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Techno-Economic Comparison of Low-Carbon Fuels for Hybrid SOFC-ICE System

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ABSTRACT

Renewable energy will be globally implemented through energy carriers in the low-carbon energy system. This paper first analyzes the chemical properties of methanol, methane, and ammonia, and then constructs detailed models of solid oxide fuel cells and homogeneous compression charge ignition engines. The lifecycle technical efficiency of methane, ammonia, and a combination of methane and ammonia is 30.8%, 30.7%, and 28.5%, respectively. The specific electric energy costs for methane, ammonia, and methanol are 1.64 CNY/kWh, 2.47 CNY/kWh, and 3.04 CNY/kWh, respectively. Currently, E-methane is more favorable compared to both ammonia and methanol, both in terms of efficiency and carbon emissions. In the future, the fuel costs for methanol, methane, and ammonia could be reduced to at least 1.02 CNY/kg, 2.47 CNY/kg, and 0.9 CNY/kg respectively. The electricity cost based on a hybrid SOFC-ICE system will be comparable to coal power generation.

Keywords: methanol, ammonia, methane, power to gas

NONMENCLATURE

Abbreviations	
SOFC	Solid Oxide Fuel Cell
ICE	Internal combustion engine
SEEC	Specific electric energy cost
Symbols	
n	Year
j	Current density
V	Voltage
F	Faraday's constant
G	Gibbs free energy

1. INTRODUCTION

Over the past twenty years, solar energy has been rapidly employed for the large-scale production of low-carbon fuels, including methanol, hydrogen, ammonia, ethanol, and more. These fuels are intended for long-distance transportation and energy storage purposes in the future. Alternative fuels play a crucial role in distributed energy systems, both from technical and economic standpoints. However, the low heating value of low-carbon fuels often falls below that of natural gas, resulting in higher specific power costs. Consequently, enhancing the energy utilization efficiency of clean fuels stands out as one of the most cost-effective approaches for curtailing carbon dioxide emissions in the short term (2021-2030).

Typically, the prime mover sizes in distributed energy systems range from 1 kW to 1 MW [1]. Solid oxide fuel cells (SOFCs) are garnering significant attention for future power generation systems due to their advantages, such as high efficiency, fuel flexibility, and the ability to operate without expensive catalysts like Pt [2]. However, operating the SOFC plant alone presents challenges in accommodating various loads within distributed energy systems. Furthermore, the chemical equilibrium in the anode has limitations, resulting in unburned fuel lingering in the anode tail gas. Given these constraints, the hybrid SOFC-combined cycle has the potential to harness the residual physical and chemical energy from the anode off-gas to further enhance power efficiency.

The hybrid SOFC-ICE system boasts superior cost-effectiveness and efficiency compared to the hybrid SOFC-gas turbine system [3]. Therefore, the application of alternative fuels in future distributed energy systems was examined from both technical and economic perspectives.

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2. MODEL CONSTRUCTION

2.1 System fueled with different e-fuels

The properties of methane, methanol, and ammonia are presented in Table 1. The hydrogen content significantly influences the performance of solid oxide fuel cells (SOFCs). The molar fraction of methane is 0.25, higher than that of methanol and ammonia, which is advantageous for SOFC performance. Additionally, the carbon content affects steam reforming and the component composition of the anode off-gas. During the transportation of alternative fuels, they are initially compressed and condensed into a liquid state. Subsequently, they are heated to a gaseous state before entering the power engine.

Methanol exhibits a higher latent heat of vaporization, at 37 kJ/mol, compared to ammonia and methane. Boiling temperature plays a role in cost considerations, the energy efficiency of transitioning from liquid to gas, and the material used in transport tanks. The volumetric heating value holds significance for steady power engines like SOFCs, engines, and combustors. Autoignition temperature and laminar burning velocity indicate fuel reactivity, implying the ease of oxygen capture for releasing chemical energy.

Table 1 Fuel properties

	Natural gas	Methanol	Ammonia
Hydrogen content	0.25; 25wt%	0.12;12.5wt %	0.18; 17.6wt%
Latent heat of vaporization	8.19 kJ/mol	37.34 kJ/mol	23.37 kJ/mol
Boling temperature at 1 atm	-160 °C	64.7 °C	-33 °C
Energy density	10.6 MJ/L 50.2 MJ/kg	18 MJ/L 22.7 MJ/kg	32.8 MJ/L 19 MJ/kg
Autoignition temperature	537°C	464°C	630 °C
Laminar burning velocity	35 cm/s	34~40 cm/s	7 cm/s

The lifecycle processes of the three fuels are illustrated in Fig. 1. Water is directed to the electrolyzers, where renewable electricity facilitates the production of hydrogen and oxygen. Hydrogen serves as the fundamental component for numerous low-carbon fuels. Methane and methanol's carbon content originates from carbon capture processes, while nitrogen atoms are sourced from the air through an air separator.

