

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.

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

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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-patterning 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 Settari 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:

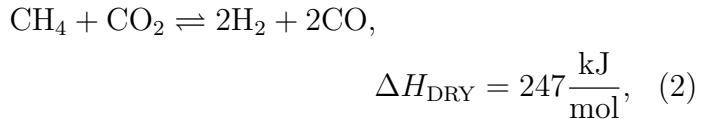
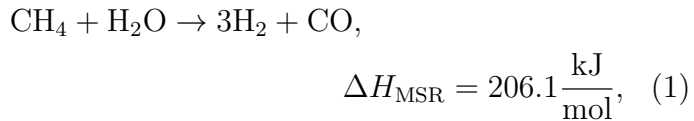
- Investigation of the macro-patterning concept applicability with the introduction of the catalytic insert radial division.
- Introduction of two separate principles for the configuration of the segments.
- Comprehensive sensitivity analysis to define the finest performing set of the evolutionary algorithm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

2. Mathematical model

The reactor geometry is designed to allow modification of the insert in a real-life scenario. The analyzed process incorporates a plug-flow reactor, maintaining axial symmetry throughout its whole volume. The reactor consists of a straight, cylindrical pipe, allowing for an accessible replacement of the catalyst insert when required. The introduced macro-patterning strategy predicts modification of the catalyst insert's morphology and its partial substitution with a non-catalytic material. Substitution of the catalyst material serves to enhance the heat transfer inside the reactor [37]. Metallic foams are chosen for application to the indicated issues [39]. To provide a relevant measure for altering the temperature distribution inside the reactor, the catalyst insert is divided into segments. Each segment may consist of a catalyst or a non-catalytic material, with their morphological parameters individually assigned. The insert's segmentation is carried out according to two separate strategies. The first strategy predicts division in the radial direction with maintaining a constant width of inlet surfaces of each cylinder (Fig. 1 b)). The second strategy predicts the application of segments with an identical area of the inlet surfaces for each of the coaxial cylinders (Fig. 1 c)). The design is prepared to contain exclusively simple geometrical shapes, allowing to maintain an insignificant computational complexity of the domain [40].

2.1. Chemical Reactions Model

The process is assumed to be dominated by three reactions, as reported in literature [41, 42, 33]. The reactions are steam reforming of methane (MSR) (Eq. (1)), dry reforming of methane (DRY) (Eq. (2)), and water-gas shift reaction (WGS) (Eq. (3)) [43]. The stoichiometric equations for the reactions are presented below:



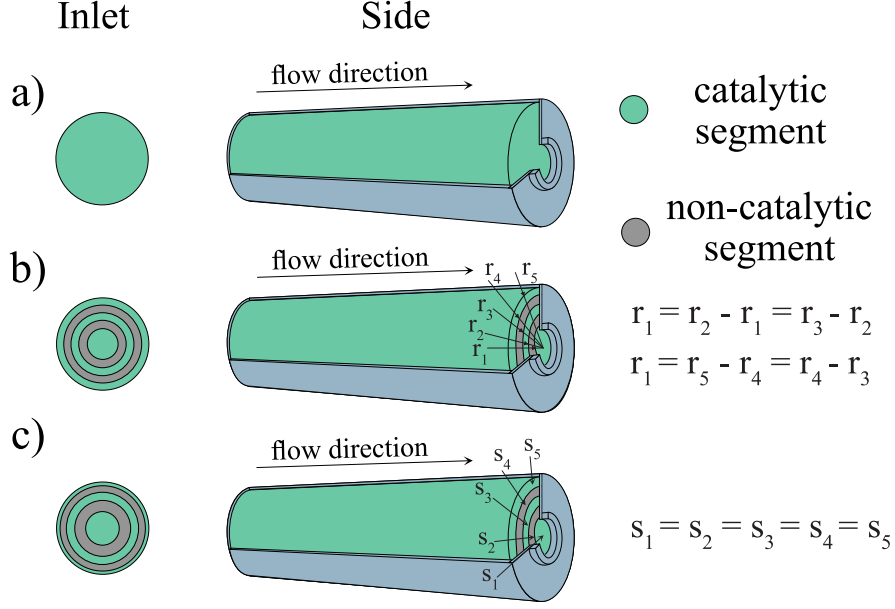
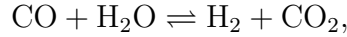


