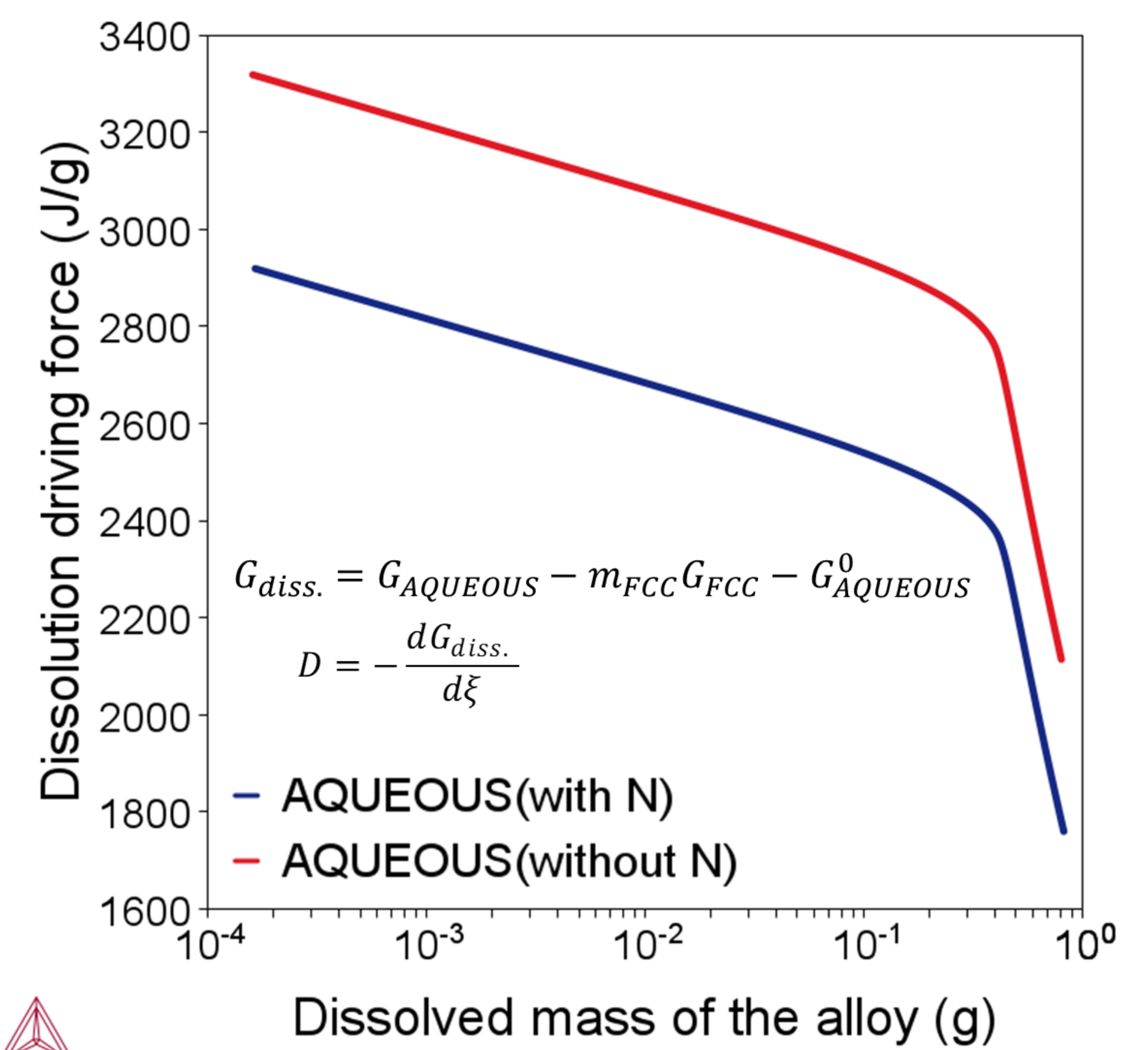


Corrosion of Multicomponent Multiphase Materials in Aqueous Solutions under Various Temperature, Pressure and Molality

