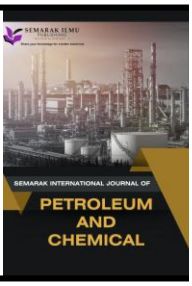
SEMARAK ILMU
PUBLISHING
202103268166(003316878-P)

Semarak International Journal of
Petroleum and Chemical

Journal homepage:
https://semarakilmu.my/index.php/sijpce/index
ISSN: 3083-9106



Thermodynamic Analysis of 2-Methylnaphthalene Steam Reforming to Hydrogen

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ARTICLE INFO

Article history:
Received 24 March 2024
Received in revised form 18 April 2025
Accepted 20 May 2025
Available online 30 June 2025

ABSTRACT

Fuel Oil Blended Stock (FOBS) is a byproduct of petroleum refining, that contains high levels of hazardous hydrocarbons, heavy metals, and sulfur compounds which present significant environmental and storage challenges. Its rich hydrocarbon content offers potential waste-to-energy that is marketable as energy sources. This study evaluates the thermodynamic feasibility of transforming FOBS using 2-methylnaphthalene as a model compound to hydrogen (H_2), employing Gibbs free energy minimization in HSC Chemistry 6.0. Key thermodynamic parameters such as temperature (300–1200°C), pressure (1–100 bar), and 2-methylnaphthalene-to-water feed ratios (0.5:0.5; 0.7:0.3; 0.8:0.2; 0.9:0.1; 0.95:0.05) were investigated to determine optimal reaction conditions. Results show that a 0.50:0.50 molar ratio of 2-methylnaphthalene to water maximizes the production of hydrogen (H_2), methane (CH_4), carbon monoxide (CO), carbon dioxide (CO_2), and other hydrocarbons (C_1-C_4). H_2 yield peaks at 29.71% at a high temperature of 1248 K at temperature 1 bar, while excessively high temperatures lead to carbon formation, underscoring the need for precise thermal control. This thermodynamic study theoretically confirmed the feasibility of converting FOBS into sustainable fuels, contributing to energy efficiency. However, further consideration of environmental sustainability is necessary, as hydrocarbon (C_1-C_4) gases are also produced alongside H_2.

Keywords:
FOBS; steam reforming; 2-methylnaphthalene; hydrogen production

1. Introduction

The rising global energy demand and growing environmental concerns have intensified the search for alternative fuel sources that maximize resource utilization while minimizing emissions. Conventional fossil fuels are major contributors to greenhouse gas emissions, air pollution, and resource depletion, underscoring the urgent need for cleaner and more sustainable energy solutions [1]. In response, various waste-derived fuels have been explored, including biofuels, synthetic fuels,

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https://doi.org/10.37934/sijpce.3.1.114

and refinery byproducts. Fuel Oil Blended Stock (FOBS) is a byproduct of petroleum refining which holds significant potential for conversion into valuable energy resources [2].

FOBS is primarily composed of residual oils generated during the refining process, with a complex mixture of aromatics, alkanes, and cycloalkanes. Then, the presence of hazardous hydrocarbons, heavy metals, sulphur, and total halogens poses significant environmental and storage challenges [3], since FOBS is continuously produced in refineries. Due to these characteristics, FOBS is categorized as high-viscosity waste and unsuitable for direct combustion, requiring conversion processes such as thermal cracking, pyrolysis, and oxidative reforming to enhance its usability as a fuel source [4].

Several thermochemical processes have been explored for FOBS upgrading. Pyrolysis, a widely studied method, involves thermal decomposition in the absence of oxygen, producing liquid bio-oils, gaseous hydrocarbons, and solid carbon residues. Pyrolysis offers flexibility in product distribution, depending on operational conditions such as temperature and heating rate [5]. However, its main drawback lies in the high oxygen and impurity content of the resulting bio-oil, requiring further upgrading for practical applications [6].

Catalytic reforming is another promising approach for FOBS conversion, where catalysts such as nickel-based or noble metal catalysts facilitate the breakdown of heavy hydrocarbons into valuable gaseous products, including hydrogen and syngas. Compared to pyrolysis, catalytic reforming can improve reaction selectivity and reduce unwanted by-product formation. However, catalyst deactivation due to coke deposition remains a significant challenge, often requiring additional regeneration steps [7].

Among these methods, steam reforming has emerged as a viable pathway for FOBS conversion due to its ability to produce high hydrogen yields at lower costs. Steam reforming, a type of gasification, occurs at high temperatures, converting waste oil-based materials into fuel gas, which can be further upgraded to syngas through the reaction of steam and hydrocarbons in the gas phase. Steam reforming offers several advantages, including low-cost hydrogen production, a higher heating value of the produced gas, and improved safety and process control [8] Indeed, steam reforming is the primary process used for natural gas for hydrogen production [9].

While several studies have investigated the upgrading and refining of FOBS, there is limited research specifically addressing its thermodynamic behaviour in steam reforming for hydrogen production. Previous studies have primarily focussed on the compositional analysis of FOBS, its refining potential and alternative conversion processes such as pyrolysis and thermal cracking. However, a comprehensive thermodynamic evaluation of FOBS steam reforming, particularly using Gibbs free energy minimization, remains unexplored. Furthermore, the role of 2-methylnaphthalene as a model compound in this process has not been extensively analysed in terms of its impact on reaction efficiency and H_2 yield. Therefore, this study aims to fill this gap by systematically assessing the thermodynamic feasibility of H_2 production from FOBS steam reforming, optimizing process conditions and providing fundamental into its potential as a sustainable H_2 source.

So, this study explores the thermodynamic feasibility of hydrogen production from the steam reforming of FOBS. To assess the feasibility of converting FOBS into a cleaner and more efficient fuel, this study employs thermodynamic modelling using HSC Chemistry 6.0, applying Gibbs free energy minimization to analyse reaction pathways and equilibrium compositions [10]. By systematically varying key parameters such as temperature, pressure, and feedstock ratios, the study aims to establish optimal process parameters that maximize hydrogen and hydrocarbon production while minimizing carbon formation and undesirable byproducts [11]. This research builds upon previous studies that have explored FOBS upgrading, refining the process by incorporating 2-methylnaphthalene as a model compound and evaluating its impact on fuel properties and reaction efficiency [10].

The thermodynamic data from this analysis serve as a foundation for further research on waste-derived fuels, especially on the thermodynamic behaviour of FOBS in the steam reforming process and its potential as a sustainable option for hydrogen production. Furthermore, this study aligns with global efforts to reduce carbon emissions and transition toward cleaner fuel alternatives, offering insights into how waste-derived fuel sources can be integrated into existing energy infrastructures with minimal modifications [12].

