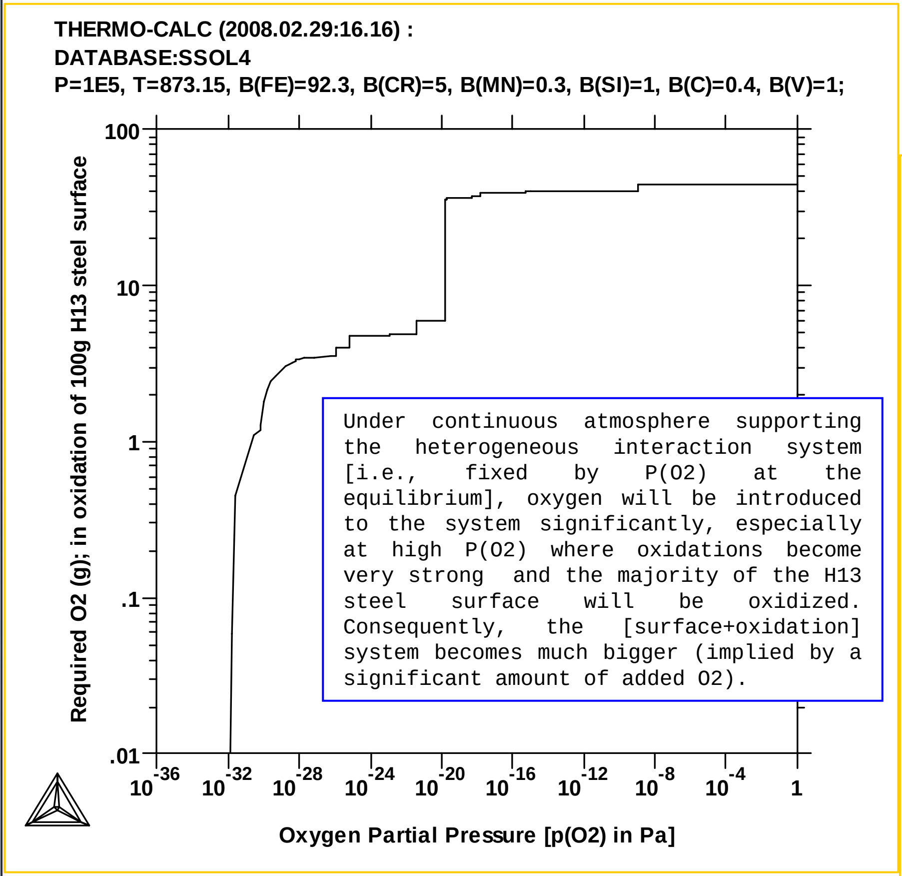


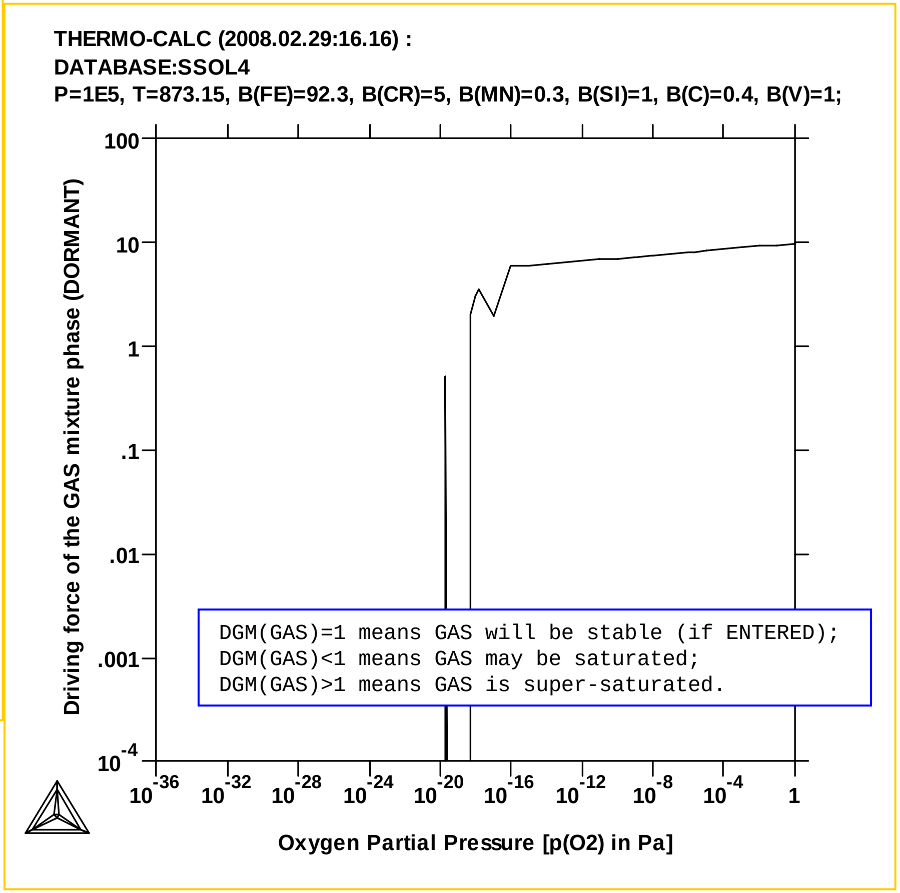
Stable phases during oxidation of H13 Hot Work Steel [Fe-5.14Cr-0.41Mn-1.02Si-0.40C-0.93V-1.46Mo-0.001S-0.009P-O], varied with the oxygen partial pressure. The calculation is made for an interaction system at temperature of 600°C and a total pressure of 1 bar.

