Reaction profile control of the continuous pulp digester

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Abstract

In this work, a model-based control strategy is presented for the Kappa number profile control of a continuous pulp digester. The strategy employs an empirically derived process model using subspace identification techniques. A state-space model predictive control algorithm is used to adjust five manipulated inputs in order to regulate five process outputs, in response to five randomly varying process disturbances (of which three are measurable). Profile sensitivity to closed-loop response is also explored. © 1999 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Kraft pulping is the most common chemical pulping process which normally utilizes a continuous digester. Yearly US wood pulp production is around 52 million tons with approximately 400 (Kamyr) continuous digesters in operation. Digesters are very capital intensive ($50–$100 million), yet their performance is of paramount importance to maximize the produced pulp quality and yield, reduce the overall operating costs and minimize the adverse environmental impacts of pulp mills. With more pulp and paper companies replacing their pulping processes with modern fiberlines using continuous digesters to meet increasing competitiveness in the global market place and tighter environmental regulations, there is an increasing need for improved control of digesters.

Continuous digesters are very complex plug-flow reactors in which the lignin that binds wood chips together is broken down through a combination of chemical and thermal effects. A number of cocurrent and counter current zones are employed in a typical configuration (see Fig. 1). Some of the challenging characteristics of these reactors which preclude efficient control include: (i) long residence times (on the order of 10 h), (ii) complex non-linear dynamic behavior, (iii) key process variables are unmeasurable in real time, and (iv) the biological feedstock varies stochastically. The key quality variable is the Kappa number (see Notation for formal definition), which represents the degree of delignification. Consequently, this quantity is directly correlated with the extent of reaction. Although accurate fundamental models of this unit operation have been available for some time (Christensen et al., 1982), recent work has extended these descriptions to include more accurate transport and reaction effects (Wisnewski et al., 1997). The models that result are distributed in nature and must be converted to a lumped form for control design, and possibly reduced in dynamic order (Wisnewski et al., 1998c).

The key idea in this work is that the Kappa number profile (and corresponding liquor concentration profile) should be tightly managed to improve the overall operation of this reactor (Kayihan, 1997a, 1998). This is completely consistent with temperature profile control in fixed bed reactors, however, in the present case, the process variable measurement is difficult, if not impossible, to obtain. In this work, a model predictive control approach will be presented for Kappa number profile control. An inferential configuration will be introduced which allows the estimation of the unmeasured Kappa profile. Hence, the available measurements and the fundamental model are utilized in an efficient manner to reproduce the profile which is to be controlled. The motivation for this approach is to maintain critical fiber
properties such as strength, which depend on the reaction path as well as the final conversion.

2. Process description

Continuous digesters are very complex vertical tubular reactors. An aqueous solution of sodium hydroxide and hydrosulfide, called white liquor, is used to react with porous and wet wood chips. Usually, continuous digesters are separated into multiple reaction and extraction zones to carry out the specific process sequence. Depending on the production needs of a pulp mill and on the state of the art of digester design at the time of installation, there may be numerous differences between digesters. However, common to all is the general sequence of transport and reaction processes that govern the overall operation. Due to the complexities of these physical and chemical phenomena and the fact that wood chips are nonuniform and constantly changing, regulating product quality in a digester is a non-trivial task.

Wet chips are steamed to remove air in the pores and fed into the impregnation vessel (IV) (see Fig. 1) together with white liquor. In the impregnation vessel, white

Fig. 1. Schematic of a continuous digester showing key reaction zones.
liquor penetrates into the chips and equilibrates with initial moisture for about 30 min depending on the production rate. In the IV, both chips and liquor move in the cocurrent downward direction.

From the IV, the chips are carried into the top section of the digester with hot liquor that brings the mixture to the desired reaction temperature. The top section of the digester, referred to as the cook zone, is a cocurrent section where the main reactions take place. Chips react with the liquor that replenish the active ingredient holdup in the pores. Spent liquor saturated with dissolved solids is instantly mixed with white liquor at the feed conditions. Other important factors are the yield of lignin, important process and the model represents a much-simplified approach due to the space velocities based on compaction and volumetric flowrates.

