



# Carbon emission reduction and hydrogen production maximization from carbon emission-based hydrogen sources

Johnson Kehinde Abifarin<sup>1</sup> · Fredah Batale Abifarin<sup>2</sup>

Received: 2 February 2024 / Accepted: 30 June 2024  
© The Author(s) 2024

## Abstract

This study aims to optimize hydrogen ( $H_2$ ) production via ethanol steam reforming (ESR) and water gas shift reaction (WGSR) pathways, focusing on minimizing  $CO$ ,  $CO_2$ , and  $CH_4$  emissions while maximizing  $H_2$  yield. Employing Taguchi grey relational analysis, we investigate the intricate balance between production conditions and multi-response gas generation. Utilizing Origin Pro software, regression modeling forecasts individual and overall gas generation. Our analysis identifies optimal conditions: a feed liquid flow rate of 2 mL/min, water-to-carbon ratio of 3, ESR temperature of 300 °C, and WGSR temperature of 350 °C. These conditions promise clean, efficient  $H_2$  production. Key results show the water-to-carbon ratio and ESR temperature contributing 59.22% and 32.69% to production conditions' impact, respectively. Graphical and mathematical models validate these findings. Moving forward, further experimental validation of optimal conditions for multi-response gas generation is recommended. This study pioneers a transformative approach towards sustainable, environmentally friendly  $H_2$  production.

**Keywords** Energy vector · Clean production · Carbon capturing · Taguchi grey relational analysis · Optimization · Sustainable energy

## Introduction

Fossil fuel emissions clog our skies, staining the very air we breathe with pollution. The relentless plunder of non-renewable resources only deepens this ecological wound, driving urgent calls for a shift towards sustainable alternatives. Enter hydrogen is a promising contender in the battle against environmental degradation (Bolt et al. 2020; Karaoglu and Yolcular 2022). With its lofty energy density, pristine purity, and infinite regenerative potential, hydrogen emerges as a beacon of hope amidst the murky landscape of energy alternatives (Satyapal et al. 2007). Yet, harnessing

its power demands a unique understanding—for hydrogen marches to the beat of its chemical drum (Karaoglu and Yolcular 2022). When unleashed within a fuel cell, hydrogen dances as a pristine performer, emitting naught but water vapor. Its celestial cleanliness positions it as the darling of power generation and transportation, offering portable electricity solutions for both vehicles and dwellings alike (Kumar and Muthukumar 2020; Xiao et al. 2022). The allure of clean, secure energy beckons from the hydrogen horizon, tantalizing us with the promise of a brighter tomorrow. With its prowess to fuel both fuel cells and internal combustion engines, hydrogen stands are poised to revolutionize our energy landscape. But despite its cosmic abundance, hydrogen remains a reluctant guest on our planet's surface, necessitating innovative production and storage solutions to unlock its full potential. To weave hydrogen into the fabric of our sustainable future, we must harvest its power from renewable sources, embracing techniques that are gentle on both our planet and our wallets. Only then can we truly harness the boundless energy of hydrogen, ushering in an era where clean, green power reigns supreme.

Responsible Editor: Ta Yeong Wu

✉ Johnson Kehinde Abifarin  
johnson.abifarin@anu.edu.au

<sup>1</sup> School of Engineering, College of Engineering, Computing, and Cybernetics, Australian National University, Canberra, Australia

<sup>2</sup> Department of Metallurgical and Materials Engineering, Ahmadu Bello University, Zaria, Nigeria

In a city battling pollution, two solutions emerged: carbon capture and utilization (CCU) (Dou et al. 2023) and carbon reduction optimization (CRO). CCU captured emissions from factories, repurposing them for various uses. Meanwhile, CRO-optimized processes reduce emissions at their source. While CCU seemed effective, CRO's proactive approach proved superior. By targeting emissions directly, CRO minimized the need for extensive infrastructure and promoted sustainable practices. Ultimately, CRO led to cleaner air and a brighter future for the city. In the expansive realm of sustainable energy, an array of diverse endeavors has been undertaken to grapple with the pressing issue of emissions during hydrogen production from traditional sources such as WGS and ESR. Casanovas et al. (2009) conducted a comprehensive study delving into the investigation of Mn promotion over Co/ZnO catalysts for ethanol steam reforming (ESR) and water gas shift (WGS) reactions, unraveling intricate insights into catalyst characteristics and performance. Nevertheless, amidst its elucidation, a conspicuous lacuna emerges, as it overlooks the crucial aspect of optimizing hydrogen production and minimizing carbon emissions, thereby constituting a significant drawback. This oversight underscores missed opportunities to enhance process efficiency and bolster environmental sustainability. On a similar note, Sharma et al. (2017) eloquently underscored ethanol steam reforming's potential for hydrogen production, yet astutely noted a glaring absence in optimization for hydrogen yield and reduction of carbon emissions, accentuating the exigency for more holistic strategies. Additionally, Chen et al. (2017) singularly focused on hydrogen generation from ESR and WGS techniques, regrettably sidestepping the imperative of addressing carbon emission reduction, thus magnifying environmental apprehensions. This recurrent theme of neglecting carbon emission mitigation alongside hydrogen yield optimization, as exemplified in Quan et al.'s (2024) evaluation of Ni–Ce/mesopore Y catalysts for ESR, speaks volumes about the prevailing trend in the literature. Furthermore, Cordaro et al.'s (2024) proposition of a model for co-generating hydrogen and electricity unveils a pertinent concern—its oversight in optimizing both hydrogen and carbon emissions, underscoring an inherent deficiency in overall efficiency and sustainability considerations. While Di Nardo et al. (2024) provided a nuanced analysis of CO<sub>2</sub> emissions across diverse steam reforming processes, their failure to optimize hydrogen yield and carbon emissions is a palpable shortcoming that merits attention. Similarly, Kim et al.'s (2024) exploration into enhancing hydrogen production from waste-derived syngas signals a clear imperative for further optimization in both hydrogen yield and carbon minimization. Ovalle-Encinia and Lin's (2024) investigation of a CO<sub>2</sub>-perm-selective membrane reactor for WGS reaction, albeit demonstrating enhanced CO conversion and H<sub>2</sub> purity, notably disregarded optimization for hydrogen

yield and carbon emissions, thus presenting an area ripe for improvement in reactor efficiency and sustainability. Against this backdrop, our study endeavors to bridge this gap by integrating comprehensive strategies aimed at minimizing emissions and maximizing hydrogen yield through both singular (Taguchi design) and multi-response (grey) optimization analyses, thereby contributing substantively to a more environmentally benign and economically sustainable paradigm in hydrogen production.

The Taguchi design methodology has proven effective in reducing experiment variability and improving the quality and efficiency of processes, products, and systems (Abifarin 2021; Roy 2010). It is commonly utilized to optimize process or production parameters for enhanced performance characteristics (Taguchi 1995). However, a limitation of Taguchi design is its inability to optimize multiple performance characteristics simultaneously (Abifarin et al. 2021a). When dealing with multiple characteristics, complications arise as they may not align in the same domain and may have conflicting objectives. To address the challenges of optimizing multiple performance characteristics, grey relational analysis (GRA) has been extensively integrated with the Taguchi design technique across various applications, including automotive (Abifarin and Ofodu 2022a; Garud and Lee 2023; Salmani et al. 2022), aerospace (Panwar and Chandna 2023; Unnikrishna Pillai et al. 2023), biomedical (Abifarin et al. 2023a,b, 2022; Hussain et al. 2023), CNC machining (Aravind et al. 2017; Esangbedo and Abifarin 2022), materials fabrication (Esangbedo and Abifarin 2023; Abifarin 2021; Tzeng et al. 2009), and energy production (Deepanraj et al. 2017; Kadier et al. 2015; Abifarin and Ofodu 2022b; Shi et al. 2023; Vasantharaj et al. 2017). The optimization results obtained through this approach are effective and efficient. Despite the exceptional advantages of Taguchi GRA in optimizing multiple performance characteristics, no study, to the best of our knowledge, has focused on maximizing hydrogen production while minimizing carbon emissions from carbon-sourced hydrogen. This paper presents a model and settings for hydrogen production from any carbon-based hydrogen source, aiming to reduce carbon emissions and increase hydrogen energy for environmental sustainability and human consumption.

