Decarbonizing Hydrogen Supply Chain via Electrifying Endothermic Processes

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Highlights

- Feasibility of electrified ammonia decomposition is investigated with wired reactors.
- A semi-detailed kinetic model for ammonia decomposition is proposed and utilized.
- Short transient time in proposed configuration enables the coupling with renewables.
- Temperature control via programmed heating assures mechanical and process integrity.
- The configuration enables the decarbonized pathway for hydrogen supply chain.

1. Introduction

CO_2 emissions in atmosphere have been continuously rising, which have detrimental impacts on climate, health and ecology. Most emissions are from manufacturing industries that use fossil-fuel based heating to supply the required endothermic heat. For instance, commercial-scale steam methane reformer plants exhibit 9 to 11 tons of CO2 per ton of hydrogen produced. Similarly, ethane and naphtha-based conventional cracker plants emits 1 – 1.8 tons of CO2 per ton of ethylene produced. For steel, cement and aluminum industries, this ratio goes to even much higher: 10-18 tons of CO2 per tons of the product. Therefore, significant efforts have been made on developing CO2-free or reduced emission technologies, especially for manufacturing industries. Some of them are based on eliminating the source of emissions via replacement of fuels or heating processes, and some are based on mitigating the impact of existing technologies (i.e., via CO2 capture post combustion or directly from air).

Here, we focus on the first route, especially on hydrogen supply chain [1], where we present an alternate option towards decarbonization via electrifying the associated endothermic processes (i.e., steam methane reforming for hydrogen production, and ammonia cracking enabling the large-scale hydrogen transport). In particular, we present a novel electrified reactors consisting of parallel wires [2 - 4] and demonstrate the technical feasibility of the concept for these processes.

2. Methods

Mathematical modeling describing the transport and reaction in electrified wired reactor is based multi-scale multiphase reduced-order model (ROM) for steam methane reforming [4] and pseudohomogeneous model [5] for ammonia cracking. The kinetic model for steam methane reforming is taken same as in [3, 5] while a global kinetic model of ammonia cracking is developed in this work using detailed microkinetics steps, which can be expressed as

$$NH_3 \rightarrow \frac{1}{2}N_2 + \frac{3}{2}H_2;\ (-r_A) = r_f\left(1 - \frac{P_N P_H^3}{K_p^2 P_A^2}\right);\quad r_f = k_{f0}\exp\left(\frac{E_a}{RT}\right)\left(\frac{K_A P_A}{den}\right)^2 \qquad 1(a)$$

$$den = K_A P_A\left(1 + \frac{\sqrt{K_H P_H}}{K_{P4}}\right) + (K_H P_H)^{3/2} \qquad 1(b)$$

where P_j represents the partial pressure of jth species (A: NH_3, H: H_2, and N: N_2); k_{f0} and E_a are the pre-exponent factor and activation energy of the forward limiting reaction, and K with various subscripts represent the chemical/adsorption equilibrium constants.

3. Selected Results

The first main result is the development of a global expression given in Eq. (1), which satisfy the various limiting features of the ammonia decomposition, such as (i) thermodynamic equilibrium constraint, (ii) forward rate being inhibited by hydrogen at high H_2 partial pressures (iii) forward rate is independent

of P_A at its high values. Additionally, the global rate is much simpler as compared to other proposed forms and describes various features of cracking reactions that are ignored in most proposed simpler (linear) forms.

Other main results are pertaining to the simulations as shown in Figure 1 below, which plots the equilibrium conversion versus feed temperature for steam methane reforming (Figure 1a) and for ammonia cracking (Figure 1b) during various reaction pathways corresponding to equilibrium, isothermal, adiabatic and electrically heated operations. It can be seen from this figure that the electrically heated pathways could lead to much higher conversion than the isothermal operation, but at the expense of higher exit temperatures. Several other results related to effect of programmed heating, space time, electric power supply rate, volume fraction of catalyst and feed composition on reactor performance will be discussed in the presentation.

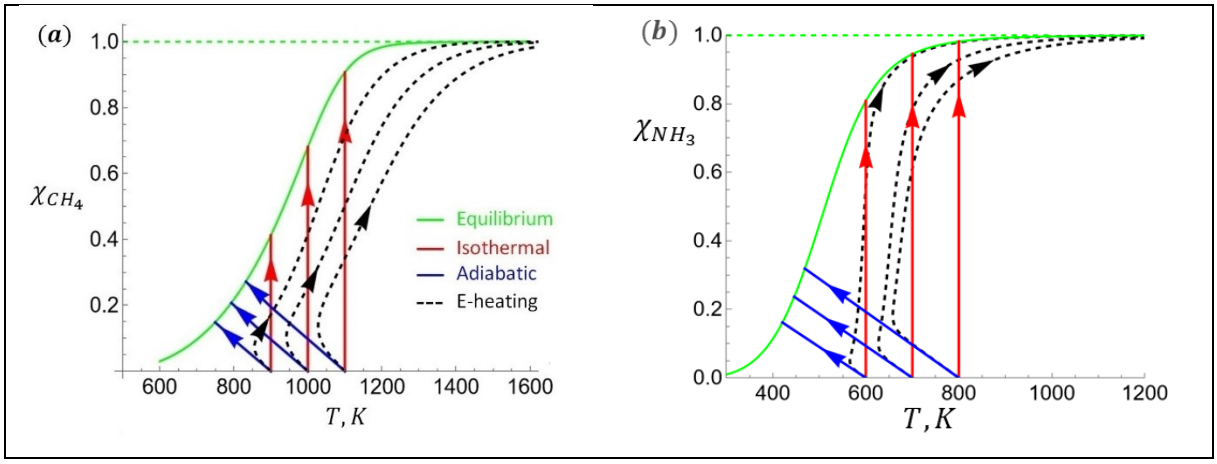

Figure 1. Various reaction pathways (equilibrium, isothermal, adiabatic and electrified operations) showing the conversion versus temperature for (a) steam methane reforming for hydrogen production and (b) ammonia cracking enabling the hydrogen transport.

4. Key Conclusions

The main conclusion of this work is demonstration of the technical feasibility of electrified wired reactors towards decarbonization of hydrogen supply chain, specifically focusing on supplying the Joule heating for associated endothermic reactions (i.e. hydrogen production from steam methane reforming and ammonia cracking for enabling the ammonia route for transportation). In particular, we show that electrified reactor configurations discussed here can replace traditional fossil-fuel based heat supply for chemical manufacturing and have various advantages such as (i) ability to couple with the renewable power (even with the intermittency issues), (ii) reduced, net-zero or negative emissions, (iii) higher thermal efficiency, (iv) uniform heating with lower start-up times, (iv) modularity, design flexibility, ease in scaleup and maintenance, (v) and most importantly, applicability to various endothermic catalytic/non-catalytic processes.

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Keywords
Process Intensification; Process Electrification; Emission reduction, Hydrogen supply chain; Steam methane reforming; Ammonia decomposition.