

Production scheduling based on Real-time Optimization and Zone Control Nonlinear Model Predictive Controller

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ABSTRACT

The motivation of this work is an application of a production scheduling based on Real-Time Optimization and Zone Control Nonlinear Model Predictive Controller on a liquid recovery unit of an LPG production plant. In this unit, the scheduling-relevant disturbances occur on a time scale relevant to the system dynamics; thus, we propose a novel combination of a well-known control strategies leading to a hierarchical two-layered strategy, where the lower layer employs a zone control nonlinear model predictive controller (NMPC) to define inventory setpoints while the upper layer uses real-time optimization (RTO) to determine optimal plant-wide flow rates from an economic perspective. Unlike a traditional RTO, the proposed upper-layer problem is parameterized by product demands, with a distinct optimization problem formulated for each demand scenario. Our novel approach allows for proactive mitigation of potential inventory issues by dynamically recalculating the distribution of plant products. This approach addresses the challenges of storage bottlenecks and inventory fluctuations, and it is more effective than the typical operator decisions from an economic perspective in the system of interest.

Keywords: Process Operations, Planning & Scheduling, Model Predictive Control, Zone Control, Real-time Optimization

INTRODUCTION

Chemical industry has a high demand for process optimization methods and tools that enhance profitability while operating near the nominal capacity. The implementation of such methods can lead to significant productivity gains, particularly when the used strategy adopts a holistic perspective considering inventory [1,2].

Products inventory, both in-process and end-of-process, serve as buffers to mitigate fluctuations in operation and demand while maintaining consistent and predictable production. Efficient product inventory management is crucial for the profitable operation of chemical plants. To ensure optimal operation, various strategies have been proposed that consider in-process storage and aim to satisfy mass balances while avoiding bottlenecks [3].

When final product demand is highly oscillatory with unexpected stoppages, end-of-process inventories must be carefully controlled within minimum and maximum bounds. This prevents plant shutdowns and ensures

compliance with legal product supply requirements. In both cases, a plant-wide perspective should be considered when making in- and end-of-process product inventory level decisions to improve overall profitability [4].

To address this problem, we propose a holistic hierarchical two-layered strategy. The upper layer uses real-time optimization (RTO) to determine optimal plantwide flow rates from an economic perspective. The lower layer employs a zone control nonlinear model predictive controller (NMPC) to define inventory setpoints. The idea is that RTO defines setpoints for flow rates that manipulate plant throughput, while NMPC maintains inventory levels within desired bounds while keeping flow rates as close as possible to the RTO-defined setpoints.

Despite the fact that the individual strategies used here have been widely studied, the use of this two-layered holistic approach is novel for this specific problem and our main contribution; however, a secondary contribution is the introduction of an ensemble of optimization problems at the RTO level. Each RTO problem is associ-

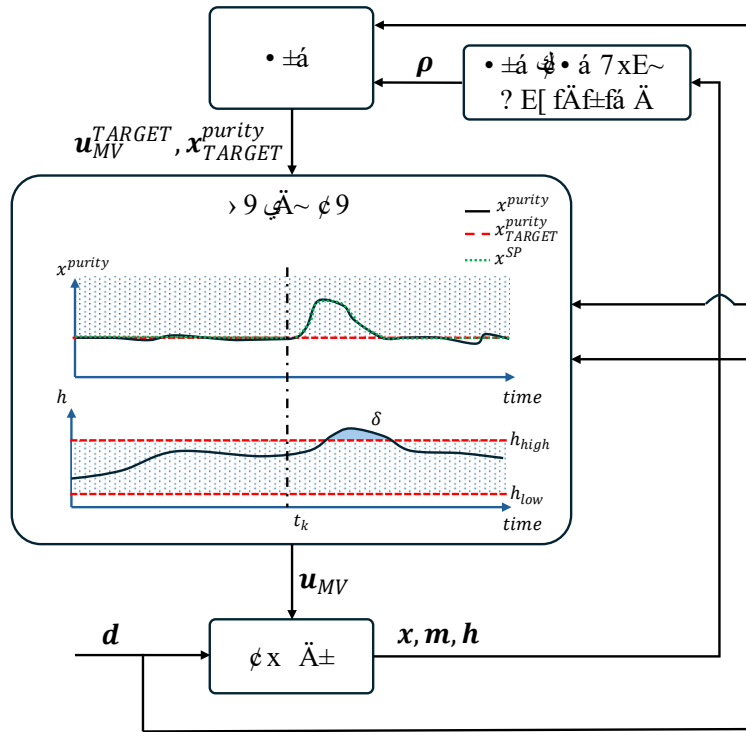


Figure 2: Block diagram of the proposed method. The variables that are sent between different blocks are indicated. The definition of the variables can be found in the Mathematical Formulation section. Inside the ZC-NMPC block, we illustrate an operating scenario and the action taken by the controller.