In conclusion, while the literature has extensively explored methods such as water–gas shift (WGS) reaction and ethanol steam reforming for hydrogen production, a notable gap remains in the simultaneous optimization of hydrogen yield and carbon emissions reduction. Our work stands out by addressing this gap and introducing novel strategies to integrate Taguchi design and grey relational analysis. By leveraging these techniques, we aim to maximize hydrogen production while minimizing carbon emissions from carbon-sourced hydrogen. This approach represents a significant advancement in the field, offering a more

comprehensive and sustainable solution to the challenges of hydrogen production. Through our study, we not only bridge the gap in the existing literature but also contribute to a cleaner, greener energy landscape, paving the way for a more environmentally friendly and economically viable approach to hydrogen production.

## Methodology

### Taguchi design analysis

The data analyzed in this study is derived from the study of Chen et al. (2017), and here is the summary of the conditions employed to obtain the data from their work: The system employed included the experimentation of producing hydrogen and enriching carbon dioxide. It included a feeding unit, a reaction unit, a condenser, and units for gas and liquid analysis. Ethanol–water mix in a flask was fed using a pump. The reaction unit had ESR and WGSR

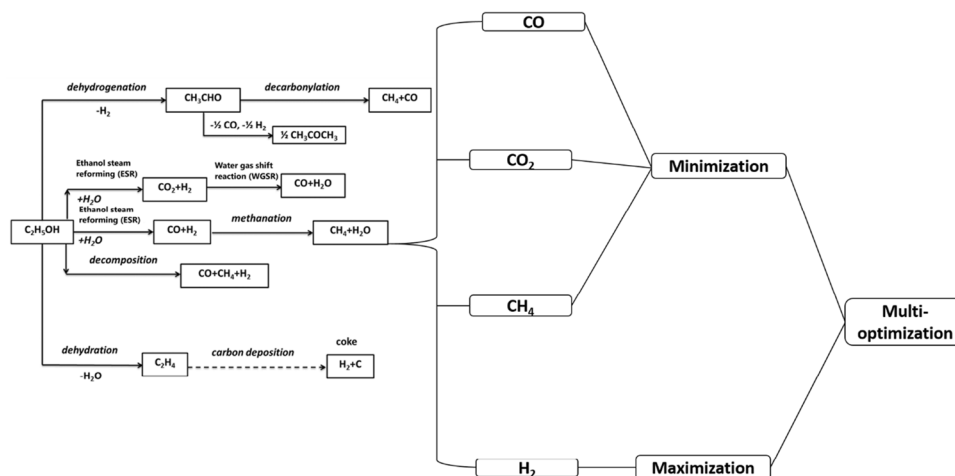
reactors, with controlled temperatures. ESR used a Ni-based catalyst, with liquid hourly space velocity (LHSV) values of 2.14 and 4.28 h<sup>-1</sup>. WGSR used a Fe–Cr-based catalyst. Gas from ESR went into WGSR. Gas and liquid analyses were done using specific instruments. Calibration ensured precise measurements. Each experiment lasted 4 h, yielding steady results.

For the trials, a Taguchi L9 orthogonal array (OA) was used, comprising nine runs as indicated in Table 1. Four response factors, CO, CO<sub>2</sub>, CH<sub>4</sub>, and H<sub>2</sub>, were used to evaluate the gases produced, as shown in Table 1. The results and models generated for the four gases are presented and discussed in “Results and discussion.” Like the study of Abifarín and Owolabi (2023), note that the production conditions employed are labeled A to D (Table 1) for the mathematical modeling of resultant gases discussed in “Results and discussion.” The design overview is depicted in Fig. 1.

**Table 1** Orthogonal array design

Design run	Hydrogen production conditions from ethanol steam reforming and water gas shift reaction pathways				Generated gases as responses			
	A: Rate of feed liquid flow (mL/min)	B: Water-to-carbon ratio	C: ESR temperature (°C)	D: WGSR temperature (°C)	CO (%)	CO <sub>2</sub> (%)	CH <sub>4</sub> (%)	H <sub>2</sub> (%)
1	2	3	400	300	1.62	21.82	6.04	66.71
2	2	4	450	350	0.48	21.18	6.07	66.81
3	2	5	500	400	0.67	23.44	1.58	70.38
4	3	3	450	400	1.85	21.96	3.6	68.69
5	3	4	500	300	1.44	21.3	1.52	70.43
6	3	5	400	350	1.14	21.25	2.75	69.51
7	4	3	500	350	3.69	18.99	4.31	67.67
8	4	4	400	400	1.23	21.52	3.29	67.53
9	4	5	450	300	2.8	20.51	1.62	70.73

**Fig. 1** Singular and multi-response gases design analytical procedure



## Multi-gas response optimization using GRA

The Taguchi design of experiments (DOE) method is adequate for evaluating optimal processing parameters for a single performance response. However, when optimizing two or more responses, a multi-objective optimization technique is necessary. Grey relational analysis (GRA) is employed to handle irregular finite data by normalizing all four gases into a single domain for Taguchi optimization analysis. Therefore, multi-gas optimization of processing parameters is conducted using the Taguchi GRA technique.

### Grey relational analysis

The preprocessing of the four experimental gas data was done to ensure that they fell between zero and one, as stated in the grey relational analysis technique. The “higher-the-better” (Eq. 1) preprocessing data methodology was applied to H<sub>2</sub>, whereas the “smaller-the-better” method was applied to CO, CO<sub>2</sub>, and CH<sub>4</sub> (Eq. 2). The reason for this choice is that a higher quantity of H<sub>2</sub> is desired for fuel efficiency maximization, while as small as possible CO, CO<sub>2</sub>, and CH<sub>4</sub> emissions are desired for emission reduction (Len and Luque 2023; Zurrer et al. 2023). Table 3 shows the preprocessed data ( $x_i^*$ ), which is commonly referred to as grey relational generation. For each of the four generated gases, an ideal sequence,  $x_0(k)$  ( $k=1, 2, \dots, 9$ ), was compared. The grey relational coefficient

was then processed by computing the deviation sequence (Eq. 3). Table 3 also displays the deviation sequence ( $\Delta_{oi}$ ) for each of the four experimental gases. Next, using Eq. 4, the grey relational coefficient (GRC) was calculated. The link between the expected and actual experimental data is depicted by the grey relational coefficient. Additionally, it provides the ability to link and calculate the statistical means of the different experimental data that are not additive. The five grey relational coefficients were then averaged to determine the grey relational grade or GRG, in Eq. 5. Table 2 also displays the GRG and GRC values. The total reaction of the four experimental gases is provided by the grey relational grade. Stated differently, the unique answer (GRG) produced by the grey computational analysis makes the hitherto impractical optimization of the four complex data possible. The level exhibiting the highest GRG is the optimization of the material’s design parameters.