7. Reaction kinetics follow the suggestions of the ‘Purdue Model’ (Christensen, 1982) but the heats of reactions are ignored.

8. Reactions and mixing during the process affect solid and liquor densities but not volumes, i.e. volumes are conserved.

9. Wood extractives are ignored and initial moisture is instantly mixed with white liquor at the feed conditions.

10. Delignification reactions occur only in the digester vessel.

4. Model equations

There are 10 partial differential equations (PDEs) which comprise the mass and energy balances for each of the zones in the digester (five wood components, four liquor compositions, one temperature). In the cook zone, where both solid and liquor phases are moving in the same direction, the equations are

\[
\frac{\partial \rho_{Si}}{\partial t} = -v_S \frac{\partial \rho_{Si}}{\partial z} + R_{Si}, \quad i = 1, \ldots, 5, \tag{1}
\]

\[
\frac{\partial \rho_{Lj}}{\partial t} = -v_L \frac{\partial \rho_{Lj}}{\partial z} + R_{Lj}, \quad j = 1, \ldots, 4, \tag{2}
\]

\[
(1 + \alpha) \frac{\partial T}{\partial t} = -v_S (1 + \omega_L/v_S) \frac{\partial T}{\partial z}. \tag{3}
\]

where the solid and liquor ‘velocities’ are given by

\[
v_S = \frac{v_S}{A(1 - \eta)}, \quad v_L = \frac{v_L}{A\eta} \tag{4}
\]

and the constant \( \alpha \) is given by

\[
\alpha = \eta C_{PL} \rho_L/(1 - \eta) C_{PS} \approx \eta/(1 - \eta). \tag{5}
\]

The corresponding PDEs for countercurrent flow zones are

\[
\frac{\partial \rho_{Si}}{\partial t} = -v_S \frac{\partial \rho_{Si}}{\partial z} + R_{Si}, \quad i = 1, \ldots, 5, \tag{6}
\]

\[
\frac{\partial \rho_{Lj}}{\partial t} = v_L \frac{\partial \rho_{Lj}}{\partial z} + R_{Lj}, \quad j = 1, \ldots, 4, \tag{7}
\]

\[
(1 + \alpha) \frac{\partial T}{\partial t} = -v_S (1 - \omega_L/v_S) \frac{\partial T}{\partial z}. \tag{8}
\]

The overall reaction rates for the solid components are specified as

\[
R_{Si} = -\theta [k_{Si} \rho_{PL1} + k_{Si} \rho_{PL2}^{1/2}] (\rho_{Si} - \rho_{Si}^e), \quad i = 1, \ldots, 5 \tag{9}
\]
with individual reaction rate expressions: 

\[ \frac{d\rho_{L_1}}{dt} = \left[ (\beta_{E_1} - \frac{1}{2}\beta_{HSL})R_{LG} + \beta_{E_1}C \right] \left( \frac{1 - \eta}{\eta} \right), \]  

(10)

\[ \frac{d\rho_{L_2}}{dt} = \left( \frac{1}{2}\beta_{HSL}R_{LG} \right) \left( \frac{1 - \eta}{\eta} \right), \]  

(11)

\[ \frac{d\rho_{L_3}}{dt} = (-\beta_3) \left( \frac{1 - \eta}{\eta} \right), \]  

(12)

\[ \frac{d\rho_{L_4}}{dt} = (-R_{LG}) \left( \frac{1 - \eta}{\eta} \right), \]  

(13)

where \( R_{LG} = R_{S_1} + R_{S_2}, \) \( R_c = R_{S_3} + R_{S_4} + R_{S_5}, \) and \( R_S = R_{LG} + R_c. \)

