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Research Paper

Optimization of the production of syngas from shale gas with economic and safety considerations

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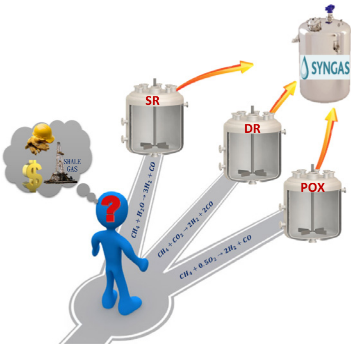
HIGHLIGHTS

- An optimization approach is presented for the production of syngas from shale gas.
- Economic and safety issues are considered.
- A solution approach that links ASPEN PLUS, MATLAB and SCRI has been implemented.
- A case study is presented to show the applicability of the proposed approach.

GRAPHICAL ABSTRACT



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ABSTRACT

Reforming is an essential technology for the monetization of shale gas through the production of syngas. Steam reforming, partial oxidation, dry reforming, or combined reforming may be used. Traditionally, H_2:CO ratio, yield or economic criteria have been used to select the type of reforming technology. The operating conditions, the nature of the reactions and compounds produced in the reforming technologies create the necessity to know the level of risk presented by these technologies. Thus, this paper introduces an approach for the optimal selection and design of reforming technologies incorporating economic aspects. A quantitative risk analysis is applied to the obtained solutions for evaluating the risk. The approach optimally selects the technology or set of technologies and operating conditions required to comply with a specific quality of syngas, maximizing the net profit. The optimization model was solved using genetic algorithms in the MATLAB® platform coupled with the ASPEN Plus® software for process and thermodynamic modeling. The results show that the steam reforming is the best technology to reach the highest quality of syngas with the lowest risk for the simulated conditions.

1. Introduction

Recently, shale gas production has drastically increased from an average growth of 2.7% per year from 1995 to 2000 to 47.9% per year from 2005 to 2011 [1]. With the continued growth, shale gas is estimated to provide up to 50% of the production of natural gas for 2040 [2]. This tendency is expected to continue because of the increasing demands for energy and feedstocks for chemical manufacturing [3]. Specifically, the interest in shale gas is attributed to technical, environmental, and economic benefits compared with other forms of fossil fuels [4]. Since shale gas can be converted into a multitude of value-added chemicals, it is anticipated to reshape the process industries in the US and around the world

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Nomenclature

Annual Sale Revenue	revenues due to sales of syngas, $/year
$\bar{C}^{out}_{R,U}$	set data of costs to technology U, $
D	carbon dioxide price, $/kg
EP	energy price (heating or cooling) $/MMJ
$\bar{f}^{inlet}_{R,U}$	set data of reactant flowrate R (D, O and S), kmol/h
$\bar{f}^{inlet}_{SG,U}$	set data of shale gas flowrate SG, kmol/h
$\bar{f}^{out}_{P,U}$	set data of flow rates to technology U, kmol/h
$\bar{f}^{optimal}_{R,U}$	set data of optimal reactants flowrates to technology U, kmol/h
$F^{inlet-well}_{r}$	flowrate of shale gas to the mixer, kmol/h
$F^{Total-inlet-SG}$	total flowrate of shale gas to be converted into syngas, kmol/h
$f^{SR-inlet}$	flowrate of shale gas sent to SR, kmol/h
$f^{POX-inlet}$	flowrate of shale gas sent POX, kmol/h
$f^{DR-inlet}$	flowrate of shale gas sent to DR, kmol/h
$J^{SR-inlet}_{w}$	flowrate of water used in SR, kmol/h
$J^{SR-inlet}_{o}$	flowrate of oxygen used in POX, kmol/h
$J^{SR-inlet}_{d}$	flowrate of carbon dioxide used in DR, kmol/h
$f^{SR-out}_{H_2}$	flowrate of hydrogen produced in SR, kmol/h
f^{SR-out}_{CO}	flowrate of carbon monoxide produced in SR, kmol/h
$f^{POX-out}_{H_2}$	flowrate of hydrogen produced in the POX, kmol/h
$f^{POX-out}_{CO}$	flowrate of carbon monoxide produced by POX, kmol/h
$f^{DR-out}_{H_2}$	flowrate of hydrogen produced in DR, kmol/h
f^{DR-out}_{CO}	flowrate of carbon monoxide produced in DR, kmol/h
f_i	incident outcome frequency events/year
FC	fixed cost, $
G	shale gas price $/kg
H	working hours in a year, h/year
i	incident outcome
I	radiation intensity, kW/m^2
$IR_{x,y}$	individual risk in the coordinates x, y
$k1$	constant Probit function
$k2$	constant Probit function
k_f	annualization factor, 1/y
NETPROFIT	net profit in the production of syngas, $/year
O	oxygen price $/kg
p	overpressure peak, N/m^2
P	damage probability
$P_{x,y,i}$	damage probability of outcome incident at coordinates x, y
P^{SR-out}	operation pressure of the steam reformer reactor, MPa
$P^{POX-out}$	operation pressure of the POX reactor, MPa
P^{DR-out}	operation pressure of the DR reactor, MPa
$\bar{P}^{inlet}_{U}$	set data of pressure to technology U, Pa
$\bar{P}^{optimal}_{U}$	set data of optimal pressures to technology U, Pa
$\bar{Q}^{out}_{U}$	set data of heat added or removed to technology U, J
Price Syngas	price of syngas, $/kg
Q^{SR}	external utility for SR, J
Q^{POX}	external utility for POX, J
Q^{DR}	external utility for DR, J
r	well of shale gas
Raw Material Costs	costs of raw materials, $
t	exposure time, s
$\bar{T}^{optimal}_{U}$	set data of optimal temperatures to technology U, K
$\bar{T}^{inlet}_{U}$	set data of temperature to technology U, K
T^{SR-out}	operation temperature of the SR reactor, K
$T^{POX-out}$	operation temperature of the POX reactor, K
T^{DR-out}	operation temperature of the DR reactor, K
S	water steam price $/kg
Technology Cost	cost of technology, $
Utilitie Costs	costs of external utilities, $
V	variable physical (overpressure, toxicity and radiation)
VC	variable cost, $
x, y	coordinates
Y	Probit value

