

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

Feridun DEMIR^{a,b,*}, Spyros A. SVORONOS^b

^a*Department of Chemical Engineering, Osmaniye Korkut Ata University, Osmaniye 80000, Turkey*

^b*Department of Chemical Engineering, University of Florida, Gainesville, Florida 32611-6005, USA*

*2nd World Congress on Petrochemistry and Chemical Engineering",
October 27-29, 2014 Las Vegas, USA*

Outline

Process description

- The Kanapaha Water Reclamation Facility (KWRF)
- Chlorination reactions

Process control objectives

Process control challenges

- Large and variable dead-time
- Disturbances
- Dynamic model for a disinfection

Approach -I-

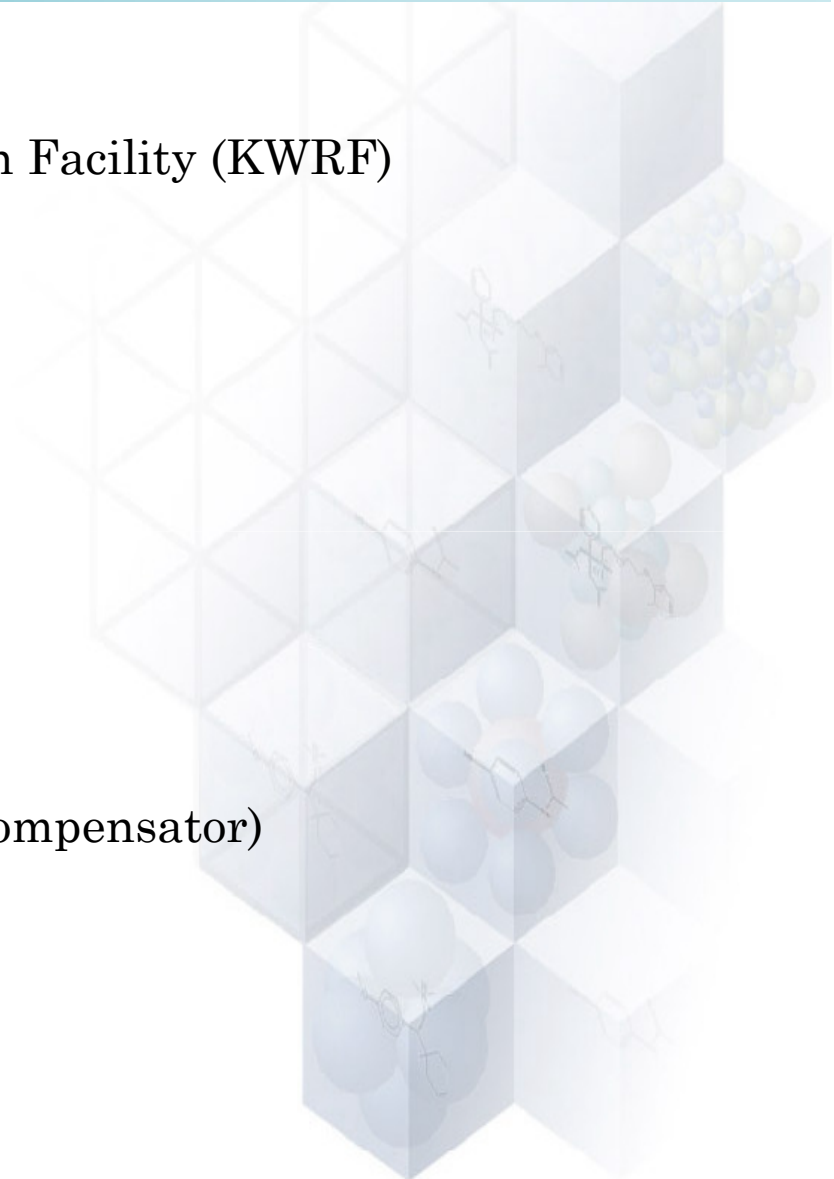
- Cascade/Ratio control

Approach-II-

- The Smith predictor (Dead-time compensator)
- Odometric transformation
- Method of characteristics

