AN INDUSTRIAL CASE STUDY ON THE COMBINED IDENTIFICATION AND OFFSET-FREE MODEL PREDICTIVE CONTROL OF A CHEMICAL PROCESS*

Steven J. Kuntz [a,1], James J. Downs [b], Stephen M. Miller [b], James B. Rawlings [a]

[a] Department of Chemical Engineering, University of California Santa Barbara

[b] Eastman Chemical Company, Kingsport, Tennessee 37662, United States

Abstract

For three decades, model predictive control (MPC) has been the flagship advanced control method in the chemical process industries. However, most implementations still use heuristic methods for designing MPC estimators, especially for offset-free MPC implementations. In this paper, we present a recently developed maximum likelihood-based method for the identification of linear augmented disturbance models for use in offset-free MPC. This method provides noise covariances that are used to derive Kalman filters and moving horizon estimators, forgoing the need for manual design and tuning of the estimator. The method is extended to handle closed-loop plant data. We also discuss design strategies for safe and inexpensive identification experiments. The proposed identification method and estimator design are evaluated in industrial-scale, real-world case study of a process at Eastman Chemical's Kingsport plant.

Keywords

System identification, identification for control, model predictive control, offset-free model predictive control, subspace identification, closed-loop identification, disturbance identification.

1. Introduction

Model predictive control (MPC) is widely used in the chemical process industries as an advanced feedback control method (Qin and Badgwell, 2003). Some important factors in the success of MPC are its inherent robustness to disturbances and plant-model mismatch, and the ability to track setpoints without offset (Rawlings, Mayne, and Diehl, 2020, pp. 46-59, 204-214). As is often noted by industrial practitioners, MPC can be quite forgiving with respect to model errors, aging of the plant, changes in environmental conditions, and changes in operating conditions. As such, practitioners have long achieved sufficient performance with heuristic or out-of-date models, without rigorous methods of identifying both plant and disturbance models. As stake holders continue to demand greater performance from their processes, they require a system of best practices for identifying plant and disturbance models.

Process modeling and estimator design

Two simple linear process modeling methods are (1) using SISO identification methods with step response data (Caveness and Downs, 2005), and (2) linearizing a physical plant model (Rawlings et al., 2020, pp. 46-59). Neither approach provides the noise covariance estimates required to design a Kalman filter (KF) or moving horizon estimator (MHE) for the MPC implementation. While subspace methods such as canonical variate analysis (CVA) can be used to estimate the process and measurement noise covariances, they cannot be used to estimate the disturbance noise covariance (Qin, 2006; Larimore, 1990). Autocovariance least squares (ALS) can identify the complete disturbance model, but it has a high computational cost for minimum variance estimates and has not seen widespread adoption (Odelson, Rajamani, and Rawlings, 2006; Zagrobelny and Rawlings, 2015). Autoregressive integrating models (i.e., ARIX, ARIMAX, and vector equivalents) can be used in place of the linear augmented disturbance model (Sun, Zhao, and Qin, 2011). However, these approaches do not directly provide state space models, which are common to MPC theory and implementation.

We present a closed-loop extension of the algorithm proposed in Kuntz and Rawlings (2022). These identification algorithms are the only existing methods for estimating both the state-space model coefficients and the disturbance noise covariances required to implement offset-free MPC.

Towards closed-loop identification experiments

Adopting closed-loop identification experiments is an opportunity for significant safety and profitability improve-

* This work was supported by the National Science Foundation (NSF) under Grant 2138985.

1 Corresponding author: S. J. Kuntz (E-mail: skuntz@ucsb.edu).

ments. Closed-loop identification experiments can then be conducted online, at and around the optimal operating point, negating the cost of opening the loop to perform the experiment. New MPCs can then be implemented on processes controlled with other methods (PID, IMC, etc.) and existing MPCs be significantly improved with re-identified models. Closed-loop experiments can be conducted via setpoint perturbations that are more predictable and reliable than open-loop input perturbations. Moreover, the control loop is never broken, so the MPC is always enforcing constraints throughout the experiment.

While there are many closed-loop identification methods available in the literature, none have seen widespread adoption (van der Veen, van Wingerden, Bergamasco, Lovera, and Verhaegen, 2013). No existing method is able to identify both the plant and disturbance models, and as a result are not suited to offset-free MPC implementations. In this paper, we extend the algorithm of Kuntz and Rawlings (2022) to handle closed-loop data and show that the resulting algorithm provides consistent estimates of the plant and disturbance models.