$$x_i(k) = \frac{y_i(k) - \min y_i(k)}{\max y_i(k) - \min y_i(k)} \quad (1)$$

$$x_i(k) = \frac{\max y_i(k) - y_i(k)}{\max y_i(k) - \min y_i(k)} \quad (2)$$

$$\Delta_{oi}(k) = \|x_0(k) - x_i(k)\| \quad (3)$$

**Table 2** Grey relational analytical results

Design run	Grey relational generation ( $x_i^*$ )				Deviation sequence ( $\Delta_{oi}$ )				Grey relational coefficient ( $\epsilon_i(k)$ )				GRG ( $\gamma_i$ )
	CO	CO <sub>2</sub>	CH <sub>4</sub>	H <sub>2</sub>	CO	CO <sub>2</sub>	CH <sub>4</sub>	H <sub>2</sub>	CO	CO <sub>2</sub>	CH <sub>4</sub>	H <sub>2</sub>	
1	0.645	0.364	0.007	0	0.355	0.636	0.993	1	0.585	0.440	0.335	0.333	0.423
2	1	0.508	0	0.025	0	0.492	1	0.975	1	0.504	0.333	0.339	0.544
3	0.941	0	0.987	0.913	0.059	1	0.013	0.087	0.894	0.333	0.974	0.852	0.763
4	0.573	0.333	0.543	0.493	0.427	0.667	0.457	0.508	0.54	0.428	0.522	0.496	0.497
5	0.701	0.481	1	0.925	0.299	0.519	0	0.075	0.626	0.491	1	0.870	0.747
6	0.794	0.492	0.730	0.697	0.206	0.508	0.270	0.304	0.709	0.496	0.649	0.622	0.619
7	0	1	0.387	0.239	1	0	0.613	0.761	0.333	1	0.449	0.397	0.545
8	0.766	0.431	0.611	0.204	0.234	0.569	0.389	0.796	0.682	0.468	0.562	0.386	0.524
9	0.277	0.658	0.978	1	0.723	0.342	0.022	0	0.409	0.594	0.958	1	0.740

**Table 3** Analysis of variance of hydrogen production conditions on the generation of hydrogen

Factor	Degree of freedom	Adjusted sum square	Adjusted mean square	Contribution (%)
Rate of feed liquid flow (mL/min)	2	3.7538	1.87688	18.27
Water-to-carbon ratio	2	10.4572	5.22861	50.88
ESR temperature (°C)	2	3.7318	1.86588	18.16
WGS temperature (°C)	2	2.6088	1.30441	12.69
Residual error	0	0	0	-
Total	8	-	10.27578	100

$$\xi_i(k) = \frac{\Delta_{\min} + \zeta \Delta_{\max}}{\Delta_{oi}(k) + \zeta \Delta_{\max}} \quad (4)$$

$$\gamma_i = \frac{1}{n} \sum_{i=1}^n \xi_i(k) \quad (5)$$

In the equation, where  $y_i(k)$  represents the starting sequence of the response mean and  $x_i(k)$  stands for the preprocessed data for the  $i$ th experiment. The sequences of deviation, reference, and comparability are denoted by  $\Delta_{oi}(k)$ ,  $x_o(k)$ , and  $x_i(k)$ , respectively. The GRC value of each gas response, calculated as a function of the minimum and maximum deviations of each response variable,  $\Delta_{\min}$  and  $\Delta_{\max}$ , is reflected in  $\xi_i(k)$ . The differentiating coefficient (0~1) is  $\zeta$ ; however, each parameter is often given a separate weight of 0.5. The value of GRG for the  $i$ th experiment is represented by  $\gamma_i$ , where  $n$  is the total number of performance characteristics.

### Variance analysis

The purpose of ANOVA is to determine whether the processing factors in the experiment design (DOE) have a substantial impact on the production efficiency being evaluated. The analysis of interactions between processing factors and their impact on dependent variables has also extensively utilized the ANOVA table (Sambasevam et al. 2023; Abifarín et al. (2021b)). It is employed to investigate the amount of contribution of production factors to the efficiency of the whole system. Here, we used ANOVA with Minitab 16 software to investigate the significance and contribution of production factors (rate of feed liquid flow,  $H_2O/C$  ratio, ESR temperature, WGSR temperature) on the individual response gases and their multi-gas characteristics.

## Results and discussion

### Hydrogen ( $H_2$ ) maximization analysis

#### Significance of hydrogen production conditions on hydrogen generation

The results from Table 3 highlight the significant influence of various hydrogen production conditions on the yield of  $H_2$ . Specifically, the water-to-carbon ratio emerges as the most influential factor, contributing 50.88% to the maximization of  $H_2$  yield. This underscores the importance of maintaining an optimal ratio of water to carbon for efficient hydrogen production in ethanol steam reforming (ESR) and water gas shift reaction (WGSR) pathways. Additionally, the rate of feed liquid flow and ESR temperature each contribute

approximately 18% to  $H_2$  yield, indicating their substantial impact on the process. Conversely, WGSR exhibits the lowest contribution, accounting for only 12.69% of  $H_2$  yield variation. These findings emphasize the necessity of prioritizing the water-to-carbon ratio as a key production condition for maximizing hydrogen output in ESR and WGSR processes. The effectiveness of the model is further confirmed by a residual error of zero, validating its accuracy in predicting  $H_2$  generation under varying production conditions. Equation 6 mathematically represents the relationship between production conditions and  $H_2$  yield, with variables  $A$ ,  $B$ ,  $C$ , and  $D$  denoting the resultant  $H_2$  values corresponding to feed liquid flow rate, water-to-carbon ratio, ESR temperature, and WGSR temperature, respectively. This comprehensive analysis elucidates the critical role of process parameters in influencing hydrogen production efficiency and underscores the importance of optimizing conditions to enhance overall process performance.

$$H_2(\%) = 55.69 + 0.338A + 1.25B + 0.0158C - 0.00029D \quad (6)$$

#### Effect of hydrogen production conditions on hydrogen production

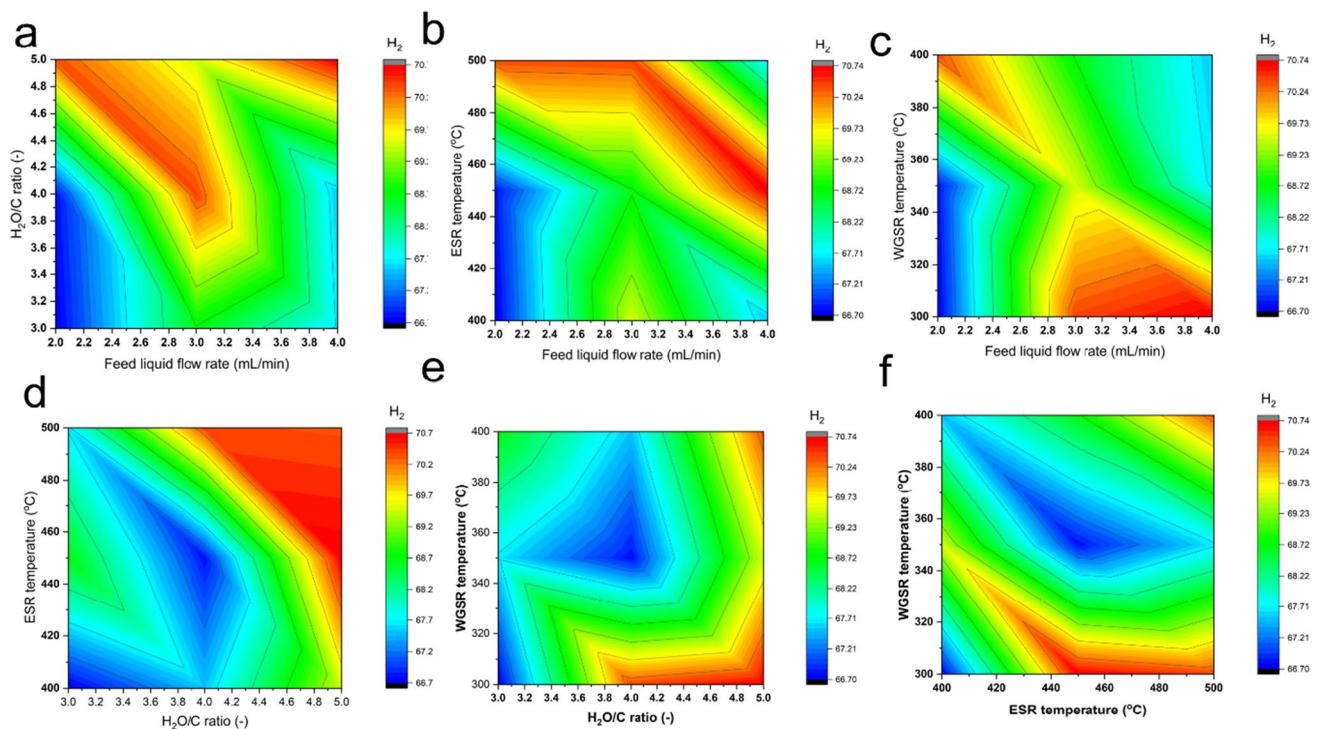
The interaction between hydrogen production conditions and their impact on  $H_2$  generation is crucial for maximizing production efficiency. Illustrated in Fig. 2, the varying shades from deep red to deep blue denote the spectrum of  $H_2$  levels, with deep red representing the highest and deep blue the lowest. Ideally, production conditions yielding a deep red hue indicate optimal  $H_2$  generation. Consequently, a higher water-to-carbon ( $H_2O/C$ ) ratio and ESR temperature, in conjunction with other hydrogen production conditions, lead to maximal  $H_2$  production. Conversely, lower values of feed liquid flow rate and WGSR temperature contribute to optimal  $H_2$  yield, while also offering energy-saving benefits. Therefore, by precisely controlling production conditions as guided by the model depicted in Fig. 2 and Eq. 6, maximum hydrogen production can be achieved via ethanol steam reforming and water gas shift reaction pathways. This underscores the importance of strategic process parameter management in enhancing  $H_2$  generation efficiency and overall process performance.

