

Le Chatelier Response: a Quantitative Application of the Le Chatelier Principle to Chemical Equilibria

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This presentation is to introduce the Le Chatelier Response (LCR) as a quantitative application of the Le Chatelier Principle (LCP) to the chemical systems and a measure of the system reaction to the stress, caused by an external thermodynamic force. While the LCP states qualitative relations between the external reasons to change equilibrium and the shift direction, the LCR is establishing a quantitative relationship between the external force and the shift value and sign, interpreting the shift power series as a function of the external force. Such an approach accounts for the system and its response complexity. The LCR influence on the shape of the system domain of states, composed of the inverse bifurcation diagrams, and on the system proneness to evolution via bifurcations is investigated. Depending upon the LCR structure, the theory leads to different shapes of inverse bifurcation diagrams for the systems with regular and with “triggering” types of chemical reactions running within the system. In more traditional, pre-bifurcation areas of the domain of states where thermodynamic simulation is applicable, the LCR structure affects simulated deviation of the system from “true” thermodynamic equilibrium. The idea of the LCR is very important in a context of recently developed discrete thermodynamics of chemical equilibria. It may also motivate and facilitate a progress in applications of discrete thermodynamics and the based on it Method of Bound Affinity to the systems with chemical as well as with quasi-chemical transformations, like the bio-population units, reactions between elemental particles at relatively high concentrations (the Big Bang is the extreme), thermodynamics of lasers, some other.