Feedback control over the chlorine disinfection process at a wastewater treatment plant using a Smith Predictor, a Method of Characteristics and Odometric Transformation

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Process description

- An advanced wastewater treatment plant in Gainesville, Florida, and uses chlorine for disinfection.

- Treats the wastewater to the standards for drinking water, and most of the water effluent is used for irrigation, reuse, and injection into groundwater.

- Current allowable capacity of 14.9 million gallons per day.

- Performs the disinfection process in two chlorine contact basins that are open to the atmosphere.
Process description

A schematic representation of the disinfection process

Sampling points for the chlorine measurements
Chlorination reactions

- Modeled based on the breakpoint chlorination by Morris and Isaac (1983) for a wastewater

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Forward-rate constant</th>
<th>Reverse-rate constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>$NH_3 + HOCl \leftrightarrow NH_2Cl + H_2O$</td>
<td>$6.6 \times 10^8 \exp\left(-\frac{1510}{T}\right)$</td>
<td>$1.38 \times 10^8 \exp\left(-\frac{8800}{T}\right)$</td>
</tr>
<tr>
<td>$NH_2Cl + HOCl \leftrightarrow NHCl_2 + H_2O$</td>
<td>$3 \times 10^5 \exp\left(-\frac{2010}{T}\right)$</td>
<td>$7.6 \times 10^{-7}\left(\frac{L}{mol \cdot s}\right)$</td>
</tr>
<tr>
<td>$NHCl_2 + HOCl \leftrightarrow NCl_3 + H_2O$</td>
<td>$2 \times 10^5 \exp\left(-\frac{3420}{T}\right)$</td>
<td>$5.1 \times 10^3 \exp\left(-\frac{5530}{T}\right)$</td>
</tr>
<tr>
<td>$2NH_2Cl \leftrightarrow NHCl_2 + NH_3$</td>
<td>$80 \exp\left(-\frac{2160}{T}\right)$</td>
<td>$24.0\left(\frac{L}{mol \cdot s}\right)$</td>
</tr>
</tbody>
</table>

- Reaction rates are in units of L/mol-s, concentrations are in mol/L and the temperature is room temperature (25°C).
Chlorination reactions

- Proposed reaction rate expressions for the reactions

\[ r_{\text{HOCl}} = -k_1 [NH_3][HOCl] + k_2 [NH_2Cl] - k_3 [NH_2Cl][HOCl] + k_4 [NHCl_2] - k_5 [NHCl_2][HOCl] + k_6 [NCl_3] - k_{\text{Disinfection}} [HOCl] \]

\[ r_{\text{NH}_3} = -k_1 [NH_3][HOCl] + k_2 [NH_2Cl] + k_7 [NH_2Cl]^2 - k_8 [NHCl_2][NH_3] \]

\[ r_{\text{NH}_2\text{Cl}} = k_1 [NH_3][HOCl] - k_2 [NH_2Cl] - k_3 [NH_2Cl][HOCl] + k_4 [NHCl_2] - k_7 [NH_2Cl]^2 + k_8 [NHCl_2][NH_3] \]

\[ r_{\text{NHCl}_2} = k_3 [NH_2Cl][HOCl] - k_4 [NHCl_2] - k_5 [NHCl_2][HOCl] + k_6 [NCl_3] + k_7 [NH_2Cl]^2 - k_8 [NHCl_2][NH_3] \]

\[ r_{\text{NCl}_3} = k_5 [NHCl_2][HOCl] - k_6 [NCl_3] \]

- The term \( k_{\text{Disinfection}}[HOCl] \) represents the chlorine consumed during the disinfection
Chlorination reactions

- A first-order kinetic model is able to describe the chlorine disinfection in the ammonia-free part of wastewater.

- The reaction rate constant, $k_{\text{Disinfection}}[\text{HOCl}]$, was estimated to be 0.0073 h$^{-1}$. 

![Simulation Result](chart)
Process control objectives

• Develop a process control strategy and design an appropriate feedback controller for the disinfection process

• Overcome the large and variable transportation lags

• Produce an effluent that meets required environmental regulations at the end of the contact basin

• Avoid the formation of organic compounds known as trihalomethanes

• Add an appropriate amount of chlorine into the influent
Process control challenges

- Significant changes of flow rate
- Quality of wastewater
- Complex reactions of chlorine residuals with ammonia in wastewater and dynamic behavior
- Biological processes (the complexity of the physical and biochemical phenomena)
- Large and variable dead-time
- Lack of adequate sensors and actuators
- Difficulty to design an appropriate process control system
  - Feed forward-feedback control
  - Linearized and optimal control, Nonlinear multiobjective model-predictive control
  - Fuzzy control, Optimization control
  - Adaptive and robust-adaptive control
  - Model predictive control
Process control objectives

Large and variable dead-time

- Primary control issue because the contact basin is too long (\(\equiv 200\) m)
- Complicates the stability analysis and the controller design
- Flow rate changes relative to daily water usage

\[
\frac{\text{Maximum flow rate}}{\text{Minimum flow rate}} \approx 10 \rightarrow \frac{\text{Maximum dead – time}}{\text{Minimum dead – time}} \approx 10
\]

- Changes from 1h to 2 or 3 h for the chlorine disinfection of wastewater treatment plant
- The average dead-time is 2 hours in the KWRF
Process control challenges

Disturbances

- Affect the output without being adjusted by the process operator or an automatic method.