### Carbon monoxide (CO) reduction analysis

#### Significance of hydrogen production conditions on carbon monoxide

After analyzing the graphical representation depicting the interaction of various hydrogen production conditions on CO gas generation, it is imperative to quantitatively assess





**Fig. 2** Interaction between the production parameters on hydrogen ( $H_2$ ) production

the effects of these production conditions on CO generation during hydrogen production from ethanol steam reforming and water gas shift reaction pathways. Utilizing ANOVA analysis, Table 4 provides insights into the percentage contribution of each production condition to CO generation. The results highlight the significant impact of the rate of feed liquid flow, contributing 50.77%, followed by the water-to-carbon ratio at 32.95%. Remarkably, the residual error exhibits zero contribution, indicating the model's exceptional goodness of fit. Regression modeling facilitated the development of a mathematical model for CO generation, as presented in Eq. 7, where variables  $A$ ,  $B$ ,  $C$ , and  $D$  correspond to the resultant generated values of CO gas concerning the rate of feed liquid flow,  $H_2O/C$  ratio, ESR temperature, and WGS temperature, respectively. This comprehensive analysis underscores the critical role of production conditions in

influencing CO generation, providing valuable insights for optimizing hydrogen production pathways while minimizing unwanted byproducts like CO.

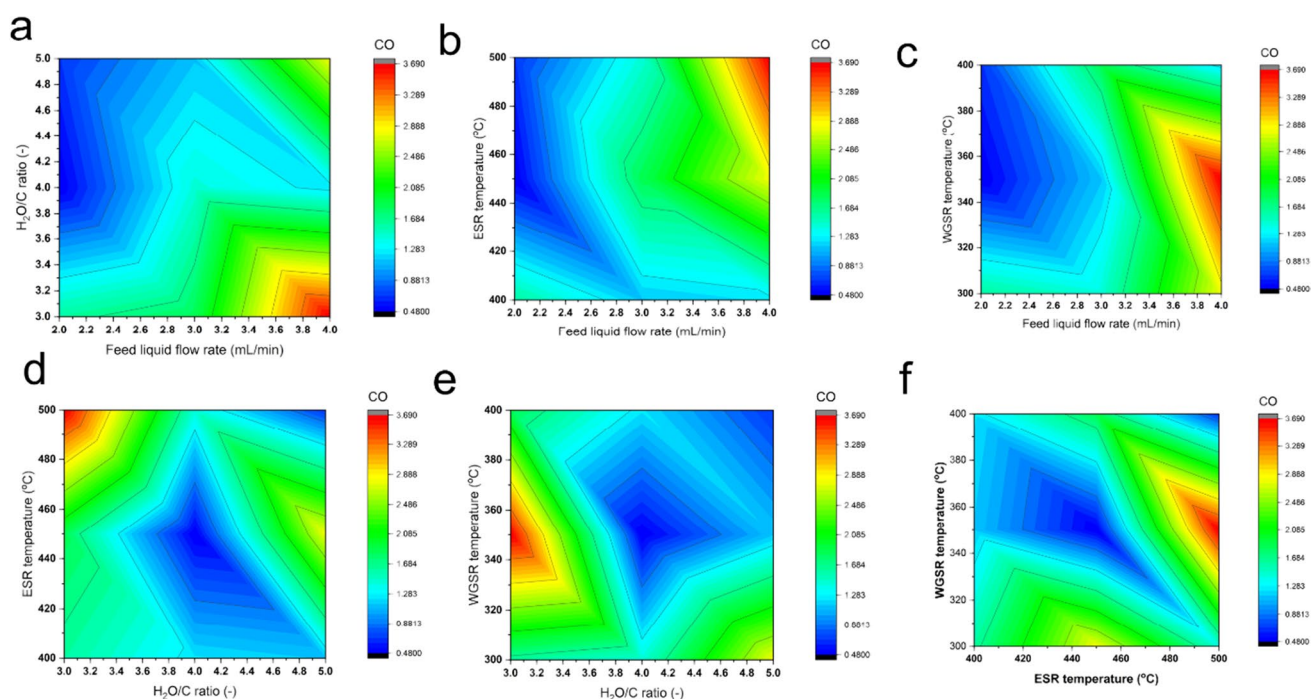
$$CO (\%) = 0.63 + 0.825A - 0.425B + 0.00603C - 0.00703D \quad (7)$$

#### Effect of hydrogen production conditions on carbon monoxide reduction

To explore the impact of hydrogen production conditions on CO generation, Origin Pro software was employed to simulate the interaction among various production parameters. Figure 3 presents the emitted percentages of CO relative to the interactions of production conditions, with different color gradients indicating varying CO levels.

**Table 4** Analysis of variance of hydrogen production conditions on carbon monoxide

Hydrogen production conditions	Degree of freedom	Adjusted sum square	Adjusted mean square	Contribution (%)
Rate of feed liquid flow (mL/min)	2	4.23136	2.11568	50.77
Water to carbon ratio	2	2.74602	1.37301	32.95
ESR temperature (°C)	2	0.55829	0.27914	6.70
WGS temperature (°C)	2	0.79869	0.39934	9.58
Residual error	0	0	0	0
Total	8	8.33436	4.16717	100



**Fig. 3** Interaction between the production parameters on carbon monoxide reduction

Notably, deep red hues signify higher CO levels, while deep blue hues denote lower CO levels. Overall, the results reveal that a high water-to-carbon ( $H_2O/C$ ) ratio coupled with a lower rate of feed liquid flow tends to result in lower CO generation when interacting with other production conditions. Interestingly, the figure illustrates that different ESR and WGS temperatures can minimize CO generation. Specifically, employing lower temperatures, such as 400 °C for ESR and 300 °C for WGS, can yield minimal CO generation, suggesting relatively low energy costs required to mitigate CO production. This graphical modeling for CO generation offers valuable insights for researchers and production engineers, enabling them to manipulate various production conditions to minimize CO generation when producing hydrogen via ethanol steam reforming and water gas shift reaction pathways.