Subsequently, at the fuel decomposition unit, under high-temperature operating conditions, the fuels can either be directly split or reformed at the anode. However, for the sake of easy SOFC efficiency calculations, certain assumptions are made. Specifically, methane, ammonia, and methanol are assumed to be fully converted into carbon dioxide and hydrogen. Methane and methanol undergo a steam process, whereas ammonia undergoes a cracking process.

The hydrogen reacts with oxygen sourced from the cathode, constrained by chemical equilibrium. This equilibrium results in some unburned hydrogen within the anode off-gas, which subsequently enters a homogeneous engine for combustion once again.

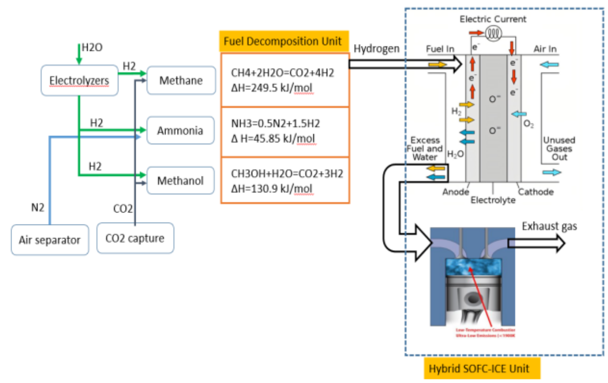

Fig. 1 low-carbon fuels applied for hybrid SOFC-ICE System diagram

2.2 Governing equations

The anode-supported solid oxide fuel cell system comprises a Ni-YSZ anode, a solid YSZ electrolyte, an LSM-YSZ cathode, and an inverter. The properties of the fuel cell model are provided in Table 2. The external characteristics are represented by the current density vs. voltage curve. The cell voltage is determined through Eq.(1), calculated by subtracting the ideal Nernst voltage from the sum of polarization loss, activation loss, and ohm loss, as derived in Eq.(2) ~Eq. (6).

The Nernst voltage is influenced by the mass flow rates of hydrogen and air, with the assumption that the mass flow is sufficiently large. Ohmic loss arises from the passage of electric ions through materials, generating heat. This loss is associated with the conductivity of the anode, cathode, and electrolyte. Concentration polarization results from the disparities between the anode or cathode and the Triple Phase Boundary (TPB). The cathode diffusion coefficient is $1.37 \times 10^{-5}\ m^2/s$, while the anode diffusion coefficient is $3.66 \times 10^{-5}\ m^2/s$ [4].

The activation loss of both the anode and cathode is described using the Butler-Volmer equation, formulated in Eq.(6). The voltage vs. current density curve was validated against Aguiar's data at temperatures of 973K, 1023K, and 1073K, as shown in Fig. 2. Within the operational voltage range of 0.6 to 0.8V, the deviation between this model and Aguiar's [4] data remains below 0.05%.

$$V_{cell} = V_{Nernst} - V_{ohm} - V_{conc,ca} - V_{conc,an} - V_{act,ca} - V_{act,an} \quad (1)$$

$$V_{Nernst} = \frac{-\Delta G}{2F} \quad (2)$$

$$V_{ohm} = j \cdot R_{ohm} \quad (3)$$

$$V_{conc,an} = \frac{RT}{2F} ln\left(\frac{P_{H_2O,TPB} P_{H_2}}{P_{H_2O} P_{H_2,TPB}}\right) \quad (4)$$

$$V_{conc,ca} = \frac{RT}{4F} ln\left(\frac{P_{O_2}}{P_{O_2,TPB}}\right) \quad (5)$$

$$j = j_0 \left\{\exp\left\{\frac{\beta zFV_{act}}{RT}\right\} - \exp\left\{-\frac{(1-\beta)zFV_{act}}{RT}\right\}\right\} \quad (6)$$

Table 2 Input parameters for fuel cell model validation

Type	Anode Supported
Anode	Ni-YSZ
Electrolyte	YSZ
Cathode	LSM-YSZ
Cell pressure [bar]	1
Operating temperature [°C]	600~800
Anode thickness [μm]	500
Cathode thickness [μm]	50
Electrolyte thickness [μm]	20
Cell length, *L* [m]	0.1
Cell width, *W* [m]	0.1
Fuel	Methane
DC-AC inverter efficiency	0.97
Fuel utilization factor	0.75

