Improving the Capability of Process Simulators to Represent Solid-Fluid Equilibria Applied to Natural Gas Liquefaction: The Methane + Neopentane System at Low Temperature

David Bluck, Seiya Hirohama, Nevin Gerek Ince, Marco Campestrini, Paolo Stringari, Freddy Garcia, Jean-Jacques Bartuel

Improving the Capability of Process Simulators to Represent Solid-Fluid Equilibria Applied to Natural Gas Liquefaction: The Methane + Neopentane System at Low Temperature

David Bluck [1], Seiya Hirohama [1], Nevin Gerek Ince [1], Marco Campestrini [2], Paolo Stringari [2], Freddy Garcia [3], Jean-Jacques Bartuel [4]

[1] AVEVA, 26561 Rancho Pkwy S, Lake Forest, CA & Houston, TX, United States
[2] MINES ParisTech, PSL University, CTP - Centre of Thermodynamics of Processes, 35 rue St Honoré 77300 Fontainebleau, France
[3] Total Energies, 2, place Jean Millier 92078 Paris La Défense CEDEX France
[4] Technip Energies, 2126 Boulevard de la Défense, CS 10266, 92741 Nanterre Cedex, France

Corresponding author e-mail: david.bluck@aveva.com or seiya.hirohama@aveva.com

Abstract

Natural gas is mainly methane, but it contains a number of other components, such as linear, branched, and cyclic hydrocarbons, aromatics, sulphur compounds, carbon dioxide, water, nitrogen, etc. Natural gas can be transported in pipelines or in its liquefied form, LNG, depending on the distance between the production site and the place of its utilization, the existence of geographical barriers, geopolitical considerations, or the need of a more flexible market. In order to be liquefied, natural gas must be cooled to about 110 K. This temperature is achieved after the natural gas is cooled in the Main Cryogenic Heat Exchanger (MCHE) at high pressure, usually higher than 50 bar, and then expanded down to the atmospheric pressure. The triple point temperatures of most of the natural gas components are higher than the temperatures that natural gas achieves in the MCHE. Consequently, if the mole fraction of these components in natural gas is higher than their solubility limits at the temperature and pressure in the MCHE, they can form solid phases in the heat exchanger. The solid formation increases the pressure drop in the MCHE and reduces the heat transfer efficiency. This means more frequent maintenance operations are required, that can have a very important negative impact on the profitability of the liquefaction plant. In order to avoid solid formation in the MCHE, an accurate knowledge of the solid-liquid, solid-vapor, and solid-liquid-vapor equilibria is mandatory to design purification units allowing reducing the content of the potential solid formers below their solubility limits before entering the MCHE. For such a purpose, the capability of the process simulators of representing accurately the phase diagram of natural gas is very important to avoid designing oversized purification units or to limit the energy and material consumption in these units.

This work is the result of a collaboration among a natural gas producer, an EPC (Engineering, Procurement, and Construction) company, a simulation software company and a research laboratory with the aim of improving the knowledge of the solubility limits of some key impurities in LNG. In this perspective, neopentane has been selected as a potential solid former because of its high triple point temperature, 256.6 K. In addition, the only two articles in the literature reporting solubility data of neopentane in methane (the main natural gas component) are not in agreement each other. A wide experimental investigation of the liquid-vapor, solid-vapor, solid-liquid, and solid-liquid-vapor equilibria for the methane + neopentane system at low temperature has been carried out and presented in Campestrini et al. 2022. This work shows how the data produced by the research laboratory are made available to industries thanks to the implementation of dedicated models and algorithms in a process simulator. In particular, an accurate model, based on the Soave-Redlich-Kwong (SRK) cubic Equation of State (EoS), has been developed for the phase equilibria of the methane + neopentane system including solid phases. In addition, a robust multi-phase flash algorithm has been developed for the solid-liquid(-liquid)-vapor equilibrium calculation. Rigorous thermodynamic phase stability analysis is used to determine the correct number of phases that will coexist at any given temperature and pressure. The new model and the phase equilibrium algorithm are integrated in the process simulator to improve the accuracy in the representation of the phase boundaries in natural gas and to allow an optimized design of the liquefaction units.

Keywords: Process Design and Development, Liquefied Natural Gas (LNG) and Liquefied Petroleum Gas (LPG), Crystallization