## Carbon dioxide (CO<sub>2</sub>) reduction analysis

### Significance of hydrogen production conditions on the generation of carbon dioxide

Like the CO analysis, ANOVA was utilized to explore the effect and significance of the employed hydrogen production conditions on CO<sub>2</sub> generation, as depicted in Table 5. It is evident that WGS temperature significantly influences CO<sub>2</sub> generation during hydrogen production, with a contribution of 45.18%, slightly higher than the contribution (44.51%) of the rate of feed liquid flow, which contrasts with the case of CO generation. Furthermore, the results indicate that the water-to-carbon ratio has a lesser effect (8.71%) compared to CO generation. The zero residual error also reflects the goodness of fit of the model. Additionally, like CO generation, varying production conditions yield different CO<sub>2</sub>

**Table 5** Analysis of variance of hydrogen production conditions on carbon dioxide

Factor	Degree of freedom	Adjusted sum square	Adjusted mean square	Contribution (%)
Rate of feed liquid flow (mL/min)	2	5.03127	2.51563	44.51
Water to carbon ratio	2	0.9842	0.4921	8.71
ESR temperature (°C)	2	0.18107	0.09053	1.6
WGS temperature (°C)	2	5.10647	2.55323	45.18
Residual error	0	-	-	-
Total	8	-	5.65149	100

values, as mathematically presented in Eq. 8, where  $A$ ,  $B$ ,  $C$ , and  $D$  represent the resultant generated values of  $\text{CO}_2$  gas for the rate of feed liquid flow,  $\text{H}_2\text{O}/\text{C}$  ratio, ESR temperature, and WGSR temperature, respectively.

$$\text{CO}_2(\%) = 19.87 - 0.903A + 0.405B + 0.00287C + 0.01097D \quad (8)$$

### Effect of hydrogen production conditions on the generation of carbon dioxide

Similar to the CO reduction analysis, the effect of hydrogen production conditions on  $\text{CO}_2$  generation was investigated, and the interaction between these conditions on the resulting percentage of  $\text{CO}_2$  was simulated, as shown in Fig. 4. The different color outlets reflect variations in  $\text{CO}_2$  percentages, with deep red indicating the highest level of  $\text{CO}_2$  and deep blue indicating the lowest level. In contrast to CO generation, when a low value of water-to-carbon ( $\text{H}_2\text{O}/\text{C}$ ) ratio and a high value of the rate of feed liquid flow interact with other production conditions, lower  $\text{CO}_2$  generation is observed. Additionally, a higher value of ESR temperature results in lower  $\text{CO}_2$  generation. The results further reveal that WGSR temperature in the range of 320 to 370 °C yields relatively low  $\text{CO}_2$  levels, indicating a lesser WGSR energy cost to produce hydrogen with minimal  $\text{CO}_2$  generation. These modeled production conditions presented in the figure provide a pathway to optimizing lower  $\text{CO}_2$  generation

during hydrogen production from ethanol steam reforming and water gas shift reaction pathways.

### Methane ( $\text{CH}_4$ ) minimization analysis

#### Significance of hydrogen production conditions on the generation of methane

The effect and significance of the employed hydrogen production conditions on generated  $\text{CH}_4$  were analyzed, as presented in Table 6. The results indicate that the water-to-carbon ratio is the most significant production condition for minimizing  $\text{CH}_4$ , contributing 42.73%, followed by the rate of feed liquid flow, with a contribution of 24.34%. Interestingly, both ESR and WGSR show approximately the same contribution (16%). This analysis underscores the importance of all four hydrogen production conditions in minimizing  $\text{CH}_4$  during the production of hydrogen from the employed pathways. The model's reliability is confirmed by a residual error of zero percentage. Furthermore, different  $\text{CH}_4$  values can be obtained when varying the production conditions, as mathematically presented in Eq. 9, where  $A$ ,  $B$ ,  $C$ , and  $D$  represent the resultant generated values of  $\text{CH}_4$  gas for the rate of feed liquid flow,  $\text{H}_2\text{O}/\text{C}$  ratio, ESR temperature, and WGSR temperature, respectively.

$$\text{CH}_4(\%) = 18.82 - 0.745A - 1.333B - 0.0156C - 0.0024D \quad (9)$$

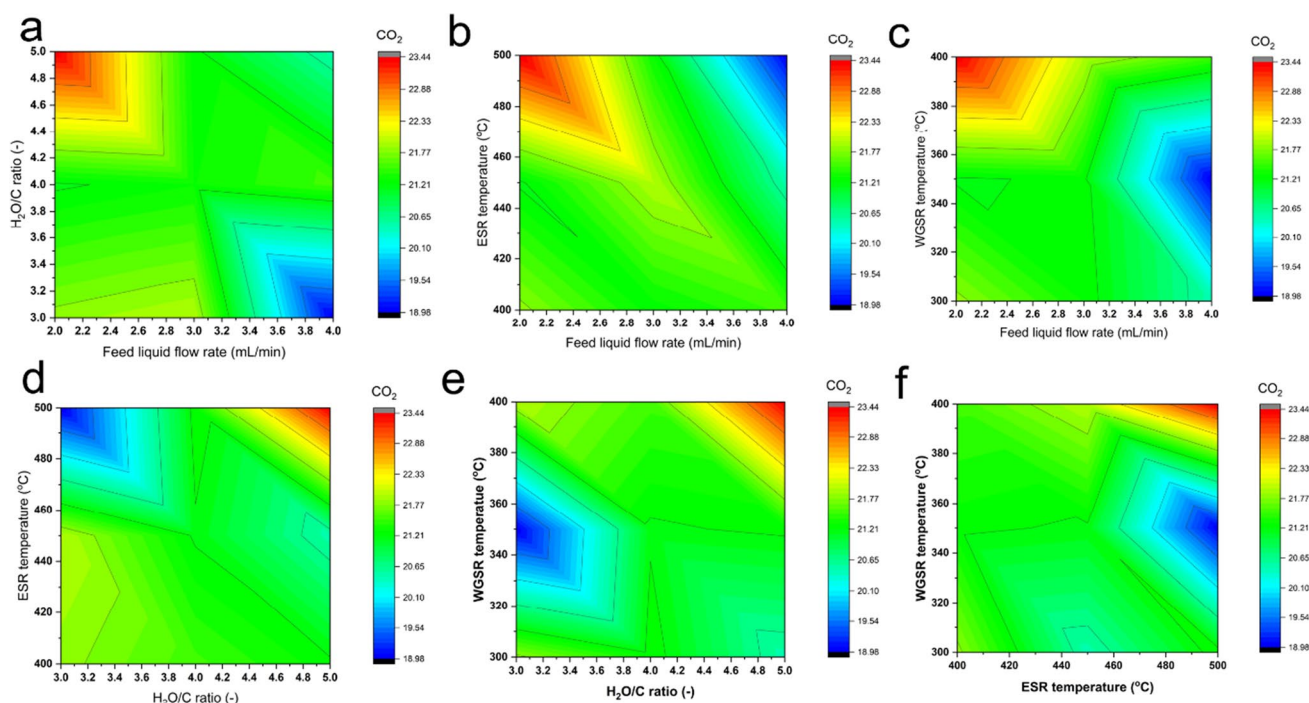


Fig. 4 Interaction between the production parameters on carbon dioxide reduction



**Table 6** Analysis of variance of hydrogen production conditions on methane

Factor	Degree of freedom	Adjusted sum square	Adjusted mean square	Contribution (%)
Rate of feed liquid flow (mL/min)	2	6.1862	3.0931	24.34
Water to carbon ratio	2	10.8589	5.42943	42.73
ESR temperature (°C)	2	4.1653	2.08263	16.39
WGSR temperature (°C)	2	4.2025	2.10123	16.54
Residual error	0	0	0	0
Total	8	-	12.70639	100