Closed-loop experimentation requires an existing controller, meaning open-loop experiments for MPC design or PID tuning are still required. To this end we suggest suboptimal but safe experiments be done using traditional step-response designs, or loops be initially closed with PID methods. The algorithm proposed herein and in Kuntz and Rawlings (2022) will still handle open-loop step responses, and a closed-loop identification experiment may be run at later times to produce refined models on demand.

Summary

In this paper, we present a unified method for identifying linear augmented disturbance models. Our method systematizes the identification of new offset-free MPC models and design of new MPC estimators, allowing practitioners save time and achieve optimal estimator performance. To validate the viability of our method in the wider chemical process industries, we performed a case study on an existing process at Eastman Chemical's Kingsport, Tennessee location. The newly identified model shows clear improvement from the older step-response model. Moreover, we used a closed-loop experimental design that is desirable to operations engineers for its simplicity, safety, and ability to produce predictably high-quality data. The case study serves as a template for the use of our method to improve existing MPC performance.

2. Problem statement

The goal of our identification algorithm is to estimate the following *linear augmented disturbance model*,

$$\begin{aligned} x^+ &= Ax + Bu + B_d d + w \\ d^+ &= d + w_d \\ y &= Cx + C_d d + v \end{aligned} \qquad \begin{bmatrix} w \\ w_d \\ v \end{bmatrix} \sim N(0, S_d) \tag{1}$$

where $x \in \mathbb{R}^n$ is the model state, $u \in \mathbb{R}^{n_u}$ is the input (manipulated variables), $y \in \mathbb{R}^{n_y}$ is the output (measured variables), $d \in \mathbb{R}^{n_y}$ is the integrating disturbance state, w and v are the process and measurement noises and w_d is the driving noise for the disturbances. We assume (w, w_d, v) is uncorrelated in time. To identify this model, we need to augment a smaller model that we refer to as the *standard model*,

$$\begin{aligned} x^+ &= Ax + Bu + w \\ y &= Cx + v \end{aligned} \qquad \begin{bmatrix} w \\ v \end{bmatrix} \sim N\left(0, \begin{bmatrix} Q_w & \\ & R_v \end{bmatrix}\right) \tag{2}$$

Again, we assume (w, v) is uncorrelated in time.

It is worth noting that the particular disturbance model parameters (B_d, C_d) are (mostly) inconsequential to the performance of the offset-free controller. Consider the following sufficient condition for offset-free performance (Rajamani, Rawlings, and Qin, 2009):

$$\operatorname{rank} \begin{bmatrix} A - I & B_d \\ C & C_d \end{bmatrix} = n + n_d \tag{3}$$

For each (A, B, C) *all* disturbance models (B_d, C_d) that satisfy (3) are equivalent up to a similarity transformation, making it unnecessary to estimate the parameters (B_d, C_d) from data. In the special case where A contains no integrators, the so-called *output disturbance model* $(B_d, C_d) = (0, I_{n_y})$ satisfies the rank condition (3). This special case is a numerically advantageous choice in our algorithm.

3. Closed-loop subspace identification

Background and notation

Subspace identification revolves around Kalman predictor and estimator forms of the model (2) (Qin, 2006). There exists a steady-state Kalman gain K and innovation error covariance R_e such that $A_K := A - KC$ is stable and

$$\hat{x}^+ = A_K \hat{x} + B_K z, \qquad e := y - C\hat{x} \overset{iid}{\sim} N(0, R_e) \tag{4}$$

where $B_K := [B,\ K]$, $\hat{x} \in \mathbb{R}^n$ are the state estimates, and $z := [u'\ y']'$ is the combined input-output data.