sequences that avoid costly set-ups and changeovers, reducing the duration and the lost product during transitions, avoiding schedules that lead to operational problems, using more precise and timely information in scheduling, etc. [1].

Traditional Formulation

A range of problem formulations is used for solving scheduling problems. Typically, a mixed-integer linear program is formulated to determine when and how the operating conditions should be modified, taking into account the timing of actions as well their feasibility [1].

In contrast, RTO optimizes an economic objective function subject to a detailed first principle steady-state model that describes the plant behavior. At each RTO sampling time, key parameters of the steady state model are updated to reduce the plant-model mismatch, using plant measurements [10]. Then, the setpoint values, obtained by the economic model optimization, are fed to the control layer below, typically a model predictive controller (MPC) [7].

MPC predicts future system behavior and calculates a sequence of control actions that minimize the deviation from the setpoints defined at the RTO level. The literature is rich in diverse MPC formulations. Here, we use zone control (ZC) MPC. This strategy is interesting when maintaining outputs within defined zones is more important

than achieving precise set point tracking. Therefore, while the outputs are within the pre-determined zone, the controller “gains” additional degrees of freedom that can be used to track other targets, such as input targets, giving the controller some flexibility [11].

Proposed Strategy

Figure 2 depicts the proposed strategy and illustrates how it works. Within the controller block (ZC-NMPC), we show a specific operating condition and the corresponding controller actions. The top plot displays the purity trajectory of one of the column's products, while the bottom plot shows the level of the associated tank. The dotted pattern in both plots indicates the desired operating zone for the controller: the product purity should be larger than the target value, and the tank level must remain within the defined low-high level limits.

In this illustrative scenario, we assume a sudden unexpected decrease in product demand at time t_k . Consequently, the tank level h begins to rise. The operator would typically respond by reducing the plant's overall feed rate to prevent tank overflow. While this action resolves the immediate issue, it can significantly impact plant profitability due to a decrease in the production of other products.

In contrast, when the proposed strategy is implemented, the controller takes two simultaneous actions.

Firstly, it increases the purity of the affected product. This higher purity typically leads to a reduced product flow rate, helping to stabilize the tank level. Secondly, the controller adjusts the operating conditions of the other columns within the plant based on the setpoints determined by the RTO level. This coordinated adjustment ensures that the tank level remains within safe operating limits while minimizing disruptions to the overall production process and maximizing plant profitability.

MATHEMATICAL FORMULATION

Before presenting the mathematical formulation of the RTO and ZC-NMPC layers, we introduce some useful simplifications used to model the liquid recovery unit.

First, we consider only 4 generic components in the system C_1 , C_2 , C_3 , and C_4 and assume constant relative volatility. The model keeps track of the fraction of the three lightest components in each tray of columns A , B , and C (i.e., from tray 1 to N_T). The fractions are represented by $\mathbf{x}$. Note that the fraction of the heaviest component (C_4) can be easily obtained from the other three.

The system inputs are divided into freely manipulated variables (column's reflux and boil-up rates) $\mathbf{u}_{MV}$ and the remaining input variables (distillate and bottoms flow rates) $\mathbf{u}_{DV}$. We also defined the process measured disturbances $\mathbf{d}$ (feed flow rate and composition, as well as product demands). We represent the system steady-state model as $\mathbf{f}$, which consists of mass balances and component mass balances, and the state and inputs feasible region as $\mathcal{X}$ and $\mathcal{U}$, respectively. Additionally, we define the operating constraints