Open loop simulation results

Closed loop simulation results



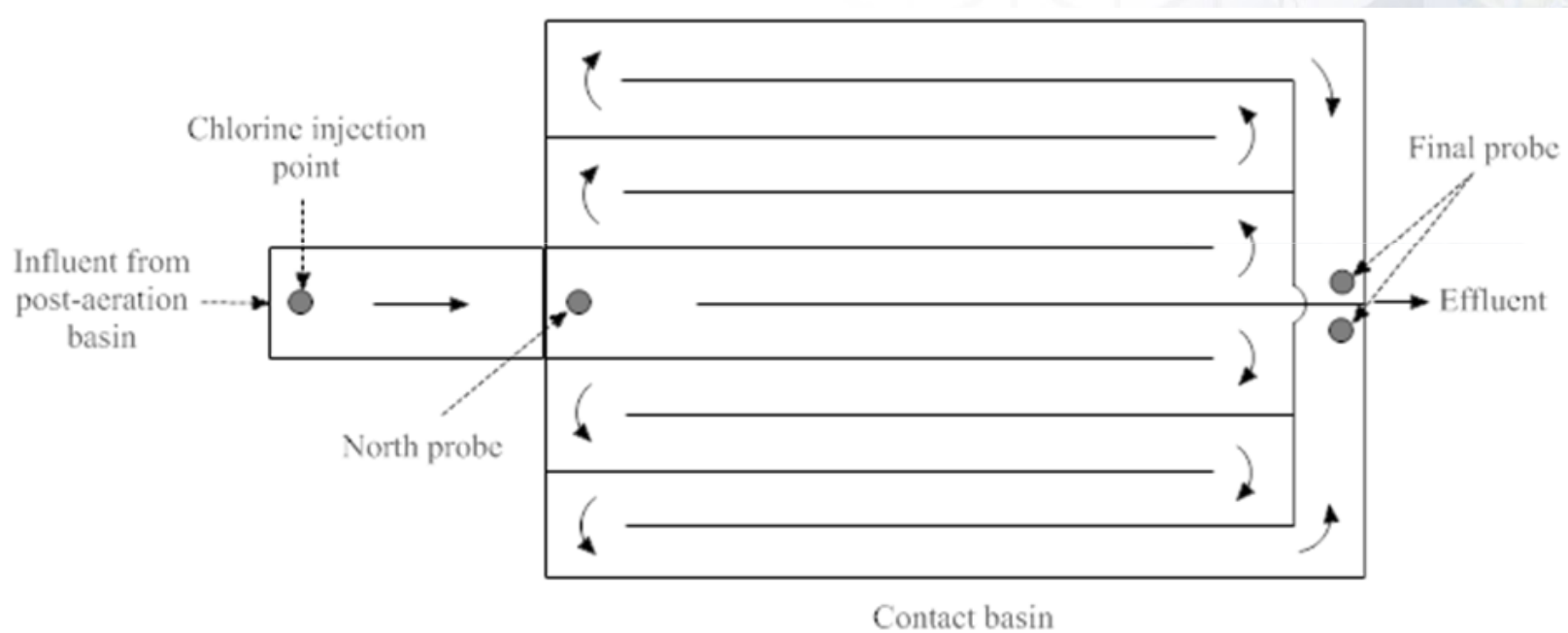
Process description

- 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

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

- 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

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

$$r_{NH_3} = -k_1 [NH_3][HOCl] + k_2 [NH_2Cl] + k_7 [NH_2Cl]^2 - k_8 [NHCl_2][NH_3]$$

$$r_{NH_2Cl} = k_1 [NH_3][HOCl] - k_2 [NH_2Cl] - k_3 [NH_2Cl][HOCl] + k_4 [NHCl_2] - k_7 [NH_2Cl]^2 + k_8 [NHCl_2][NH_3]$$

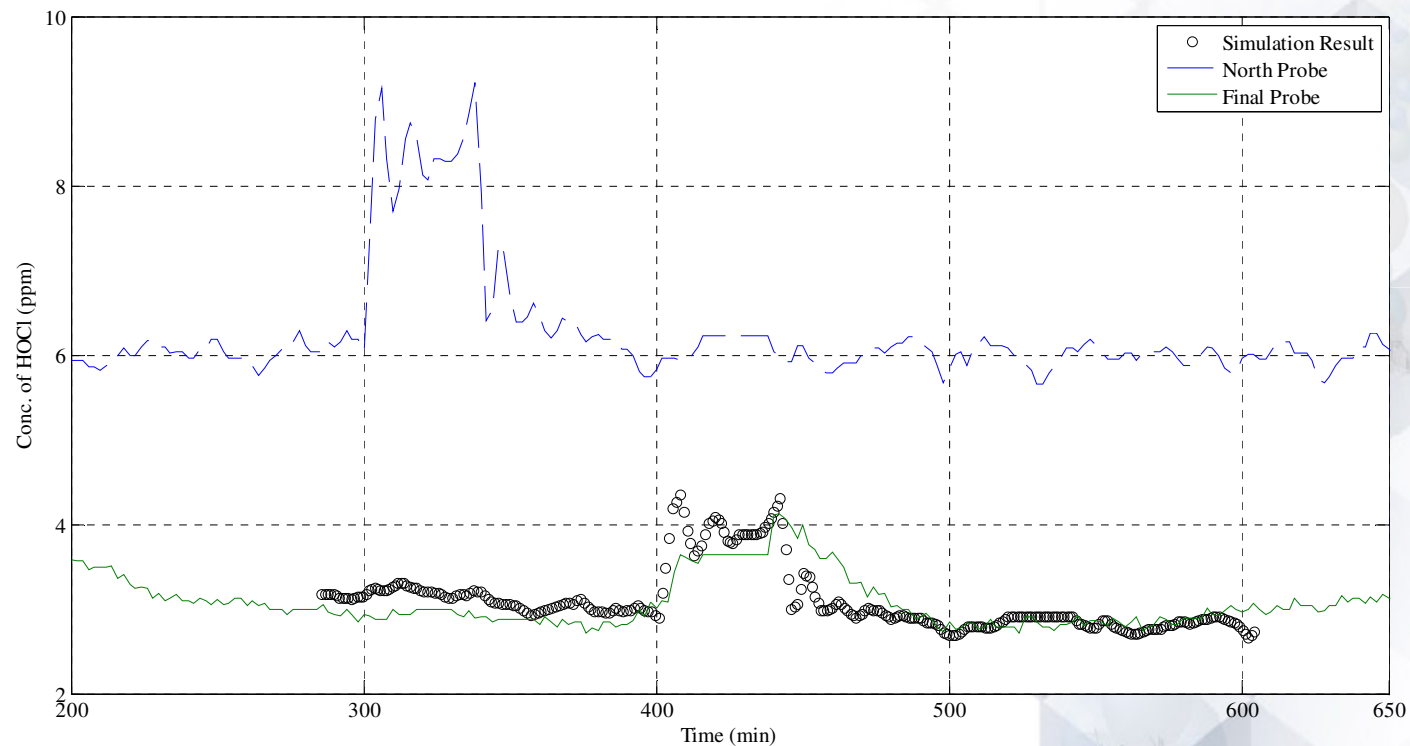
$$r_{NHCl_2} = k_3 [NH_2Cl][HOCl] - k_4 [NHCl_2] - k_5 [NHCl_2][HOCl] + k_6 [NCl_3] + k_7 [NH_2Cl]^2 - k_8 [NHCl_2][NH_3]$$

$$r_{NCl_3} = k_5 [NHCl_2][HOCl] - k_6 [NCl_3]$$

- The term $k_{Disinfection} [HOCl]$ 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, $k_{Disinfection}[HOCl]$, was estimated to be 0.0073 h^{-1}