[5], hydrogen production from shale gas is a clear example [6]. Other examples include the production of syngas [7], ethylene [8], ethylen using flue gases [9], propylene [10], methanol [11], gas to liquid processes [12], transportation fuels [13], Fischer Tropsh products [14] and other petrochemicals [15]. In all of these monetization pathways, reforming of shale gas into synthesis gas (syngas) is a central chemical pathway. The selection of type and operating variables for reforming is essential in the optimal design of the process, and this impacts the technical, economic, environmental and safety attributes of the process [16].

There are four primary types of reforming that can be used to transform shale/natural gas into syngas. The alternatives are steam reforming (SR), partial oxidation (POX), dry deforming (DR) and combined reforming (CR). These reforming approaches require different reactants (oxygen, steam, carbon dioxide), external utilities (heating and cooling) and operating conditions (pressure and temperature) to produce syngas with different H_2:CO ratios, costs of production and levels of security due to the material inventories and operating conditions. In SR, shale/natural gas reacts with steam in the presence of a catalyst [17] as follows:

$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad \Delta H_{298} = 206\ \mathrm{kJ/mol}$$

The reforming reaction is highly endothermic and requires a large amount of energy [18]. It is particularly attractive for the production of hydrogen or the production of syngas with a high H_2:CO ratio. Partial oxidation is an exothermic reaction, using oxygen as an oxidizing agent. It has advantages for usage for production of hydrogen and syngas at small and medium capacities [19] and H_2:CO ratios around 2 [20] through the following reaction [21]:

$$CH_4 + \frac{1}{2}O_2 \rightarrow CO + 2H_2 \quad \Delta H_{298} = -36\ \mathrm{kJ/mol}$$

Dry reforming is a catalytic endothermic reaction that converts methane and carbon dioxide into syngas. It is particularly attractive in managing greenhouse gas emissions through CO_2 to produce syngas at low H_2:CO ratios (around 1), which is suitable for several applications [22] or may be combined with other reforming technologies [23]:

$$CH_4 + CO_2 \rightarrow 2CO + 2H_2 \quad \Delta H_{298} = 247\ \mathrm{kJ/mol}$$

Other methodologies proposed for the production of syngas are based on the use of biomass as raw material [24], these have focused on the improvement and modification of existing processes to improve the quality of syngas [25]. Also, adaptable gasification processes to changes in feedstocks have been reported; in this sense, Haro et al. [26] presented an algorithm for calculating the gas composition and thermophysical properties for different feedstocks used in gasification. Ongen [27] studied the methane rich syngas production by gasification of waste plastics form a cable materials company. Purification of syngas obtained from