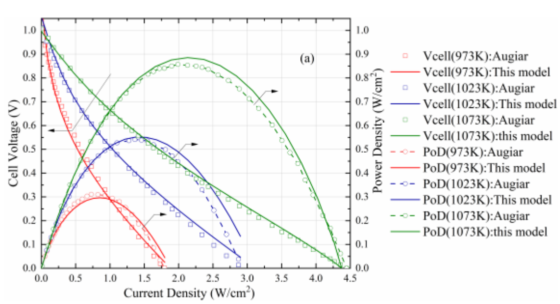

Fig. 2 The V-J curve verification

In the case of a homogeneous charge compression ignition engine (HCCI engine), it's necessary to heat the inlet fuel and air to a minimum of 200°C, rather than starting from room temperature. The composition of components is uniform within the engine and under dilute conditions. The reactions occurring within the cylinder are governed by mechanical equations and the distribution of components. In this context, the mechanical data is selected from GRI-MECH 3.0, which encompasses 325 elementary reactions involving 53 species. The in-cylinder pressure is computed using a heat release model, represented by Eq. (7).

$$AHRR = \left(-P\frac{dV}{dt} - \frac{dQ}{dt} - \frac{d(m \cdot e)}{dt} + \sum_i m_i h_i\right) \quad (7)$$

Where Q represents the heat of the elementary reaction, and e, m, and h correspond to the internal energy, mass, and enthalpy of each species, respectively. The indicated thermal efficiency of the engine is calculated using Eq.(8).

$$\eta_{\mathrm{th}} = \frac{\text{Power}}{\text{Fuel power}} \quad (8)$$

2.3 Economic evaluation

The economic assessment encompasses both the fuel production and transportation processes, as well as the hybrid SOFC-ICE device. The expenses involve various aspects, including depreciation costs, operational costs, maintenance costs, investment interest costs, insurance costs, and taxation costs, all outlined in Table 3. where n is life cycle, 10 years. φ is fuel flux, $\mathrm{N}m^3/h$, N_h is annual operation time, 8000 hf_{mai} is maintenance cost factor, 0.06. i is interest rate, 0.0926. f_{ins} is insurance cost factor, 0.2. f_{tax} is insurance cost factor, 0.054. Specific electric energy cost is obtained from Eq.(9) [5].

Table 3 economic model

Depreciation cost	$\dot{\mathrm{M}}_{dep} = M_{cap}/n$
Operation cost	$\dot{\mathrm{M}}_{ope} = c\varphi N_h$
Maintenance cost	$\dot{\mathrm{M}}_{mai} = (M_{cap}/n) \cdot f_{mai}$
Investment interest cost	$\dot{\mathrm{M}}_{int} = (M_{cap}/n) \cdot \mathrm{i}$
Insurance cost	$\dot{\mathrm{M}}_{ins} = (M_{cap}/n) \cdot f_{ins}$
Taxation cost	$\dot{\mathrm{M}}_{tax} = (M_{cap}/n) \cdot f_{tax}$

$$\mathrm{SEEC} = \frac{\dot{\mathrm{M}}_{dep} + \dot{\mathrm{M}}_{ope} + \dot{\mathrm{M}}_{mai} + \dot{\mathrm{M}}_{int} + \dot{\mathrm{M}}_{ins} + \dot{\mathrm{M}}_{tax}}{(W_{SOFC} + W_{engine}) \cdot N_h} \quad (9)$$

3. REUSLTS AND DISCUSSION

3.1 Technology analysis

As depicted in Fig. 1, methane, ammonia, and methanol originate from renewable sources such as electricity, water, air, and carbon capture. An analysis was conducted on their lifecycle efficiency and carbon dioxide emissions. Utilizing the mathematical model of the SOFC and HCCI engine, the power efficiency results of the prime movers are illustrated in Fig. 3. The molar fraction of gas directed to the engine is presented in Table 4.

In cases where methane powers the SOFC, its efficiency stands at 0.55, surpassing that of methanol and ammonia due to its higher hydrogen content. At an equivalence ratio of 0.1, the fuel composition of the anode off-gas is detailed in Table 4. The power efficiency of methanol off-gas is 0.363, akin to methane and greater than ammonia. Despite ammonia having a higher in-cylinder pressure than methanol in Fig. 4, its fuel power is more substantial, resulting in a thermal efficiency of only 0.349. The hybrid ammonia system achieves the highest efficiency of 0.59 due to its lower heating value of 18.6 MJ/kg. Methane and methanol exhibit similar performance. Consequently, the specific power fuel consumption among the three fuels is highest for ammonia at 341.27 g/kWh.

