



## Full Length Article

# Numerical simulation on the effect of operating conditions and syngas compositions for synthetic natural gas production via methanation reaction



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## HIGHLIGHTS

- Synthetic natural gas (SNG) production via methanation is numerically investigated.
- Methanation is sensitive to the reaction temperature.
- Hot spot in the reactor causes decreases in CO conversion and CH<sub>4</sub> yield.
- Best CO conversion can be obtained from isothermal reactor.
- Enhanced H<sub>2</sub>/CO ratio is required for SNG production using syngases as feedstock.

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## ABSTRACT

The synthetic natural gas (SNG) production via methanation reaction was investigated in this study. A fixed-bed tubular reactor was used as the physical model and axisymmetric non-isothermal governing equations for the gas flow, energy transfer and species transport were solved numerically. The operating conditions (inlet pressure, inlet temperature, feed rate, and heat transfer) and the reactant gas composition effects on the reaction were studied. CO conversion, CH<sub>4</sub> yield, H<sub>2</sub> efficiency and CO<sub>2</sub> yield were used to characterize the reaction performance. It was found that CO methanation is sensitive to the reaction temperature. Based on the operating conditions used in this study, CO conversion from 0% at reactant inlet temperature ( $T_{in}$ ) of 300 °C abruptly increases to 100% at  $T_{in}$  = 380 °C. As  $T_{in}$  is greater than 380 °C, a hot spot exists in the reactor, leading to decreases in CO conversion and CH<sub>4</sub> yield. It was also found that under the same operating condition, 60% decrease in CO conversion could result from an adiabatic reactor compared with the isothermal reactor. CO conversion and CH<sub>4</sub> yield can be enhanced by increasing the reaction pressure and H<sub>2</sub>/CO ratio, and decreasing the space velocity. With the addition of product species (CH<sub>4</sub>, CO<sub>2</sub>, and H<sub>2</sub>O) as the reactants, a decrease in CO conversion was found except for the addition of H<sub>2</sub>O. It was found that the CH<sub>4</sub> yield was decreased by product species addition.

Low CO conversion and CH<sub>4</sub> yield were obtained when coal- or biomass-derived syngas was used as the feedstock for methanation reaction due to low H<sub>2</sub>/CO ratio. To enhance SNG production via syngas methanation, it is suggested that the water-gas shift reaction be employed to increase the H<sub>2</sub>/CO ratio before carrying out methanation reaction.

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## 1. Introduction

Because of the increasing demand for natural gas and the need to reduce greenhouse gases [1,2], synthetic gas (syngas) conversion into synthetic natural gas (SNG) has attracted much attention in recent years [3,4]. The conventional route for SNG production

involves the gasification of coal or biomass to obtain syngas in which the major components are H<sub>2</sub> and CO [5]. After purification, the catalytic methanation reaction is used to convert the CO and H<sub>2</sub> into SNG. The CO methanation reaction has been extended to the storage of electrical energy produced from renewable sources based on the power to gas (PtG) concept [6,7]. In PtG excess electricity produced from a renewable source can be used to electrolyze steam and CO<sub>2</sub> into syngas via a reversible solid oxide cell (RSOC) operated in solid oxide electrolysis cell (SOEC) mode.

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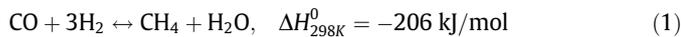
E-mail address: [rychein@dragon.nchu.edu.tw](mailto:rychein@dragon.nchu.edu.tw) (R.-Y. Chein).