We will use the following notation in this section. Given a signal $\{a(k)\}$ and integers p, f, we write the "past" and "future" horizons of lengths p and f as

$$\begin{aligned} A_p(k) &:= \begin{bmatrix} a(k-1)' & \dots & a(k-p)' \end{bmatrix}' \\ A_f(k) &:= \begin{bmatrix} a(k)' & \dots & a(k+f-1)' \end{bmatrix}' \end{aligned}$$

and we write the following block matrices

$$\mathcal{G}_f := \begin{bmatrix} 0 & & & \\ G_1 & 0 & & \\ \vdots & \ddots & \ddots & \\ G_{f-1} & \dots & G_1 & 0 \end{bmatrix}, \qquad \mathcal{O}_f := \begin{bmatrix} C \\ CA_K \\ \vdots \\ CA_K^{f-1} \end{bmatrix}$$

$$\mathcal{K}_p := \begin{bmatrix} B & A_K B & \dots & A_K^{p-1} B \end{bmatrix}$$

$$\mathcal{H}_{f,p} := \begin{bmatrix} G_1 & G_2 & \dots & G_p \\ \vdots & \vdots & & \vdots \\ G_f & G_{f+1} & \dots & G_{f+p-1} \end{bmatrix} = \mathcal{O}_f \mathcal{K}_p$$

where $G_i := CA_K^{i-1}B_K$ are the impulse response coefficients of (4). For any two signals $\{a(k)\}_{k\in\mathbb{I}_a}$ and $\{b(k)\}_{k\in\mathbb{I}_b}$, we denote the sample covariance operator as $S\{a,b\} = \frac{1}{N_{ab}}\sum_{k\in\mathbb{I}_a\cap\mathbb{I}_b} a(k)b(k)'$ where N_{ab} is the number of elements in $\mathbb{I}_a\cap\mathbb{I}_b$, and the index sets $\mathbb{I}_a,\mathbb{I}_b$ are implied from context. We assume $p,f \geq n$ throughout.

Estimating the impulse response coefficients

First, we seek to estimate the coefficients G_i. Given any p large enough so that $A_K^p \approx 0$, we can recursively solve (4) to write the state as follows,

$$\hat{x}(k) = A_K^p\hat{x}(k-p) + \mathcal{K}_p Z_p(k) \approx \mathcal{K}_p Z_p(k) \tag{6}$$

We can also write the following higher-order ARX (HOARX) model,

$$y(k) \approx C\mathcal{K}_{\overline{p}} Z_{\overline{p}}(k) + e(k) \tag{7}$$

where $\overline{p} := \max\{f,p\}$. Notice that the coefficients are a linear function of the first $\overline{p}$ impulse response coefficients, $C\mathcal{K}_{\overline{p}} = \begin{bmatrix} G_1 & G_2 & \ldots & G_{\overline{p}} \end{bmatrix}$. The ML estimates of the impulse response coefficients in the HOARX model (7) are given by

$$\widehat{C\mathcal{K}_{\overline{p}}} = S\{y, Z_{\overline{p}}\}S^{-1}\{Z_{\overline{p}}, Z_{\overline{p}}\} \tag{8}$$

The estimates (8) are unbiased.[2] Moreover, the estimate errors $\mathcal{E}_{\text{HOARX}} := \widehat{C\mathcal{K}_{\overline{p}}} - C\mathcal{K}_{\overline{p}} = [\hat{G}_1 - G_1, \ldots, \hat{G}_{\overline{p}} - G_{\overline{p}}]$ are independent of the innovation sequence $e(k)$ and regression vectors $Z_{\overline{p}}(k)$.

Estimating the state sequence

In the notation above we can write the following extended state-space model

$$Y_f(k) \approx \mathcal{H}_{f,p}Z_p(k) + \mathcal{G}_f Z_f(k) + E_f(k) \tag{9}$$

For closed-loop data, the future data term $\mathcal{G}_f Z_f(k)$ is correlated with the error vector $E_f(k)$ (Qin, 2006). Noting that the future data coefficients $\mathcal{G}_f$ is simply a linear function of the HOARX coefficients, i.e. $\mathcal{G}_f = \mathcal{L}(C\mathcal{K}_{\overline{p}})$, the future data term in the model (9) can be "pre-estimated" as follows,

$$\tilde{Y}_f(k) := Y_f(k) - \hat{\mathcal{G}}_f Z_f(k) \approx \mathcal{H}_{f,p}Z_p(k) + \mathcal{E}_{\text{ESS}}(k) \tag{10}$$

where $\hat{\mathcal{G}}_f = \mathcal{L}(\widehat{C\mathcal{K}_{\overline{p}}})$, and $\mathcal{E}_{\text{ESS}} := \mathcal{L}(\mathcal{E}_{\text{HOARX}})Z_f + E_f$ is zero-mean since $\mathcal{E}_{\text{HOARX}}$ and Z_f are independent.