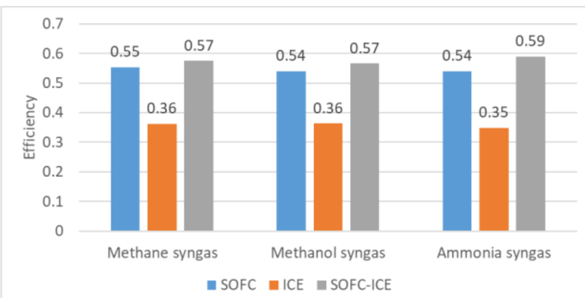

Fig. 3 Power efficiency of prime movers fueled with syngas

Table 4 Fuel composition of anode off-gas fueled with methane, methanol and ammonia.

Fuel for SOFC	CH4 (CO2:H2)	CH3OH (CO2:H2)	NH3 (N2:H2)
	1:4	1:3	1:3
Anode off-gas for HCCI engine			
CO2 (%)	5.92	7.74	0
H2 (%)	5.92	5.8	5.8
N2 (%)	55.62	54.55	62.28
O2 (%)	14.79	14.51	14.51
H2O (%)	17.75	17.4	17.41
Fuel power(kW)	15.88	15.48	15.74

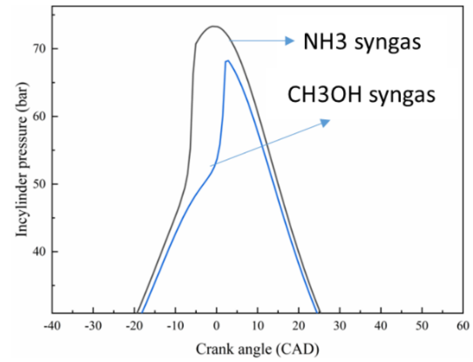

Fig. 4 incylinder pressure of NH3 and CH3OH anode off-gas

In terms of carbon emissions, methanol has the highest emissions at 779 g/kWh. Methane follows with carbon emissions of 597 g/kWh in Fig. 5. As we are aware, the carbon emission from the electricity grid is estimated at 838 g/kWh [6]. In China, utilizing E-methanol and E-methane would result in a reduction of 305 kg and 1246 kg per person for every 5317 kWh consumed. However, E-methanol is not as favorable when compared to the electricity grid network. While ammonia doesn't emit carbon dioxide directly, it's worth noting that N2O and NOx emissions associated with ammonia are higher than those of methanol and methane.

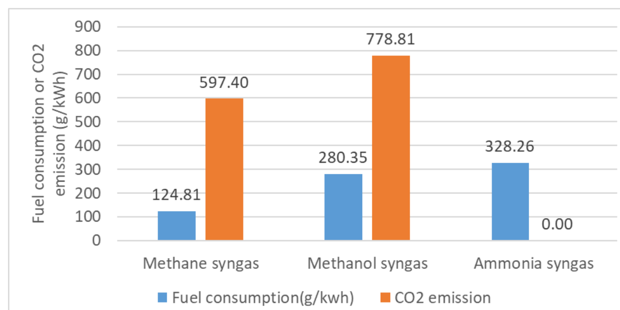

Fig. 5 fuel consumption and carbon dioxide emission

The fuel production efficiency of ammonia takes into account the water electrolyzer and air separator. For methanol and methane, the efficiency considerations involve power-to-hydrogen and carbon capture processes. Power-to-hydrogen conversion using a PEM (Proton Exchange Membrane) achieves an efficiency of around 70%. The efficiency for power-to-methanol conversion is 54% [7] while power-to-ammonia conversion efficiency is 52% [8]. Power-to-methane conversion also has an efficiency of 54% [9].

The thermal efficiency of the prime movers is calculated using the mathematical model discussed earlier. Consequently, the lifecycle efficiencies for methane, ammonia, and methanol are determined to be 30.8%, 30.7%, and 28.5%, respectively in Table 5.

Table 5 lifecycle efficiency and carbon emission.

E-Fuels	Fuel production efficiency	Power efficiency	Overall efficiency	Carbon emission (g/kWh)
NH3	52%	59%	30.7%	N2O, NOx
CH3OH	50%	57%	28.5%	916
CH4	54%	57%	30.8%	775

3.2 Economic analysis

The fuel cost is comprised of production and transportation costs [10], as detailed in Table 6. Methane carries the highest cost, followed by methanol and ammonia. Notably, LNG transportation is the most costly due to its boiling temperature of -163°C. Among the three, methanol production cost is the highest.