Figure 1: The investigated macro-patterining designs: a) conventional reactor with homogeneous and continuous catalytic insert, b) catalytic insert divided in the radial direction (equal width of inlet surface), c) catalytic insert divided in the radial direction (equal area of inlet surface)



$$\Delta H_{\text{WGS}} = -41.15 \frac{\text{kJ}}{\text{mol}}. \quad (3)$$

The reformer is supplied with a mixture of H_2 , CO_2 , and CH_4 . The composition of the feedstock is determined the steam-to-carbon ratio (SC) parameter, defining the ratio of steam to methane provided at the reactor's inlet. The process conditions are remarkably influenced by the SC value, as the reactions' rates depend directly on the composition of the inlet gases [44]. A proper setting of the SC is crucial for the prevention of the carbon deposition phenomenon [45]. Adverse process conditions can result in carbon particles precipitating on the catalyst surface [46]. A proper setting of the ratios and the process' temperature are proven to have the most significant influence on the alleviation of the poisoning hazard [47]. The enthalpy changes ΔH are taken from literature [37, 48]. Knowledge of their rates is

essential to allow the inclusion of the reactions into the model. According to the research conducted by Brus et al. [49], the effective rate of MSR and DRY reactions can be expressed with a common equation:

$$R_{\text{eff}} = \dot{w}_{\text{cat}} A_{\text{MSR}} \exp \left(-\frac{E_a}{RT} \right) p_{\text{CH}_4}^\alpha (p_{\text{H}_2\text{O}} + p_{\text{CO}_2})^\beta. \quad (4)$$

The individual reaction rates for the MSR and DRY reactions can be distinguished as follows:

$$R_{\text{MSR}} = R_{\text{eff}} \frac{p_{\text{H}_2\text{O}}}{p_{\text{CO}_2} + p_{\text{H}_2\text{O}}}, \quad (5)$$

$$R_{\text{DRY}} = R_{\text{eff}} \frac{p_{\text{CO}_2}}{p_{\text{CO}_2} + p_{\text{H}_2\text{O}}}. \quad (6)$$

The reforming reaction is reported to occur rather slowly [50]. However, the WGS reaction has a more unpredictable nature [51]. Thus, the preparation of a formula, returning proper values regardless of the process conditions, is not feasible. According to Ahmed and Föger, the WGS reaction can be assumed to maintain equilibrium under specific conditions [52]. The equilibrium assumption has been successfully applied in other numerical analyses [53, 54, 55]. The assumption also meets a good agreement between the calculations and the experimental data [56, 57, 58]. Taking into account the provided literature review, the WGS reaction is assumed to be in the equilibrium state in the presented analysis. The process conditions are designed to satisfy the equilibrium assumption. Following the statements, CO, CO₂, H₂ and H₂O have to satisfy the equilibrium equation, expressed by the following formula:

$$K_{\text{WGS}} = \frac{k_{\text{WGS}}^+}{k_{\text{WGS}}^-} = \frac{p_{\text{CO}_2} p_{\text{H}_2}}{p_{\text{CO}} p_{\text{H}_2\text{O}}} = \exp \left(-\frac{\Delta G_{\text{WGS}}^0}{RT} \right). \quad (7)$$

The WGS reaction rate can be further expressed using Eq. (8):

$$R_{\text{WGS}} = k_{\text{WGS}}^+ p_{\text{CO}} p_{\text{H}_2\text{O}} + k_{\text{WGS}}^- p_{\text{H}_2} p_{\text{CO}_2}. \quad (8)$$

The value of R_{WGS} can be acquired through the analysis of the reforming process stoichiometry and balancing the chemical species [59, 60]. Balancing the reaction's stoichiometry allows for the calculation of the partial pressures

included in Eq. (7), leading to the relation describing the WGS reactions' rate (Eq. (9)) [49].

$$R_{\text{WGS}} = \frac{n_{\text{CH}_4}^{\text{outlet}}}{V} = \frac{n_{\text{CH}_4}^{\text{inlet}} \cdot xcr}{V} ycr. \quad (9)$$

Following, the methane conversion rate xcr and carbon monoxide conversion rate ycr can be specified with:

$$xcr = 1 - \frac{n_{\text{CH}_4}^{\text{inlet}} - R_{\text{MSR}}V}{n_{\text{CH}_4}^{\text{inlet}}}, \quad (10)$$

$$ycr = \frac{K_{\text{WGS}} + 3xcr - \sqrt{\chi - \omega}}{2(K_{\text{WGS}} - 1)}, \quad (11)$$

where:

$$\chi = (K_{\text{WGS}}SC + 3xcr)^2, \quad (12)$$

$$\omega = 4K_{\text{WGS}}xcr(K_{\text{WGS}} - 1)(SC - xcr). \quad (13)$$

Coupling Eq. (10) with Eq. (9) and applying simple mathematical transformations results in the formulation of a final expression for the WGS reaction's rate:

$$R_{\text{WGS}} = R_{\text{MSR}}ycr. \quad (14)$$

The mass consumption and production rates of the reforming process reactions (Eqs. (1) - (3)), are summarized in the Table 1. The values are further applied to the mass transfer equation (Eq. (19)), as a part of its source terms. The heat generation rates by the described reactions are calculated depending on the rates of the reactions (Eqs. (5), (6), (14)) and the values of enthalpy change ΔH [41, 49]. The heat generation rates are given below:

$$Q_{\text{MSR}} = -\Delta H_{\text{MSR}}R_{\text{MSR}}, \quad (15)$$

$$Q_{\text{DRY}} = -\Delta H_{\text{DRY}}R_{\text{DRY}}, \quad (16)$$

$$Q_{\text{WGS}} = -\Delta H_{\text{WGS}}R_{\text{WGS}}. \quad (17)$$

2.2. Heat and Mass Transfer Model

The fundamental transport equations are incorporated into the mathematical model. Considering the computational domain defined for the needs of the analysis, the equations are implemented for two dimensions. Therefore, the model's equations are solved along the axis and radius of the reactor's geometry. The volume-averaging method was chosen for the derivation of the governing equations implemented in the model used for this analysis. The process parameters are locally averaged for each representative volume and included in the mathematical formulas [61]. Values of continuity (Eq. (18)), mass transfer (Eq. (19)), momentum (Eqs. (21) and (22)) and energy equations (Eq. (27)) characterize the transport phenomena occurring during the reforming process. The equations are derived for the laminar flow. The analyzed fluids are considered to be Newtonian and incompressible. Thus, the continuity equation takes the following form [62, 63]:

$$\frac{\partial(\rho_0 U_x)}{\partial x} + \frac{1}{r} \frac{\partial(r \rho_0 U_r)}{\partial r} = 0, \quad (18)$$

The species conservation is calculated using molar fractions of species taking part in the reaction (Equation (19)). The formulated equation is derived from Fick's law of diffusion [33]. The mass sources and sinks S_j depend on the MSR, DRY, and WGS rates and molar masses of the species taking part in the reaction [20, 64]. The exact equations defining the values of S_j are described in Table 1.

$$\begin{aligned} \rho_0 \left(U_x \frac{\partial Y_j}{\partial x} + U_r \frac{\partial Y_j}{\partial r} \right) &= \frac{\partial}{\partial x} \left(\rho_0 D_{j,\text{eff}} \frac{\partial Y_j}{\partial x} \right) \\ &+ \frac{1}{r} \frac{\partial}{\partial r} \left(r \rho_0 D_{j,\text{eff}} \frac{\partial Y_j}{\partial r} \right) + S_j. \end{aligned} \quad (19)$$

The effective mass diffusivity of species $D_{j,\text{eff}}$ was calculated using the equation explained below (Eq. (20)) [65]:

$$D_{j,\text{eff}} = (1 - \sqrt{1 - \varepsilon}) D_j. \quad (20)$$

The diffusion of substance j in the gas mixture D_j is computed using Fuller's method and Blanc's law. The gases' properties are taken from the literature [66]. The values assumed for the flow model describe the local phase

Table 1: Mass sources/sinks

species	mass generation MSR	mass generation WGS	mass generation DRY	summarized generation
H ₂	$3R_{\text{MSR}}M_{\text{H}_2}$	$R_{\text{WGS}}M_{\text{H}_2}$	$2R_{\text{DRY}}M_{\text{H}_2}$	$3R_{\text{MSR}}M_{\text{H}_2} + R_{\text{WGS}}M_{\text{H}_2} + 2R_{\text{DRY}}M_{\text{H}_2}$
CO	$R_{\text{MSR}}M_{\text{CO}}$	$-R_{\text{WGS}}M_{\text{CO}}$	$2R_{\text{DRY}}M_{\text{CO}}$	$R_{\text{MSR}}M_{\text{CO}} - R_{\text{WGS}}M_{\text{CO}} + 2R_{\text{DRY}}M_{\text{CO}}$
CO ₂	0	$R_{\text{WGS}}M_{\text{CO}_2}$	$-R_{\text{DRY}}M_{\text{CO}_2}$	$R_{\text{WGS}}M_{\text{CO}_2} - 2R_{\text{DRY}}M_{\text{H}_2}$
CH ₄	$-R_{\text{MSR}}M_{\text{CH}_4}$	0	$-R_{\text{DRY}}M_{\text{H}_2}$	$-R_{\text{MSR}}M_{\text{CH}_4} - R_{\text{DRY}}M_{\text{H}_2}$
H ₂ O	$-R_{\text{MSR}}M_{\text{H}_2\text{O}}$	$-R_{\text{WGS}}M_{\text{H}_2\text{O}}$	0	$-R_{\text{MSR}}M_{\text{H}_2\text{O}} - R_{\text{WGS}}M_{\text{H}_2\text{O}}$

average of the gas control volume. The momentum conservation depends directly on the insert's morphology. The materials composing the insert are considered porous. Therefore, parameters describing the material structure have to be included in the equations. The parameters are porosity ε , permeability K_p , and inertial coefficient c_{ine} [38]. A separate momentum equation is formulated for each of the computational domain dimensions (Eqs. (21) and (22)).

