Robust Simulation and Optimization Methods for Natural Gas Liquefaction Processes

by

Harry Alexander James Watson

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Abstract

Natural gas is one of the world's leading sources of fuel in terms of both global production and consumption. The abundance of reserves that may be developed at relatively low cost, paired with escalating societal and regulatory pressures to harness low carbon fuels, situates natural gas in a position of growing importance to the global energy landscape. However, the nonuniform distribution of readily-developable natural gas sources around the world necessitates the existence of an international gas market that can serve those regions without reasonable access to reserves. International transmission of natural gas via pipeline is generally cost-prohibitive beyond around two thousand miles, and so suppliers instead turn to the production of liquefied natural gas (LNG) to yield a tradable commodity. While the production of LNG is by no means a new technology, it has not occupied a dominant role in the gas trade to date. However, significant growth in LNG exports has been observed within the last few years, and this trend is expected to continue as major new liquefaction operations have and continue to become operational worldwide.

Liquefaction of natural gas is an energy-intensive process requiring specialized cryogenic equipment, and is therefore expensive both in terms of operating and capital costs. However, optimization of liquefaction processes is greatly complicated by the inherently complex thermodynamic behavior of process streams that simultaneously change phase and exchange heat at closely-matched cryogenic temperatures. The determination of optimal conditions for a given process will also generally be nontransferable information between LNG plants, as both the specifics of design (e.g. heat exchanger size and configuration) and the operation (e.g. source gas composition) may have significantly variability between sites. Rigorous evaluation of process concepts for new production facilities is also challenging to perform, as economic objectives must be optimized in the presence of constraints involving equipment size and safety precautions even in the initial design phase. The absence of reliable and versatile software to perform such tasks was the impetus for this thesis project.

To address these challenging problems, the aim of this thesis was to develop new models, methods and algorithms for robust liquefaction process simulation and opti-

mization, and to synthesize these advances into reliable and versatile software. Recent advances in the sensitivity analysis of nondifferentiable functions provided an advantageous foundation for the development of physically-informed yet compact process models that could be embedded in established simulation and optimization algorithms with strong convergence properties. Within this framework, a nonsmooth model for the core unit operation in all industrially-relevant liquefaction processes, the multistream heat exchanger, was first formulated. The initial multistream heat exchanger model was then augmented to detect and handle internal phase transitions, and an extension of a classic vapor-liquid equilibrium model was proposed to account for the potential existence of solutions in single-phase regimes, all through the use of additional nonsmooth equations.

While these initial advances enabled the simulation of liquefaction processes under the conditions of simple, idealized thermodynamic models, it became apparent that these methods would be unable to handle calculations involving nonideal thermophysical property models reliably. To this end, robust nonsmooth extensions of the celebrated inside-out algorithms were developed. These algorithms allow for challenging phase equilibrium calculations to be performed successfully even in the absence of knowledge about the phase regime of the solution, as is the case when model parameters are chosen by a simulation or optimization algorithm. However, this still was not enough to equip realistic liquefaction process models with a completely reliable thermodynamics package, and so new nonsmooth algorithms were designed for the reasonable extrapolation of density from an equation of state under conditions where a given phase does not exist. This procedure greatly enhanced the ability of the nonsmooth inside-out algorithms to converge to physical solutions for mixtures at very high temperature and pressure.

These models and submodels were then integrated into a flowsheeting framework to perform realistic simulations of natural gas liquefaction processes robustly, efficiently and with extremely high accuracy. A reliable optimization strategy using an interior-point method and the nonsmooth process models was then developed for complex problem formulations that rigorously minimize thermodynamic irreversibilities. This approach significantly outperforms other strategies proposed in the literature or implemented in commercial software in terms of the ease of initialization, convergence rate and quality of solutions found. The performance observed and results obtained suggest that modeling and optimizing such processes using nondifferentiable models and appropriate sensitivity analysis techniques is a promising new approach to these challenging problems. Indeed, while liquefaction processes motivated this thesis, the majority of the methods described herein are applicable in general to processes with complex thermodynamic or heat transfer considerations embedded. It is conceivable that these models and algorithms could therefore inform a new, robust generation of process simulation and optimization software.

Thesis Supervisor: Paul I. Barton
Title: Lammot du Pont Professor of Chemical Engineering