According to Ho and Kalman (1966), $\mathcal{H}_{f,p}$ must have rank less than or equal to n, so we estimate it using reduced-rank regression. According to Larimore (1990); Anderson (1999), the ML estimate of $\mathcal{H}_{f,p}$ of rank n for the model (10) is given by

$$\hat{\mathcal{H}}_{f,p} = S\{\tilde{Y}_f, Z_p\}J_n'J_n$$

where J_n denotes the first n rows of $J = U'S^{-1/2}\{Z_p, Z_p\}$, and U are the left singular vectors of the following singular value decomposition,

$$S^{-1/2}\{Z_p,Z_p\}S\{Z_p,Y_f\}S^{-1/2}\{Y_f,Y_f\} = USV'$$

[2] This neglects numerical errors introduced by the approximation $A_K^p \approx 0$.

Given these estimates, we have the rank factorization $\hat{\mathcal{H}}_{f,p} = \hat{O}_f\hat{\mathcal{K}}_p$ where $\hat{O}_f = S\{\tilde{Y}_f, Z_p\}J_n'$ and $\hat{\mathcal{K}}_p = J_n$. Moreover, the estimate $\hat{\mathcal{K}}_p$ is a consistent and asymptotically normal estimator of $\mathcal{K}_p$ (up to similarity transformation). Therefore, we have consistent and asymptotically normal estimates of the states,

$$\tilde{x} = J_n Z_p \tag{11}$$

Estimating the state-space parameters

Treating the state sequence (11) as the true states, ML estimates of the parameters of (2) are

$$\begin{bmatrix}\hat{A} & \hat{B}\end{bmatrix} = S\{\tilde{x}^+, t\}S^{-1}\{t,t\} \tag{12a}$$

$$\hat{C} = S\{y,\tilde{x}\}S^{-1}\{\tilde{x},\tilde{x}\} \tag{12b}$$

$$\hat{Q}_w = S\{\tilde{x}^+,\tilde{x}^+\} - S\{\tilde{x}^+,t\}S^{-1}\{t,t\}S\{t,\tilde{x}^+\} \tag{12c}$$

$$\hat{R}_v = S\{y,y\} - S\{y,\tilde{x}\}S^{-1}\{\tilde{x},\tilde{x}\}S\{\tilde{x},y\} \tag{12d}$$

where $t = [\tilde{x}', u']'$. Since $\tilde{x}$ are consistent estimates and independent of the errors (w,v), the estimates (12) are consistent. This completes the closed-loop identification of the model (2) from an input-output sequence.

4. Closed-loop disturbance model identification

Choosing the disturbance model

As previously discussed, the disturbance model (B_d, C_d) can be chosen to maximize interpretability of the model (1). We propose general guidelines for choosing the disturbance model below.

- If $\hat{A}$ does not contain integrators, use an output disturbance model.
- If $\hat{A}$ contains integrators and $n_u = n_y$, use an input disturbance model, $(B_d, C_d) = (B, 0)$.
- Otherwise, use some combination of input and output disturbances, i.e. $(B_d, C_d) = (B\tilde{I}_1, \tilde{I}_2)$ where $\tilde{I}_1$ and $\tilde{I}_2$ are diagonal matrices with zeros and ones on the diagonal and collectively n_y nonzero elements.

Models in these forms retain interpretability while ensuring that the rank condition (3) is satisfied.

Estimating the disturbance sequence

Given a model of the form (2), a disturbance model (B_d, C_d), and a state sequence $\{\tilde{x}(k)\}_{k=p}^N$, we treat the disturbance sequence $\{d(k)\}_{k=0}^{N-1}$ as accounting for the long-range model errors. That is, the long-range output is

$$y(k) = \hat{C}\hat{A}^{k-p}\tilde{x}(p) + \sum_{j=0}^{k-1}\hat{C}\hat{A}^{k-j-1}\hat{B}u(j) + \sum_{j=0}^{k-1}\hat{C}\hat{A}^{k-j-1}(B_d d(j) + w(j)) + C_d d(k) + v(k)$$

and the *predicted* long-range output is

$$\hat{y}(k) := \hat{C}\hat{A}^{k-p}\tilde{x}(p) + \sum_{j=0}^{k-1} \hat{C}\hat{A}^{k-j-1}\hat{B}u(j) \tag{13}$$

Next, we define the long-range prediction error as $z(k) := y(k) - \hat{y}(k)$ which gives

$$z(k) = \sum_{j=0}^{k-1} \hat{C}\hat{A}^{k-j-1}(B_d d(j) + w(j)) + C_d d(k) + v(k)$$