$$\frac{\rho_0}{\varepsilon_0^2} \left(U_x \frac{\partial U_x}{\partial x} + U_r \frac{\partial U_x}{\partial r} \right) = -\frac{\partial P}{\partial x} + \frac{\mu}{\varepsilon} \left[\frac{\partial^2 U_x}{\partial x^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial U_x}{\partial r} \right) \right] - \frac{\mu}{K_p} U_x - \frac{\rho_0 c_{\text{ine}}}{\sqrt{K_p}} U_x \sqrt{U_x^2 + U_r^2}, \quad (21)$$

$$\frac{\rho_0}{\varepsilon_0^2} \left(U_x \frac{\partial U_r}{\partial x} + U_r \frac{\partial U_r}{\partial r} \right) = -\frac{\partial P}{\partial r} + \frac{\mu}{\varepsilon} \left[\frac{\partial^2 U_r}{\partial x^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial U_r}{\partial r} \right) - \frac{U_r}{r^2} \right] - \frac{\mu}{K_p} U_r - \frac{\rho_0 c_{\text{ine}}}{\sqrt{K_p}} U_r \sqrt{U_x^2 + U_r^2}. \quad (22)$$

The permeability K_p of the specific segment is calculated using (23), basing on the information about its porosity ε [67]:

$$K_p = \frac{\varepsilon(1 - (1 - \varepsilon)^{1/3})}{36((1 - \varepsilon)^{1/3} - (1 - \varepsilon))} d_p^2, \quad (23)$$

where d_p stands for an average pore diameter. The inertial coefficient c_{ine} was calculated using [68]:

$$c_{\text{ine}} = 0.0095 g_s^{-0.8} \sqrt{\frac{\varepsilon}{3(\tau - 1)}} (1.18 \sqrt{\frac{(1 - \varepsilon)}{3\pi} \frac{1}{g_s}})^{-1}, \quad (24)$$

where tortousity τ and and shape function g_s are expressed with following equations [67, 68]:

$$\tau = \frac{\varepsilon}{1 - (1 - \varepsilon)^{1/3}}, \quad (25)$$

$$g_s = 1 - \exp\left(-\frac{1 - \varepsilon}{0.04}\right). \quad (26)$$

The energy conservation equation (Eq. (27)) describes the process of heat transfer during the reaction. The equation includes local thermal conditions, the materials' parameters, and the heat sources calculated using Eqs. (15) - (17).

$$\rho_0 C_p \left(U_x \frac{\partial T_{\text{loc}}}{\partial x} + U_r \frac{\partial T_{\text{loc}}}{\partial r} \right) = \frac{\partial}{\partial x} \left(\lambda_{\text{eff}} \frac{\partial T_{\text{loc}}}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \lambda_{\text{eff}} \frac{\partial T_{\text{loc}}}{\partial r} \right) + Q_s. \quad (27)$$

Due to the application of metallic foam, a proper relation describing the λ_{eff} of the material is essential [68]. The model chosen for calculating the value of the λ_{eff} was proposed by Boomsma and Poulikakos and further corrected by Dai et al. [69, 70]. The outcome relation allows for the derivation of equations describing the thermal conductivity of metallic foams. According to the literature review, an adequate model including the morphology of metallic foams is prepared [71].

$$\lambda_{\text{eff}} = \frac{\sqrt{2}l}{2(R_A + R_B + R_C + R_D)}, \quad (28)$$

where $R_A - R_D$ stand for the thermal resistances of the porous media cell subsections [37, 70].

3. Numerical model

To solve systems of the defined equations a discretization of the previously prepared continuous computational domain is necessary. The numerical model is prepared using the Finite Volume Method [72]. A uniform computational grid with evenly spaced nodes is formed, to assure a minimal complexity of the calculations, [40]. The grid's dimensions are established at 150 elements in the longitudinal and 25 elements in the radial directions, resulting in square-shaped elements. A single grid sector is presented in Fig. 2

3.1. Transport Equations

Integration of the fundamental transport equations of the reforming process over the created control volumes is conducted [73]. The partial differential equations covering the species conservation (Eq. (19)), the momentum

Table 2: Coefficients and terms for substitution in Eq. (29)

Eq.	ϕ	Ψ_x	Ψ_r	Γ	\bar{S}
(19)	Y_j	$\rho_0 U_x$	$\rho_0 U_r$	$\rho_0 D_{j,\text{eff}}$	S_j
(21)	U_x	$\frac{\rho_0}{\varepsilon_0^2} U_x$	$\frac{\rho_0}{\varepsilon_0^2} U_r$	$\frac{\mu}{\varepsilon_0}$	$-\frac{\partial P}{\partial x} - \frac{\mu}{K_p} U_x - \frac{\rho_0 c_{\text{ine}}}{\sqrt{K_p}} U_x \sqrt{U_x^2 + U_r^2}$
(22)	U_r	$\frac{\rho_0}{\varepsilon_0^2} U_r$	$\frac{\rho_0}{\varepsilon_0^2} U_r$	$\frac{\mu}{\varepsilon_0}$	$-\frac{\partial P}{\partial r} - \frac{\mu}{K_p} U_r - \frac{\rho_0 c_{\text{ine}}}{\sqrt{K_p}} U_r \sqrt{U_x^2 + U_r^2} - \frac{\mu U_r}{\varepsilon_0 r^2}$
(27)	T	$\rho_0 C_p U_x$	$\rho_0 C_p U_r$	λ_{eff}	Q_s

