**Application of Iterative Real-time Optimization in an Intensified Continuous Plant at Pilot Plant Scale.**

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**Highlights**

* A lithiation process performed in an intensified tubular reactor is optimized.
* Modifier adaptation with quadratic approximation (MAWQA) is used.
* MAWQA identifies the plant optimum in the presence of plant-model mismatch.
* Concentrations are measured using an online NMR developed by BAM, Berlin.

**1. Introduction**

It is always of great interest to identify the optimal point of a plant and to operate it at this point. Usually, the optimal operating point of a plant is identified by solving a model-based optimization problem. Developing an accurate mathematical model and estimating its parameters require a large amount of time and effort. Sometimes it may not be possible at all to develop an accurate model due to the complex phenomena that take place in the plant. Modifier adaptation with quadratic approximation (MAWQA) [1] is an iterative optimization scheme which uses measurements from the plant to drive the plant to its true optimum in spite of the presence of significant plant-model mismatch.

**2. Methods**

In MAWQA, the iterative gradient-modification optimization (IGMO) method is combined with a derivative free optimization (DFO) method to estimate the plant gradients along with an additional surrogate model. We refer to [1] for a detailed description of the MAWQA algorithm. The process under consideration is a lithiation reaction that takes place in a tubular reactor in a containerized pilot plant. The pilot plant setup has been developed in the European project F3-Factory [2]. The reaction mechanism and its kinetic parameters are not precisely known. The overall reaction is depicted in Figure 1.



Figure 1: Overall lithiation reaction scheme

Due to the unavailability of the complete reaction information, the mathematical model of the process is incomplete and does not represent the behavior of the plant accurately.

The aim of the controller is to operate the process at its economically optimal operating point. This is enabled by real-time concentration measurements from a novel online NMR device that was developed by BAM, Berlin [3], in the context of the EU-funded project CONSENS [4].

The maximized plant profit function is: $profit= \frac{M\_{4}C\_{4} w\_{4}}{ρ} \sum\_{i}^{3}u\_{i}- \sum\_{i}^{3}w\_{i} u\_{i}.$ $M\_{4}, C\_{4}$ are molar mass $[\frac{kg}{mol}]$ and concentration $[\frac{mol}{m^{3}}]$ of Li-NDPA. $u\_{1}, u\_{2}, u\_{3}$ are feed flowrates [$\frac{kg}{h}]$ of Aniline, Li-HMDS and FNB. $w\_{1}, w\_{2}, w\_{3},w\_{4}$ are relative costs of reactants Aniline, Li-HMDS and FNB and product Li-NDPA. $ρ$ is the density $[\frac{kg}{m^{3}}]$ of the reaction mixture.

**3. Results and discussion**



Figure 2: Plant cost over MAWQA iterations in the validation experiment performed at the pilot plant in INVITE, Leverkusen

The evolution of the plant profit during the iterative optimization using the NMR measurements is shown in Figure 2. The blue line indicates the real plant profit as computed from the measurements whereas red line represents the plant profit as computed from the nominal model which has both structural and parametric plant-model mismatch. After an unknown change of the feed concentration of Li-HMDS, the algorithm managed to improve the plant profit (blue line) significantly. In contrast, the plant profit function that was predicted by the model drops as a fixed value for the feed concentration is assumed.

**4. Conclusions**

In summary, it was validated that the combination of the NMR measurements with the iterative optimization algorithm MAWQA could drive the plant to an optimal operation despite significant deviations between the plant model and the true plant behavior. MAWQA reacted quickly to changes in the process conditions and responded by making input moves to identify the true process optimum. Measurement delays caused by low sample flow rates and long piping between the reactor and the NMR device can be compensated using the methods proposed in [5].

**References**

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