Surface Redox Reactions (III)

Thermo-Calc Software

Example: Oxidation of H13 Hot Work Steel



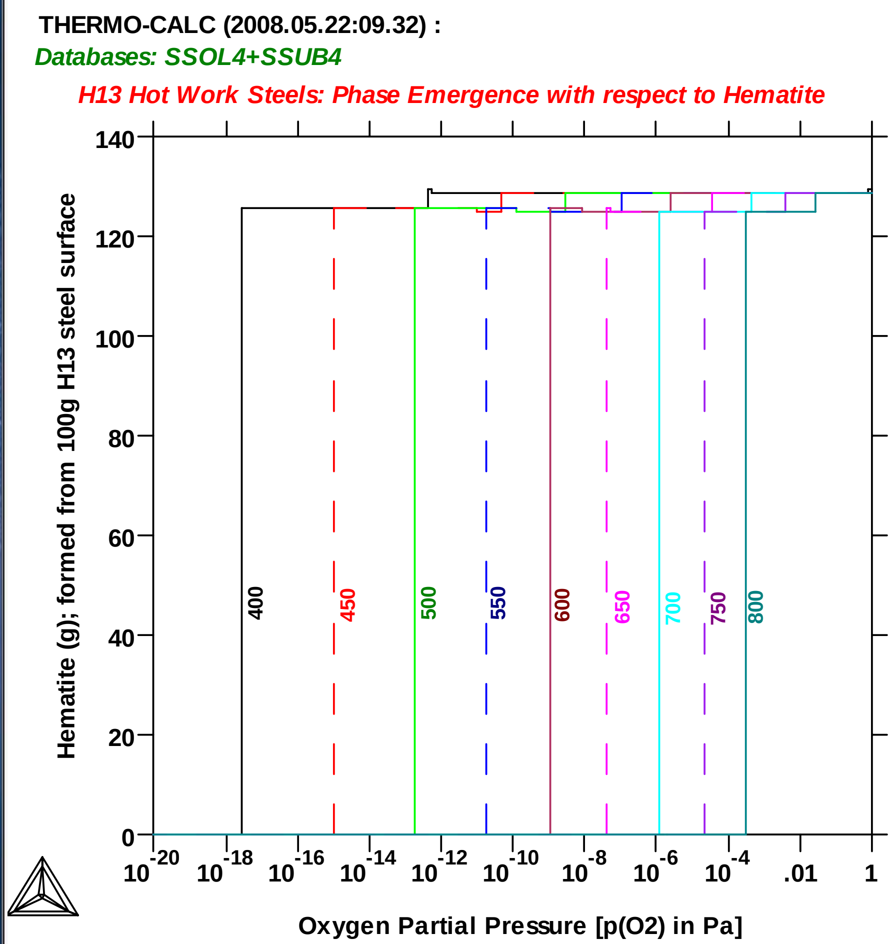


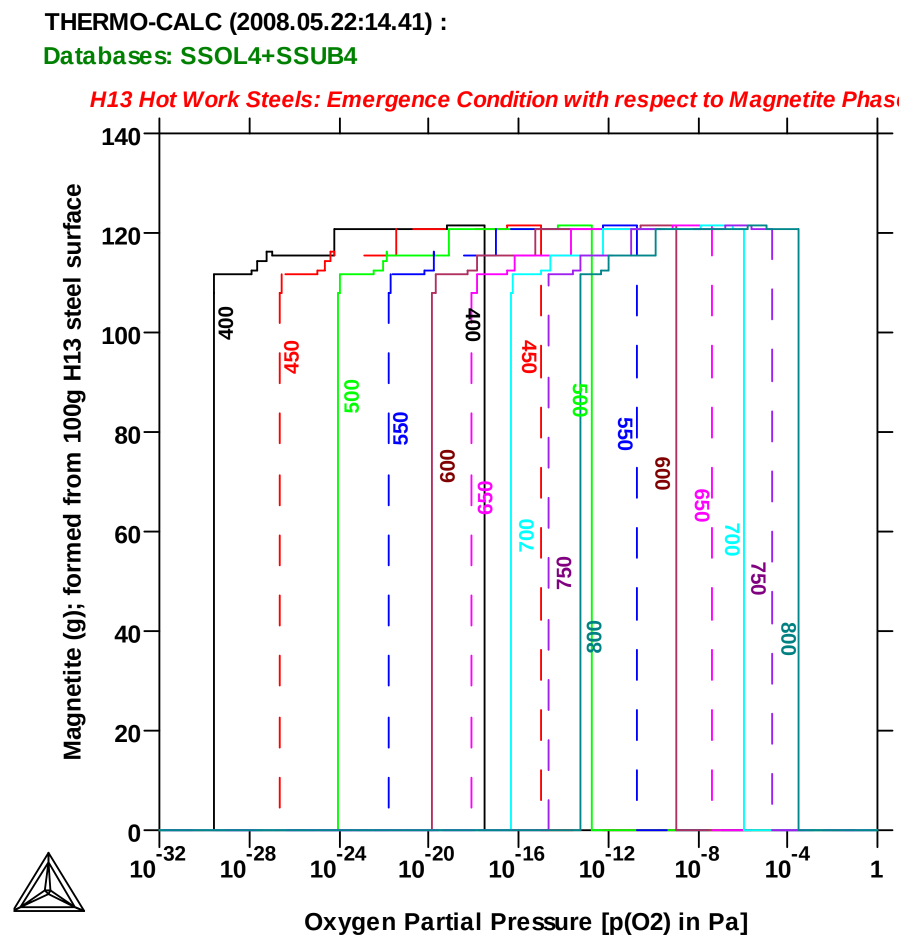
Required O2 Input and Driving force of the dormant GAS phase during oxidation of H13 Hot Work Steel [Fe-5.14Cr-0.41Mn-1.02Si-0.40C-0.93V-1.46Mo-0.001S-0.009P-O], varied with the oxygen partial pressure. The calculation is made for an interaction system at temperature of 600ºC and a total pressure of 1 bar.