2. Methodology

2.1 Model compound of FOBS

The thermodynamic analysis of the process was performed using the total Gibbs free energy minimization approach. This method evaluates reaction behaviour and product formation trends under varying feed ratios, pressures, and temperatures. While experimental studies are often constrained by limited parameter ranges, thermodynamic modelling provides a broader perspective on how different conditions influence reaction outcomes. In this study, HSC Chemistry 6.0 was utilized for equilibrium data generation and thermodynamic calculations [2].

Gibbs free energy minimization is a widely used algorithm in thermodynamic studies for predicting equilibrium conditions. It accounts for the total Gibbs free energy of all chemical species present, making it a reliable tool for computational modelling.

Due to the complex composition of FOBS, a model compound was chosen for simulation analysis. The selected hydrocarbon should represent key hydrocarbon groups found in commercial fuels, including cycloalkanes, iso-alkanes, aromatics, and n-alkanes. In this study, 2-methylnaphthalene was selected as the model compound for FOBS conversion due to its significant presence in crude oil and petroleum-derived fuels.

2-methylnaphthalene is a polycyclic aromatic hydrocarbon (PAH) with the molecular formula $C_{11}H_{10}$, classified as an alkylated derivative of naphthalene. It appears as a crystalline white solid and belongs to the benzenoid PAH group, consisting of two fused benzene rings without heteroatoms or additional substituents [4]. It has a molar weight of 142.2 g/mol and a density of approximately 1.02 g/cm^3. As a significant pollutant and a common hydrocarbon in petroleum-derived fuels, 2-methylnaphthalene is one of the 16 PAHs designated as priority pollutants by the U.S. Environmental Protection Agency (EPA) due to its toxicity and environmental persistence. Studies indicate that 2-methylnaphthalene and its derivatives are among the most abundant hydrocarbons dissolved in water from fuel oil spills, posing substantial ecological risks [13]. Research on marine fuel oil spills further confirms that alkyl naphthalene, including 2-methylnaphthalene, is predominant in the water-accommodated fraction of spilt oil.

2.2 Thermodynamic Analysis

To determine the equilibrium composition of chemical species, a non-stoichiometric approach was adopted. This method simplifies convergence by directly minimizing Gibbs free energy, eliminating the need to define exact reaction pathways or initial equilibrium compositions. The Gibbs free energy (G) is influenced by temperature (T), pressure (P), and the molar quantities of the species (η_i) involved. Its differential form is expressed in Eq. (1) and Eq. (2).

$$dG = V\,dP - S\,dT + \sum \mu_i d\eta_i \tag{1}$$

For an isothermal and isobaric system, the equation simplifies to:

$$\sum \mu_i d\eta_i = 0 \tag{2}$$

By indicating that the system achieves equilibrium when Gibbs free energy reaches its minimum. The effects of T, P, and feed ratios were analyzed in the conversion of the FOBS model compound (2-methylnaphthalene) into fuel using HSC Chemistry 6.0. The software was utilized to calculate equilibrium compositions at specific T, P, and feed compositions. The Gibbs routine within HSC Chemistry minimizes constraints by selecting the most thermodynamically stable species combination and identifying equilibrium compositions for a given mass balance, pressure, and temperature. The input species in this study were 2-methylnaphthalene ($C_{11}H_{10}$) and water (H_2O), with the following major products identified at equilibrium:

i. Hydrogen (H_2)
ii. Carbon dioxide (CO_2)
iii. Carbon monoxide (CO)
iv. Methane (CH_4)
v. Ethylene (C_2H_4)
vi. Ethane (C_2H_6)
vii. Propylene (C_3H_6)
viii. Propane (C_3H_8)
ix. Butene (C_4H_8)
x. Solid carbon (C)

To ensure the accuracy and replicability of the thermodynamic modelling, several key assumptions were made. It was assumed that all reactions proceed until thermodynamic equilibrium is reached, allowing the system to fully transform under the given conditions. The gaseous species were treated as ideal gases, meaning non-ideal interactions at higher pressures were neglected. Additionally, the model focused solely on equilibrium thermodynamics, excluding reaction kinetics, catalyst effects, and mass transfer limitations. Only the primary species typically observed in hydrocarbon steam reforming were considered, while side reactions and minor by-products were not included. The system was modelled as a closed batch reactor, with no exchange of material between the reactor and its surroundings. Furthermore, for simplification, the specific heat capacities of all species were assumed to remain constant across the temperature range. These assumptions provided a controlled framework for analyzing the thermodynamic behaviour of the FOBS steam reforming process. Then, the three main thermodynamic parameters influencing FOBS conversion are T, P, and feed ratio (2-methylnaphthalene: water). The following ranges were considered for optimization:

i. Temperature: 573 - 1473 K
ii. Pressure: 0-100 bar
iii. Feed ratio (2-methylnaphthalene: water): (0.50:0.50), (0.70:0.30), (0.80:0.20), (0.90:0.10), (0.95:0.05)

3. Results and Discussions

3.1 Equilibrium Constant and Possible Reaction Pathways

The reaction between 2-methylnaphthalene ($C_{11}H_{10}$) and water (H_2O) under controlled thermodynamic conditions plays a crucial role in converting Fuel Oil Blended Stock (FOBS) into valuable fuel components. The feasibility of these reactions is assessed through Gibbs free energy change (ΔG) and the equilibrium constant (K). A negative ΔG indicates a spontaneous reaction, while a positive ΔG suggests thermodynamic limitations. Additionally, the natural logarithm of K (ln K) provides insight into the favourability of product formation under different conditions. Table 1 summarizes the enthalpy change (ΔH), Gibbs free energy change (ΔG), and equilibrium constants for proposed reactions at 298 K. These reactions include steam reforming, thermal cracking, hydrogenation, and the water-gas shift reaction. The thermodynamic data help in predicting the most favourable conditions for fuel production.

