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Assessment of thermodynamic models for the design, analysis and optimisation of gas liquefaction systems

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HIGHLIGHTS

- Six thermodynamic models used for evaluating gas liquefaction systems are compared.
- Three gas liquefaction systems are modelled, assessed and optimised for each equation of state.
- The predictions of thermophysical properties and energy flows are significantly different.
- The GERG-2008 model is the only consistent one, while cubic, virial and statistical equations are unsatisfying.

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ABSTRACT

Natural gas liquefaction systems are based on refrigeration cycles – they consist of the same operations such as heat exchange, compression and expansion, but they have different layouts, components and working fluids. The design of these systems requires a preliminary simulation and evaluation of their performance. However, the thermodynamic models used for this purpose are characterised by different mathematical formulations, ranges of application and levels of accuracy. This may lead to inconsistent results when estimating hydrocarbon properties and assessing the efficiency of a given process. This paper presents a thorough comparison of six equations of state widely used in the academia and industry, including the GERG-2008 model, which has recently been adopted as an ISO standard for natural gases. These models are used to (i) estimate the thermophysical properties of a Danish natural gas, (ii) simulate, and (iii) optimise liquefaction systems. Three case studies are considered: a *cascade* layout with three pure refrigerants, a single *mixed-refrigerant* unit, and an *expander*-based configuration. Significant deviations are found between all property models, and in all case studies. The main discrepancies are related to the prediction of the energy flows (up to 7%) and to the heat exchanger conductances (up to 11%), and they are *not* systematic errors. The results illustrate the superiority of using the GERG-2008 model for designing gas processes in real applications, with the aim of reducing their energy use. They demonstrate as well that particular caution should be exercised when extrapolating the results of the conventional thermodynamic models to the actual conception of the gas liquefaction chain.

1. Introduction

1.1. Background

Production of liquefied natural gas (LNG) is an energy-intensive process that represents about 4% of the gas energy content. Minimising the energy use of this system has received increasing interest in the design procedure [1,2]. Liquefied natural gas is natural gas that has been converted to liquid form, while compressed natural gas (CNG) is natural gas in a gaseous state and at high pressure. At typical storage conditions (−160 °C for LNG and 250 bar for CNG), the energy density of LNG is about 22 MJ per litre, which is about 2.4 times greater than that of CNG [3]. The higher heating value of LNG and CNG ranges between 52 and 54 MJ/kg, which is about 3% lower than that of pure methane, but higher than those of crude oil, coal and biomass. These properties make LNG suitable for storage and long-distance transportation, and its use in marine applications seems promising in the future, because of the new limits on nitrogen and sulphur oxides emissions established by the International Marine Organization (IMO) within the Annex VI of the MARPOL treaty [4].

The liquefaction process consists of the following steps. Natural gas is received at ambient temperature and above atmospheric

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Nomenclature

A_0	empirical parameter
B	second virial coefficient
B_0	empirical parameter
C	third virial coefficient
C_0	empirical parameter
D_0	empirical parameter
E_0	empirical parameter
K	number of terms
N	number of substances
R	ideal gas constant, J mol^{-1} K^{-1}
R^*	obsolete ideal gas constant, J mol^{-1} K^{-1}
T	temperature, K or °C
T_c	critical temperature, K or °C
T_r	reduced temperature
V	volume, m^3
Z	compressibility factor
$\bar{x}$	molar composition (vector of molar fractions)
a	attraction-related parameter
a	empirical parameter
a	molar Helmholtz free energy
b	empirical parameter
b	volume-related parameter
c	empirical parameter
c	volume-translation parameter
c_p	isobaric heat capacity, J mol^{-1} K^{-1}
d	empirical parameter
i	ith component
n	empirical parameter
p	pressure, Pa
p_c	critical pressure, bar
p_r	reduced pressure
t	empirical parameter
x	molar fraction

Abbreviations

BWR	Benedict, Webb and Rubin
BWRS	Benedict, Webb, Rubin and Starling
COP	Coefficient of Performance
EOS	Equation of State
FOM	Figure of Merit
LK	Lee and Kesler
LKP	Lee, Kesler and Plöcker
LNG	Liquefied Natural Gas
MINLP	Mixed Integer Non-Linear Programming
NG	Natural Gas
PC	Perturbated Chain
PR	Peng-Robinson
SAFT	Statistical Association Fluid Theory
SRK	Soave-Redlich-Kwong

Greek letters

α	empirical parameter
α	reduced Helmholtz free energy
$\Delta\alpha$	departure function for the reduced molar Helmholtz free energy
Δ	deviation
δ	empirical constant(s)
δ	reduced density
η	energy efficiency
γ	empirical parameter
ω	acentric factor
τ	inverse reduced temperature
υ	molar volume, m^3 mol^{-1}
ϑ	empirical parameter

Superscripts

o	ideal-gas state
r	residual contribution

Subscripts

o	property of the pure substance
r	reducing property

pressure. It is then precooled, condensed and subcooled down to −160 °C, and is finally flashed off to the storage conditions. Heat removal in these cryogenic conditions is ensured by refrigeration, which implies the need for input power and heat rejection to the ambient conditions. Natural gas is a mixture containing light- (methane and ethane), medium- (propane and butane) and heavy-weight (pentane and others) hydrocarbons, together with impurities (carbon dioxide, water and nitrogen), which are removed upstream. This mixture is zeotropic: at a constant pressure, it condenses along a temperature glide and the compositions of the two phases in the vapour-liquid region are never the same.

1.2. Literature review

Several refrigeration processes for gas liquefaction have been developed over the last half-century. The scientific literature shows a large number of studies on the modelling, analysis and optimisation of gas liquefaction systems. Several handbooks, such as the ones of McDermott and Ranney [5] and of Mokhatab and Poe [6], as well as the papers of Lim et al. [7] and of Chang [8], present the cycles that have attracted most interest up-to-now. As discussed in Venkatarathnam and Timmerhaus [9], they can be subdivided into the cascade, mixed refrigerant and expander-based processes. The selection, in practice, of a particular process depends on considerations such as the system performance (compression duty), cost (equipment), size (heat exchangers), simplicity (item inventory) and safety (working fluid) [10,11]. It is therefore not possible to propose a suitable process for all applications, as different fields of application have different requirements. For example, mixed-refrigerant and expander-based processes may be preferred for small-scale applications [12] because of their lower equipment inventory, while cascade, dual [13] and propane-precooled [14,15] mixed-refrigerant systems are preferred for systems where high efficiency is the prime criterion. Mixed-refrigerant processes attract a lot of attention because of their high efficiency and their use in many industrial applications, but the high number of degrees of freedom when designing such systems results in a complex problem. Mortazavi et al. [16] suggest the use of alternative expansion techniques to enhance the performance of the C3MR process. Li et al. [17] present an optimisation methodology for optimising the design parameters of gas liquefaction processes applicable to hydrogen and methane. Khan et al. [18] propose a novel method for selecting the most appropriate refrigerant composition, which is applied to a single and propane precooled mixed system. In the same line, Xu et al. [19] suggest a correlation between the refrigerant composition and ambient conditions to design more efficient PRICO processes.

Several papers present a performance comparison of gas liquefaction processes. Remeljej and Hoadley [12] assess four LNG processes for small-scale production, suggesting that expander-based