Surface Redox Reactions (III)

Thermo-Calc Software

Example: Oxidation of H13 Hot Work Steel



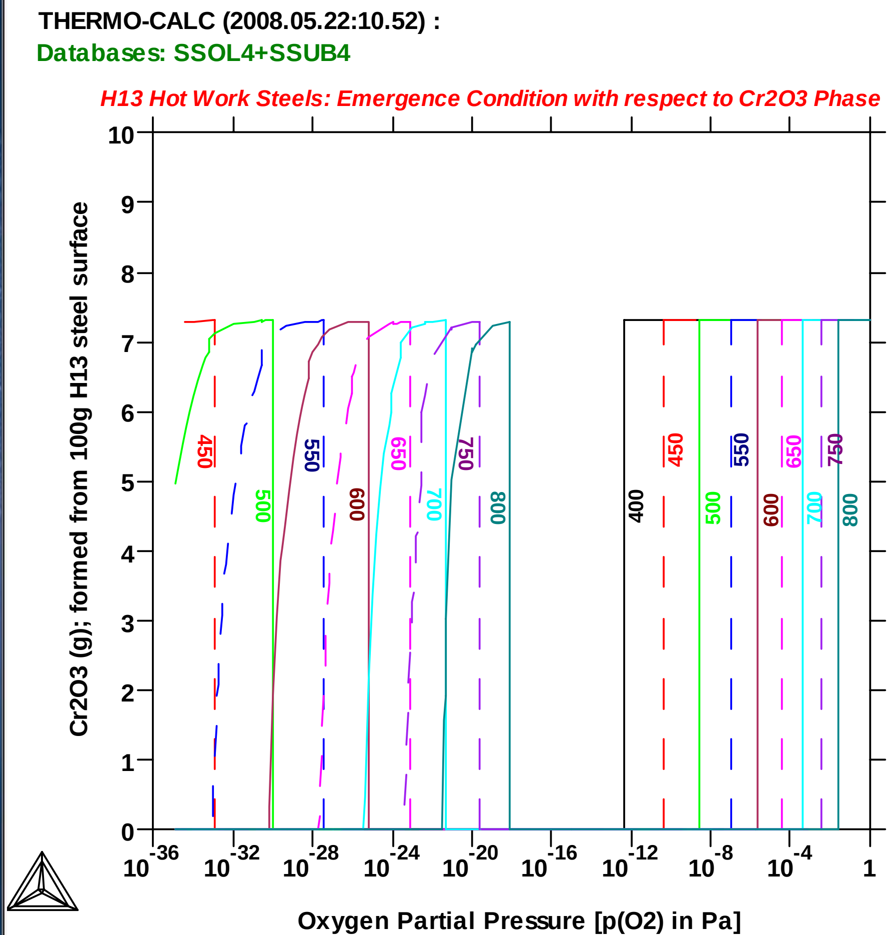


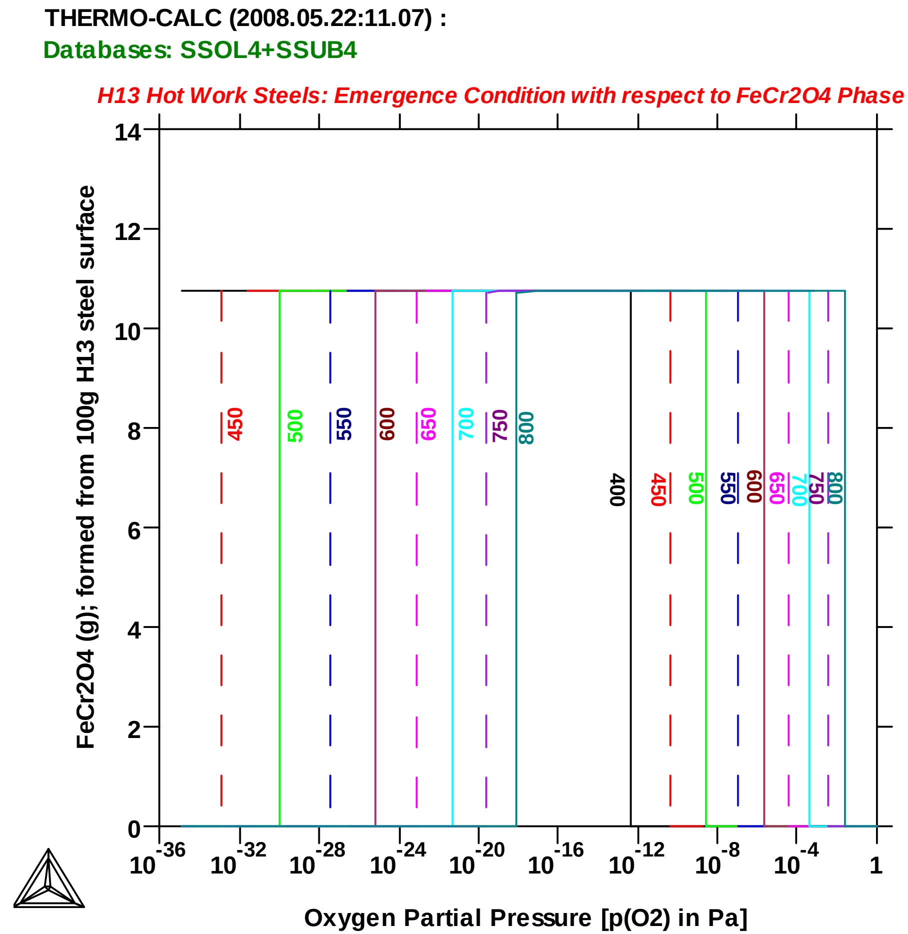
Emergence Conditions with respect to and Fe_2O_3 (Hematite) and Fe_3O_4 (Magnetite) during oxidation of H13 Hot Work Steel [Fe-5.14Cr-0.41Mn-1.02Si-0.40C-0.93V-1.46Mo-0.001S-0.009P-O], at 9 different temperatures (between 400 and 800ºC, with an interval of 50ºC) and 1 bar.

Surface Redox Reactions (III)