At the mixing zone of the impregnation vessel the liquor balance and the density dilutions, due to moisture in wet chips, are

\[ v_{L_0} = v_L - \frac{\rho_{So}}{\rho_w} w_o v_{So}, \]  

(14)

and

\[ \rho_{L_j} = \frac{v_{L_0}}{v_L} \rho_{L_0}, \quad j = 1, \ldots, 4. \]  

(15)

The PDE model equations are numerically approximated using finite differences to yield the standard CSTR approximation to the distributed parameter system. Let the CSTR count for any section be \( n = 1, \ldots, N \) where numbering starts from the top. Then, residence times for chips and liquor are

\[ \tau_S(n) = \Delta z [1 - \eta(n)]/\nu_S, \]  

(16)

and

\[ \tau_L(n) = \Delta z \eta(n)/\nu_L. \]  

(17)

For the countercurrent zones the corresponding equations are

\[ \frac{d\rho_{Si}}{dt} = \left[ \rho_{Si}(n - 1) - \rho_{Si}(n) \right]/\tau_S(n) + R_{Si}(n), \]  

\[ i = 1, \ldots, 5, \]  

(18)

\[ \frac{d\rho_{Lj}}{dt} = \left[ \rho_{Lj}(n + 1) - \rho_{Lj}(n) \right]/\tau_L(n) + R_{Lj}(n), \]  

\[ j = 1, \ldots, 4, \]  

(19)

and

\[ \frac{dT(n)}{dt} = \frac{v_S + v_L}{\Delta z} [T(n - 1) - T(n)]. \]  

(20)

See the Notation for the explanation of variables, and the relevant parameter values are available in Kayihan, (1998).

5. Model predictive control design

Although there are a variety of techniques for model-based control, one of the most flexible formulations is model predictive control. This flexibility arises from the variety of process model forms which can be incorporated (impulse response, state–state, etc.), as well as the direct handling of constraints. In MPC, the control computation is posed as an optimization problem, thus yielding and implicit control law. As additional data is collected, the control algorithm is updated and the steps of model prediction and control computation are repeated, giving rise to a ‘receding horizon’ implementation. Though the main ideas of MPC existed in the literature since the middle 1960s and early 1970s (Dreyfus, 1965), the advantages of MPC were not widely known or explored until the late 1970s and early 1980s (Cutler and Ramaker, 1979). The optimization problems which result from using linear models with two-norm objective functions are quadratic programs, although for unconstrained systems an analytical (least squares) solution can be derived. Using a state–space representation for the models, open-loop and closed-loop observers were incorporated in the MPC framework to improve the regulatory control (Li et al., 1989; Ricker, 1990; Lee et al., 1994). The multivariable and constraint handling capabilities of MPC have been demonstrated on several industrial challenge problems such as the Tennessee Eastman challenge problem (Ricker and Lee, 1995), the Shell Standard control problem (Yu et al., 1994), and the Amoco FCCU challenge problem (Kalra and Georgakis, 1996).

The source of a model for MPC can come from two generic sources: fundamental process knowledge or
identified directly from process data. In this work, we adopt the latter approach. The area of linear model identification for single-input–single-output (SISO) and multiple-input–single-output (MISO) models is well developed (Ljung, 1987). Recently, new techniques for the identification of multiple-input–multiple-output (MIMO) models have been developed which directly identify compact, state-space models from input/output data (Van Overschee and De Moor, 1994). The basic idea of these so called subspace identification techniques is to determine, from input/output data, a discrete-time state-space model of the following form:

\[
x_{k+1} = Ax_k + Bu_k + \eta_k,
\]

\[
y_k = Cx_k + \eta_k,
\]

where \( \eta_k \) and \( \eta_k \) are unobservable, Gaussian-distributed, zero mean, white noise vector sequences. In this formula, \( x \) represents the model states, \( u \) is the manipulated input, and \( y \) is the process output. The time index \( k \) denotes a discrete (sampled) system. Input/output data is used to construct an optimal multi-step prediction equation in which the matrices relating the: (i) past outputs; (ii) past inputs; and (iii) future inputs, are identified via linear least squares estimation. These matrices are then used to construct an extended observability matrix. Using a Kalman filter formulation of the multi-step prediction equation and the extended observability matrix, the system matrices for the Kalman filter equation are generated in a straightforward manner.