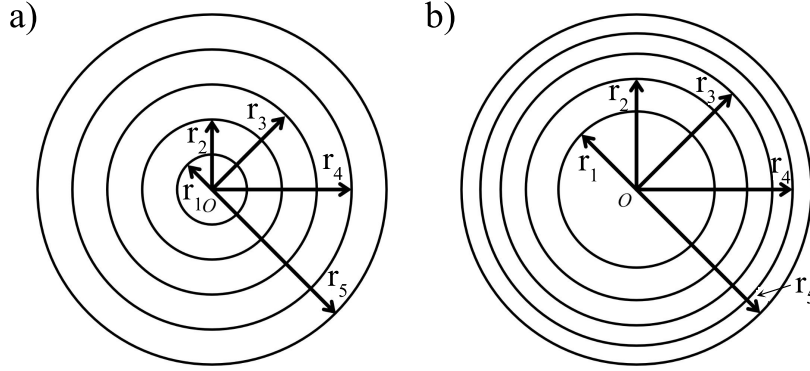


Figure 3: The coaxial segments configurations: a) equal width of rings, b) equal inlet and outlet surface

The exact dimensions of the particular rings for Fig. 3 b) are calculated using the system of equations (30), as follows:

$$\begin{cases} 2\pi r_1^2 = \frac{2}{5}\pi R^2 \\ 2\pi (r_2^2 - r_1^2) = \frac{2}{5}\pi R^2 \\ 2\pi (r_3^2 - r_2^2) = \frac{2}{5}\pi R^2 \\ 2\pi (r_4^2 - r_3^2) = \frac{2}{5}\pi R^2 \\ 2\pi (r_5^2 - r_4^2) = \frac{2}{5}\pi R^2 \end{cases} \quad (30)$$

The values resulting from solving the Eqs. (30) are presented in Tab. 3.

The computational domain is indicated with the red dashed line (Fig. 4). Segments can be described with the following parameters - porosity, average

Table 3: Rings' dimensions		
Radius	Equal width (cm)	Equal surface (cm)
r_1	1	$\sqrt{5}$
r_2	2	$\sqrt{10}$
r_3	3	$\sqrt{15}$
r_4	4	$2\sqrt{5}$
r_5	5	5

pore size, as well as their catalytic properties, which are directly correlated to the porosity value. The analyzed model is steady and the flow of gases is assumed to be laminar and occurring in one direction. Fluids taking part in the process are assumed to be Newtonian. The presented numerical analysis is a quasi-three-dimensional case. Due to the axial symmetry of the reactor's tube, a computational domain can be constrained to a two-dimensional cross-section of the reformer. Implementation of proper boundary conditions allows assuming the process occurs in the same manner throughout the reactor's whole volume [73].

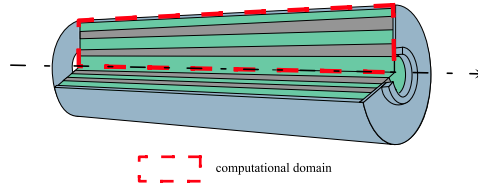


Figure 4: Quasi 3-dimensional computational domains for the rings configurations

3.3. Boundary Conditions and Materials

To complete the preparation of the numerical analysis, setting the properties of the materials and the boundary conditions is vital. Proper setting of SC value is essential for this analysis, due to the threat of carbon deposit formation [74]. If the ratios are chosen incorrectly, the carbon deposition phenomenon may occur, poisoning the reactor's catalyst [75]. Choosing an appropriate steam-to-carbon ratio allows for avoiding the described hazard.

The value of SC for this analysis was set to be equal to 2.0 [-], preventing this occurrence [43, 47]. The catalyst insert's segments are assumed to consist of one of two materials. The first material is a catalytic composite of nickel and yttria-stabilized-zirconia (Ni/YSZ). The second material, serving the purpose of heat transport medium, is chosen to be steel foam. The metallic foam segments are introduced for the unification of the temperature distribution inside the reactor. Suppression of the reforming reaction, combined with a considerable heat exchange surface for foams, is expected to let the gases mixture reheat effectively [76]. The value of λ_{solid} is set at $22 \text{ W m}^{-1} \text{ K}^{-1}$ for the catalytic material [77], while the value of λ_{solid} for the steel foam is established at $30 \text{ W m}^{-1} \text{ K}^{-1}$ [78]. The dimensionless cubic node length e is set to be equal to 0.0339, as explained by Boomsma and Poulikakos [69]. The temperature of the fuel flowing inside the unit is considered to reach the temperature of the reformer instantly. The symmetry boundary conditions are set at the symmetry axis, while the no-slip boundary condition is applied at the wall of the reformer. The boundary conditions necessary for the solution of the governing equations are summarized below.