Rewriting this as a linear model,

$$\mathbf{z} = \mathcal{A}\mathbf{d} + \mathcal{B}\mathbf{w} + \mathbf{v}, \qquad \mathcal{B}\mathbf{w} + \mathbf{v} \sim N(0, \mathcal{V}) \tag{14}$$

where $\mathbf{z} := [z(p)', \ldots, z(N)']'$ is the sequence of long-range prediction errors, $\mathbf{d} := [d(p)', \ldots, d(N)']'$ is the sequence of disturbances, $\mathbf{w} := [w(p)', \ldots, w(N)']'$ and $\mathbf{v} := [v(p)', \ldots, v(N)']'$ are the process and measurement noise sequences, and

$$\mathcal{B} := \begin{bmatrix} 0 & & & \\ B_1 & 0 & & \\ \vdots & \ddots & \ddots & \\ B_{N-1} & \ldots & B_1 & 0 \end{bmatrix}, \qquad B_j := \hat{C}\hat{A}^{j-1},$$

$$\mathcal{A} := \mathcal{B}(I \otimes B_d) + (I \otimes C_d), \qquad \mathcal{V} := \mathcal{B}(I \otimes Q_w)\mathcal{B}' + I \otimes R_v$$

The model (14) has a MLE solution due to Rao (1971) and (Magnus and Neudecker, 2019, p. 313):

$$\hat{\mathbf{d}} = (\mathcal{A}'\mathcal{V}_0^{\dagger}\mathcal{A})^{\dagger}\mathcal{A}'\mathcal{V}_0^{\dagger}\mathbf{z} \tag{15}$$

where $\mathcal{V}_0 := \mathcal{V} + \mathcal{A}\mathcal{A}'$. This is an $O(N^3)$ computation with $O(N^2)$ memory requirements. Notice that when $B_d = 0$ and $C_d = I$, we have $\mathcal{A} = I$, $\mathcal{V}_0 = \mathcal{V} + I$ invertible, and

$$(\mathcal{A}'\mathcal{V}_0^{\dagger}\mathcal{A})^{\dagger}\mathcal{A}'\mathcal{V}_0^{\dagger} = \mathcal{V}_0\mathcal{V}_0^{-1} = I$$

Therefore (15) is equivalently written

$$\hat{d}(k) = z(k) \tag{16}$$

which is an $O(N)$ computation without additional memory requirements. It is clear that whenever the system is free of integrators, the simplified solution (16) is computationally advantageous. A similarity transformation can be used to find the desired disturbance model after the output disturbance model is found (Rajamani et al., 2009).

Estimating the noise covariances

Given the estimated states and disturbances, one can stack the equations (1) to write a simple covariance estimation problem,

$$\tilde{e}(k) := \begin{bmatrix} \tilde{x}(k+1) \\ \hat{d}(k+1) \\ y(k) \end{bmatrix} - \begin{bmatrix} \hat{A} & B_d & \hat{B} \\ 0 & I & 0 \\ \hat{C} & C_d & 0 \end{bmatrix} \begin{bmatrix} \tilde{x}(k) \\ \hat{d}(k) \\ u(k) \end{bmatrix} \overset{iid}{\sim} N(0, S_d)$$

The ML estimate of S_d is therefore $\hat{S}_d = S\{\tilde{e}, \tilde{e}\}$ (Anderson, 2003, Thm. 8.2.1). Thus, we have found the complete set of parameters for the model (1), which concludes our description of the algorithm.

5. Case study

Process of interest

To evaluate the proposed closed-loop identification algorithm and experimental design, a case study was conducted on a reactor at Eastman Chemical's plant in Kingsport, Tennessee. The chosen process is similar to that used in Caveness and Downs (2005). The process produces dimethyl terephthalate (DMT) by reacting terephthalic acid (TPA) with methanol (MeOH). Water is a byproduct of the reaction. The primary equilibrium reaction can be represented as

$$\text{TPA} + 2\text{MeOH} \rightleftharpoons \text{DMT} + 2\text{H}_2\text{O}$$

TPA is a solid and enters the reactor in a slurry with methanol, and additional methanol enters as a vapor. The reactor has two phases. The reaction takes place in a liquid phase, and the DMT product, water, excess methanol, and side products leave the reactor as a vapor and move forward to a DMT purification section. Xylene is added as reflux to minimize the carryover of an impurity that results from the half reaction of TPA and methanol. Xylene does not participate in the reaction. A schematic of the reactor is shown in Figure 1.

