Study on the effects of inert on Water-Gas Shift Reaction

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A. Background

For equilibrium reactions, addition of inert compounds can shift the equilibrium to either the forward or backward reaction. The extent to which addition of inert affects the equilibrium is calculated by applying principle of reaction equilibrium and in turn dependent on the solution thermodynamics of the system. Thus the thermodynamic model used to predict solution behavior can impact the equilibrium conversion. To illustrate this, a simple case study based on Paiva (2008) is illustrated in this work. Water gas shift reaction is simulated in an equilibrium reactor operated isothermally using two different thermodynamic models to describe the system. The same reaction is further simulated with addition of inert (Xenon). The results are compared to arrive at an appropriate inference.

B. Description of Flow Sheet

The feed, consisting of 50 mol% water and 50 mol% carbon monoxide, flows at the rate of 360 kmol/h at a temperature of 326.85^{o}C and 100 bar pressure. The feed is fed into a equilibrium reactor operated isothermally. In a similar process the feed consisting of water and carbon monoxide is mixed with equi-molar amount (180 kmol/h) of inert gas (Xenon) and then sent to an equilibrium reactor. The process is simulated using two thermodynamic models (Raoult's Law and Chao-Seader) to understand the effect of non-ideal nature of the components on reaction equilibria. This process flowsheet is based on Paiva (2008).

C. Results and Conclusions

The equilibrium conversion of each simulation case are tabulated below

	Equilibrium conversion	
	No inert	**With inert**
Raoult's Law (ideal model)	84.14%	81.34%
Chao-Seader (non-ideal model)	83.76%	82.93%

It is seen that the thermodynamic model has an impact upon the equilibrium state of the reaction. The effect of exothermic reaction is dependent on the thermodynamic model used to describe the system. Thus as detailed in Paiva (2008), the effect of inert on reaction equilibrium needs to ascertained with the sound know-how of the solution thermodynamics of the system. This case study shows that free and open source simulator can be used as an effective learning tool to simulate and thereby demonstrate the importance of usage of appropriate thermodynamic models in process simulation.

D. Reference

Paiva J. C. M. (2008), Does the Addition of Inert Gases at Constant Volume and Temperature Affect Chemical Equilibrium? *Journal of Chemical Education*, Vol. 85 No.8, 1133-1135