Major advantages of subspace identification methods are that very little prior knowledge of the system is required to start the algorithms, and the algorithms themselves are based on numerically stable, noniterative linear algebra operations. The subspace algorithm N4SID (Van Overschee and De Moor, 1994), is implemented in MATLAB’s System Identification Toolbox, and has been found to be numerically robust. One disadvantage to the subspace identification approaches is that a large amount of data is required to obtain accurate models. The process of generating and collecting data could be so economically expensive for some processes that the method is rendered impractical.

For the present case study, 500 h of simulation data is used to identify a 25th order, state-space model. The manipulated inputs and process disturbances are varied as random signals. Noisy measurements of the Kappa \# and secondary measurements are taken every 10 min. A state-space model of the following form, using the N4SID algorithm in MATLAB’s System Identification Toolbox (Ljung, 1991), is identified between the inputs/measured disturbances and the Kappa \# and secondary measurements:

\[
x_{k+1} = Ax_k + Bu_k + \eta_k,
\]

\[
Ay_k = Cx_k + \eta_k.
\]

In the above equation, the input/measured disturbance vector is denoted as \( u \), and the primary/secondary output vector is denoted \( y \). The inputs and outputs are differenced from the previous time step so that the stochastic input to the system, \( \eta \), is zero-mean and stationary.

A 25th-order empirical model is quite reasonable given: (i) the digester exhibits significant time delay resulting in high-order discrete states, (ii) the various process inputs and outputs are distributed along the axial length of the digester, and (iii) the number of distinct input/output channels is 40. These results are also comparable to those of Amirthalingam and Lee (1997) in which the Purdue Digester Model was studied.

A linear model predictive controller, based on optimal state-estimation, is constructed following the work of Lee et al. (1992). Using information from time step \( k-1 \), the system states at time step \( k \) are predicted utilizing the model and then corrected with the current output measurements:

\[
\hat{x}_{k|k-1} = \Phi \hat{x}_{k-1|k-1} + \Gamma_u \hat{u}_{k-1} + \Gamma_y \hat{v}_{k-1},
\]

\[
\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_f (\hat{y}_k - \hat{z}_l \hat{x}_{k|k-1}).
\]

The output measurement vector consists of the available, noisy measurements of the primary and secondary outputs. The state vector consists of the 25 empirical model states plus the five process outputs.

The MPC prediction equation is developed by constructing the individual \( p \)-step-ahead prediction equations for the primary control variable. A simple iterative calculation yields the following multi-step-ahead, state prediction equation

\[
\hat{x}_{k+l|k} = \Phi^l \hat{x}_{k|k} + \sum_{i=0}^{l-1} \Phi^i \Gamma_u \sum_{i=0}^{l-2} \Phi^i \Gamma_u \cdots \Phi^0 \Gamma_u \Delta U_k
\]

\[
+ \sum_{i=0}^{l-1} \Phi^i \Gamma_y \Delta V_k,
\]

where

\[
\Delta U_k = [\Delta u_k^T \Delta u_{k+1}^T \cdots \Delta u_{k+1}^T].
\]

The multi-step-ahead prediction of the primary output is found by extracting the estimate of the primary output from the augmented state vector:

\[
\hat{y}_{k+l|k} = \hat{z}_p \hat{x}_{k+l|k}.
\]