Table 1
Possible reactions in 2-methylnaphthalene-water

Reaction	Type of Reaction	Equation	ΔH_{298K} (kJ/mol)	ΔG_{298K} (kJ/mol)
1	Steam Reforming	$C_{11}H_{10} + 11H_2O \rightarrow 11CO + 16H_2$	1802.45	890.32
2	Thermal Cracking	$C_{11}H_{10} \rightarrow CH_4 + C_2H_4 + 9C$	-192.72	-236.55
3	Thermal Cracking	$C_{11}H_{10} \rightarrow C_3H_6 + C_4H_8 + 7C$	-176.34	-152.88
4	Hydrogenation of Ethylene	$C_2H_4+H_2 \rightarrow C_2H_6$	-137.081	-101.207
5	Hydrogenation of propylene	$C_3H_6+H_2 \rightarrow C_3H_8$	-124.762	-86.72
6	Hydrogenation of Butene	$C_4H_8+H_2 \rightarrow C_4H_{10}$	-148.36	-84.79
7	Methane decomposition	$CH_4 \leftrightarrow 2H_2 + C$	74.60	50.53
8	Dehydrogenation of ethane	$C_2H_6 \leftrightarrow C_2H_4 + H_2$	137.08	101.18
9	Water gas shift reaction	$CO + H_2O \leftrightarrow H_2 + CO_2$	−41.14	−28.60
10	Boudouard Reaction	$2CO \leftrightarrow CO_2 + C$	−172.42	−120.00
11	Methanation	$CO + 3H_2 \leftrightarrow CH_4 + H_2O$	−205.89	−141.93
12	Methanation	$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O$	−164.75	−113.33
13	Reduction of CO	$H_2 + CO \leftrightarrow H_2O + C$	−131.29	−91.40
14	Reduction of CO_2	$CO_2 + 2H_2 \leftrightarrow 2H_2O + C$	−90.15	−62.80

The reaction between 2-methylnaphthalene ($C_{11}H_{10}$) and water (H_2O) under controlled thermodynamic conditions plays a crucial role in converting Fuel Oil Blended Stock (FOBS) into valuable fuel components. The feasibility of these reactions is analysed through Gibbs free energy change (ΔG) and equilibrium constant (K). Negative ΔG values indicate spontaneity, while positive ΔG values suggest thermodynamic constraints. The natural logarithm of K (ln K) determines the favourability of product formation under varying conditions [13].

Table 1 summarizes the enthalpy change (ΔH), Gibbs free energy change (ΔG), and equilibrium constants for proposed reactions at 298 K. These reactions include steam reforming, thermal cracking, hydrogenation, and the water-gas shift reaction. The thermodynamic data help in predicting the most favourable conditions for fuel production.

These reactions demonstrate as well that temperature influences the thermodynamic equilibrium of key FOBS conversion reactions. As temperature increases, equilibrium shifts favour the formation of hydrogen and lighter hydrocarbons, confirming the endothermic nature of many reactions. Thermal cracking contributes to the decomposition of 2- methylnaphthalene into smaller hydrocarbons, supporting higher energy fuel production [14]. Additionally, hydrogenation reactions maintain relatively stable equilibrium constants across moderate temperatures, facilitating hydrogen production and carbon reduction while limiting undesirable by-products.

These thermodynamic insights confirm that higher temperatures enhance hydrogen and hydrocarbon formation, whereas lower temperatures tend to favour liquid-phase hydrocarbons. By optimizing reaction conditions, FOBS can be efficiently converted into sustainable fuels with minimal carbon byproducts, supporting cleaner energy applications and industrial sustainability.

3.2 Effects of Temperature and Feed Ration on Product Yield At 1 Bar

Figure 1 illustrates the equilibrium composition of chemical species formed during the conversion of Fuel Oil Blended Stock (FOBS) at varying temperatures (573–1473 K) and a constant pressure of 1 bar. The identified products include (a) H_2, (b) $C_{11}H_{10}$, (c) CO_2, (d) H_2O, (e) CO, (f) H_2S, (g) C, (h) C_2H_2, (i) C_2H_4, and (j) C_2H_6. Hydrogen (H_2) production is most favourable at higher temperatures, peaking at 1248 K for a 2-methylnaphthalene: water molar ratio of 0.50:0.50, yielding 29.71%. This behaviour is driven by the endothermic steam reforming reaction, where equilibrium shifts favour H_2 formation as temperature increases. Steam reforming is the most widely used method for industrial hydrogen production due to its high yield and efficiency [1]. However, beyond 1248 K, hydrogen production declines due to competing reactions and decomposition of intermediates [2]. This observation aligns with previous studies that highlight the thermal degradation of hydrocarbons at extreme temperatures.

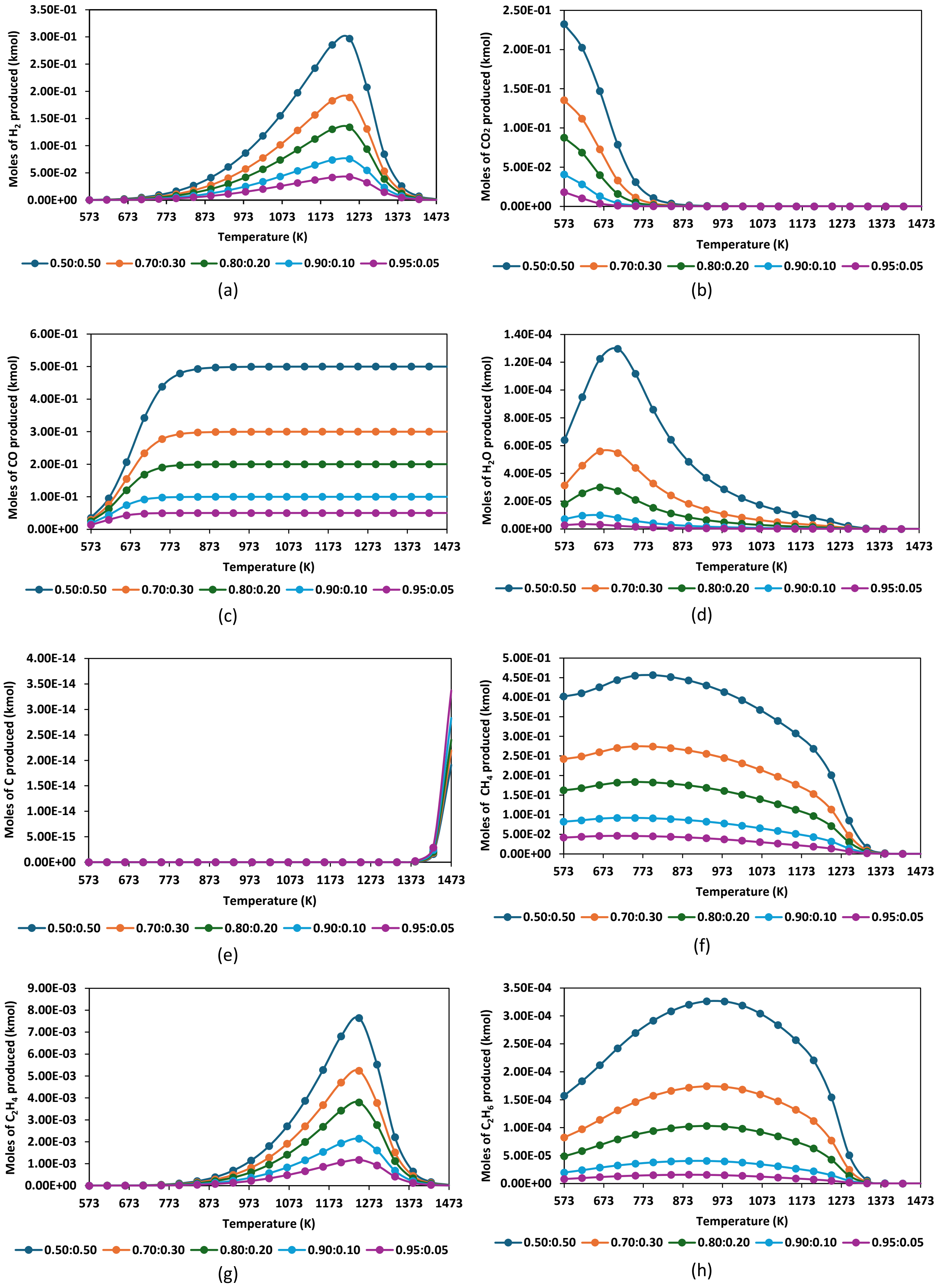
Carbon dioxide (CO_2) production follows an opposite trend, peaking at moderate temperatures (573–873 K) and declining at higher temperatures. The water-gas shift reaction, responsible for CO_2 formation, is exothermic, meaning lower temperatures favour its products [9]. At higher temperatures, the equilibrium shifts back toward reactants, reducing CO_2 yield. This suggests that temperature control is crucial for optimizing CO_2 removal in FOBS processing [3].

