MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX TECHNICAL SYSTEMS
MAGDEBURG
PROCESS SYSTEMS ENGINEERING

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Master Thesis Topic

Optimal system design and scheduling for ammonia production from renewables under uncertainty

Background and motivation

Defossilization confronts the chemical industry in particular with increasing challenges. One of the most important bulk products of the chemical industry is ammonia, whose production is solely responsible for more than 1% of global anthropogenic CO_2 emissions. Due to the primary use of ammonia for fertilizer production and the resulting correlation with population growth, a steady increase in ammonia demand is projected for the coming years. A promising approach to reduce CO_2 emissions associated with ammonia production is to generate the necessary electricity using renewable energy sources, such as solar and wind. However, their inherent dynamic energy availability poses challenges when coupled with chemical production plants. One approach to investigate the interaction between fluctuating renewables and chemical processes is to model the production network in the form of a mathematical optimization problem. Due to their computational efficiency, large-scale linear programming (LP) or mixed-integer linear programming (MILP) formulations are commonly used for this purpose. By optimizing various decision variables, optimal plant design and scheduling can be determined based on the availability of wind and solar resources. Additionally, a wide range of parameters is necessary to characterize the chemical production system, including process investment costs, wind speeds, solar irradiance, purchase and sales prices. These parameters are usually derived from literature data and fixed before optimization. However, parameters like costs or forecasts concerning the availability of renewables are not deterministic in reality but rather subject to uncertainty. Mathematical methods of optimization under uncertainty can be applied to deal with such deviations from the nominal parameter values. In particular stochastic programming and robust optimization are widely used methods to address parameter uncertainty in optimization problems and to identify solutions that satisfy all constraints under all possible realizations of uncertain parameters.
This project builds on previous and current work in the MPI PSE group centered on renewables-to-chemicals processes and superstructure optimization.

Objective

The purpose of this project is the identification of an optimal design and scheduling for a Power-to-Ammonia plant under consideration of uncertainty. Therefore, an existing deterministic optimization problem needs to be transformed into formulations considering uncertainty. Uncertainty is considered by solving the optimization problem once in the form of a stochastic programming problem and once in the form of a robust optimization problem.

Work plan

- Literature review: optimization under uncertainty (stochastic programming, robust optimization, probability distributions, uncertainty sets, statistical indicators), application of optimization under uncertainty in the area of Power-to-Ammonia/energy conversion systems
- Familiarize with time discretized superstructure optimization regarding ammonia production systems (modeling with the Python package Pyomo)
- Identification of interesting uncertain parameters with respect to Power-to-Ammonia superstructure optimization
- Reformulation of an existing deterministic Power-to-Ammonia optimization problem into a stochastic programming optimization problem and a robust optimization problem and solving the optimization problems under consideration of uncertainty
- Systematic comparison of the deterministic solution (design and scheduling) with the solutions under consideration of uncertainty (stochastic programming and robust optimization)

Requirements

- B.Sc. completed in chemical engineering, process engineering, or similar
- Experience in computational modeling and optimization
- Familiarity with formulating large-scale optimization problems is helpful
- Good skills with Python
- Interest in further developing software skills and knowledge regarding mathematical optimization
- Dedication and enthusiasm for research
- Ability to work systematically and independently

Start: according to arrangement

Duration: 20 weeks

Supervision: Alexander Klimek

Applications

Please email your application with CV and overview of grades to Alexander Klimek:

klimek@mpi-magdeburg.mpg.de

The Max Planck Society has set itself the goal of employing more severely disabled people. Applications from severely disabled people are expressly encouraged. The Max Planck Society strives for gender equality and diversity. Furthermore, the Max Planck Society aims to increase the proportion of women in areas where they are underrepresented. Women are therefore explicitly encouraged to apply. Please note the information on the collection of personal data at: https://www.mpi-magdeburg.mpg.de/data-protection-for-applicants.

Literature

C. Ganzer and N. Mac Dowell. “A comparative assessment framework for sustainable production of fuels and chemicals explicitly accounting for intermittency”. In: *Sustainable Energy & Fuels* 4.8 (2020), pp. 3888-3903. DOI: 10.1039/C9SE01239G.

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