Thermo-Calc Software

Example: Oxidation of H13 Hot Work Steel



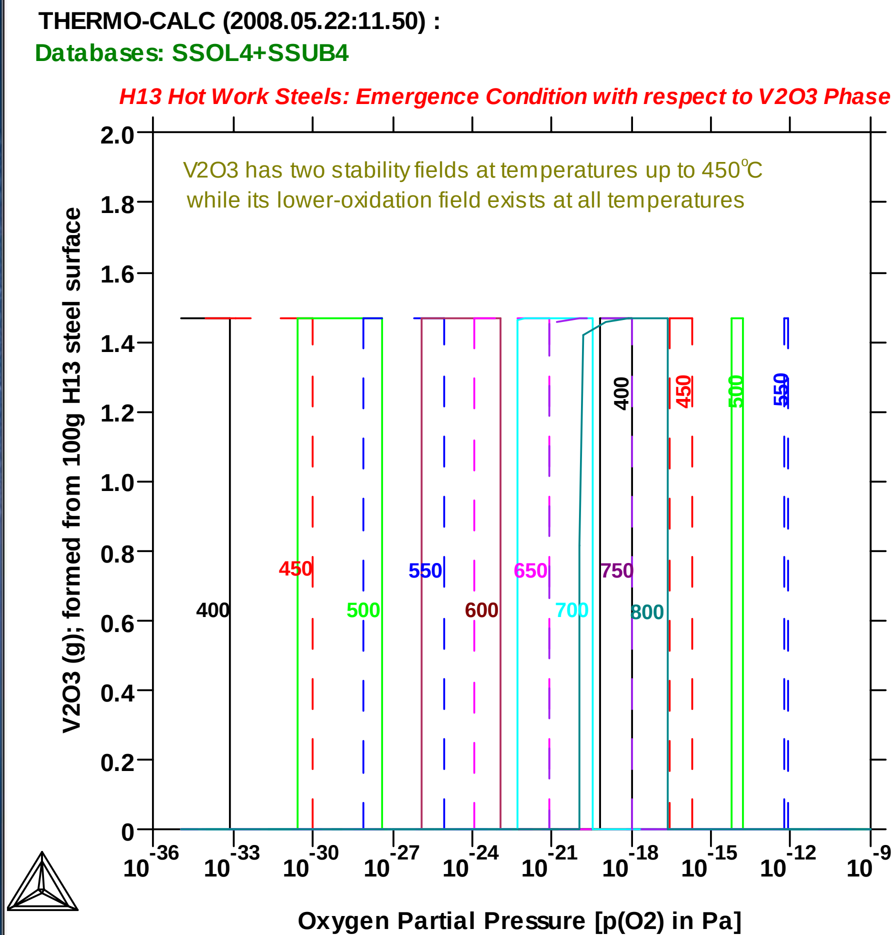


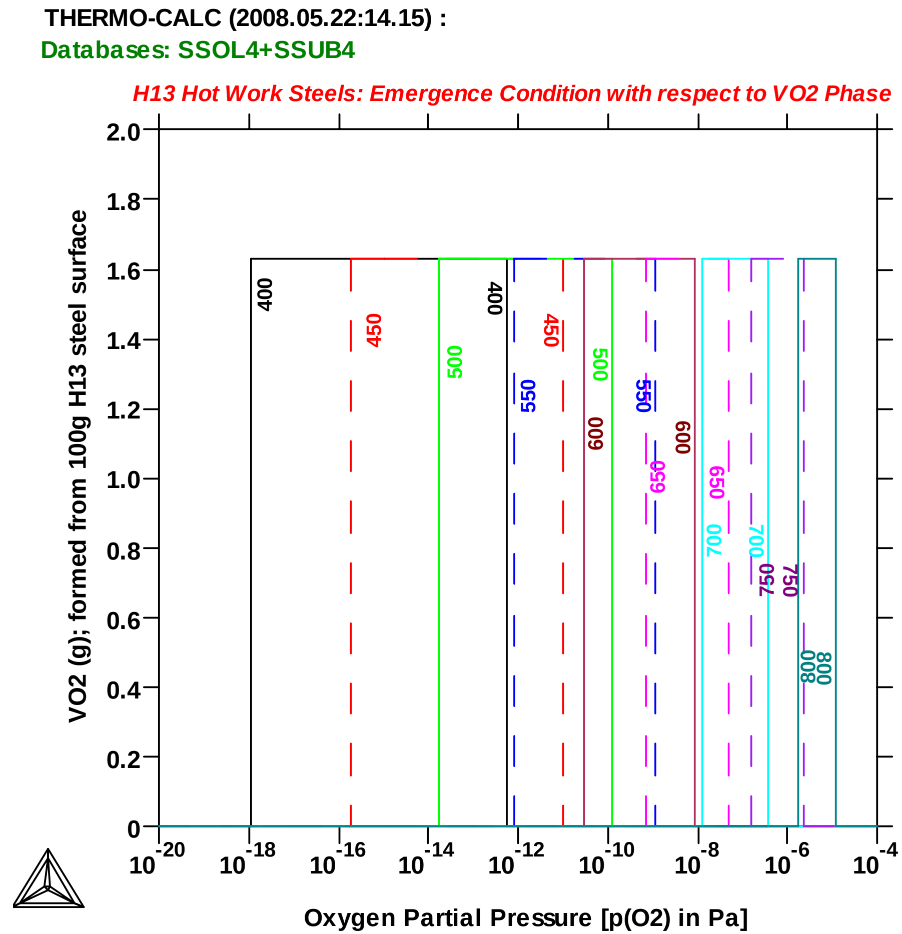
Emergence Conditions with respect to Cr_2O_3 and $FeCr_2O_4$ during oxidation of H13 Hot Work Steel [Fe-5.14Cr-0.41Mn-1.02Si-0.40C-0.93V-1.46Mo-0.001S-0.009P-O], at 9 different temperatures (between 400 and 800ºC, with an interval of 50ºC) and 1 bar.

Thermo-Calc Software

Surface Redox Reactions (III)