Carbon monoxide (CO) production increases steadily with temperature and stabilizes beyond 873 K, as reactions such as steam reforming and the Boudouard reaction favour CO formation at elevated temperatures [4]. Conversely, water formation is highest at 708 K before declining with rising temperatures. This behaviour aligns with the exothermic methanation reaction, where equilibrium shifts toward reactants at high temperatures [13]. These results emphasize the delicate balance required to optimize the hydrogen-to-carbon monoxide ratio, which is essential for syngas applications.

Carbon (C) formation is negligible below 1373 K but rises significantly at higher temperatures, particularly at 2-methylnaphthalene-rich conditions (0.95:0.05). Since 2-methylnaphthalene is the primary carbon source, excess carbon formation at high temperatures is expected, as highlighted in studies on the hydrogenation of naphthalene derivatives [10]. Similarly, methane (CH_4) production peaks at moderate temperatures (573–798 K) but declines beyond 1173 K due to CH_4 decomposition, where CH_4 breaks into hydrogen and solid carbon at extreme temperatures, a process well-documented in thermodynamic analyses of FOBS [12].

Ethylene (C_2H_4) formation is maximized at 1248 K for a 0.50:0.50 molar ratio, primarily due to the thermal cracking of 2-methylnaphthalene. At higher temperatures, competing reactions and decomposition limit C_2H_4 yields, similar to findings from studies on fuel additives and their thermal stability [10]. Ethane (C_2H_6) production follows a similar trend, peaking at 933 K before declining as equilibrium shifts back toward reactants. The hydrogenation reaction responsible for C_2H_6 formation favours lower temperatures, making it susceptible to decomposition beyond its optimal range, as demonstrated in light cycle oil [15].

Propene (C_3H_6), propane (C_3H_8), butene (C_4H_8) and butane (C_4H_{10}) yields increase at high temperatures (1248–1273 K) due to endothermic decomposition reactions. However, beyond this range, thermal decomposition and secondary reactions reduce hydrocarbon yields. This trend highlighted the importance of precise temperature regulation in maximizing hydrocarbon fuel production from FOBS, a critical aspect noted in the study of thermal processes in petrochemical applications [2].