Thermal Boundary Conditions

- inlet temperature $T = T_{\text{in}} = 900 \text{ K}$ at $x = 0$ and $0 \leq r < R$,
- outlet temperature $\partial T / \partial x = 0$ at $x = L$ and $0 \leq r < R$,
- symmetry boundary condition $\partial T / \partial r = 0$ at $0 \leq x < L$ and $r = 0$,
- wall heat flux $\partial T / \partial r = \text{const}$ at $0 \leq x < L$ and $r = R$.

The thermal boundary condition set at the reactor's wall is chosen to be of a second type. Constant heat flux is assumed on the reactor's wall, and the wall itself is the medium for heat exchange between the reactor and the system boundaries. The wall thickness is set to be equal to 0.001 m and is assumed to consist of the same material as the metallic foams. Thus, the value of λ_{solid} for the reactor's wall is equal to $30 \text{ W m}^{-1} \text{ K}^{-1}$ [78]. The boundary conditions essential for the calculation of the species conservation equations are presented below.

Mass Transport Boundary Conditions

- inlet mole fractions $Y_j = Y_{j,\text{in}}$ at $x = 0$ and $0 \leq r < R$,

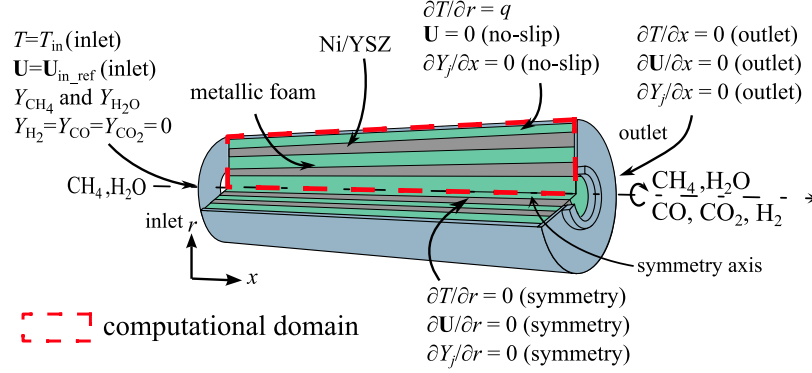


Figure 5: Boundary conditions applied in the analysis

- outlet mole fractions $\partial Y_j / \partial x = 0$ at $x = L$ and $0 \leq r < R$,
- symmetry boundary condition $\partial Y_j / \partial r = 0$ at $0 \leq x < L$ and $r = 0$,
- no-slip boundary condition $Y_j = 0$ at $0 \leq x < L$ and $r = R$.

To complete the numerical model's setting, the boundary conditions for solving the momentum conservation equations are needed. The conditions are applied in the manner listed below.

Momentum Boundary Conditions

- inlet velocity $U = U_{\text{in}} = 0.15 \text{ m s}^{-1}$ at $x = 0$ and $0 \leq r < R$,
- outlet velocity $\partial U / \partial x = 0$ at $x = L$ and $0 \leq r < R$,
- symmetry boundary condition $\partial U / \partial r = 0$ at $0 \leq x < L$ and $r = 0$,
- no-slip boundary condition $U = 0$ at $0 \leq x < L$ and $r = R$.

All of the boundary conditions are summarized in Fig. 5.

4. Genetic algorithm

The conducted optimization includes the application of an evolutionary algorithm, to define the optimal design of the catalytic insert for the coaxial segments. The genetic algorithm (GA) is selected to be the optimization procedure used for the needs of the analysis. The algorithm analyses subsequent,

finite populations of test specimens, which parameters are inherited from the specimens acquiring the best results in the preceding generation. The results are evaluated by user-defined fitness functions [79]. The functions are exclusive to a certain problem. If more than one function is defined, the functions have to be combined into a single value, which will be further processed by the genetic algorithm itself [80]. The remaining part of the genetic algorithm operation is the mutation procedure. The mutation is used as an additional procedure for preventing the local extremum trap and a measure for the introduction of genes that were not present in the initial population or are just not possible to acquire on the way of the crossover procedure [81]. Coupling of the prepared numerical analysis with the algorithm requires proper parametrization of reactor parameters [80]. The catalyst insert is set to contain 5 coaxial segments. Each of the segments is assumed to consist of either a catalytic composite of nickel with yttria-stabilized-zirconia (Ni/YSZ) or a stainless steel foam [71]. The insert regions may differ in their morphological parameters regardless of the constituting material. The parameters altered by the algorithm are segment catalytic character, porosity ε and average pore diameter d_p . The porosity values available for application in the analysis are constrained to the range between 0.5 and 0.8. The lower boundary is set at 0.5, as lower porosity values resulted in over-significant pressure drops during the preliminary calculations. The choice of 0.8 as the upper boundary is motivated by lower accessibility to the manufacturing methods determined for metallic foams of higher porosities [82]. The average pore diameters d_p are calculated for each segment, based on the values of the porosity [71]. The upper boundary of the d_p range is restricted by the model conditions. According to the volume-averaging method, the size of a single pore is not allowed to exceed the size of a single numerical grid element. Therefore, the upper boundary is limited to 0.002 m [61]. Furthermore, segment porosity ε has a direct influence on the catalyst density. The catalyst density \dot{w}_{cat} is calculated using Eq. (31):