The reactor operates under pressure, which is controlled by manipulating a valve in the vapor line. Heat is supplied to the reboiler by circulating hot oil through the shell side of the exchanger. A temperature controller manipulates the flow of hot fluid supplying the circulation loop to control the temperature of the heating fluid entering the reboiler. Liquid level is controlled by manipulating the xylene reflux. Any change in the material balance that affects the composition of methanol in the reactor has a large influence on reactor temperature. Infinite-horizon MPC is used to control the reactor temperature, T, and the production rate (ultimately set by the slurry feed, F_2) and to maintain the methanol feed, F_1, at a desired rate. The MPC also handles constraints on two quality-control variables, r_1 and r_2, and on the hot oil controller valve position (used to infer a temperature pinch/constraint on hot oil temperature, T_H). The manipulated variables are the PID loop setpoints for the inlet flowrate and utility temperature controllers, denoted $(\overline{F}_1, \overline{F}_2, \overline{T}_H)$.

The control objectives are to (1) achieve offset-free setpoint tracking and disturbance rejection, and (2) avoid violating box constraints on the measured and manipulated variables. For several decades the reactor has run on an MPC designed with a step response model (to be referred to as the "old MPC model") and hand-tuned estimator, as described in Caveness and Downs (2005). The inlet flowrate "measurements" are "wrap-around" variables and are supplied as their PID setpoints, passed through first-order filters. The MPC runs at a sample time of 5 seconds.

Identification

To identify the process, we used a closed-loop experimental design based on pulses to the normal MPC setpoints. Eight setpoint pulses were applied, each lasting about 30 minutes, with 30 minute "rests" between the pulses to allow the process to settle back to the normal operating point.

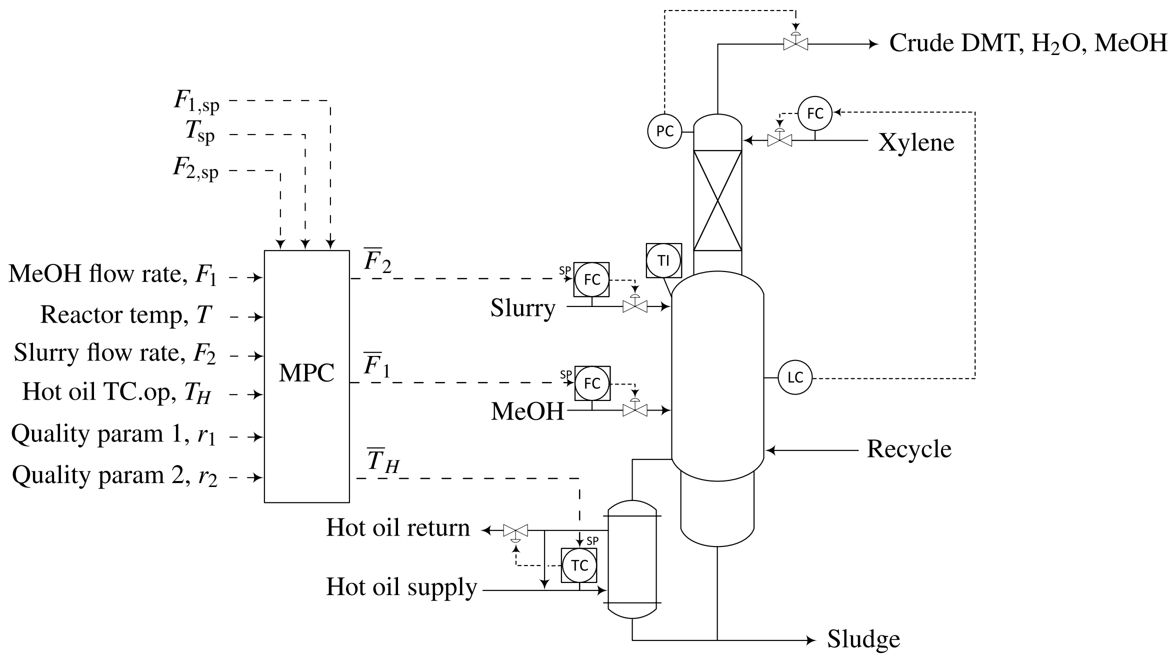

Figure 1: Schematic of the DMT reactor and MPC control strategy.