The following MPC prediction equation for a \( p \)-step-ahead output prediction and a \( q \)-step-ahead control action computation is developed

\[
\hat{y}_{k+l|k} = \hat{z}_p \hat{x}_{k+l|k} + \hat{z}_p \Delta U_k + \hat{z}_p \Delta V_k.
\]
This equation is used to predict the primary control variable \( p \) time steps into the future. The future control action, \( \Delta U_k \), is computed such that the following quadratic objective function is minimized

\[
\min_{\Delta U_k} \| A^r (Y_{k+1|k} - R_{k+1|k}) \|_2^2 + \| A^u \Delta U_k \|_2^2
\]  

subject to the constraints on the manipulated variables. The weighting matrices \( A^r \) and \( A^u \) are used to assign the relative importance in output deviation (from the reference) and the manipulated input moves, respectively. The first control move of \( \Delta U_k \) is implemented and the optimization is repeated at the next time step.

### 6. Results

Using the benchmark model described earlier, a realistic digester simulation is carried out using noisy process measurements and random measured and unmeasured disturbance sequences. For the following control studies, the following process variables are employed (see Fig. 1):

- **Output:** [Kappa \# at the end of the cook, mcc, and emcc zones, upper and lower extract residual EA densities]
- **Manipulated input:** [upper extract flowrate, temperatures of cook, mcc, and emcc heaters, mcc trim white liquor flowrate]
- **Measured disturbances:** [chip flowrate, chip moisture, white liquor EA density]
- **Unmeasured disturbances:** [chip lignin density, dilution flowrate]

The open-loop system response is depicted in Fig. 2a where the entire Kappa \# deviation profile is shown. It should be noted that the Kappa \# deviation excursions in the middle of the digester are quite large, and actually exhibit a maximum deviation from nominal somewhere in the mcc zone. Note, the Kappa \# profile extends from the top of digester to the end of emcc zone, and represents the 150 CSTRs that comprise the lumped approximation of the original PDEs.

To establish a basis for comparison for the MPC scheme, the conventional control results using PI feedback and a constant alkali-to-wood ratio feedforward policy are reviewed (Kayihan, 1998). The corresponding output plots are shown in Fig. 2b. Although the feedback policy is effective in maintaining the final (emcc) Kappa \# nearly constant, and the feedforward policy reduces the overall magnitude of Kappa \# profile deviation, it is clear that large excursions still exist for the internal Kappa \#s.

Next, the empirically derived state–space model is used in the previously described state space MPC framework to result in a centralized 5 input by 5 output controller design. A key limitation is the lack of reliable tuning rules for complex, constrained, multivariable systems. In tuning the MPC controller for this study, the tuning parameters proposed in Kayihan (1998) were initially adopted, but were fine-tuned to reflect the state–space model employed in this study (as compared to the step response model in Kayihan (1998)). The relevant tuning parameters are summarized below:

- Prediction horizon: 50
- Move horizon: 5
- Input penalty weight: diag\([1000 1 1000 1 1]\]
- Output penalty weight: diag\([5 5 5 5 5]\]
- Update filter: diag\([0.8 0.8 0.8 0.8 0.8]\)

The closed-loop response is depicted below in Fig. 3a. One immediately recognizes that this control policy has resulted in a tightly controlled Kappa \# profile, as well tighter regulation of the effective alkali concentration. This is accomplished with a reasonable amount of control action (not depicted).

In order to evaluate the impact of process measurements on the MPC controller performance, an inferential formulation is considered in which the model alone is used for prediction of the internal Kappa \# values (cook and mcc zones). These results are summarized in Fig. 3b. Although the Kappa \# profile performance is deteriorated due to the presence of unmeasured disturbances, the overall performance exceeds classical feedback (plus feedforward). This is accomplished at the expense of additional manipulations and additional measurements. It is worth noting that the primary manipulated variable adjustment is the emcc temperature. This can be improved if one considers the inferential estimation of the unmeasured disturbances as well (Wisnewski and Doyle, 1997).