Example: Oxidation of H13 Hot Work Steel



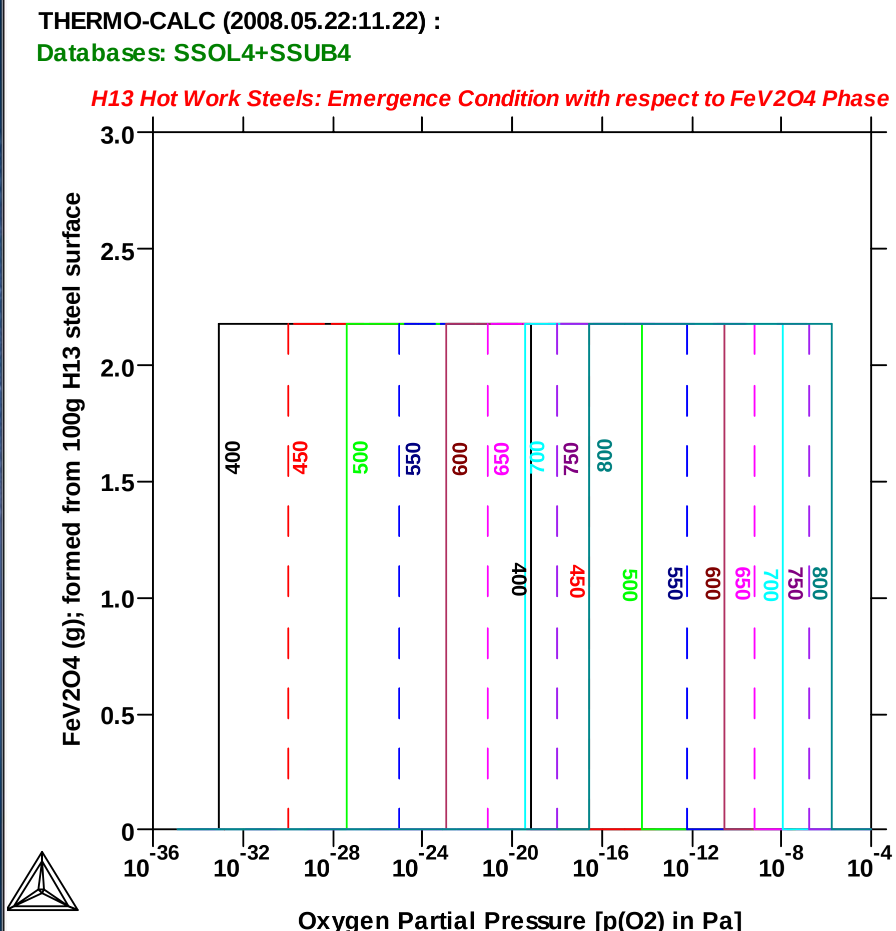


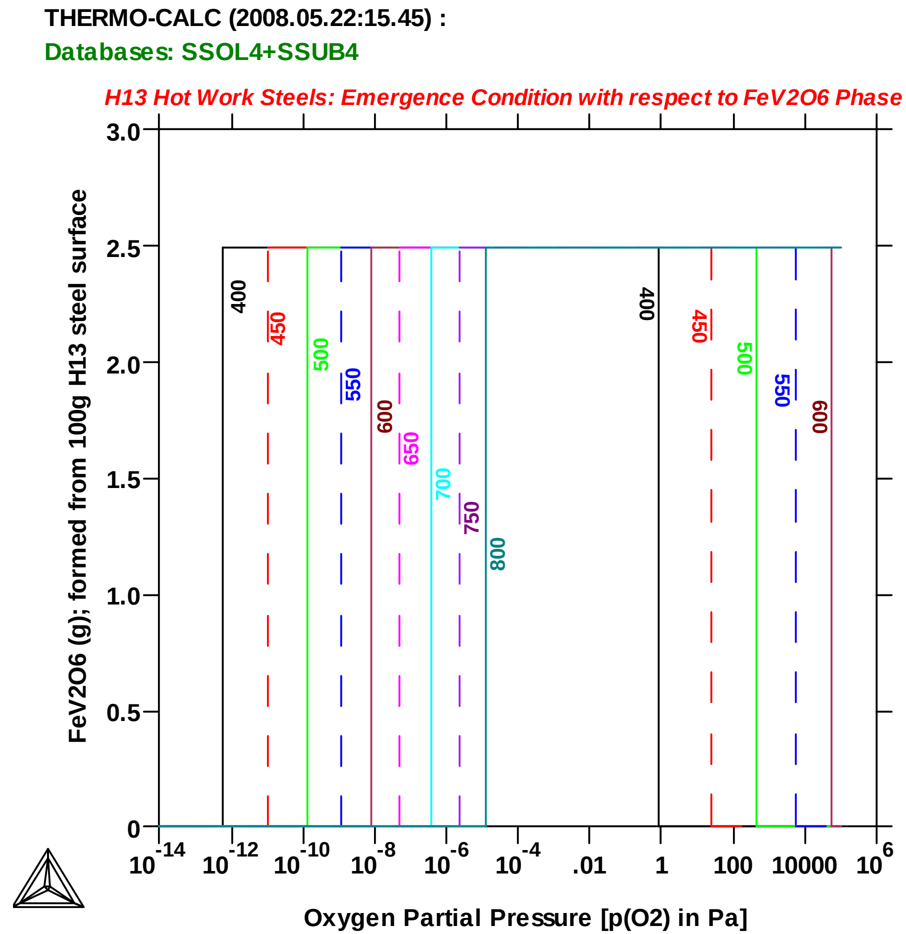
Emergence Conditions with respect to V_2O_3 and VO_2 during oxidation of H13 Hot Work Steel [Fe-5.14Cr-0.41Mn-1.02Si-0.40C-0.93V-1.46Mo-0.001S-0.009P-O], at 9 different temperatures (between 400 and 800ºC, with an interval of 50ºC) and 1 bar.

Surface Redox Reactions (III)