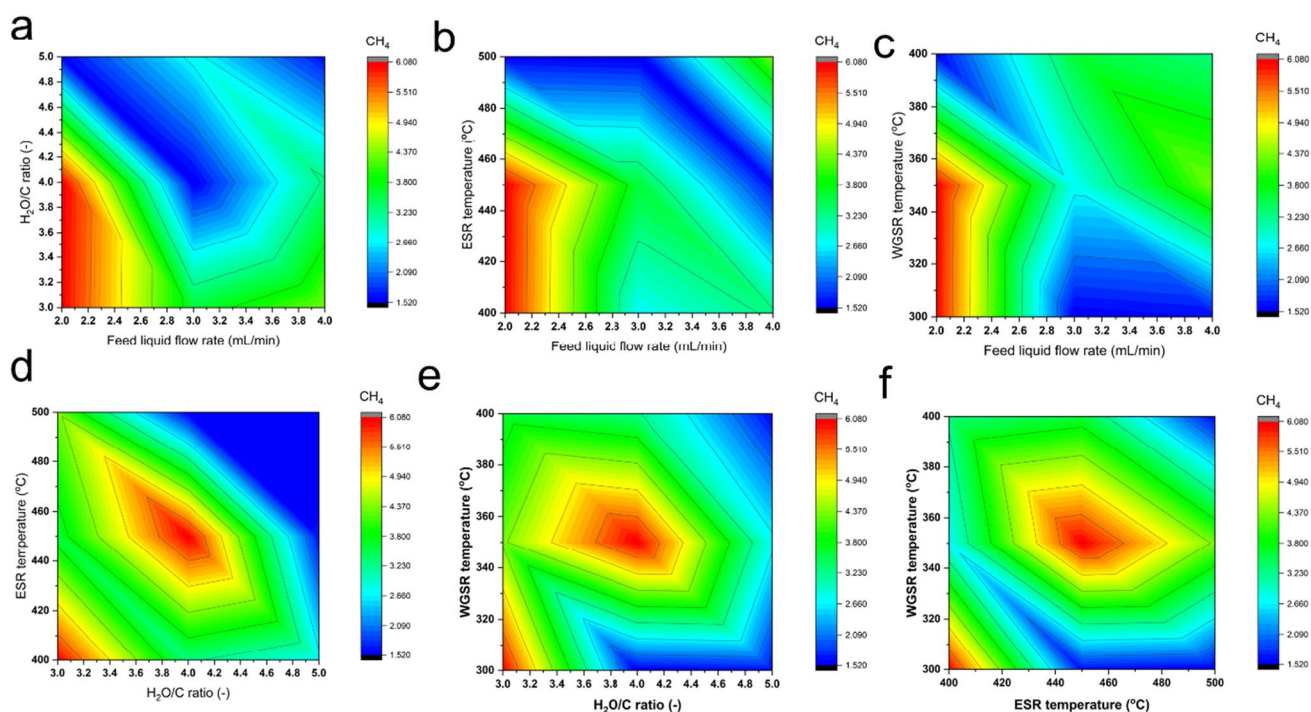
### Effect of hydrogen production conditions on the generation of methane

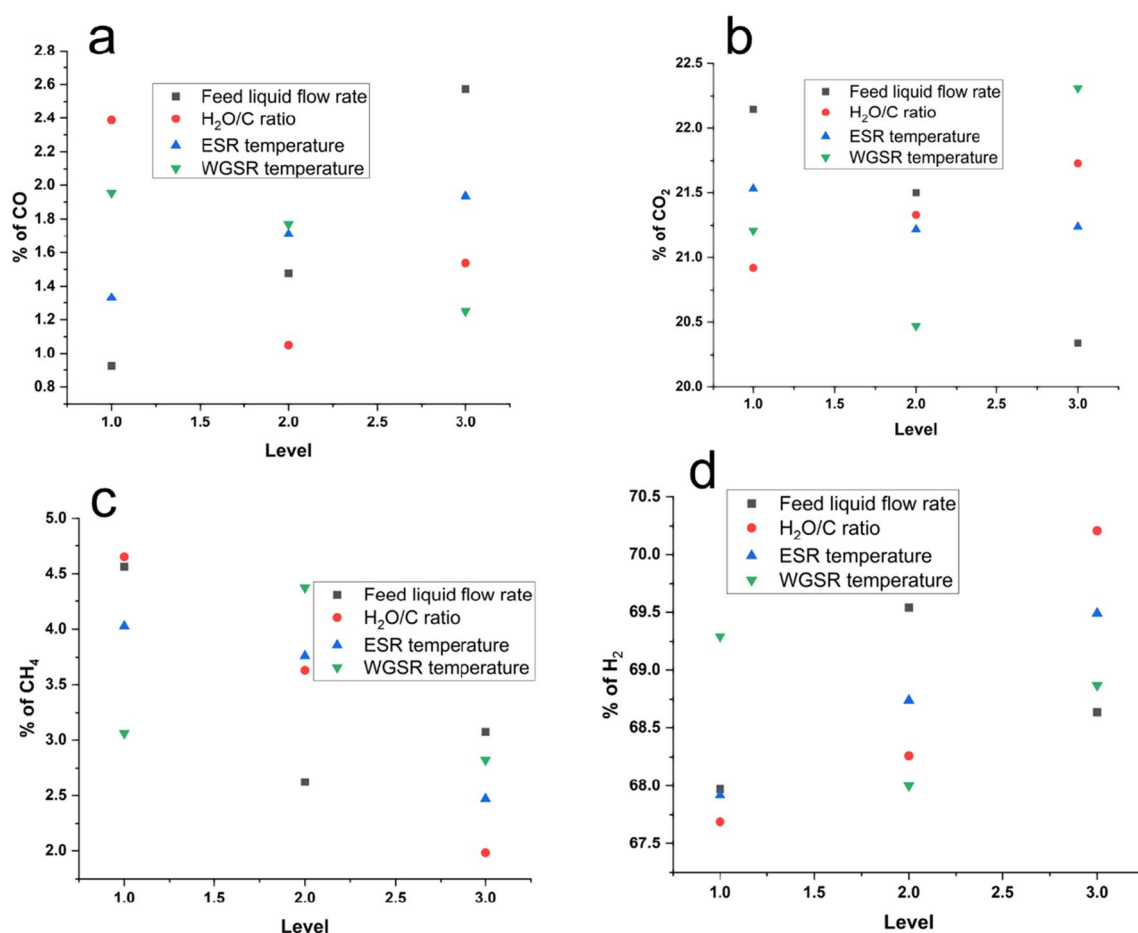
A similar analysis was conducted to assess the effect of hydrogen production conditions on the generation of  $\text{CH}_4$ , with the interaction between these conditions simulated and presented in Fig. 5. Different color outlets in the figure represent variations in  $\text{CH}_4$  percentages, where deep red indicates the highest level of  $\text{CH}_4$  and deep blue indicates the lowest. It was observed that higher values of the water-to-carbon ( $\text{H}_2\text{O}/\text{C}$ ) ratio and ESR temperature when interacting with other hydrogen production conditions result in the minimization of  $\text{CH}_4$ . Additionally, different values of the rate of feed liquid flow interacting with other production conditions can also lead to the minimization of  $\text{CH}_4$ . This suggests that a lower liquid flow rate (for energy cost minimization) can be applied to minimize  $\text{CH}_4$  generation during the production

of hydrogen from ethanol steam reforming and water gas shift reaction pathways. Interestingly, it was found that both lower and higher WGSR temperature ranges can yield minimum  $\text{CH}_4$  values. However, to save on hydrogen production costs and minimize  $\text{CH}_4$ , a WGSR temperature as low as 300 °C is recommended. This graphical model aids in decision-making regarding  $\text{CH}_4$  minimization during hydrogen production from ethanol steam reforming and water gas shift reaction pathways.

### Singular response optimization analysis on hydrogen production conditions on the resultant gases

The resultant gases outlined in Table 1 underwent Taguchi design analysis for individual response optimization, as depicted in Fig. 6. This analysis distinctly illustrates the production conditions yielding optimal gases, aiming