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 ($\cong 200$ 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

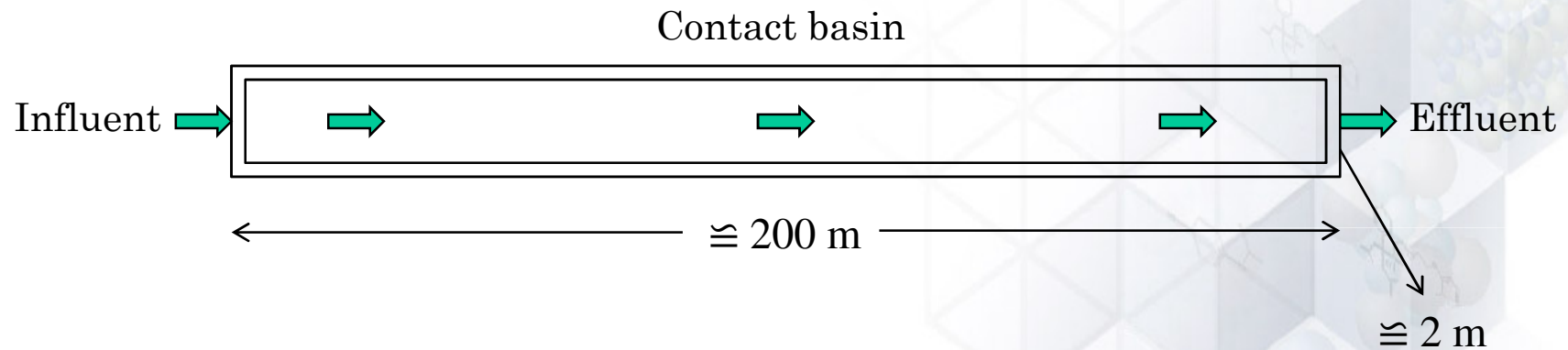
Disturbances

- 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

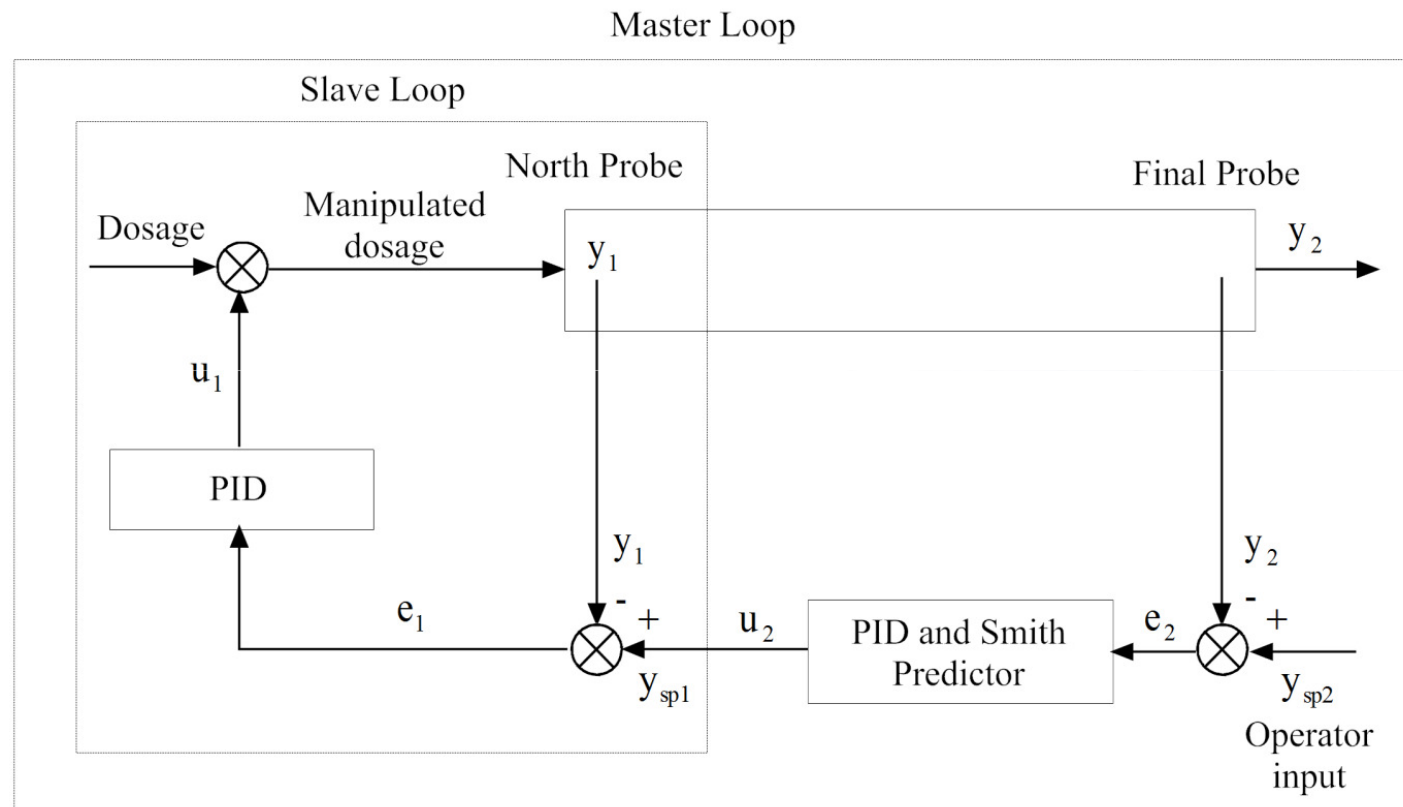
Dynamic model for a disinfection

Assumption: Plug flow reactor



Approach -I-

Cascade/Ratio control (Ratio of Cl_2 dosage to influent flow rate)

