



## **Optimal site-wide planning of a NH<sub>3</sub> network – A study on uncertain logistic constraints –**

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### **Highlights**

- Optimal scheduling for physically coupled production plants.
- Application to an NH<sub>3</sub> network at an integrated petrochemical production site.
- Investigation of uncertain logistics in the supply chain on the optimal schedule.

### **1. Introduction**

Many companies in the process industries operate in a highly competitive market environment and are thus obliged to improve continuously their production in terms of energy and material efficiency and to become greener [1]. In general, the value chain of chemical production consists of several, sometimes many production steps and complex interactions between these production steps exist, which lead to highly integrated and physically coupled systems of systems [2]. In large (petro-) chemical production sites, complex networks of flows of material and carriers of energy link the production plants. For an optimal operation of the overall system, mathematical modeling of the constituent systems and a joint optimization has to be employed to find site-wide optimal and feasible operating conditions according to different objectives such as material efficiency, reduction of carbon footprint, or economic performance indicators. The scope of such an optimization can, however, not be limited to the units and buffers of the production site, but it also has to consider exogenous influences such as fluctuating market prices for energy and raw materials and the logistics of their provision and distribution. Recently, there has been an increased interest in expanding the domain of optimization and thus enlarging the scope of the formulated optimization problems to include these aspects [3].

### **2. Method and case study**

In [4], a mixed-integer linear program (MILP) optimization model with an expanded scope that includes demand side management (DSM), network optimization, plant optimization, and logistic constraints has been proposed for site-wide scheduling of integrated petrochemical production sites. It has been parametrized to generate a one month optimal schedule for the NH<sub>3</sub> network of INEOS in Köln, a large petrochemical production site in Germany. The logistic constraints cover the deliveries to and the shipping of raw materials and base chemicals from the site via barges on the



river Rhine and via train vessels. The nature of the solution of MILP is that the resulting schedule operates at the bounds, e. g., a tank is emptied just before a barge arrives. In practice, however, many exogenous influences and thus also the logistic constraints are not known precisely ahead of time. For instance, in Germany in the summer of 2018, the river Rhine was at such low water levels that barges could only carry a fraction of their usual load or were even not able to deliver at all. Many chemical companies that are dependent on barge deliveries had to reduce their capacities or even had to shut down complete plants or production complexes.

### 3. Investigated scenario

In this contribution, we investigate the sensitivity of the optimal schedule for the operation of the INEOS in Köln production site with respect to this kind of events. We analyze the situation of a delayed barge, which is a common situation in daily operation. With the help of the formulated optimization model, we identify which measures should be taken in a critical situation. We investigate which process or plant has to reduce its load first or which production capacities can be shifted in order to ensure a seamless operation of the coupled production plants.

### 4. Conclusions

The analysis of the sensitivity of the optimal schedule for the operation of the NH<sub>3</sub> network at INEOS in Köln reveals important insights into where the site runs into critical limitations in a situation of unforeseen uncertain events such as delayed ships. The analysis is applicable to answer similar what-if scenarios for structurally related questions such as unforeseen equipment failures or plants shutdowns. The proposed optimization model offers a powerful tool to guide the planners' decisions at large (petro-) chemical production sites in the process industries.

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### References

- [1] R. Baños, F. Manzano-Agugliaro, F. G. Montoya, C. Gil, A. Alcayde, and J. Gómez, "Optimization methods applied to renewable and sustainable energy: A review," *Renew. Sustain. Energy Rev.*, vol. 15, no. 4, pp. 1753–1766, May 2011.
- [2] S. Engell and C. Sonntag, Eds., *Proposal of a European Research and Innovation Agenda on Cyber-physical Systems of Systems, 2016-2025*. CPSoS EU Project, 2016.
- [3] P. M. Castro, I. E. Grossmann, and Q. Zhang, "Expanding scope and computational challenges in process scheduling," *Comput. Chem. Eng.*, vol. 114, pp. 14–42, Jun. 2018.
- [4] S. Wenzel, Y.-N. Misz, K. Rahimi-Adli, B. Beisheim, R. Gesthuisen, and S. Engell, "An optimization model for site-wide scheduling of coupled production plants with an application to the ammonia network of a petrochemical site," (under review).