Graphical Abstract

Coaxial multi-criteria optimization of a methane steam reforming reactor for effective hydrogen production and thermal management

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Highlights

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- Introduction of a novel approach to the macro-patterning concept.
- Sensitivity analysis conducted for the evolutionary algorithm parameters.
- Enhancement of thermal conditions via a modification of the catalyst insert.
- Increase in hydrogen productivity.

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Abstract

The advancement in environmental awareness is the recent driving factor of the energy industry development. The market sentiments dictate the commercialization of unconventional energy sources. Thus, generation via hydrogen conversion gains popularity. The presented research regards the enhancement of the steam reforming reaction, used for the production of hydrogen via the conversion of hydrocarbons. The reforming process characterizes by a strong endothermic nature. The rapid course of the reaction leads to the creation of temperature gradients of a considerable magnitude. The presented research strives to alleviate the negative consequences of the reaction character. An original strategy by the name of macro-patterning is suggested as a remedy. The presented research proposes an updated concept, predicting the introduction of coaxial segments to the catalytic insert. The segments may consist of catalytic material or metallic foam applied for local suppression of the reaction. The morphology of specific segments may be altered independently, to allow for additional control of the reforming reaction. The objective of the research is to define the optimal segment composition. The optimization process is based on an in-house procedure implementing a genetic algorithm. The acquired results appear to validate the macro-pattering concept. A significant unification of the temperature field is obtained, with a simultaneous increase in hydrogen productivity.

Keywords: hydrogen, evolutionary algorithms, reforming, design optimization

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1. Introduction

Hydrogen technologies are one of the promising directions of the clean energy sector development [1]. The research on hydrogen is conducted to provide a reliable alternative to the currently dominant fossil fuel energy sources [2, 3]. Hydrogen might be used as an energy carrier for internal combustion or fuel cells, both resulting in steam being the main product [4, 5]. However, with the application of hydrogen technology, some crucial issues arise. The first issue regards hydrogen acquisition, as it does not occur on Earth in its pure form. The second matter is hydrogen storage, with currently no effective measures of long-term storage [6, 7]. The two most common processes for on-the-spot production of hydrogen are water electrolysis and the reforming of hydrocarbons [8, 9]. Water electrolysis is a process predicting the breaking of chemical bonds between oxygen and hydrogen in particles of water. The current state of the electrolysis development is far from meeting economical requirements [10]. The only reasonable use of water electrolysis is to deplete surplus energy generated from renewable sources during low market demand and short-term storage of hydrogen for further use during increased demand for energy [11]. The second measure for hydrogen production is the reforming reaction [12, 13]. The reforming process is a catalytic reaction used for the conversion of hydrocarbons for the production of hydrogen [14, 15]. The reforming process can be successfully applied to the conversion of biofuels, allowing the reforming process to be considered a renewable hydrogen source [16, 17]. Furthermore, the process can be successfully applied as a measure of carbohydrate-based waste gases or plastic recycling, establishing it as a prominent for hydrogen generation [18, 19]. The reforming technology brings a series of issues regarding the thermal conditions occurring inside the reactor. The strong endothermic nature of the process results in the occurrence of thermal stresses and may lead to a shortening of the reactor's lifespan [20]. The presented research aims to reduce the drawbacks of the process, by enhancement of the thermal conditions. The majority of researchers focused on the parametric study and optimization of the reaction conditions, resulting in improvements only to a certain extent [21, 22]. Further development of the process is pursued by the introduction of new materials and design concepts, including new catalyst structures [23, 24], the introduction of new kinds of catalyst supports [25], or by rethinking the design of the reactor itself [26, 27, 28]. A captivating opportunity is described in a work by Palma et al. [29], who introduced a structured catalyst for the intensification of the reforming reaction. The research confirms the improvement of the reaction rate, resulting from the enhancement of the axial and radial temperature distribution. The research reported by Yun et al. [30] focuses on the enhancement of heat transfer, by modification of the design, to acquire a maximized heat transfer area. The proper handling of heat in the reforming process is confirmed to enhance the overall process conduction [31]. Furthermore, a rapid temperature decay at the upstream region of the reactor results in thermal stresses forming in the reactor. Thus, leading to its uneven degradation and reduction of the unit's lifetime [32]. A unification of the temperature distribution may not only improve the conditions but also achieve easier control of the process [33]. The presented research aims to alleviate the negative consequences of the strong endothermic character of the process, via the introduction of radial division of the catalytic insert. The concept originates from the approach proposed by Settar et al. [34]. The research predicted an introduction of macro-patterned active surfaces with an introduction of metallic foam matrices, focusing on providing advantageous thermal conditions for the reaction [35, 36]. The presented research extends the concept to fill the whole reactor's volume with a catalytic composite of nickel and yttria-stabilized zirconia (Ni/YSZ), to maximize the reaction region in the reactor. Further, the reforming unit is divided into segments in the radial direction, instead of the longitudinal division [37]. Non-catalytic metallic foam is used as a substitute for parts of the catalyst, to adjust the intensity of the reaction proceeding, leading to the unification of the thermal field inside the reactor. To define the optimal alignment of the catalyst, an evolutionary algorithm is coupled with an in-house reforming simulation [38]. The presented analysis includes:

- Investigation of the macro-patterning concept applicability with the introduction of the catalytic insert radial division.
- Introduction of two separate principles for the configuration of the segments.
- Comprehensive sensitivity analysis to define the finest performing set of the evolutionary algorithm parameters.
- Analysis of the results robustness, via measuring the hydrogen productivity of specimens defined by the specific algorithms.

2. Mathematical model

3. Numerical analysis

4. Conclusions

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