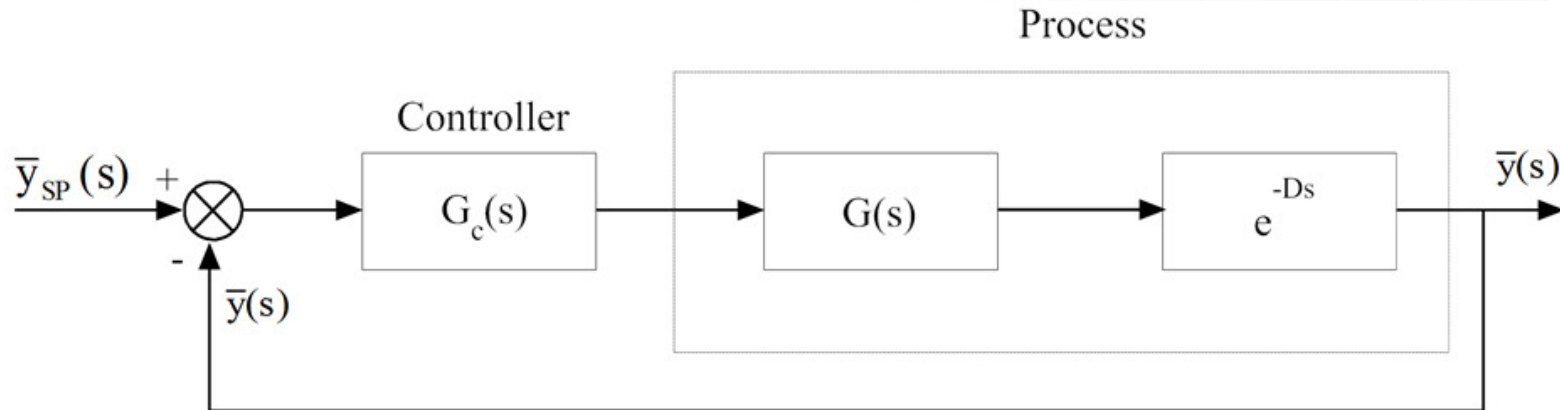


- Improve the system performance in the presence of long dead times between the control and process variables

Approach-II-

The Smith predictor (Dead-time compensator)

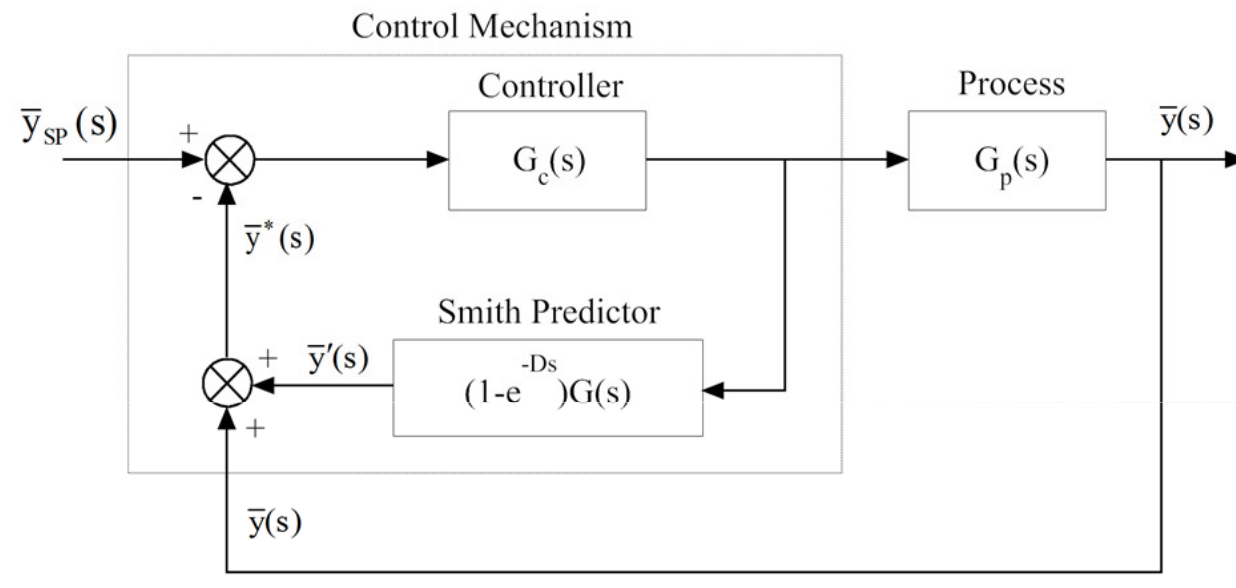
- Cancel out the dead-time and obtain a delay-free transfer function
- The Smith predictor structure used in this study was derived by George Stephanopoulos (1984)