- Sunlight and rainfall are some disturbances in the KWRF because contact basin is open to the atmosphere.

- Sunlight affects the chlorine chemistry due to UV and reduces the final chlorine content.

- Rainfall reduces the chlorine concentration via dilution, affecting the chlorine levels at the end of the contact basin.
Process control challenges

Dynamic model for a disinfection
Assumption: Plug flow reactor

Contact basin

Influent ➔ Effluent

≈ 200 m

≈ 2 m
Cascade/Ratio control (Ratio of Cl₂ dosage to influent flow rate)

Approach -I-

- Improve the system performance in the presence of long dead times between the control and process variables
Approach-II-

The Smith predictor (Dead-time compensator)

- Cancel out the dead-time and obtain a delay-free transfer function
- The Smith predictor structure used in this study was derived by George Stephanopoulos (1984)

Block diagram for a feedback control
Approach-II-

- The Smith predictor structure

- Delay-free feedback block diagram
Odometric transformation

- First introduced by Svoronos and Lyberatos (1992) and Harmon et al. (1990)
- They claimed that
  “Variability in the effective time constant can be considerably reduced if one considers, instead of time, the cumulative amount of a quantity generated, consumed, or fed as the independent dynamic model variable”

**Odometric variable (β)**

\[
\frac{\partial \beta}{\partial t} = v(t) \quad \Rightarrow \quad \beta(t) = \int_0^t v(t)
\]

\[
\frac{\partial C_l}{\partial \beta} = -\frac{\partial C_l}{\partial z} + \frac{1}{v(\beta)} r_l(C(\beta, z))
\]

- Transforms the dynamics of the system to an equivalent constant time delay model
- Replaces time with a new odometric variable (β)
- (β) represents the displacement of flow or cumulative distance traveled by water
Method of characteristics

- Many PDEs occur when modeling the chlorine disinfection reactions
- Solves PDEs by reducing them to a set of ODEs
- General expressions of a PDE as follows (P and Q are constants)

\[ P \frac{\partial z}{\partial x} + Q \frac{\partial z}{\partial y} = R(x,y) \]

\[ x = r + s \cos(\theta) \]
\[ y = s \sin(\theta) \]

\[ \theta = \tan^{-1} \left( \frac{Q}{P} \right) \]

\[ z(x,y) = z(x - y \cot(\theta)) + \int_{0}^{y \cos \theta} R(x - y \cot(\theta) + s' \cos(\theta), s' \sin(\theta)) \frac{ds'}{\sqrt{P^2 + Q^2}} \]
Applying transformation techniques

- Transforms the system dynamics to a constant time delay model and ODEs

\[
\frac{\partial C_i}{\partial \beta} = -\frac{\partial C_i}{\partial z} + \frac{1}{v(\beta)} r_i \left(C(\beta,z)\right)
\]

\[
\frac{\partial c_i(\beta_o + \frac{\sigma}{\sqrt{2}}, \frac{\sigma}{\sqrt{2}})}{\partial \sigma} = \frac{1}{\sqrt{2}} \frac{1}{v(\beta_o + \frac{\sigma}{\sqrt{2}})} r_i \left(c \left(\beta_o + \frac{\sigma}{\sqrt{2}}, \frac{\sigma}{\sqrt{2}}\right)\right)
\]

\[
\beta = \beta_o + \sigma \sin(\theta) \\
z = \sigma \cos(\theta) \\
\theta = 45°
\]
Smith predictor scheme for the master controller in terms of ($\beta$)
Process control equations

- Set point for the slave controller
  \[ u(\beta) = y_{sp1}(\beta) \]

- Discrete change in the odometric variable
  \[ \Delta \beta = \frac{D}{N} \]

- Signal \((y_k)\) produced by the Smith Predictor
  \[
y_k(\beta) = \left(1 - \frac{\Delta \beta}{\tau}\right)y_k(\beta - \Delta \beta) + K_{gain}(u(\beta - \Delta \beta) - u(\beta - D - \Delta \beta))\frac{\Delta \beta}{\tau}
  \]
  \[
y_2^*(\beta) = y_2(\beta) + \left(1 - \frac{\Delta \beta}{\tau}\right)y_k(\beta - \Delta \beta) + K_{gain}(u(\beta - \Delta \beta) - u(\beta - D - \Delta \beta))\frac{\Delta \beta}{\tau}
  \]

- Feedback error for the master loop
  \[ e(\beta) = y_{sp2}(\beta) - y_2^*(\beta) \]