$$\dot{w}_{\text{cat}} = \rho_{\text{cat}} \cdot (1 - \varepsilon_0), \quad (31)$$

where ρ_{cat} is equal to $5.3448 \cdot 10^6 \text{ g m}^{-3}$. The chemical reaction kinetics model derived for the implemented numerical simulation regards a Ni/YSZ composite with a 60:40 Ni to YSZ ratio [71]. Nickel serves the catalytic purpose, while YSZ serves as a scaffold. Therefore, the basic catalyst density for the Ni/YSZ element should be calculated concerning the ratio of the

materials. The solid nickel density equals to $8.908 \cdot 10^6 \text{ g m}^{-3}$ [83]. The value of ρ_{cat} is calculated by applying the given ratio to the value of the solid nickel density [71]. The definition of the relations allows commencing the operation of the GA. The algorithm starts its operation with the preparation of the initial generation, with the specimens' parameters fully randomized. First, the segments' character is randomized. The algorithm is expected to generate catalytic and non-catalytic segments in a ratio of 50:50, as the randomization procedure uses a uniform distribution for its seed [84]. When the specific segment's character is determined, the algorithm randomizes its porosity ε and average pore size d_p values. As the final initialization step, the GA calculates the catalyst density for each of the segments designated to consist of Ni/YSZ composite. Having defined the initial parameters, the reforming simulation code is executed for each of the generated reactors. The overall operation of the algorithm prepared for the needs of the research is presented in Fig. 6.

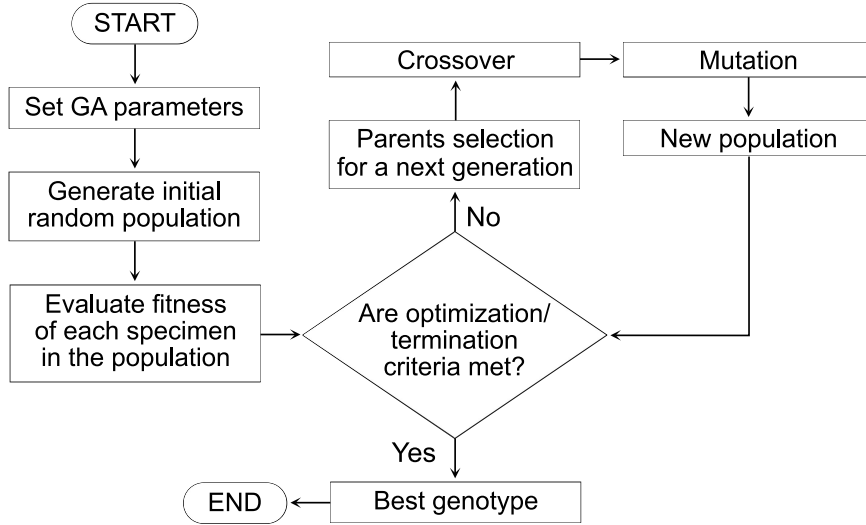


Figure 6: Summary of the genetic algorithm procedure

The conducted investigation regards optimization of the temperature field distribution inside the reactor, simultaneously maintaining a considerable methane conversion rate [38]. Therefore, the research is considered a multi-objective optimization, as the fitness analysis is required to investigate two separate factors. The first factor is temperature distribution. The main objective is to reduce the temperature gradients occurring throughout the

reactor's volume during the reaction. The strong endothermic character of the process has a consequence in large temperature decreases in the regions in which the fuel concentration is significant. The constant transition of the temperature field leads to the establishment of thermal stresses, leading to premature degradation of the catalyst material [85]. The presented research predicts the search for an optimal distribution of catalytic and non-catalytic segments and proper selection of their porosity ε and average pore size d_p . The first function f_{CH_4} regards the methane conversion rate. The fuel conversion rate is calculated using the molar fractions of the methane at the inlet and the outlet of a specific reactor. The f_{CH_4} value is calculated using Eq. (32):

$$f_{CH_4} = \frac{(frac_{CH_4in} - frac_{CH_4out})}{frac_{CH_4in}}, \quad (32)$$