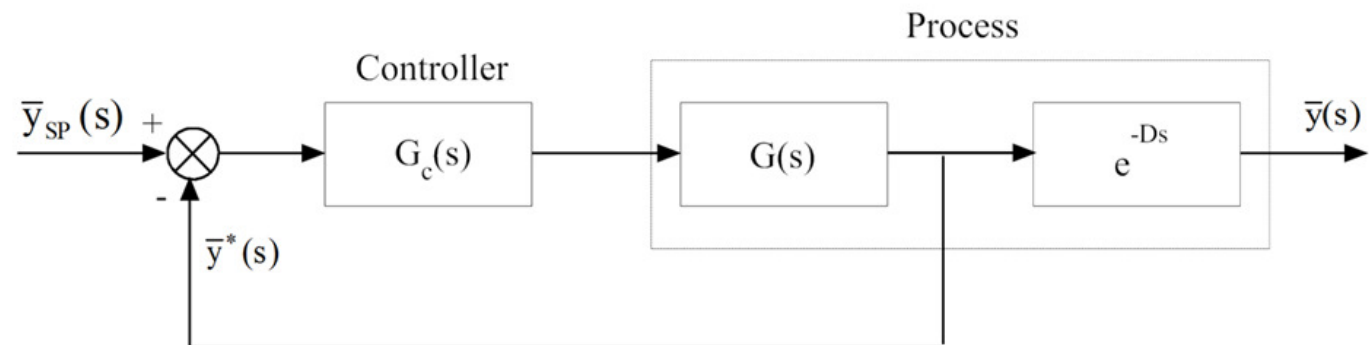
Block diagram for a feedback control

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)

$$\frac{\partial \beta}{\partial t} = v(t) \quad \rightarrow \quad \beta(t) = \int_0^t v(t) dt$$

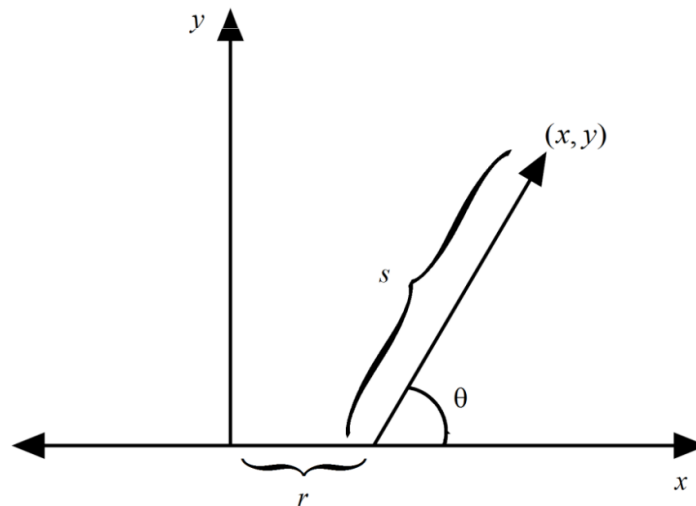
$$\frac{\partial C_i}{\partial \beta} = -\frac{\partial C_i}{\partial z} + \frac{1}{v(\beta)} r_i(\underline{C}(\beta, z))$$

- 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)

$$P \frac{\partial Z}{\partial x} + Q \frac{\partial Z}{\partial y} = R(x, y)$$



$$x = r + s \cdot \cos(\theta)$$

$$y = s \cdot \sin(\theta)$$

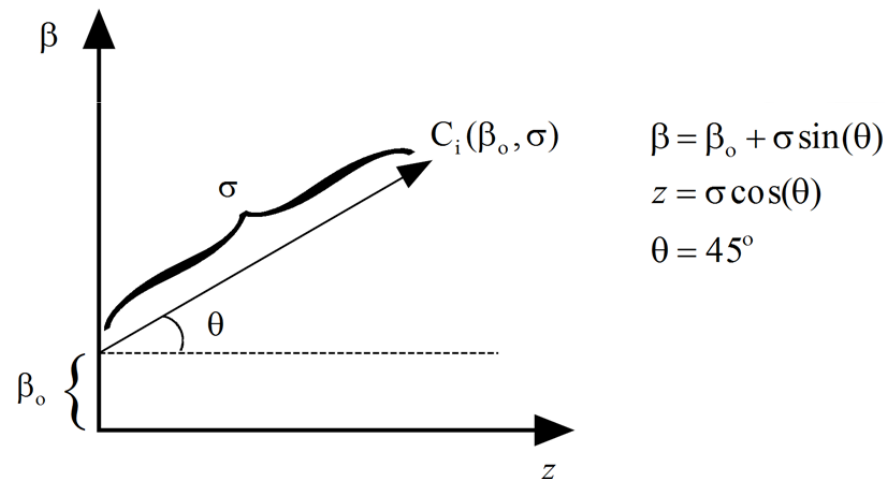
$$\theta = \tan^{-1} \left(\frac{Q}{P} \right)$$

$$z(x, y) = z(x - y \cot(\theta)) + \int_0^{y \sec(\theta)} R(x - y \cot(\theta) + s' \cos(\theta), s' \sin(\theta)) \frac{ds'}{\sqrt{P^2 + Q^2}}$$