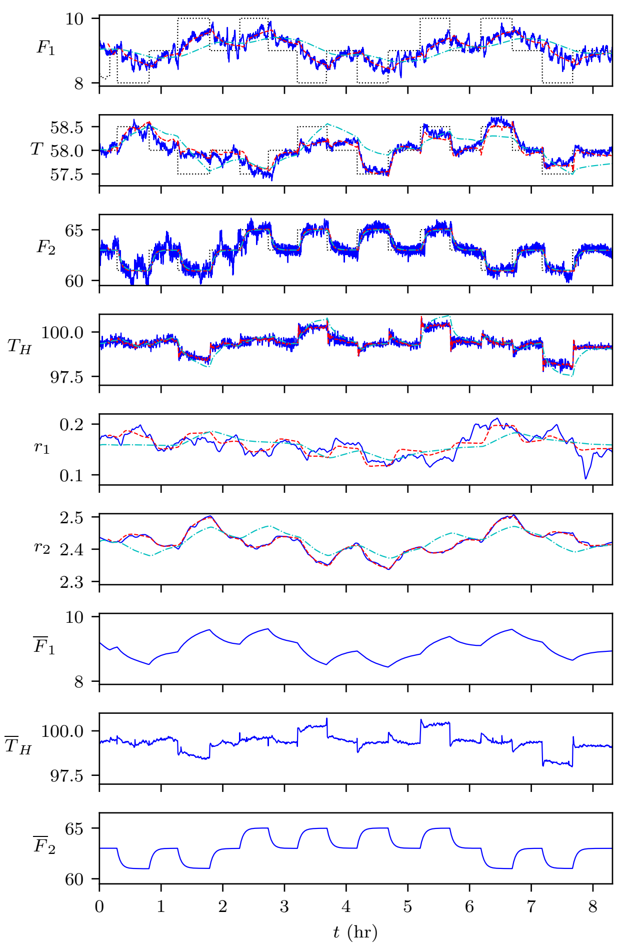

Figure 2: Anonymized data (solid blue), MPC setpoints (dotted black), old model predictions (dot-dashed cyan), and new model predictions (dashed red) for the closed-loop experiment. Predictions are computed from (13). The model was fit with $n = 19$, $p = 100$, and $f = 100$.

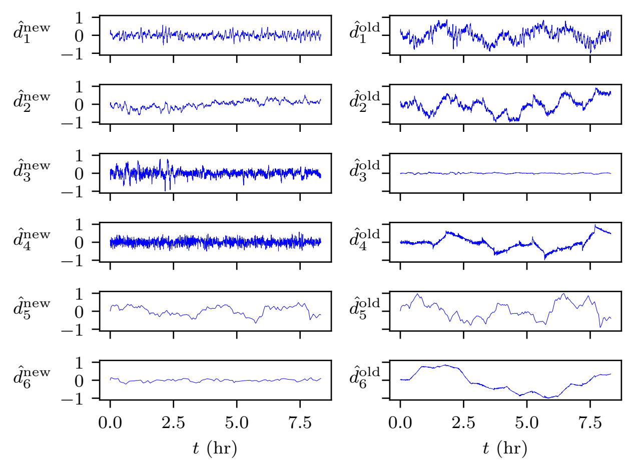

Figure 3: Disturbance estimates generated using steady-state Kalman filter with (left) new model and (right) old model.

The setpoint pulses correspond to a full factorial design of the three controlled variables.[3] The pulses were designed to keep the manipulated and measured variables within constraints, and they were checked against historical data to ensure production would not be negatively affected.

The process response, the model predictions of the existing MPC model, and the model predictions for the newly identified model are shown in Figure 2. Each process variable was shifted and scaled to anonymize the data. Over the series of changes to the MPC setpoints, the temperature T and the methanol flow rate F_1 consistently failed to reach their targets. This is due to plant-model mismatch with the old MPC model, as that model incorrectly predicts that the tempera-

[3] Because the manipulated and controlled variables form a square system, we could perturb the setpoints without worrying about correlation in the manipulated variables.

ture will reach setpoint, and the model-predicted transitions of methanol flow rate are much more sluggish than in reality. As illustrated in Figure 2, the newly identified model closely matches the process. In particular, the temperature predictions of the new model are significantly improved over those of the old model.