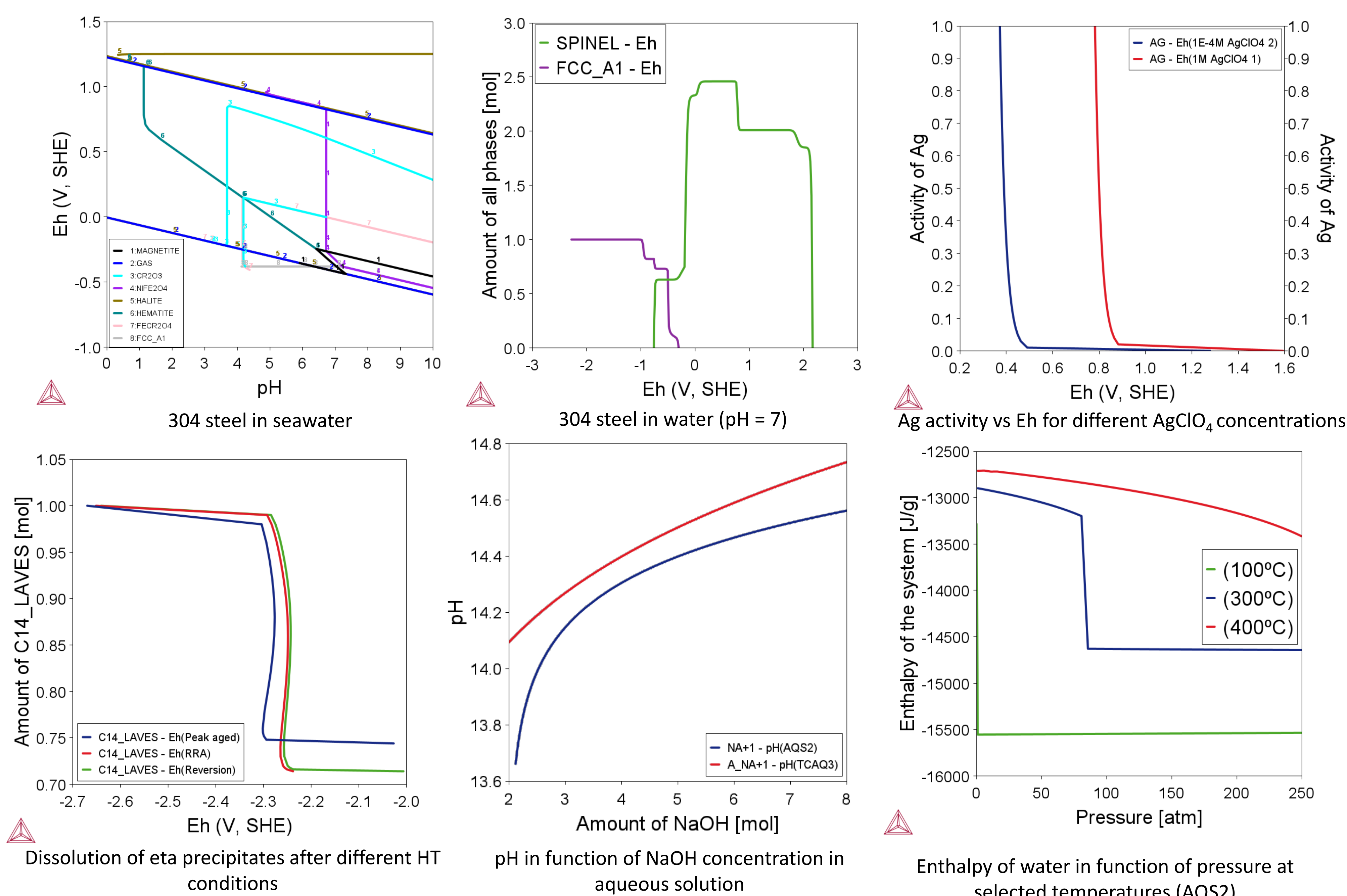
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Abstract

The potential-pH diagrams of elements in the presence of water developed by Marcel Pourbaix in 1945 remain the most important tool to understand the thermodynamics of aqueous corrosion. During the 1950s and early 1960s, Pourbaix and his collaborators produced potential-pH diagrams for all the elements and published the "Atlas of Electrochemical Equilibria" in French in 1963 and in English in 1966. Nevertheless, they are mostly limited to single metal components, to specific temperature and pressure conditions and to simple aqueous solution. Thus, it is not directly applicable in the corrosion study of heterogeneous multicomponent materials in a range of T & P. Several models to describe the aqueous phase have been presented in the literature and implemented in thermodynamic databases. The most important ones are the Specific Interaction Theory Model (SIT), which may be regarded as the combination of the Debye-Hückel Limiting Law (DHLL) and the regular-solution model, the Revised HKF Model (Helgeson-Kirkham-Flowers) and the Generalized Pitzer's Formalism (PITZ). Combining aqueous database with different compatible thermodynamic databases consisting of solution phases and compounds are readily to predict the thermodynamic tendency for dissolution of various phases in multicomponent and multiphase materials under different conditions of T, P, Eh, ph, or overall composition. They can also be coupled with other equilibrium and kinetic calculations that are used to first determine the phases that are present in the alloy after, for example, heat treatment, and then calculate the corrosion tendency of these phases and predict the potential protective oxides to design corrosion-resistant materials.