$$\mathbf{g}(\mathbf{x}) = \begin{bmatrix} x_1^{purity} \\ x_2^{purity} \\ x_3^{purity} \\ x_4^{purity} \end{bmatrix} = \begin{bmatrix} x_{B,C1,N_T} - 0.07 \\ x_{B,C3,N_T} - 0.07 \\ (1 - \sum_{j=\{C1,C2,C3\}} x_{B,j,N_T}) - 0.002 \\ 0.95 - (1 - \sum_{j=\{C1,C2,C3\}} x_{C,j,1}) \end{bmatrix}, \quad (1)$$

where the first three algebraic equations from top to bottom represent the impurity constraints on the top product (tray N_T) of column B whereas the remaining algebraic equations represents a constraint on the purity of the bottom product of the third column C . The calculation " $1 - \sum \mathbf{x}$ " is made in order to obtain the fraction of the lightest component C_4 .

For the dynamic model, we need to define the holdup of all trays of the three columns, $\mathbf{m}$, as well as the levels in the tanks 1, 2, and 3, $\mathbf{h}$. The dynamic model $\mathbf{F}$ consists of (i) dynamic mass and component balances as well as, for each column, P-controllers relating the reboiler (stage 1) and condenser (stage N_T) with the respective variables in $\mathbf{u}_{DV}$; and (ii) dynamic mass balances of the tanks. The steady-state and dynamic models were based on [12].

Real-time Optimization (RTO) Layer

The RTO problem is posed as follows:

$$\begin{aligned} \max_{\mathbf{x}, \mathbf{u}_{MV}, \mathbf{u}_{DV}} \quad & \varphi \\ \text{s. t.} \quad & \mathbf{f}(\mathbf{x}, \mathbf{u}_{MV}, \mathbf{u}_{DV}; \mathbf{d}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{x}) \leq \mathbf{0} \\ & \mathbf{x} \in \mathcal{X} \\ & \mathbf{u}_{MV}, \mathbf{u}_{DV} \in \mathcal{U} \end{aligned} \quad (2)$$

All variables have been previously defined, with the exception of the economic objective function

$$\varphi = (\rho_1 D_A + \rho_2 D_B + \rho_3 D_C + \rho_4 B_C) - \rho_5 \sum_{i=\{A,B,C\}} V_i, \quad (3)$$

where D_i and V_i are the distillate and boil-up rates of column i , which are contained in $\mathbf{u}_{DV}$ and $\mathbf{u}_{MV}$, respectively. The weight vector $\boldsymbol{\rho} := [\rho_1, \rho_2, \rho_3, \rho_4, \rho_5]$ is determined based on the operating condition:

$$\boldsymbol{\rho} := \begin{cases} \text{if } h_{low} \leq \mathbf{h} \leq h_{high} & [0 \ 0 \ 0 \ 0 \ 0.01] \\ \text{if } h_1 \geq h_{high} & [0 \ -1 \ 0 \ 0 \ 0.01] \\ \text{if } h_2 \geq h_{high} & [0 \ 0 \ -1 \ 0 \ 0.01] \end{cases} \quad (4)$$

Each of these rules represent one desired operating scenario. The second rule, for example, indicates that in the case that the level of the tank storing the product of the second column reaches a high level condition, we want to minimize the second column distillate flow rate. Note that $\boldsymbol{\rho}$ is determined prior to the RTO execution based on the tank levels. Note also that the set of rules presented here is used only to illustrate how one can choose $\boldsymbol{\rho}$ based on the operating conditions. This set can be easily extended in order to encompass different operating scenarios depending on the practitioner needs.

Zone Nonlinear Model Predictive Control Layer

After solving Equation (2), the RTO solution is sent to the ZC-NMPC layer as purity targets $\mathbf{x}_{TARGET}^{purity}$, calculated using the relations in Equation (1), and manipulated variables targets $\mathbf{u}_{MV}^{TARGET}$. The control problem is:

$$\begin{aligned} \min_{\mathbf{u}_{MV}, \mathbf{x}_{i,k}^{SP}} \quad & \sum_{k=1}^{P_H} \left(\sum_{i=1}^4 (x_{i,k}^{purity} - x_{i,k}^{SP})^2 \right) \\ & + \gamma_1 \sum_{j=1}^6 (u_{MV,j,k} - u_{MV,j}^{TARGET})^2 \\ & + \gamma_2 \sum_{l=1}^3 \delta_l^2 \\ \text{s. t.} \quad & \begin{bmatrix} \mathbf{x}_{k+1} \\ \mathbf{m}_{k+1} \\ \mathbf{h}_{k+1} \end{bmatrix} = \mathbf{F}(\mathbf{x}_k, \mathbf{m}_k, \mathbf{h}_k, \mathbf{u}_{MV,k}, \mathbf{u}_{DV,k}; \mathbf{d}) \\ & |\mathbf{u}_{MV,k} - \mathbf{u}_{MV,k-1}| \leq \Delta u_{max} \\ & h_{low} \leq h_{l,k} + \delta_l \leq h_{high}, \quad l \in \{1,2,3\} \\ & 0 \leq x_{1,k}^{SP} \leq x_{1,TARGET}^{purity} \\ & 0 \leq x_{2,k}^{SP} \leq x_{2,TARGET}^{purity} \\ & 0 \leq x_{3,k}^{SP} \leq x_{3,TARGET}^{purity} \\ & x_{4,TARGET}^{purity} \leq x_{4,k}^{SP} \leq 1 \\ & \mathbf{x}_k \in \mathcal{X} \quad \mathbf{u}_{MV,k}, \mathbf{u}_{DV,k} \in \mathcal{U} \end{aligned} \quad (5)$$

where the subscript k indicates time. The variables in Equation (5) have been already defined except: x^{SP} that represents the setpoint of the purity targets that, due to zone control formulation, become variables in the problem. This means that x^{SP} can be freely changed by the controller given that the setpoints remain in the admissible zone purity; $\delta_{1,2,3}$ are slack variables for the tank level constraints. The plots in Figure 2 visually demonstrate the effect of slack variables. The high-level constraint on the tank level is briefly violated (indicated by the blue area in the plot). However, this violation incurs a penalty within the objective function. As a result, the controller actively seeks to decrease the tank level as quickly as possible to minimize this penalty and return to within the acceptable operating range.

In addition to the variables above, the control formulation has the parameters P_H that represents the controller prediction horizon, γ_1 and γ_2 that are weights of different terms in the objective function, and Δu_{max} that represents the maximum allowable input change.

Plant profitability is significantly enhanced by the target tracking term in the objective function of Equation (5). Since the RTO layer determined these target values to maximize overall plant profitability (i.e., maximize φ), the controller prioritizes keeping the manipulated variables as close as possible to these targets due to the inclusion of this term. This ensures that controller actions not only address immediate operational issues, such as the tank level violation, but also contribute to maintaining optimal economic performance across the entire plant.

CASE STUDY DESCRIPTION & RESULTS

As the case study, we chose a representative operation scenario where the demand of one of the tanks is suddenly interrupted at a given point in time as shown in Figure 3. The simulations start at a suboptimal point both from a steady-state economic perspective as well as from a product quality perspective, where the top product of the distillation column does not meet the purity constraint ($x_{B,C1,N_T} \not\leq 0.07$).

If the controller was not in place, the operator would first try to change the column operation to keep the product within the quality targets. After achieving the targets, they would handle the tank level problem. In the case of the demand decrease in Tank 2, they would monitor the level, and once it reaches a given threshold, they would decrease the unit load, significantly affecting the plant's profitability.

On the other hand, the controller reacts to both simultaneously. As the simulation begins, it immediately brings the fraction of C_1 at the top of column B within the admissible bounds (Figure 4 - middle plot). However, since the level is decreasing rapidly before the demand change at $t = 100$ min, the controller decisions lead to

purer distillate stream. The goal is to decrease the product flow rate. After the demand disturbance, we observe a short period where the top stream impurity increases, affecting the product quality.

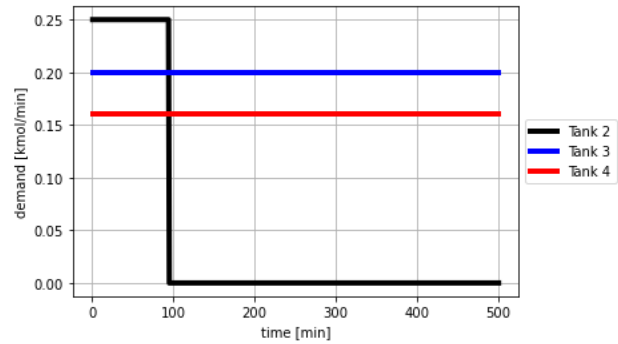


Figure 3. Change in the demand of Tank 2 at 99 minutes. Demands are in kmol/min

The proposed strategy then starts counteracting this effect immediately by increasing the reflux (Figure 4 - bottom plot). Next, the reflux rate is adjusted such that level constraint on Tank 2 is not violated. This effect can be seen in the slope change of the tank level trajectory (Figure 4 - top plot). Note that at time 500 minutes, the tank reaches the high-level threshold and the plant load will have to be decreased. However, this happens much later in comparison to the operator-based strategy, which can also give more time to the plant planning team to resolve the issue causing the demand problem.

