REVISTA MATÉRIA V.19 N.04

ISSN 1517-7076 Letter 11571, pp.400-401, 2014

A conservation law for self-hydrolysis process of aqueous sodium borohydride

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ABSTRACT

A conservation law is obtained for self-hydrolysis process of aqueous sodium borohydride, which gives an explicit relationship between the concentrations of NaBH4 and hydrogen ions during the global reaction.

Keywords: Sodium borohydride, Self-hydrolysis, Analytical model, Hydrogen storage.

1. INTRODUCTION

Excellent catalytic performance of CoO nanocrystals on the catalytic hydrolysis of alkaline $NaBH_4$ solutions was observed experimentally, hydrogen generation from the hydrolysis of sodium borohydride (NaBH4) solution has drawn much attention recently, due to its high theoretical hydrogen storage capacity and potentially safe operation [1]. However, hydrolysis of NaBH4 for hydrogen generation is a complex process [1-3], and it is highly needed to have an explicit formulation to reveal concentration change in the reaction process.

The hydrolysis of NaBH4 is an exothermic reaction that yields hydrogen (H2) gas and water-soluble sodium metaborate (NaBO2). The global reaction of H_2O and NaBH4 is given in the form [2].

$$NaBH_4(aq) + 2H_2O \rightarrow 4H_2 + NaBO_2(aq) + Heat \quad (1)$$

The rate of hydrolysis is a complicated reaction that is strongly dependent on solution temperature, NaBH4 concentration, the molar concentration of dissolved hydrogen ions, H+ [2]:

$$\frac{dx}{dt} = Ax^{a_1}y^{b_1} \quad (2)$$

$$\frac{dy}{dt} = B\exp\left(\frac{a_2(x_0 - x)}{x_0}\right)y^{b_2} \quad (3)$$

where x is NaBH4 concentration, y is H^+ concentration, x_0 the initial concentration of NaBH4, A and B are constants depending upon temperature, α_1 and β_1 represent the order of reaction for [NaBH4] and [H+], respectively. α_2 and β_2 are the exponential constant and the order of reaction for [H+], respectively.

The system, Eqs. (2) and (3), can be effectively solved by some an analytical method, such as the variation iteration method, the homotopy perturbation method, and the parameter-expansion method [4,5]. This paper aims to searching for a conservation law for self-hydrolysis process of aqueous sodium borohydride (NaBH4) for hydrogen generation purpose.

2. CONSERVATION LAW

From Eqs. (2) and (3), we have

$$\frac{dx}{dy} = \frac{Ax^{\alpha_1} y^{b_1}}{B\exp(\frac{\alpha_2(x_0 - x)}{x_0}) y^{b_2}}$$

(4)

or

$$B\exp\alpha_2 x^{-\alpha_1}\exp(-\alpha_3 x)dx = Ay^{b_1 - b_2}dy$$

(5)

where $\alpha_3 = \alpha_2 / x_0$.

Integrating Eq. (5) results in

$$y^{b_1 - b_2 + 1} = \frac{B(b_1 - b_2 + 1)\exp\alpha_2}{A}\int x^{-\alpha_1}\exp(-\alpha_3 x)dx$$

(6)

Eq. (6) is the conservation law for the self-hydrolysis process, which implies whatever the process continues, the concentrations of NaBH4 and hydrogen ions must follow Eq. (6).

3. CONCLUSIONS

This work focuses on concentration changes of NaBH4 and H+ of the self-hydrolysis of sodium borohydride, the conservation law, Eq.(6), reveals the relationship between concentrations of NaBH4 and H+ in the global reaction process. The integration constant involving in Eq.(6) can be determined by the initial concentrations, and the conservation law can be used to predict the reaction process by the pH value of the solution , which is a measure of the molar concentration of dissolved hydrogen ions.

4. ACKNOWLEDGMENTS

The work is supported by Priority Academic Program Development of Jiangsu Higher Education Institutions (PAPD), National Natural Science Foundation of China under grant No. 61303236 and No.11372205 and Project for Six Kinds of Top Talents in Jiangsu Province under grant No. ZBZZ-035, Science & Technology Pillar Program of Jiangsu Province under grant No. BE2013072, Jiangsu Province Key Laboratory No.KJS1314 and Jiangsu Planned Projects for Postdoctoral Research Funds1401076B.

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