The comprehensive costs are presented in Table 7. For methanol, operating costs constitute 8.47%, for ammonia, it's 6.72%, and for methane, it's 4.71%. The specific electric energy cost follows a similar order, with methanol being the highest, followed by ammonia and then methane. The current cost of coal-based power is 0.57 CNY/kWh in China [11]. Presently, under the given fuel, device, and investment costs, the electricity costs are 3.04 CNY/kWh for methanol, 2.47 CNY/kWh for ammonia, and 1.64 CNY/kWh for methane in Fig. 6.

Looking ahead, if methane costs are reduced to 2.47 CNY/kg, methanol to 1.02 CNY/kg, and ammonia to 0.9 CNY/kg, the cost trends are depicted in Fig. 7.

Table 6 Fuel cost

Fuel type	Production cost(RMB/MJ	Transportation cost(RMB/MJ)	Fuel cost(RMB/MJ)	Fuel cost(RMB/kg)
Traditional natural gas	0.08	0.00518	0.08518	4.26
E-CH4	0.131	0.00518	0.13618	6.81
E-CH3OH	0.227	0.00476	0.23176	5.26
E-NH3	0.188	0.00371	0.19171	3.64

Table 7 lifecycle economic parameters

Fuel type		E-CH4	E-CH3OH	E-NH3
Fuel cost(CNY/kg)		6.81	5.26	3.64
SOFC power (kW)		388	315	164
ICE power (kW)		17	16	16
Lifecycle efficiency		30.8%	28.5%	30.7%
Capital investment（k$）	SOFC	139.6		
	ICE	11.46		
	Heat exchangers	82.5		
	inverter	25.4		
	SUM	258.96		
Operating cost($)		276	914	1521
Depreciation cost($)		25896		
Maintenance cost($)		1554		
Investment interest cost ($)		2398		
Insurance cost($)		5179		
Taxation cost($)		1398		
SEEC(CNY/kWh)		1.64	3.04	2.47

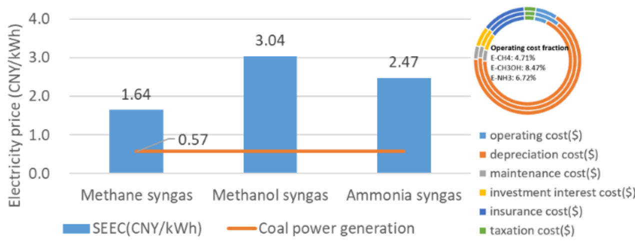

Fig. 6 Specific electric energy cost of methane, methanol and ammonia.

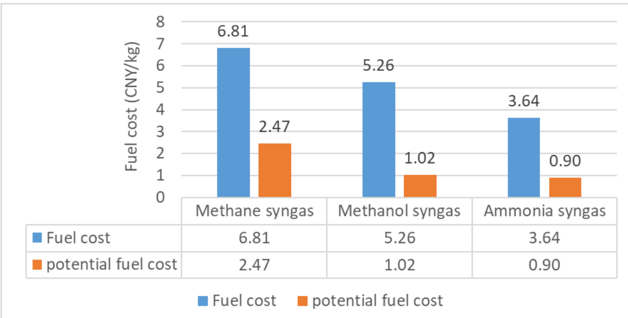

Fig. 7 Comprative fuel cost

3.3 Conclusions

Renewable energy is poised to be globally adopted as an energy carrier within the framework of low-carbon energy systems. This study initially examines the chemical properties of methanol, methane, and ammonia, and subsequently develops detailed models for both solid oxide fuel cells and homogeneous compression charge ignition engines.

The efficiency of solid oxide fuel cells remains comparable across the three fuels, while the engine efficiency for ammonia is the lowest at 34.9%. However, due to ammonia's higher fuel power, the hybrid power efficiency reaches the highest point at 59%, whereas methanol and methane perform equally at 57%. Taking into account fuel production efficiency of 54%, 52%, and 50% for methane, ammonia, and methanol respectively, the resulting lifecycle technical efficiencies are 30.8%, 30.7%, and 28.5%.

In terms of transportation, liquid methane bears the highest cost, and methanol exhibits the highest production cost. The specific electric energy costs are 3.04 CNY/kWh for methanol, 2.47 CNY/kWh for methane, and 1.64 CNY/kWh for ammonia.

At present, E-methane demonstrates greater comparative advantages over ammonia and methanol in terms of efficiency, carbon emissions, and economics. Looking ahead, it's anticipated that the costs of methanol, methane, and ammonia fuels will reduce to at least 1.02 CNY/kg, 2.47 CNY/kg, and 0.9 CNY/kg respectively. Consequently, with a hybrid SOFC-ICE system, the electricity costs will be competitive with coal power generation.

ACKNOWLEDGEMENT

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