Applying transformation techniques

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

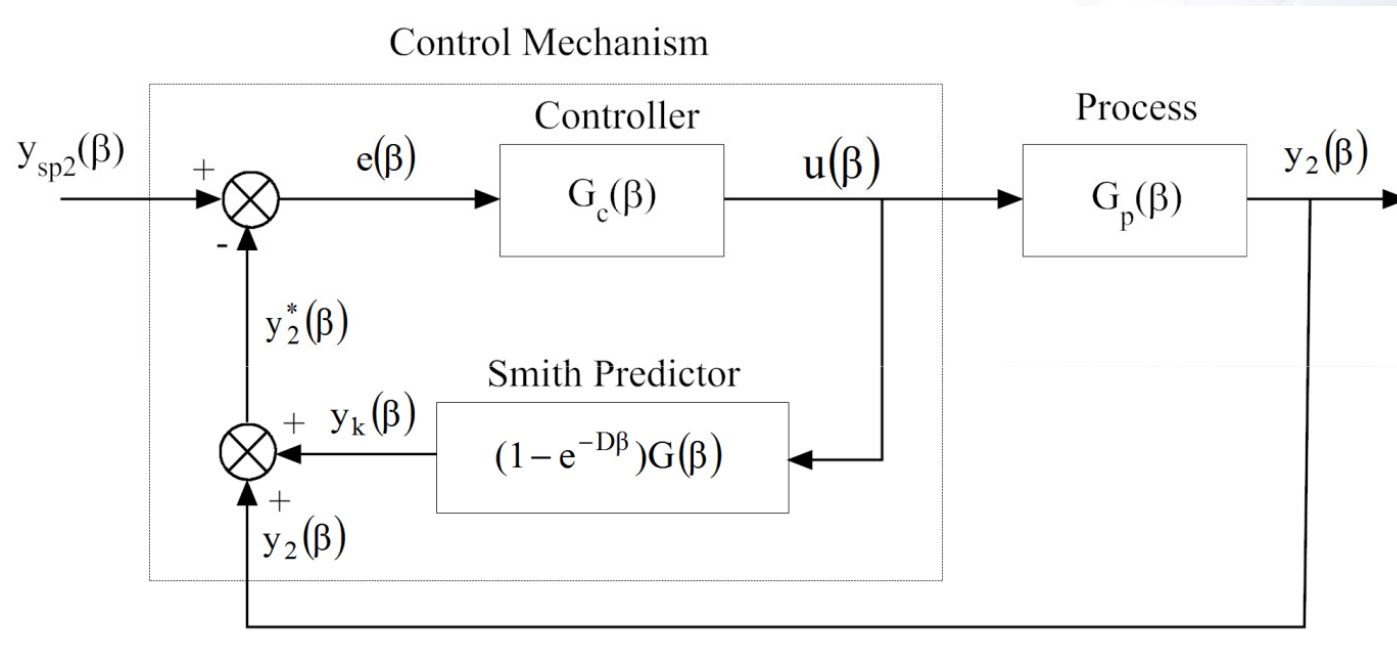
$$\frac{\partial C_i}{\partial \beta} = -\frac{\partial C_i}{\partial z} + \frac{1}{v(\beta)} r_i(\underline{C}(\beta, z))$$



$$\frac{\partial c_i\left(\beta_0 + \frac{\sigma}{\sqrt{2}}, \frac{\sigma}{\sqrt{2}}\right)}{\partial \sigma} = \frac{1}{\sqrt{2}} \frac{1}{v\left(\beta_0 + \frac{\sigma}{\sqrt{2}}\right)} r_i\left(\underline{c}\left(\beta_0 + \frac{\sigma}{\sqrt{2}}, \frac{\sigma}{\sqrt{2}}\right)\right)$$

Smith predictor scheme

Smith predictor scheme for the master controller in terms of (β)



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 (τ), and the delay (D) were determined from the step response data

Results

Closed-loop simulation (tuning)

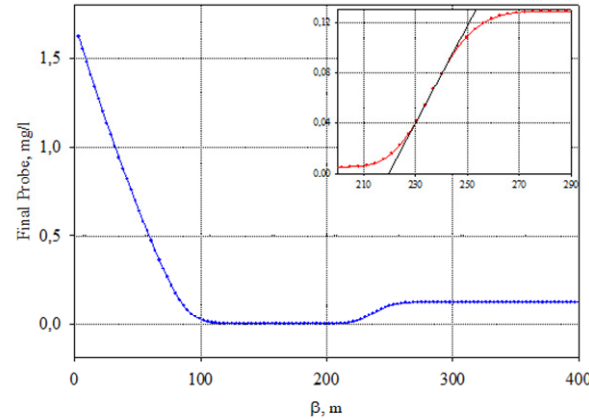
- The daily change in flow rate of wastewater was assumed to be sinusoidal
- The PID form of the master controller was used with the dead-time compensation for the tuning process
- One fixed tuning was evaluated for the different time increments, the number of reactors, and the corresponding apparent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