**Nomenclature**

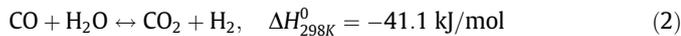
$C_F$	Forchheimer drag coefficient	$r$	radial direction
$c_p$	gas specific heat, $\text{J kg}^{-1} \text{K}^{-1}$	$T$	temperature, K
$D_{ij}$	binary molecular diffusion coefficient, $\text{m}^2 \text{s}^{-1}$	$\vec{V}$	velocity, $\text{m s}^{-1}$
$D_i^T$	thermal diffusion coefficient of species $i$ , $\text{m}^2 \text{s}^{-1}$	$v_0$	averaged inlet velocity, $\text{m s}^{-1}$
$d_p$	catalyst particle diameter, m	$X$	species conversion
$F_i$	molar flow rate of species $i$ , $\text{mol s}^{-1}$	$Y$	species yield
$h$	heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$	$x_j$	mole fraction of species $j$
$K$	catalyst bed permeability, $\text{m}^{-2}$	$z$	axial direction
$K_j$	surface adsorption equilibrium constant of species $j$ , $\text{Pa}^{-1}$		
$K_{eq,i}$	equilibrium constant of reaction $i$		
$k$	rate constant of reaction $i$ , $\text{mol Pa}^{0.5} \text{kg}_{\text{cat}} \text{s}^{-1}$ , or $\text{mol Pa kg}_{\text{cat}} \text{s}^{-1}$	<i>Greek symbols</i>	
$L$	length of reactor, m	$\varepsilon$	catalyst bed porosity
$m_{\text{cat}}$	catalyst weight, g	$\eta$	efficiency
$M_j$	molecular weight of species $j$ , $\text{g mol}^{-1}$	$\lambda$	thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
$m_j$	mass fraction of species $j$	$\mu$	viscosity, $\text{kg m}^{-1} \text{s}^{-1}$
$N_G$	number of species in the gas mixture	$\nu$	Stoichiometric coefficient
$p$	pressure, Pa	$\rho$	density, $\text{kg m}^{-3}$
$Q$	volumetric flow rate, $\text{m}^3 \text{s}^{-1}$	<i>Subscript</i>	
$q_c$	energy source term due to the chemical reaction, $\text{W m}^{-3}$	in	inlet
$R$	universal gas constant, $8.314 \text{ J mol}^{-1} \text{K}^{-1}$	m	gas mixture
$R_b$	reactor radius, m	out	outlet
$R_j$	production/destruction rate of species $j$ , $\text{kg m}^{-3} \text{s}^{-1}$	R	reaction
$r_i$	kinetic rate of reaction $i$ , $\text{mol kg}_{\text{cat}} \text{s}^{-1}$	ref	reference state
		cat	catalyst

The produced syngas is fed into a methanation reactor where it is converted into SNG. The produced SNG is then injected into the natural gas network. When high electricity consumption peaks appear, the RSOC is switched to the solid oxide fuel cell (SOFC) mode to produce electricity using the syngas produced via the tri-reforming of methane [8,9]. In addition to the above applications, methanation is one of the techniques for reducing the CO amount in the hydrogen-rich reformed gas in fuel cell applications [10,11]. More understanding of the methanation reaction is essential for improving this technology for various applications.

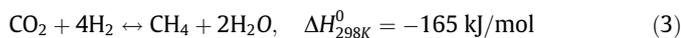
Complete CO methanation reaction is described as [12],  
CO methanation:



Water-gas shift (WGS):



CO<sub>2</sub> methanation:



In recent decades great efforts have been made to develop highly efficient methanation catalysts. The necessary requirements are high activity at low temperature and high stability at high temperature. In general, the CO methanation reaction can be catalysed using many metals such as ruthenium (Ru), rhodium (Rh), platinum (Pt), iron (Fe), nickel (Ni), and cobalt (Co) [13]. Although noble metals are very selective to methane at relatively low temperatures [14,15], they are too expensive to be used in large-scale SNG production. Therefore, nickel has been recognized as the most appropriate catalyst because of its selectivity, activity and price [16]. Many studies have focused on the selection of promoters, supports and preparation methods to increase the activity and stability of Ni-based catalysts for CO methanation [17–20]. Considerable studies have been carried out to investigate the kinetics of methanation with Ni-based catalysts. Various kinetic models have been

developed based either on the Langmuir-Hinshelwood adsorption theory or empirical approaches [21–23]. As pointed out by Kopyscinski et al. [23], the determination of accurate kinetic parameters can be challenging because methanation is a strongly exothermic and fast reaction.

In addition to experimental works, syngas methanation modelling and simulation have been reported in the literature because these approaches have the advantages of easily examining the influence of operating conditions on the reactor performance. Among the modelling works, thermodynamic analysis is a useful tool for providing guidelines in experimental study. In the study of Gao et al. [24], a detailed thermodynamic equilibrium analysis of the methanation reaction using Gibbs free energy method minimization was reported. Their results indicated that a high CH<sub>4</sub> yield can be obtained at low temperatures and high pressures. They also found that there is no significant carbon deposition under such operating conditions. In the study of Molino and Braccio [25], thermodynamic evaluation for SNG production from biomass was performed. Their results showed that methane productivity can be enhanced using a WGS reactor prior to the methanation reaction. They also pointed out that higher methanation performance can be obtained when an isothermal reactor was used instead of the adiabatic reactor. The study of Koysoumpa et al. [26] focused on the acid gas removal from the coal-derived syngas using allothermal gasification before the SNG production. They carried out their analysis for allothermal coal gasification and CO methanation based on Gibbs free energy minimization for the H<sub>2</sub>/CO ratio and CH<sub>4</sub> content estimations.

Detailed CO methanation numerical simulations were also reported in the literature. In the study of Kang et al. [27], the model of continuous stirred tank reactor (CSTR) was adopted for the dynamic simulation of CO methanation reaction. Their results indicated that a lower temperature and higher pressure are favorable for the enhancement of the methanation reaction performance. In the study of Parlikkad et al. [28], one-dimensional heterogeneous and pseudo-homogeneous models were used to simulate

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