The remaining fitness function f_T evaluates the extent of the unification of the temperature distribution inside the catalytic insert. Essentially, the thermal fitness objective is to find the ΔT value, being a representative temperature difference for a specific reactor. To assure reliability and accuracy of the mathematical formula, the thermal fitness is established to perform the temperature distribution analysis for each of the grid elements separately [38]. The algorithm iterates through each of the created control volumes and calculates the temperature difference between the central node T_P and each of the neighboring control volumes T_N , T_E , T_S , T_W (Fig. 7). Further, each of the control volumes has its specific temperature difference $\Delta T_{loc_{i,j}}$ assigned. The $\Delta T_{loc_{i,j}}$ value is chosen to be the highest temperature difference among the values calculated for each of the neighboring control volumes. The $\Delta T_{loc_{i,j}}$ for each of the cells is based on the following formula:

$$\Delta T_{loc_{i,j}} = \max \{ |T_{P_{i,j}} - T_{N_{i,j}}|, |T_{P_{i,j}} - T_{E_{i,j}}|, |T_{P_{i,j}} - T_{S_{i,j}}|, |T_{P_{i,j}} - T_{W_{i,j}}| \}. \quad (33)$$

Having computed the set of the $\Delta T_{loc_{i,j}}$ for the whole numerical grid, the algorithm selects the highest value among computed $\Delta T_{loc_{i,j}}$ and saves it as a global ΔT value representing a specific reactor (Eq. (34)).

$$\Delta T = \max \{ T_{loc_{1,1}}, T_{loc_{1,2}}, \dots, T_{loc_{i,j}} \}, \quad (34)$$

where i and j indices represent the numerical grid's dimensions. The final thermal fitness value f_T is computed using the following formula:

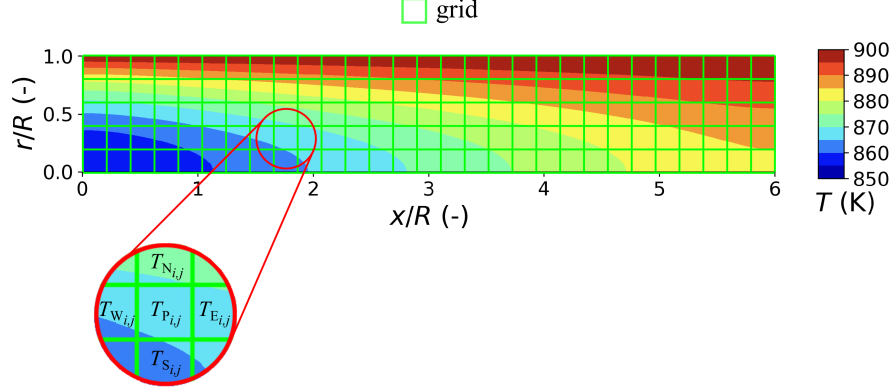


Figure 7: Temperature field evaluation strategy

$$f_T = 1 - \frac{\Delta T}{\Delta T_{\max}}, \quad (35)$$

where ΔT_{\max} stands for the highest temperature difference value reported for a single generation. The acquired f_{CH_4} and f_T values are further combined into a single fitness value f , using the weighted-sum method [86]:

$$f = \sum_{i=1}^N w_i f_i. \quad (36)$$

where N represents the number of the specimens. The weights w_i are established at 0.2, 0.4, 0.5, 0.6, and 0.8. Each of the analyses being carried out applied each of the weights to both of the fitness functions to allow the conduction of a sensitivity analysis, depending on the assumed importance of the defined fitness functions. The conducted numerical investigation includes a search for an optimal arrangement of coaxial segments, simultaneously performing a sensitivity analysis of the weights applied for the fitness calculation.

5. Numerical analysis

6. Conclusions

The conducted numerical investigation regards radial segmentation of the catalyst insert. Two different configurations of coaxial segments are proposed. The radial segments may either have equal widths of the inlet surfaces or equal areas of the inlet surfaces. Each of the possible segment configurations' performance is tested against five different sets of fitness function weights. The weight sensitivity analysis is conducted to assure the best possible practices during future numerical analyses of the macro-patterned reforming reactor design optimization. Analyzing the results leads to the following conclusions:

1. Fitness weights set at 0.4 for the methane conversion and 0.6 for thermal fitness tend to deliver better results, compared with the remaining algorithms.
2. Radial segments with equal widths of the inlet surface return results of a higher quality than radial segments with equal areas of the inlet surfaces (Strategy III & V).
3. The highest values of hydrogen productivity are acquired for the reactor with equal width of inlet surfaces (Strategy IV), proving it to be the most valid approach to the optimization of the catalytic insert design.
4. The introduction of the macro-patterning concept is proven to enhance the effectiveness of the reforming reaction. The hydrogen productivity is almost tripled for the best solution when compared with the reference case.

The conducted research indicates the influence of altering the steam reforming thermal conditions on the overall process proceeding. The possible improvement of the process effectiveness on the unification of the temperature distribution is confirmed. The proposed macro-patterning concept proves the possibility of acquiring even higher methane conversion rates, using the same amount of catalyst as in the case of the reference case. However, the macro-patterned reactors would have to suffer in the compactness, as to acquire the exact level of conversion, a slight extension of their dimensions is required. The enlargement of the reactors is whatsoever not a tremendous drawback,

when considering the possible elongation of the unit's lifetime, due to the reduction of the thermal stresses magnitude.

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