- Velocity form of the discrete control law for the master loop
  \[
u(\beta) = u(\beta - \Delta \beta) + K_c\left((e(\beta) - e(\beta - \Delta \beta)) + \frac{\Delta \beta}{\tau_i} e(\beta) + \frac{\tau_D}{\Delta \beta} (e(\beta) - 2e(\beta - \Delta \beta) + e(\beta - 2\Delta \beta))\right)
  \]
Results

Simulation

- The flow rate of the wastewater, the residence time, and the rate constant of the disinfection reactor were obtained experimentally from the KWRF.
- Coded in VISUAL BASIC

Open loop simulation (apparent process parameters)

- The dynamic model solved by approximating the reactor small with \( N \) continuous-stirred-tank reactors (CSTR).
- Various time increments (\( \Delta t = 0.5, 5, 10, \) and 20 s) were used while integrating.
- The apparent process parameters, the process gain \( (K_{gain}) \), the time constant \( (\tau) \), and the delay \( (D) \) were determined from the step response data.
Closed-loop simulation (tuning)

- The daily change in flow rate of wastewater was assumed to be sinusoidal
- The PID form of the master controller was used with the dead-time compensation for the tuning process
- One fixed tuning was evaluated for the different time increments, the number of reactors, and the corresponding apparent process parameters.
- The master PID controller was tuned and fixed to the following constant settings:

\[
\begin{align*}
K_c &= 0.5 \\
\tau_I (\beta) &= 100 \text{ m} \\
\tau_D (\beta) &= 0
\end{align*}
\]
Open loop simulation results

Reactor num. \((N) = 50\)

Reactor num. \((N) = 100\)

Reactor num. \((N) = 500\)

Reactor num. \((N) = 1000\)

Open loop simulation results \((\Delta t = 0.5)\)
Open loop simulation results

Reactor num. \( (N) = 50 \)

Reactor num. \( (N) = 100 \)

Reactor num. \( (N) = 200 \)

Reactor num. \( (N) = 300 \)

Open loop simulation results \( (\Delta t = 5) \)
Open loop simulation results

Reactor num. \((N) = 50\)

Reactor num. \((N) = 100\)

Reactor num. \((N) = 150\)

Open loop simulation results \((\Delta t = 10)\)
Open loop simulation results

- The delay calculated from the open loop response is similar to the delay calculated theoretically using the odometric transformation
### Process parameters

- Results from the open loop simulation program ($\Delta t = 0.5, 5, 10, 20$)

<table>
<thead>
<tr>
<th>Reactor Number</th>
<th>Process Gain, $K_{gain}$</th>
<th>$\tau$ (m)</th>
<th>Delay ($D$) (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.061696</td>
<td>33</td>
<td>72</td>
</tr>
<tr>
<td>100</td>
<td>0.061366</td>
<td>21</td>
<td>80</td>
</tr>
<tr>
<td>500</td>
<td>0.061555</td>
<td>10</td>
<td>85</td>
</tr>
<tr>
<td>1000</td>
<td>0.06142</td>
<td>7</td>
<td>87</td>
</tr>
</tbody>
</table>

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</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.061785</td>
<td>32</td>
<td>73</td>
</tr>
<tr>
<td>100</td>
<td>0.062154</td>
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<td>80</td>
</tr>
<tr>
<td>200</td>
<td>0.0622</td>
<td>10</td>
<td>85</td>
</tr>
<tr>
<td>300</td>
<td>0.062153</td>
<td>7</td>
<td>87</td>
</tr>
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<th>Delay ($D$) (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.062066</td>
<td>29</td>
<td>74</td>
</tr>
<tr>
<td>100</td>
<td>0.062247</td>
<td>16</td>
<td>81</td>
</tr>
<tr>
<td>150</td>
<td>0.062231</td>
<td>8</td>
<td>86</td>
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<tbody>
<tr>
<td>50</td>
<td>0.062314</td>
<td>22</td>
<td>79</td>
</tr>
<tr>
<td>90</td>
<td>0.062267</td>
<td>7</td>
<td>87</td>
</tr>
</tbody>
</table>
Flow rate of the wastewater

Assumed sinusoidal change in the flow rate of wastewater over time
The closed loop performance is poor

$K_{gain} = 0.06155$, reactor num. $= 500$, $\tau = 10$, $t = 0.5$, $D = 85$. 
Closed loop simulation result

The performance is improved because the deviation values of the final probe measurements are close to zero

\[ K_{gain} = 0.06215, \ \text{reactor num.} = 200, \ \tau = 10, \ t = 5, \ D = 85. \]
Closed loop simulation result

More improved control performance

$K_{gain} = 0.06225$, reactor num. = 100, $\tau = 16$, $t = 10$, $D = 81$
Closed loop simulation result

**GOOD CONTROL**

The deviation values of the final probe measurements is zero

\[ K_{gain} = 0.06231, \ \text{reactor num.} = 50, \ \tau = 22, \ t = 20, \ D = 79 \]
Conclusions

• Cascade control with a dead-time compensation strategy was suitable for application with an odometric transformation.

• The odometric transformation permits the design of a Smith Predictor with a constant dead-time.

• The joint application of the method of characteristics and the odometric transformation successfully control the performance.
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Article