Thermo-Calc Software

Example: Oxidation of H13 Hot Work Steel





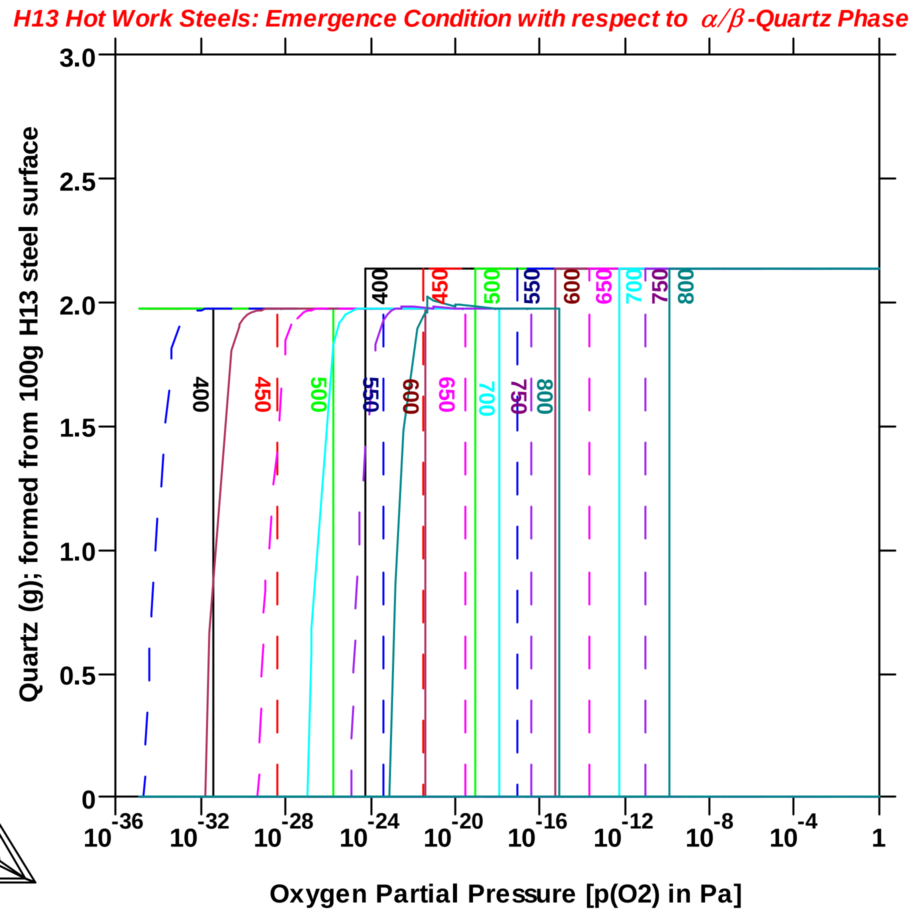
Emergence Conditions with respect to FeV_2O_4 and FeV_2O_6 during oxidation of H13 Hot Work Steel [Fe-5.14Cr-0.41Mn-1.02Si-0.40C-0.93V-1.46Mo-0.001S-0.009P-O], at 9 different temperatures (between 400 and 800ºC, with an interval of 50ºC) and 1 bar.

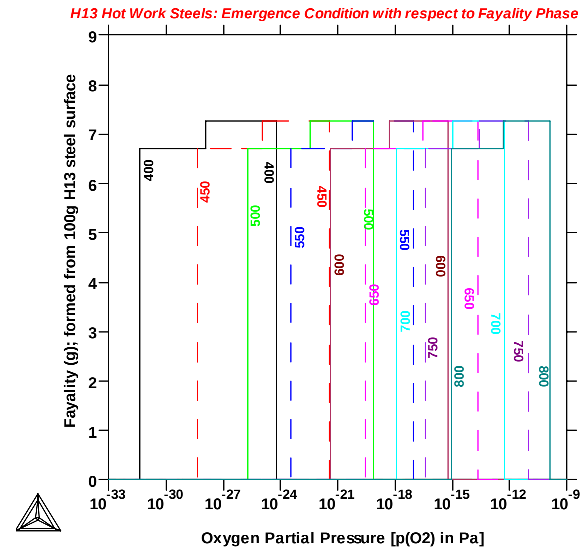
Surface Redox Reactions (III)

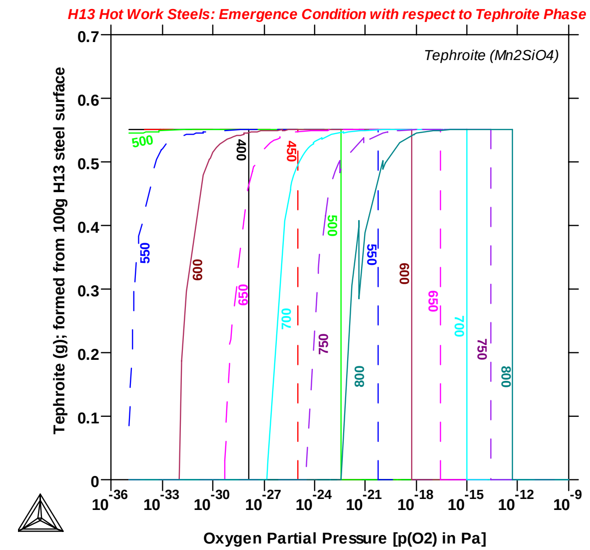
Example: Oxidation of H13 Hot Work Steel

THERMO-CALC (2008.05.22:10.46) :