Using the new and old models, we computed steady-state Kalman filter gains and applied them to the identification dataset to compute the filtered disturbance estimates $\hat{d}$. These disturbances are plotted in Figure 3, with each disturbance centered and re-scaled to facilitate comparison between the new and old model disturbance estimates. While the old model disturbance estimates are correlated with the inputs (right), the new model estimates are uncorrelated with the inputs (left). This suggests the new model disturbances are intrinsic rather than arising from plant-model mismatch. There are significant reductions in some of the disturbance covariances, suggesting the new model has changed significantly, although it is hard to predict how this will impact the estimator performance or overall closed-loop performance.

6. Conclusion

We present a method for identifying linear augmented disturbance models from closed-loop data, which provides all necessary information to design the MPC estimator. The method is tested on an existing reactor at Eastman Chemical's Kingsport, Tennessee plant. We show the method is able to fit process models from both filtered and unfiltered measurements. Moreover, the ability to use closed-loop data allows practitioners to safely and cheaply identify and re-identify their processes.

There are many possibilities in future case studies of this technology, including comparisons across competing methods (ALS, EM) and computational studies. To follow up on the present case study, the same closed-loop experiment (setpoint deviations) will be performed using the newly identified model. We will compare the closed-loop performance of MPC using the two different models over a steady-state period and setpoint tracking period in order to determine if model re-identification leads to improved tracking performance.

References

T. W. Anderson, "Asymptotic distribution of the reduced rank regression estimator under general conditions," vol. 27, no. 4, pp. 1141–1154, Aug. 1999.

——, *An Introduction to Multivariate Statistical Analysis*, 3rd ed. New York: John Wiley & Sons, 2003.

M. H. Caveness and J. J. Downs, "Reactor control using infinite horizon model predictive control," AIChE Spring Meeting, Atlanta, GA, April 2005.

B. L. Ho and R. E. Kalman, "Efficient construction of linear state variable models from input/output functions," *Regelungstechnik*, vol. 14, pp. 545–548, 1966.

S. J. Kuntz and J. B. Rawlings, "Maximum likelihood estimation of linear disturbance models for offset-free model predictive control," in *American Control Conference*, Atlanta, GA, June 8–10, 2022, pp. 3961–3966.

W. E. Larimore, "Canonical variate analysis in identification, filtering, and adaptive control," in *Proceedings of the 29th Conference on Decision and Control*, 1990, pp. 596–604.

J. R. Magnus and H. Neudecker, *Matrix Differential Calculus with Applications in Statistics and Econometrics*, 3rd ed. Hoboken, NJ: John Wiley & Sons Ltd., 2019.

B. J. Odelson, M. R. Rajamani, and J. B. Rawlings, "A new autocovariance least-squares method for estimating noise covariances," vol. 42, no. 2, pp. 303–308, Feb. 2006.

S. J. Qin, "An overview of subspace identification," vol. 30, pp. 1502–1513, 2006.

S. J. Qin and T. A. Badgwell, "A survey of industrial model predictive control technology," vol. 11, no. 7, pp. 733–764, 2003.

M. R. Rajamani, J. B. Rawlings, and S. J. Qin, "Achieving state estimation equivalence for misassigned disturbances in offset-free model predictive control," vol. 55, no. 2, pp. 396–407, Feb. 2009.

C. R. Rao, "Unified theory of linear estimation," vol. 33, no. 4, pp. 371–394, 1971.

J. B. Rawlings, D. Q. Mayne, and M. M. Diehl, *Model Predictive Control: Theory, Design, and Computation*, 2nd ed. Santa Barbara, CA: Nob Hill Publishing, 2020, 770 pages, ISBN 978-0-9759377-5-4.

Z. Sun, Y. Zhao, and S. J. Qin, "Improving industrial MPC performance with data-driven disturbance modeling," in *2011 50th IEEE Conference on Decision and Control and European Control Conference*, Dec. 2011, pp. 1922–1927.

G. van der Veen, J.-W. van Wingerden, M. Bergamasco, M. Lovera, and M. Verhaegen, "Closed-loop subspace identification methods: an overview," vol. 7, no. 10, pp. 1339–1358, 2013.

M. A. Zagrobelny and J. B. Rawlings, "Identifying the uncertainty structure using maximum likelihood estimation," in *American Control Conference*, Chicago, IL, July 1–3, 2015, pp. 422–427.