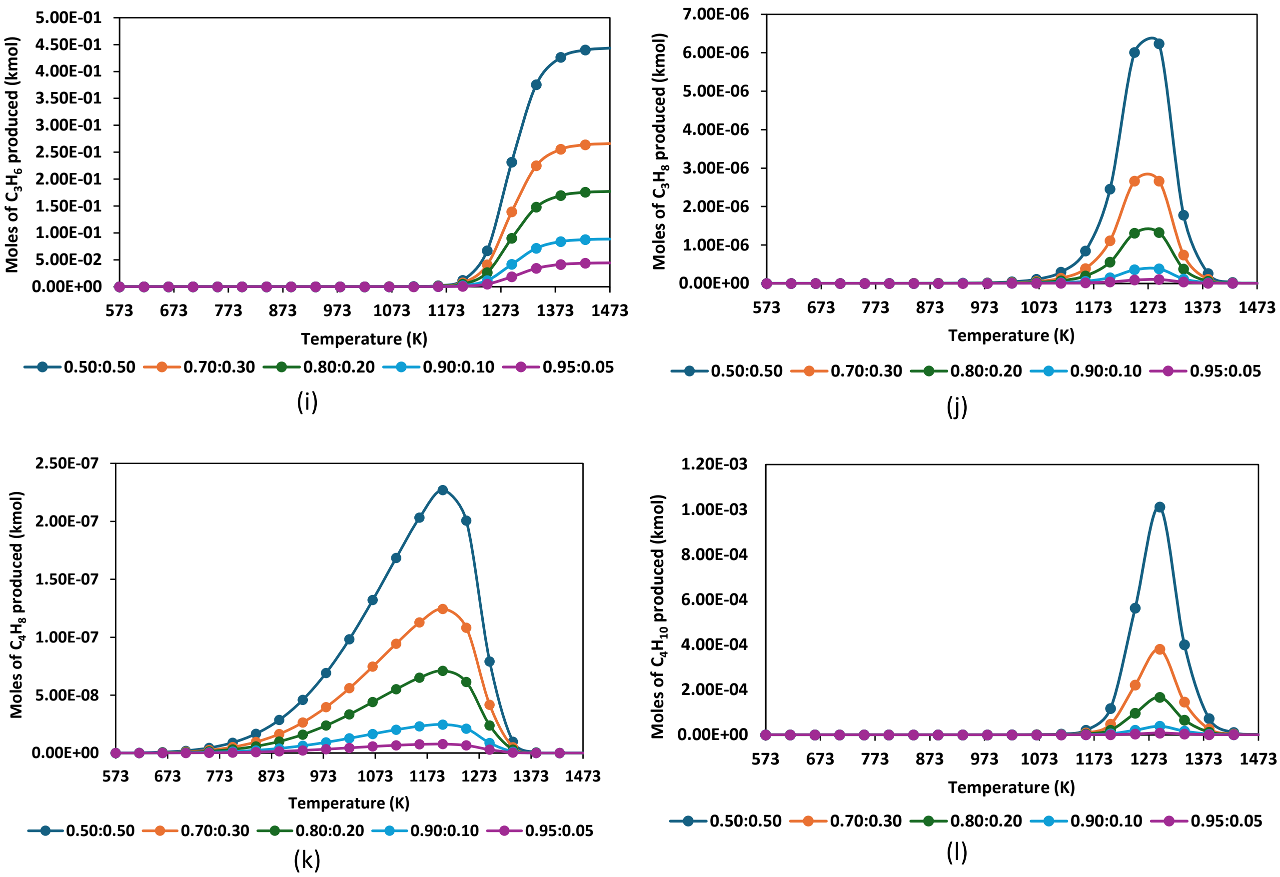

Moles of H_2 produced (kmol)
3.50E-01
3.00E-01
2.50E-01
2.00E-01
1.50E-01
1.00E-01
5.00E-02
0.00E+00
Moles of CO_2 produced (kmol)
2.50E-01
2.00E-01
1.50E-01
1.00E-01
5.00E-02
0.00E+00
Moles of CO produced (kmol)
6.00E-01
5.00E-01
4.00E-01
3.00E-01
2.00E-01
1.00E-01
0.00E+00
Moles of H_2O produced (kmol)
1.40E-04
1.20E-04
1.00E-04
8.00E-05
6.00E-05
4.00E-05
2.00E-05
0.00E+00
Moles of C produced (kmol)
4.00E-14
3.50E-14
3.00E-14
2.50E-14
2.00E-14
1.50E-14
1.00E-14
5.00E-15
0.00E+00
Moles of CH_4 produced (kmol)
5.00E-01
4.50E-01
4.00E-01
3.50E-01
3.00E-01
2.50E-01
2.00E-01
1.50E-01
1.00E-01
5.00E-02
0.00E+00
Moles of C_2H_4 produced (kmol)
9.00E-03
8.00E-03
7.00E-03
6.00E-03
5.00E-03
4.00E-03
3.00E-03
2.00E-03
1.00E-03
0.00E+00
Moles of C_2H_6 produced (kmol)
3.50E-04
3.00E-04
2.50E-04
2.00E-04
1.50E-04
1.00E-04
5.00E-05
0.00E+00
573
673
773
873
973
1073
1173
1273
1373
1473
Temperature (K)
0.50:0.50
0.70:0.30
0.80:0.20
0.90:0.10
0.95:0.05

(a) (b)

(c) (d)

(e) (f)

(g) (h)



(i) (j) (k) (l)

Fig. 1. Product produced at variant temperature at 1 bar: (a) H_2, (b) CO_2, (c) CO, (d) H_2O, (e) C, (f) CH_4, (g) C_2H_4, (h) C_2H_6, (i) C_3H_6, (j) C_3H_8, (k) C_4H_8 and (l) C_4H_{10}

Overall, Figure 1 illustrates the complex interplay between temperature and product distribution in FOBS conversion, emphasizing the importance of optimizing reaction conditions to enhance hydrogen and hydrocarbon yields while minimizing undesirable by-products. These insights are critical for refining FOBS-to-fuel strategies and improving the efficiency of waste-to-energy technologies that highlight the strong influence of temperature on hydrogen production efficiency, particularly through steam reforming of FOBS-derived hydrocarbons. The optimal temperature (1248 K) not only maximizes H_2 yield (29.71%) but also minimizes the formation of undesirable solid carbon, which is critical for preventing catalyst deactivation and reactor fouling in industrial applications. These results provide a practical guideline for optimizing process conditions in hydrogen production facilities, potentially enhancing the economic viability of waste-to-energy technologies. Moreover, the reduction in CO_2 yield at higher temperatures suggests that strategic temperature control could be leveraged to improve carbon management strategies, aligning with global efforts to reduce greenhouse gas emissions. This finding could be particularly relevant for integrating FOBS reforming into carbon capture and utilization systems and making the process more environmentally sustainable.

3.3 Effects of Temperature and Feed Ratio on Hydrocarbons Distributions

Temperature fluctuations and feedstock ratios have a significant impact on the distribution of hydrocarbon products like methane, ethylene, ethane, propane, and butene. These products are all produced by chemical reactions. Thermal cracking, hydrogenation, and dehydrogenation are the three reactions that lead to the formation of these compounds. In each of these reactions, equilibrium conditions shift depending on the temperature and the composition of the reactants. Through the optimization of these parameters, fuel yields can be increased while undesirable by-products can be reduced [3, 12].

Figure 1 (f) shows methane (CH_4) production at moderate temperatures (573–873 K) with a 0.50:0.50 2- methylnaphthalene: water molar ratio. At these temperatures, exothermic methanation reactions (R11 and R12) produce CH_4, while methane decomposition (R7) dominates above 1173 K, reducing yield. This observation is critical as it highlights the trade-off between maximizing CH_4 production and preventing its thermal breakdown into hydrogen and solid carbon, which can lead to reactor fouling and lower fuel efficiency [16, 17].

Because of endothermic thermal cracking (R2), the formation of ethylene (C_2H_4), which is depicted in Figure 1 (g), is at its highest at a temperature of 1248 K. Excessive temperatures above 1300 degrees Celsius lead to secondary decomposition, which in turn reduces selectivity and efficiency in fuel applications. To keep the C_2H_4, yield stable, temperature regulation is necessary [14, 18].

Figure 1 (h) shows that exothermic hydrogenation (R4) peaks ethane (C_2H_6) production at 933 K, but equilibrium shifts away from product formation at higher temperatures. Unlike CH_4 and C_2H_4, C_2H_6 yield is pressure-sensitive, favouring hydrogenation and hydrocarbon stability [10]. This suggests that pressure regulation could be a key strategy in optimizing ethane yield, especially for applications requiring stable hydrocarbon fractions.

Figures 1 (j) and (k), endothermic reactions (R5, R6) increase propane and butene production at 1248 -1273 K, but further heating causes thermal decomposition and lowers yield. When the hydrogen concentration is higher, the propane yield is increased, while when the heat is excessive, the butene availability is decreased [19, 20]. This indicates that optimizing temperature within a narrow range is crucial for maximizing these hydrocarbons, which are essential components of liquid fuel formulations.

The breakdown of hydrocarbons causes an increase in carbon deposits above 1273 degrees Celsius, which affects fuel efficiency. Using catalysts or modifying the conditions under which reactants are fed could reduce the amount of carbon that is formed and improve selectivity. Future research will focus on catalyst-assisted reactions and advanced reactor designs to convert 2-methylnaphthalene into sustainable fuels by optimizing temperature and feedstock ratios [13, 21].

3.4 Effects of Pressure and Temperature on Product Yield with Constant Ratio

The effect of pressure and temperature on the conversion of 2-methylnaphthalene with water at a constant 0.50:0.50 molar ratio was further investigated to optimize the yields of key products, including hydrogen, carbon monoxide, carbon dioxide, water, carbon, methane, and other hydrocarbons. This analysis provides a systematic understanding of critical reaction parameters that significantly influence product distribution [9]. Figure 2 presents the equilibrium composition of products at varying temperatures and pressures for a reactant ratio of 0.5:0.5. The identified species include (a) H_2, (b) CO_2, (c) CO, (d) H_2O, (e) C, (f) CH_4, (g) C_2H_4, (h) C_2H_6, (i) C_3H_6, (j) C_3H_8, (k) C_4H_8, and (l) C_4H_{10}.