$$K_c = 0.5$$

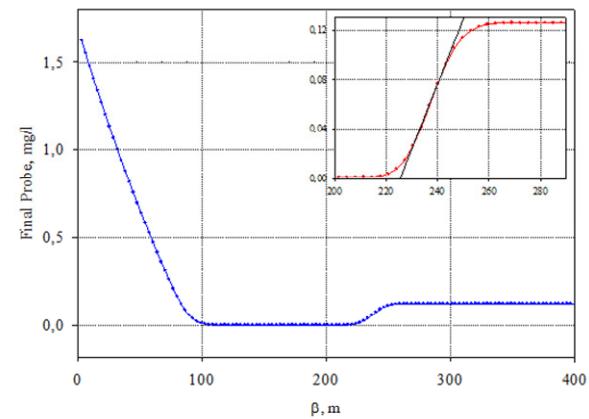
$$\tau_I(\beta) = 100 \text{ m}$$

$$\tau_D(\beta) = 0$$

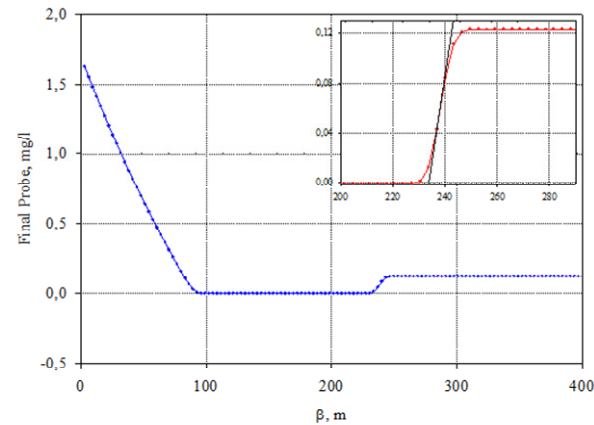
Open loop simulation results



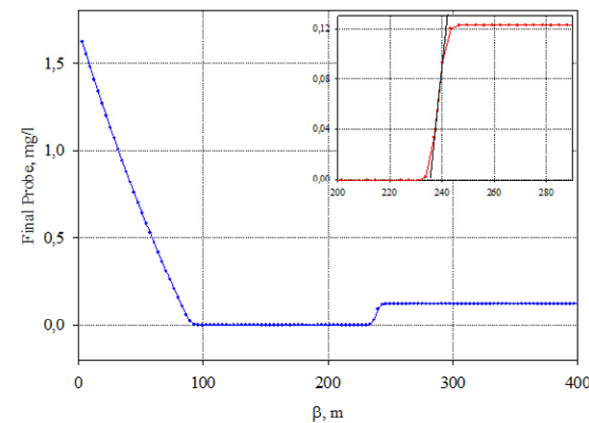
Reactor num. (N) = 50



Reactor num. (N) = 100



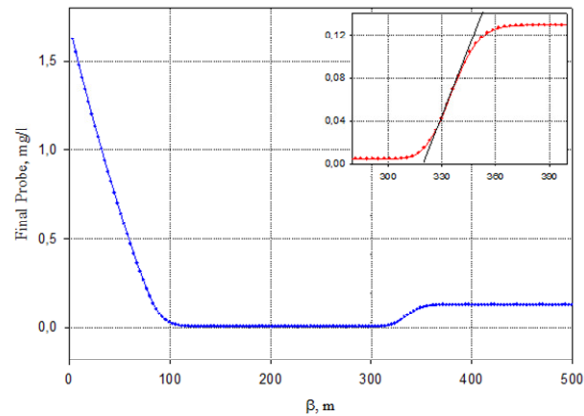
Reactor num. (N) = 500



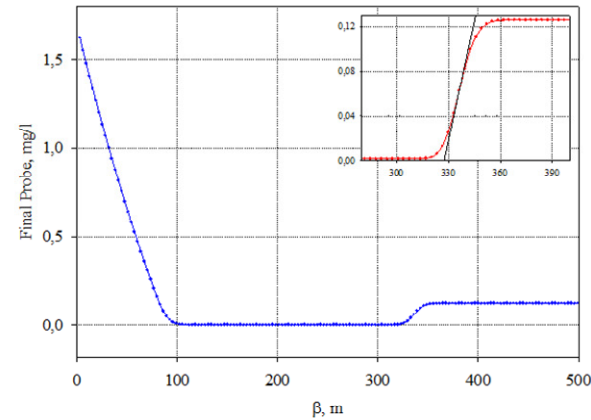
Reactor num. (N) = 1000

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

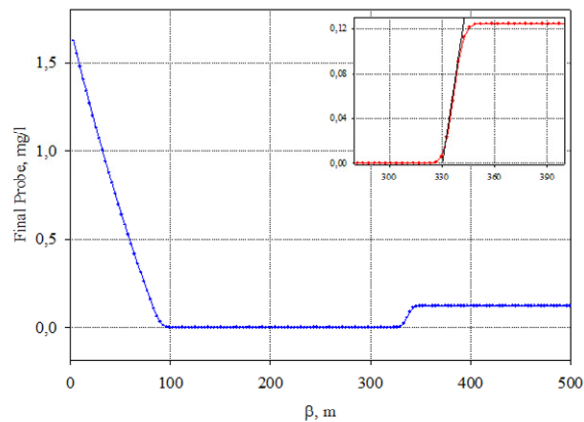
Open loop simulation results



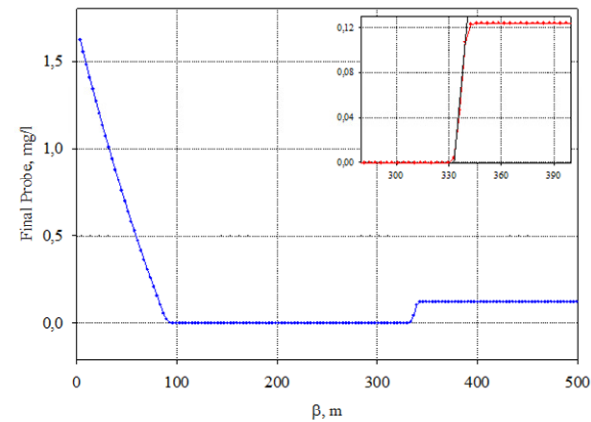
Reactor num. (N) = 50



Reactor num. (N) = 100



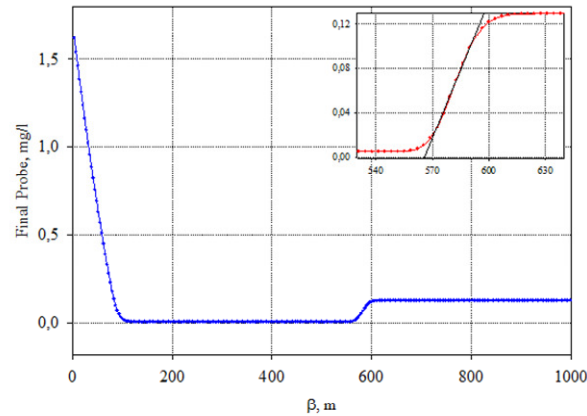
Reactor num. (N) = 200



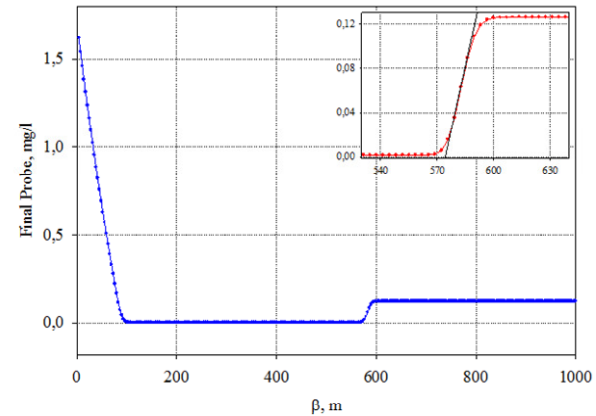