**Fig. 5** Interaction between the production parameters on methane ( $\text{CH}_4$ ) production



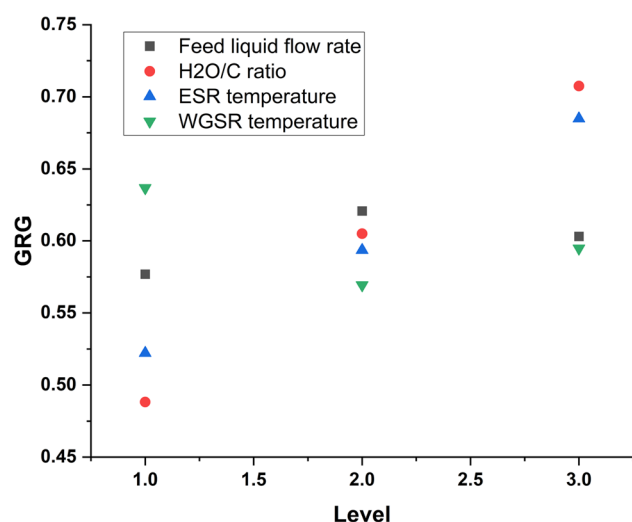
**Fig. 6** The effect of hydrogen production conditions on individual performance responses. **a** Carbon monoxide (CO). **b** Carbon dioxide (CO<sub>2</sub>). **c** Methane (CH<sub>4</sub>). **d** Hydrogen (H<sub>2</sub>)

to minimize undesired gases (CO, CO<sub>2</sub>, and CH<sub>4</sub>) while maximizing the desired gas (H<sub>2</sub>). Figure 6a showcases the optimal conditions for minimizing CO gas, revealing a rate of feed liquid flow of 2 mL/min, water-to-carbon ratio of 4, ESR temperature of 400 °C, and WGS temperature of 300 °C. Figure 6b illustrates CO<sub>2</sub> minimization, indicating optimal conditions of a liquid flow rate of 4 mL/min, water-to-carbon ratio of 3, ESR temperature of 500 °C, and WGS temperature of 350 °C. For methane reduction, Fig. 6c displays optimal conditions with a liquid flow rate of 3 mL/min, water-to-carbon ratio of 5, ESR temperature of 500 °C, and WGS temperature of 400 °C. Lastly, Fig. 6d reveals the maximization of hydrogen production at optimal conditions of a liquid flow rate of 2 mL/min, water-to-carbon ratio of 3, ESR temperature of 400 °C, and WGS temperature of 350 °C. These observations highlight different optimal production conditions for the resultant gases, complicating conclusions on singular responses given the undesirability of carbon-based gases and the desirability of hydrogen. Consequently, the subsequent section delves into the results presented

with Taguchi grey relational analysis, which effectively addresses this complexity and indecision challenge.

#### Multi-response optimization analysis on hydrogen production conditions on the resultant gases

Grey relational analysis (GRA) is commonly utilized to address problems characterized by limited information arrangements, particularly in scenarios with ambiguous frameworks lacking starkly contrasted layouts. Within the grey system, all data is represented by white, while the absence of data is depicted as black. Figure 7 presents a graphical representation of multi-response gases, aiming to minimize Co, CO<sub>2</sub>, and CH<sub>4</sub> gases while maximizing hydrogen production simultaneously. The results indicate that the optimal hydrogen production conditions are a liquid flow rate of 2 mL/min, water-to-carbon ratio of 3, ESR temperature of 300 °C, and WGS temperature of 350 °C. Intriguingly, these optimal conditions for multi-response gas optimization differ from those for individual optimization. Furthermore, they do not align with the design run



**Fig. 7** Effect of hydrogen production conditions on the multi-response gases (GRG)

employed in the work of Chen et al. (Chen et al. 2017). This discrepancy underscores the importance of conducting both singular and multi-response optimization analyses, serving as the primary motivation for this study.

To comprehensively assess the significance and percentage contribution of each production condition to the multi-response gases, an analysis of variance (ANOVA) was conducted for the grey relational grade (GRG) values at a confidence level of 95%, detailed in Table 7. The findings revealed that the water-to-carbon (H<sub>2</sub>O/C) ratio emerged as the most influential production condition, with a substantial contribution of 59.22%, followed closely by the ESR temperature at 32.69%. Notably, while the WGSR temperature and rate of feed liquid flow also demonstrated significance, their contributions were comparatively lower than those of the conditions. These results offer conclusive optimized hydrogen production conditions to minimize undesired gases and maximize desired gas (H<sub>2</sub>) production. These conditions are particularly recommended for hydrogen production via ethanol steam reforming and water gas shift reaction pathways. The observed absence of residual error in the GRA ANOVA underscores the high level of confidence in the developed

model. It is worth noting that varying the output GRG values of individual production conditions can yield different proportions of GRG, as expressed in Eq. 10. *A*, *B*, *C*, and *D* represent the resultant generated values of GRG for the rate of feed liquid flow, H<sub>2</sub>O/C ratio, ESR temperature, and WGSR temperature, respectively.

$$\text{GRG} = -0.463 + 0.0131A + 0.1097B + 0.001627C - 0.000419D \quad (10)$$

## Conclusion

In a groundbreaking endeavor, this study pioneers the application of multi-response Taguchi grey relational analysis to tackle the intricate challenges surrounding optimal hydrogen production conditions. With a dual aim of maximizing hydrogen yield while minimizing CO, CO<sub>2</sub>, and CH<sub>4</sub> emissions for enhanced energy efficiency, sustainability, and cleanliness, this research delves deep into the interplay of various production parameters. Leveraging Origin Pro software, we meticulously model the interactions between these parameters and their impact on individual gas outputs as well as overall multi-response gas generation. Through rigorous regression modeling, we unveil mathematical models for each gas, offering invaluable insights into the intricate dynamics at play. By elucidating the diverse hydrogen production conditions conducive to optimized gas yields, our study empowers the application of grey relational analysis to derive conclusive conditions for minimizing undesirable emissions and maximizing H<sub>2</sub> production via ethanol steam reforming and water gas shift reaction pathways. Notably, our findings pinpoint optimal production conditions—rate of feed liquid flow at 2 mL/min, water-to-carbon ratio at 3, ESR temperature at 300 °C, and WGSR temperature at 350 °C—as key drivers of clean and efficient hydrogen production. Highlighting the pivotal roles of water-to-carbon ratio and ESR temperature, which contribute 59.22% and 32.69% respectively, our research provides a roadmap for sustainable and high-yield hydrogen production. With our developed graphical and mathematical models demonstrating exceptional goodness of fit, underscored by zero residual

**Table 7** Analysis of variance of hydrogen production conditions on grey relational grade (GRG)

Factor	Degree of freedom	Adjusted sum square	Adjusted mean square	Contribution (%)
Rate of feed liquid flow (mL/min)	2	0.002922	0.001461	2.39
Water to carbon ratio	2	0.072267	0.036134	59.22
ESR temperature (°C)	2	0.039895	0.019947	32.69
WGSR temperature (°C)	2	0.006954	0.003477	5.70
Residual error	0	0	0	0
Total	8	0.122039	0.061019	100

error, this study heralds a new era of design reliability. Moving forward, we advocate for experimental validation of the obtained multi-response optimal conditions, paving the way for transformative advancements in hydrogen production technology.

**Author contribution** Johnson Kehinde Abifarin contributed to the study's conception and design. Material preparation, data collection, and analysis were performed by Johnson Kehinde Abifarin and Fredah Batale Abifarin. The first draft of the manuscript was written by Johnson Kehinde Abifarin, and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