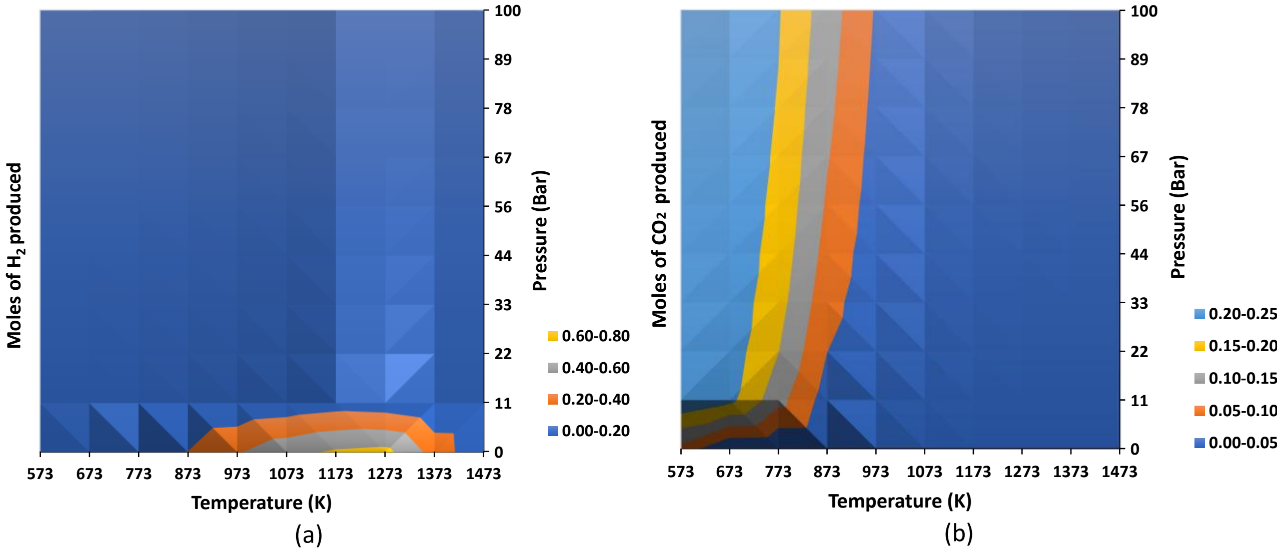
Hydrogen production is maximized at high temperatures (1173-1273 K) and low pressures (0.01–1 bar). Elevated temperatures provide the necessary thermal energy to drive endothermic reactions such as steam reforming, while lower pressures shift equilibrium toward hydrogen formation. However, as pressure increases beyond 10 bar, hydrogen yield declines due to equilibrium constraints, as observed in studies of thermodynamics involving hydrocarbons [10].

Carbon dioxide production is highest at lower temperatures (573-873 K) and elevated pressures due to the exothermic water-gas shift reaction, which is thermodynamically favoured at high pressures [4]. As temperature increases beyond 873 K, the equilibrium constant decreases, leading to a reduction in CO_2 yield.

Carbon monoxide production remains stable across different pressures but increases significantly at temperatures above 973 K, aligning with endothermic CO-producing reactions [3]. Water formation peaks at moderate-to-high temperatures (873–1273 K) and high pressures, where condensation reactions play a crucial role in stabilizing yields [13].

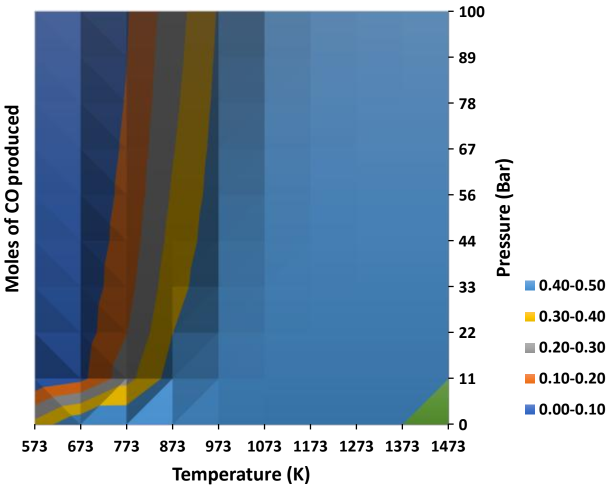
Carbon formation is negligible below 1373 K but increases at higher temperatures, particularly under 2-methylnaphthalene-rich conditions [10]. Methane, ethylene, and other hydrocarbon yields demonstrate complex dependencies on both temperature and pressure, with methane production being highest at moderate temperatures (573–798 K) and low-to-moderate pressures [18]. Precise pressure and temperature control are essential for optimizing fuel yields while minimizing undesirable by-products. Ethane (CH_4) production is optimal at 573–873 K and moderate pressures (11–33 bar), but decomposes into hydrogen above 1073 K. Ethylene (C_2H_4) and ethane (C_2H_6) are optimized at 1173–1273 K (ethylene) and 773–1173 K (ethane), with ethylene requiring moderate pressures (11–16 bar) and ethane favouring high pressures (44–77 bar). Propane (C_3H_8) and propene (C_3H_6) reach peak yields at 1273 K (propane) and 1373 K (propene), with propane favouring high pressures (77.78–100 bar). Butane (C_4H_{10}) and butene (C_4H_8) production is highest at 1273 K and 1173 K, respectively, under high pressures (77.78–100 bar). At excessive temperatures, decomposition reactions dominate, reducing hydrocarbon yields.

Moreover, the formation of longer-chain hydrocarbons such as propene and butene is strongly influenced by pressure variations, where moderate pressures favour alkene stability, preventing excessive cracking reactions [22]. These results highlight the importance of temperature and pressure optimization in enhancing hydrocarbon selectivity and minimizing carbon deposition in 2-methylnaphthalene reforming processes [23].