CONCLUSIONS

This work demonstrates the application of a hierarchical two-tier control strategy combining Real-Time Optimization (RTO) and Zone Control Nonlinear Model Predictive Control (ZC-NMPC) to a liquid recovery unit of an LPG production plant. Results indicate that this approach has the potential to effectively address production scheduling challenges, and significantly reduce excessive inventory fluctuations. By dynamically adjusting plant flow rates based on real-time economic objectives and uncertain demand scenarios, the proposed strategy significantly outperforms traditional operator-based decisions in terms of economic performance.

Future work will be divided in two stages. First, the proposed method will be compared to a single layer economic ZC-MPC as well as to the typical operator decisions. Both strategies will serve as a baseline for the performance proposed method. Second, we will further develop the method envisioning a practical implementation. For example, the RTO layer will be replaced by a look-up table and, since the optimal purity targets typically lie on the constraints to avoid product give-away, the possibility of replacing the nonlinear control structure by a linear

control one will also be studied. Furthermore, the controller performance will be analyzed in face of different operating scenarios to evaluate its robustness and potential economic benefits.

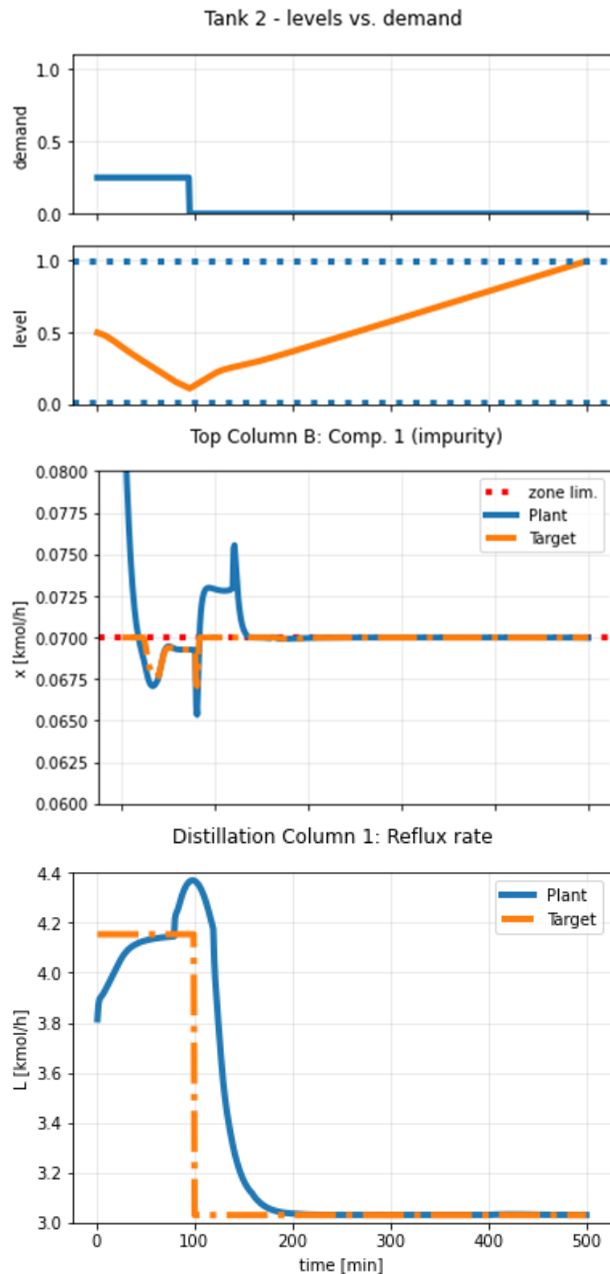


Figure 4. Case Study Results.

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