**Funding** Open Access funding enabled and organized by CAUL and its Member Institutions

## Declarations

**Ethical approval and consent to participate** Not applicable.

**Consent for publication** Not applicable.

**Competing interests** The authors declare no competing interests.

**Open Access** This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

## References

- Abifarin JK (2021) Taguchi grey relational analysis on the mechanical properties of natural hydroxyapatite: effect of sintering parameters. *Int J Adv Manuf Technol* 117(1–2):49–57
- Abifarin JK, Ofodu JC (2022a) Modeling and grey relational multi-response optimization of chemical additives and engine parameters on performance efficiency of diesel engine. *Int J Grey Syst* 2(1):16–26
- Abifarin JK, Ofodu JC (2022b) Determination of an efficient power equipment oil through a multi-criteria decision making analysis. *Vojnotehnički Glasnik* 70(2):433–446
- Abifarin JK, Owolabi OA (2023) New insight to the mechanical reliability of porous and nonporous hydroxyapatite. *J Aust Ceram Soc* 59(1):43–55
- Abifarin JK, Obada DO, Dauda ET, Oyedele EO (2021a) Taguchi grey relational optimization of the multi-mechanical characteristics of kaolin reinforced hydroxyapatite: effect of fabrication parameters. *Int J Grey Syst* 1(2):20–32
- Abifarin JK, Suleiman MU, Abifarin EA, Fidelis FB, Oyelakin OK, Jacob DI, Abdulrahim MY (2021b) Fabrication of mechanically enhanced hydroxyapatite scaffold with the assistance of numerical analysis. *Int J Adv Manuf Technol* 1–14
- Abifarin JK, Prakash C, Singh S (2022) Optimization and significance of fabrication parameters on the mechanical properties of 3D printed chitosan/PLA scaffold. *Mater Today: Proc* 50:2018–2025
- Abifarin FB, Musa Z, Abifarin JK (2023a) Mechanical processing of hydroxyapatite through sintering and multiobjective optimization technique for biomedical application. *MRS Advances* 8(9):532–537
- Abifarin JK, Abifarin FB, Oyedele EO, Prakash C, Zahedi SA (2023b) Computational analysis on mechanostuctural properties of hydroxyapatite–alumina–titanium nanocomposite. *J Korean Ceram Soc* 60(6):950–958
- Aravind S, Shunmugesh K, Biju J, Vijayan JK (2017) Optimization of micro-drilling parameters by Taguchi grey relational analysis. *Mater Today: Proc* 4(2):4188–4195
- Bolt A, Dincer I, Agelin-Chaab M (2020) Experimental study of hydrogen production process with aluminum and water. *Int J Hydrogen Energy* 45(28):14232–14244
- Casanovas A, De Leitenburg C, Trovarelli A, Llorca J (2009) Ethanol steam reforming and water gas shift reaction over Co–Mn/ZnO catalysts. *Chem Eng J* 154(1–3):267–273
- Chen CC, Tseng HH, Lin YL, Chen WH (2017) Hydrogen production and carbon dioxide enrichment from ethanol steam reforming followed by water gas shift reaction. *J Clean Prod* 162:1430–1441
- Cordaro P, Braga B, Corotti D, Gallego A, Silveira JL (2024) Electricity and hydrogen production by cogeneration system applied in a fuel station in Brazil: energy analysis of a combined SOFC and ethanol steam reforming model. *Fuel* 356:129615
- Deepanraj B, Sivasubramanian V, Jayaraj S (2017) Multi-response optimization of process parameters in biogas production from food waste using Taguchi–grey relational analysis. *Energy Convers Manag* 141:429–438
- Di Nardo A, Portarapillo M, Russo D, Di Benedetto A (2024) Hydrogen production via steam reforming of different fuels: thermodynamic comparison. *Int J Hydrogen Energy* 55:1143–1160
- Dou B, Wu K, Zhang H, Chen B, Chen H, Xu Y (2023) Sorption-enhanced chemical looping steam reforming of glycerol with CO<sub>2</sub> in-situ capture and utilization. *Chem Eng J* 452:139703
- Esangbedo MO, Abifarin JK (2022) Cost and quality optimization Taguchi design with grey relational analysis of halloysite nanotube hybrid composite: CNC machine manufacturing. *Materials* 15(22):8154
- Esangbedo MO, Abifarin JK (2023) Determination and managerial implications of machine conditions for high-grade industrial polycaprolactam (nylon 6). *Sci Rep* 13(1):10779
- Garud KS, Lee MY (2023) Grey relational based Taguchi analysis on heat transfer performances of direct oil spray cooling system for electric vehicle driving motor. *Int J Heat Mass Transf* 201:123596
- Hussain SA, Panchal M, Allamraju KV, Rajak U, Verma TN, Brindhadevi K (2023) Optimization of wear behavior of heat-treated Ti-6Al-7Nb biomedical alloy by response surface methodology. *Environ Res* 116193
- Kadier A, Abdesahian P, Simayi Y, Ismail M, Hamid AA, Kalil MS (2015) Grey relational analysis for comparative assessment of different cathode materials in microbial electrolysis cells. *Energy* 90:1556–1562
- Karaoglu S, Yolcular S (2022) Optimization of hydrogen generation process from the hydrolysis of activated Al–NaCl–SiC composites using Taguchi method. *Int J Hydrogen Energy* 47(66):28289–28302
- Kim HM, Jeong CH, Cheon BS, Negi SS, Won W, Jeong DW (2024) Improving the performance of a Co–CeO<sub>2</sub> catalyst for hydrogen production via water gas shift reaction by addition of transition metal oxides. *Energy Fuels*



- Kumar D, Muthukumar K (2020) An overview on activation of aluminium-water reaction for enhanced hydrogen production. *J Alloy Compd* 835:155189
- Len T, Luque R (2023) Addressing the CO<sub>2</sub> challenge through thermocatalytic hydrogenation to carbon monoxide, methanol and methane. *Green Chem* 25(2):490–521
- Ovalle-Encinia O, Lin JY (2024) Modeling analysis of water-gas-shift reaction on catalyst-packed ceramic-carbonate dual-phase membrane reactor for hydrogen production. *Int J Hydrogen Energy* 64:39–49
- Panwar R, Chandna P (2023) Parameter optimization of FSW aviation-grade AA8090 using Taguchi grey relational analysis. *Aircr Eng Aerosp Technol* 95(5):715–724
- Quan C, Gao Z, Liu X, Miskolczi N (2024) Ethanol steam reforming for hydrogen production under Ni/Ce catalysts. *J Energy Inst* 112:101446
- Roy RK (2010) A primer on the Taguchi method. Society of Manufacturing Engineers
- Salmani H, Khalkhali A, Ahmadi A (2022) Multi-objective optimization of vehicle floor panel with a laminated structure based on V-shape development model and Taguchi-based grey relational analysis. *Struct Multidiscip Optim* 65(3):95
- Sambasevam KP, Sateria SF, Baharin SNA, Azman NJ, Wakid SA, Shahabuddin S (2023) An optimization of fungal chitin grafted polyaniline for ammonia gas detection via Box Behnken design. *Int J Biol Macromol* 238:124079
- Satyapal S, Petrovic J, Read C, Thomas G, Ordaz G (2007) The US Department of Energy's National Hydrogen Storage Project: progress towards meeting hydrogen-powered vehicle requirements. *Catal Today* 120(3–4):246–256
- Sharma YC, Kumar A, Prasad R, Upadhyay SN (2017) Ethanol steam reforming for hydrogen production: latest and effective catalyst modification strategies to minimize carbonaceous deactivation. *Renew Sustain Energy Rev* 74:89–103
- Shi T, Chen Q, Peng X, Feng J, Guo Y (2023) Multi-objective optimization of the oil-free centrifugal air compressor in hydrogen fuel cell vehicles based on grey relational analysis. *Int J Hydrogen Energy*
- Taguchi G (1995) Quality engineering (Taguchi methods) for the development of electronic circuit technology. *IEEE Trans Reliab* 44(2):225–229
- Tzeng CJ, Lin YH, Yang YK, Jeng MC (2009) Optimization of turning operations with multiple performance characteristics using the Taguchi method and grey relational analysis. *J Mater Process Technol* 209(6):2753–2759
- Unnikrishna Pillai J, Shunmugavel M, Thangaraj M, Goldberg M, Singh R, Littlefair G (2023) Effects of machining parameters on enhancing Alpha-Beta titanium alloy using Taguchi-grey relational analysis for aerospace applications. *Proc Inst Mech Eng Part E: J Process Mech Eng* 237(2):118–127
- Vasantharaj K, Jerold M, Deepanraj B, Velan M, Sivasubramanian V (2017) Assessment of a sulfidogenic system utilizing microalgal biomass of *Chlorella pyrenoidosa* as an electron donor: Taguchi based grey relational analysis. *Int J Hydrogen Energy* 42(42):26545–26554
- Xiao F, Yang R, Liu Z (2022) Active aluminum composites and their hydrogen generation via hydrolysis reaction: a review. *Int J Hydrogen Energy* 47(1):365–386
- Zurrer T, Lovell E, Han Z, Liang K, Scott J, Amal R (2023) Harnessing the structural attributes of NiMg-CUK-1 MOF for the dual-function capture and transformation of carbon dioxide into methane. *Chem Eng J* 455:140623

**Publisher's Note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.