Databases: SSOL4+SSUB4





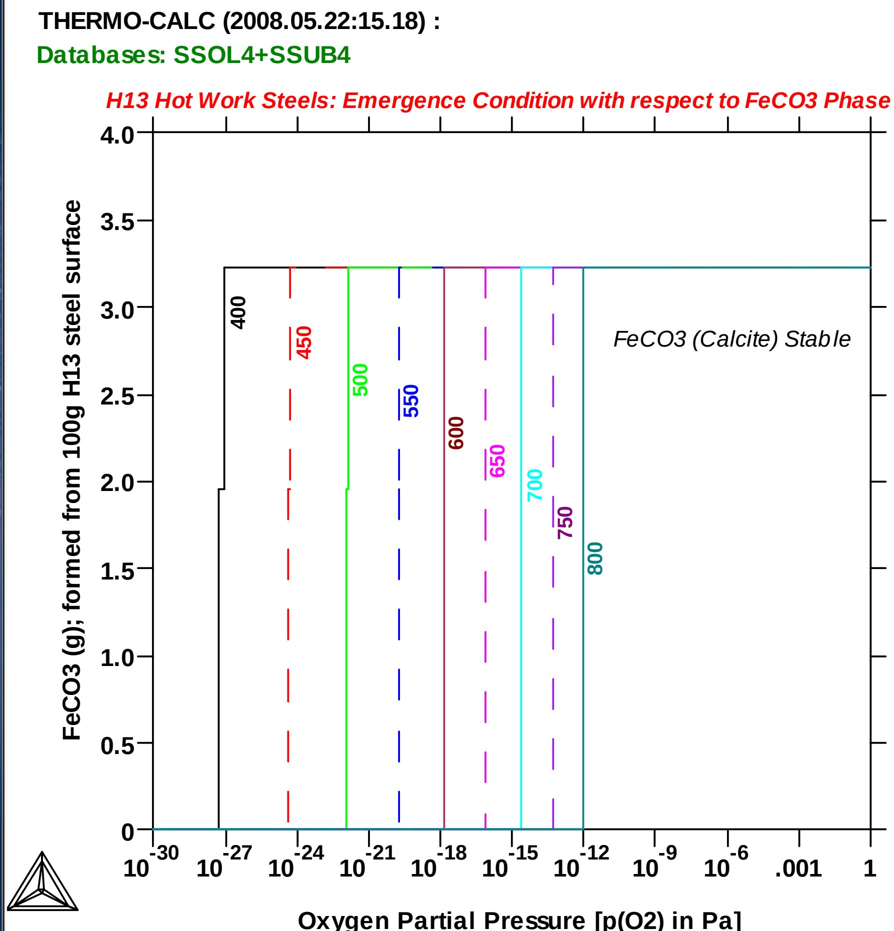


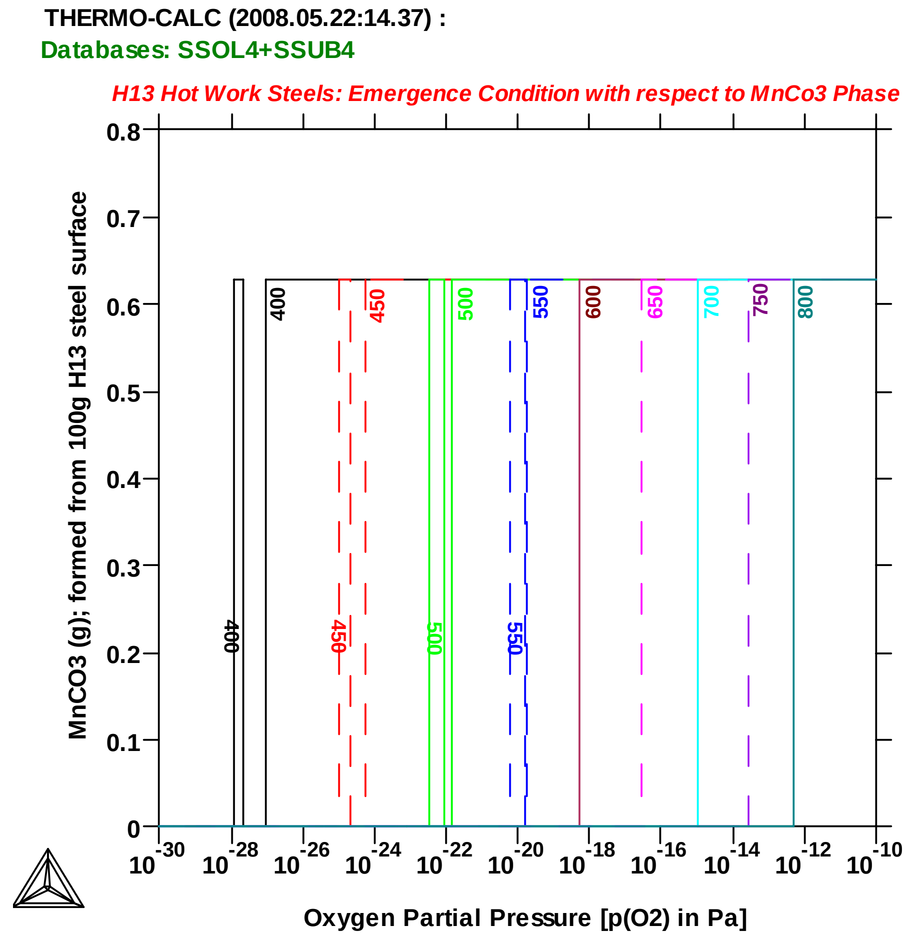
Emergence Conditions with respect to SiO_2 (α/β-Quartz), $FeSiO_4$ (Fayality) and $MnSiO_4$ (Tephroite) during oxidation of H13 Hot Work Steel [Fe-5.14Cr-0.41Mn-1.02Si-0.40C-0.93V-1.46Mo-0.001S-0.009P-O], at 9 different temperatures (between 400 and 800^{o}C, with an interval of 50^{o}C) and 1 bar.

Surface Redox Reactions (III)

Thermo-Calc Software

Example: Oxidation of H13 Hot Work Steel





Emergence Conditions with respect to $FeCO_3$ (Calcite) and $MnCO_3$ during oxidation of H13 Hot Work Steel [Fe-5.14Cr-0.41Mn-1.02Si-0.40C-0.93V-1.46Mo-0.001S-0.009P-O], at 9 different temperatures (between 400 and 800ºC, with an interval of 50ºC) and 1 bar.