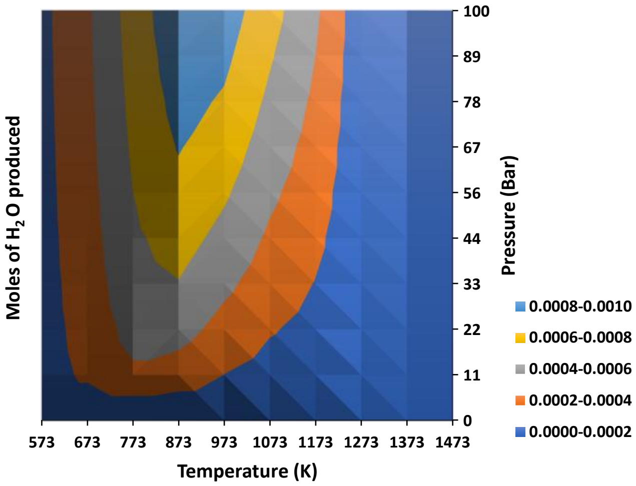


(a)

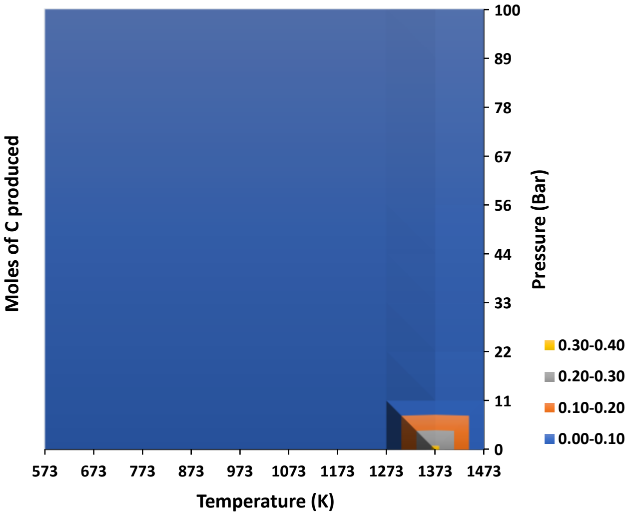
(b)


Moles of CO produced
Pressure (Bar)
100
89
78
67
56
44
33
22
11
0
573 673 773 873 973 1073 1173 1273 1373 1473
Temperature (K)
0.40-0.50
0.30-0.40
0.20-0.30
0.10-0.20
0.00-0.10

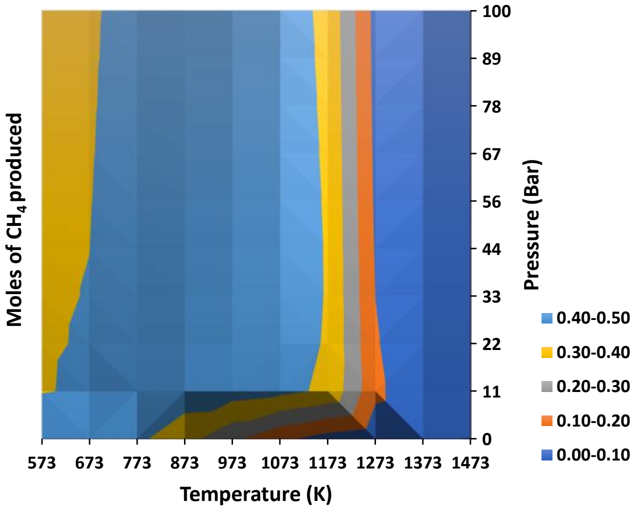
(c)


Moles of H_2O produced
Pressure (Bar)
100
89
78
67
56
44
33
22
11
0
573 673 773 873 973 1073 1173 1273 1373 1473
Temperature (K)
0.0008-0.0010
0.0006-0.0008
0.0004-0.0006
0.0002-0.0004
0.0000-0.0002

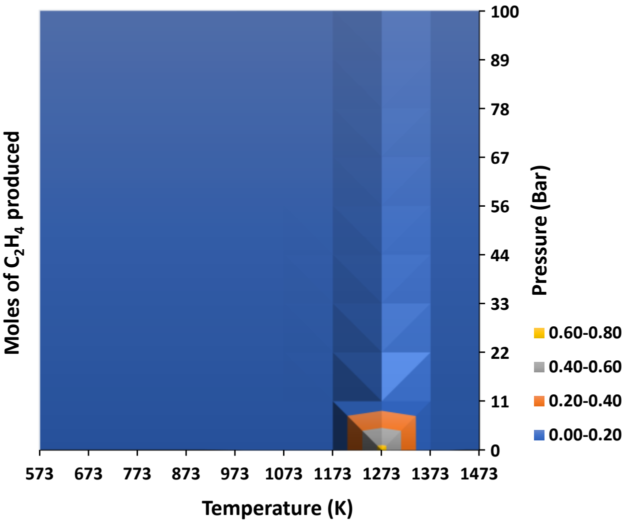
(d)


Moles of C produced
Pressure (Bar)
100
89
78
67
56
44
33
22
11
0
573 673 773 873 973 1073 1173 1273 1373 1473
Temperature (K)
0.30-0.40
0.20-0.30
0.10-0.20
0.00-0.10

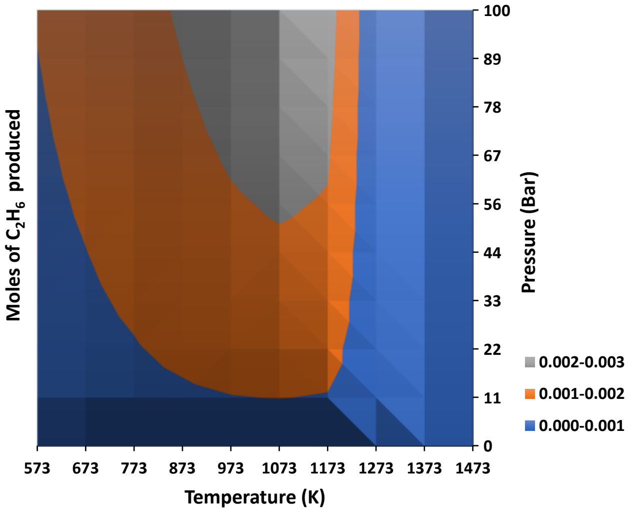
(e)


Moles of CH_4 produced
Pressure (Bar)
100
89
78
67
56
44
33
22
11
0
573 673 773 873 973 1073 1173 1273 1373 1473
Temperature (K)
0.40-0.50
0.30-0.40
0.20-0.30
0.10-0.20
0.00-0.10