An obvious issue which arises in the study of Kappa \# profile control is the choice of the ‘optimal’ profile
Fig. 2. Kappa profile to random variation in measured and unmeasured disturbances: (a) open-loop response, (b) conventional PI feedback plus feedforward control.
Fig. 3. Closed-loop response of Kappa profile to random variation in measured and unmeasured disturbances using model predictive control: (a) full output measurement, (b) partial output measurement.
Table 1
Performance summary of various profile shapes derived from adjustments in the setpoint of the K # (cook and mcc) relative to the base case. Values are reported as the variability of the emcc Kappa # (standard deviation) divided by the base case variability

<table>
<thead>
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<th>K # mcc</th>
<th>K # cook</th>
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<tbody>
<tr>
<td>5</td>
<td>15</td>
</tr>
<tr>
<td>-5</td>
<td>10</td>
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<td>-20</td>
<td>25</td>
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Fig. 4. Steady-state Kappa # profiles corresponding to three different operating policies.

shape. Using the benchmark model, this was analyzed for a variety of setpoints for the cook zone and mcc zone. The underlying assumption is that the final Kappa # (emcc zone) is dictated by operating policy, and the only two degrees of freedom are the interior two Kappa # setpoints. The results of several operating conditions are summarized in Table 1 (and Fig. 4). The data are presented as scaled values of the standard deviation of the final Kappa # (emcc) relative to the nominal operating point. Values less than one indicate improved performance (reduced Kappa # variability).

If one considers two specific curves from this table (K # cook = -25; K # cook = -15 & K # mcc = 10), one can see the variation introduced in the Kappa # profile at steady-state (Fig. 4). An analysis of the output profiles is not very revealing, as they are nearly indistinguishable from the base case, but one could argue that in many process applications, a 6% reduction in standard deviation variability ( ~ 12% reduction in variance) is quite significant. The ‘price’ for this reduced variability, as is always the case, must be reflected in the input moves. Hence, for a practical application, one must weight the competing advantages of quality improvements versus utility costs.

A final note is in order regarding the practical ‘constraints’ on such a profile optimization. The overall target profile is typically dictated by fiber quality characteristics. It might be envisioned that such characteristics could be maintained within quality specification limits for some range of K # mcc and K # cook setpoints. Given such bounds, one could perform the optimization described above to satisfy an additional operating objective (such as minimized utility consumption or minimized K # variability).

7. Summary

Simulation results are presented for the closed-loop control of the Kappa # profile in a continuous digester. Five manipulated variables and three measurements were employed to estimate two unmeasured outputs. The results demonstrate that the final Kappa # variability can be significantly reduced in such a framework. This will also impact other quality variables such as fiber strength attributes. This framework was used to explore ‘optimal’ profiling of the digester with respect to the final Kappa # variability. A detailed analysis is required to fully weigh the impact of such designs on utility costs and other quality objectives. While the results in this paper are encouraging, it is clear that extensions to the proposed approach could be employed to estimate the unmeasured process disturbances. Future work will address this issue, as well as the application of this technique to grade transition control.

Acknowledgements

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Greek letters

A
digester cross section area (same for all zones), m²

E_{Ai}
activation energies, (i = 1, ..., 5), kJ/gmol

E_{Bi}
activation energies, (i = 1, ..., 5), kJ/gmol

K*
Kappa number = 654* lignin mass/total solid mass

k_{Aoi}
pre-exponential factors, m³³/³/³g/lq/min/kg_{E,A}

k_{Boi}
pre-exponential factors, m³³/³/³g/lq/min/kg_{E,A} kg_{E,A}^{1/2}

R
gas constant, kJ/gmol °K

R_{Li}
reaction rate of liquor component j, (kg/min)/(m³ of liquor)

R_{Si}
reaction rate of solid component i, (kg/min)/(m³ of solid)

t_c
cook zone heater temperature, K

t_v
Emcc zone heater temperature, K

t_m
Mcc zone heater temperature, K

v_L
liquor space velocity, m/min

v_S
chips space velocity, m/min

W_o
chip moisture fraction (based on total mass)

References