Dissolution driving force of a Fe12Ni18Cr steel with and without N in an aqueous solution containing 0.01 M H₂SO₄.

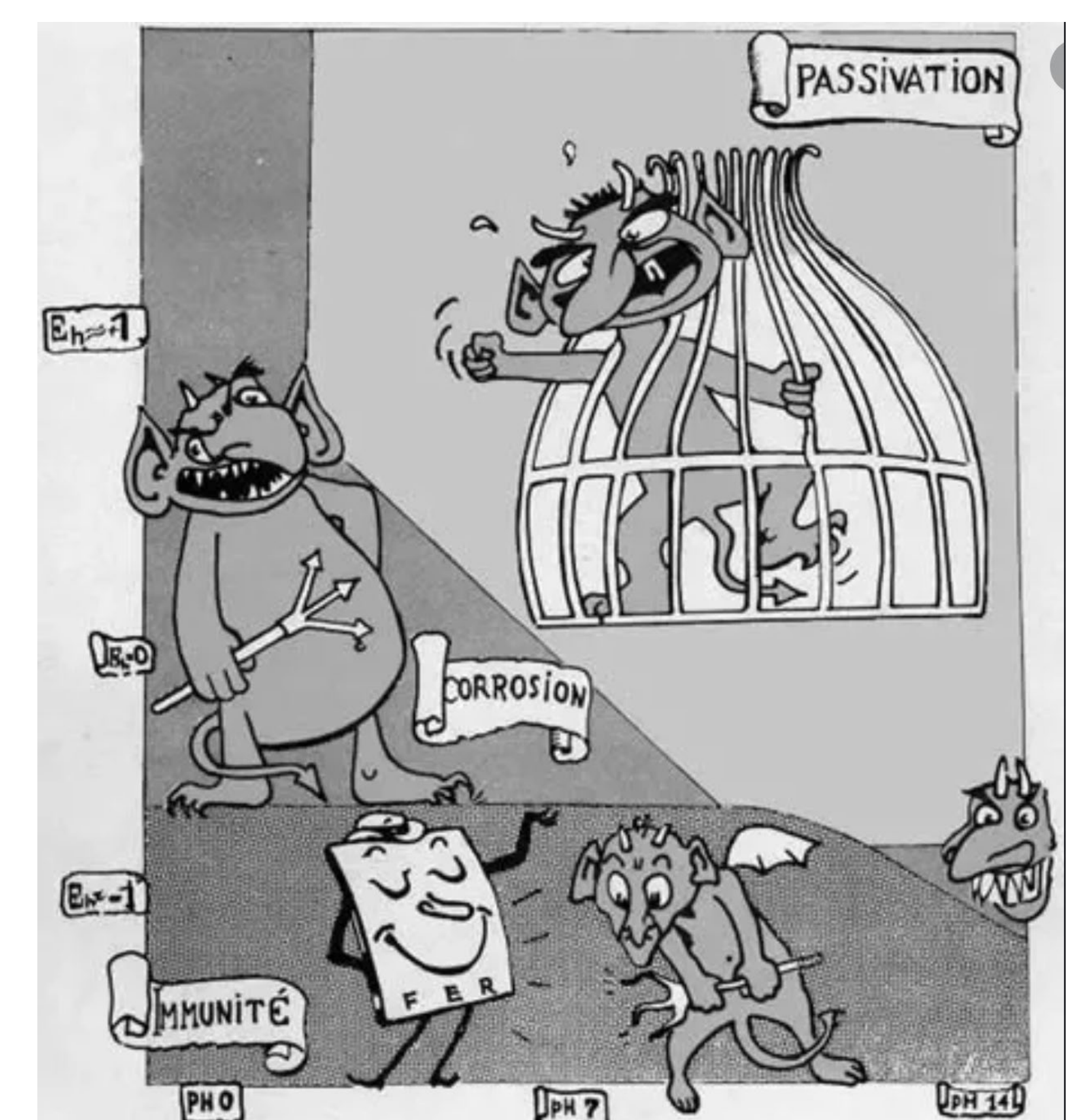


Applications

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

GES Model	Full Model Name	Applicable PTX	Databases
DHLL	Debye-Hückel Limiting Law	1 atm, 0 - 100 °C, dilute	TCAQ, PAQ, AQS
SIT	Specific Ionic Interaction Theory	1 - 200 atm, 0 - 100 °C, 3M	TCAQ, PAQ
PITZ	Generalized Pitzer's Formalism	1 atm, 0 - 100 °C, up to saturation	
HKF	Revised Helgeson-Kirkham-Flowers Model	0 - 5 kbar, 0 - 1000 °C, up to saturation	AQS

Table 1. Applicable P-T-X ranges of different thermodynamic models for aqueous solutions.



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