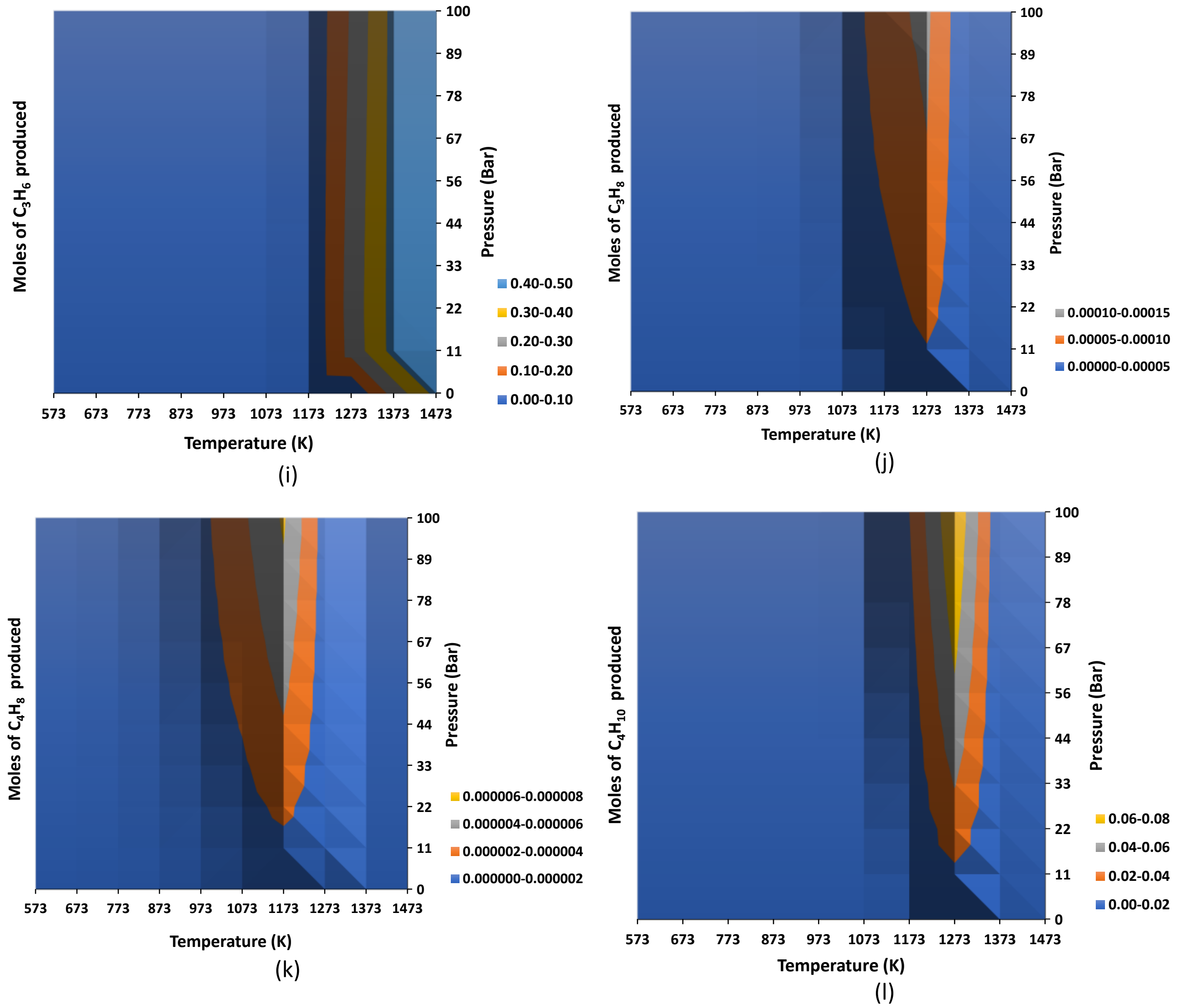
(f)


Moles of C_2H_4 produced
Pressure (Bar)
100
89
78
67
56
44
33
22
11
0
573 673 773 873 973 1073 1173 1273 1373 1473
Temperature (K)
0.60-0.80
0.40-0.60
0.20-0.40
0.00-0.20

(g)


Moles of C_2H_6 produced
Pressure (Bar)
100
89
78
67
56
44
33
22
11
0
573 673 773 873 973 1073 1173 1273 1373 1473
Temperature (K)
0.002-0.003
0.001-0.002
0.000-0.001

(h)



(i) (j) (k) (l)

Fig. 2. Product produced at variant temperature and pressure at reactant ratio 0.5:0.5: (a) H_2, (b) CO_2, (c) CO, (d) H_2O, (e) C, (f) CH_4, (g) C_2H_4, (h) C_2H_6, (i) C_3H_6, (j) C_3H_8, (k) C_4H_8 and (l) C_4H_{10}.

Based on the temperature and pressure influence the conversion efficiency of 2-methylnaphthalene into hydrogen and other hydrocarbons. Maximizing hydrogen production at high temperatures (1173–1273 K) and low pressures (0.01–1 bar) underscores the importance of optimizing operating conditions to improve yield while minimizing energy consumption. Steam reforming of 2-methylnaphthalene could serve as a potential alternative hydrogen production route, reducing reliance on conventional fossil fuels. However, the observed decline in hydrogen yield at pressures above 10 bar highlights a key limitation in high-pressure operation, necessitating further research on catalyst-assisted processes to enhance equilibrium shifts toward hydrogen production. Future studies should explore advanced catalyst formulations that lower activation energy and improve hydrogen selectivity under varying pressure conditions. Furthermore, carbon deposition at temperatures above 1373 K presents a major challenge, as excessive carbon formation can deactivate catalysts and reduce process efficiency.

4. Conclusions

This study provided a detailed thermodynamic evaluation of FOBS steam reforming using Gibbs free energy minimization and resulted in providing data for optimizing H_2 and hydrocarbon production. By systematically analysing the effects of temperature, pressure and feedstock ratios, this research identified critical operational parameters that influenced the product distribution and conversion efficiency. The finding revealed that a 2-methylnaphthalene-to-water ratio of 0.5:0.5 at 1248 K yields the highest H2 gas production (29.71%) while excessive naphthalene concentrations increase solid carbon formation which leads to reducing overall process efficiency.

A major contribution of this research is its systematic approach to evaluating FOBS reforming conditions which then able to bridge the critical gap in understanding waste-to-energy processes. The thermodynamic data obtained serves as a valuable guide for optimizing FOBS as a viable feedstock for hydrogen production. This framework is particularly relevant for industrial applications, as it can enhance efficiency, reduce energy consumption, and improve waste management strategies. Furthermore, the theoretical modelling presented in this study extends beyond fundamental analysis, offering practical insights for the development of efficient waste-to-energy systems. By refining steam reforming conditions, this research paves the way for integrating FOBS-derived hydrogen into existing energy infrastructures. Future works should explore catalyst-assisted reforming, reactor design improvements and techno-economic assessments to enhance process viability, further supporting global efforts to transition towards low-carbon energy solutions.

Acknowledgement

The authors would like to extend their most profound appreciation to the Ministry of Higher Education Malaysia (MOHE) for the financial support through Fundamental Research Grant Scheme (FRGS/1/2020/TK0/UTM/02/97) and Universiti Teknologi Malaysia for the financial support under Research University Grant (Vote 23H01).

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