Reactor num. (N) = 300

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

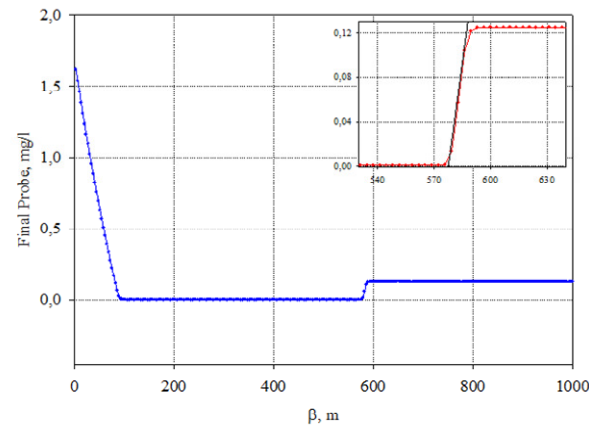
Open loop simulation results



Reactor num. (N) = 50



Reactor num. (N) = 100

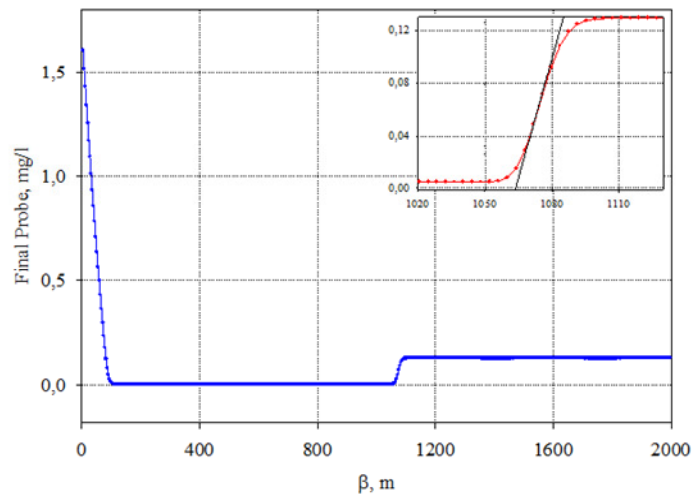


Reactor num. (N) = 150

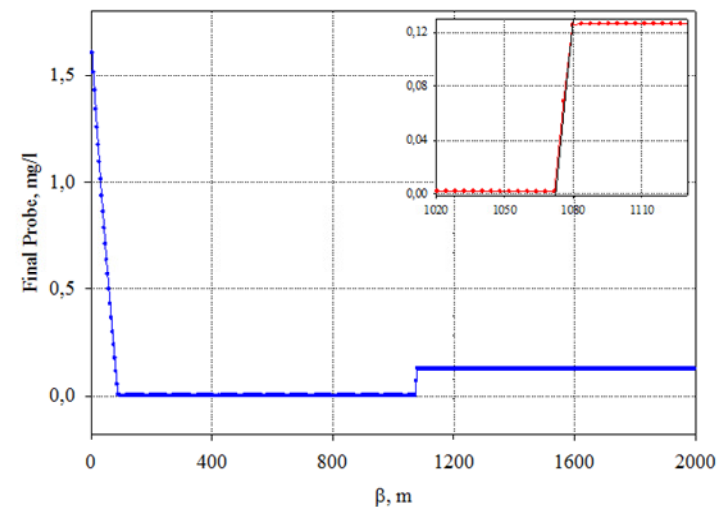
Open loop simulation results ($\Delta t = 10$)

Open loop simulation results

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



Reactor num. (N) = 50



Reactor num. (N) = 90

Open loop simulation results ($\Delta t = 20$)

Process parameters

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

Reactor Number	Process Gain, K_{gain}	τ (m)	Delay (D) (m)
50	0.061696	33	72
100	0.061366	21	80
500	0.061555	10	85
1000	0.06142	7	87

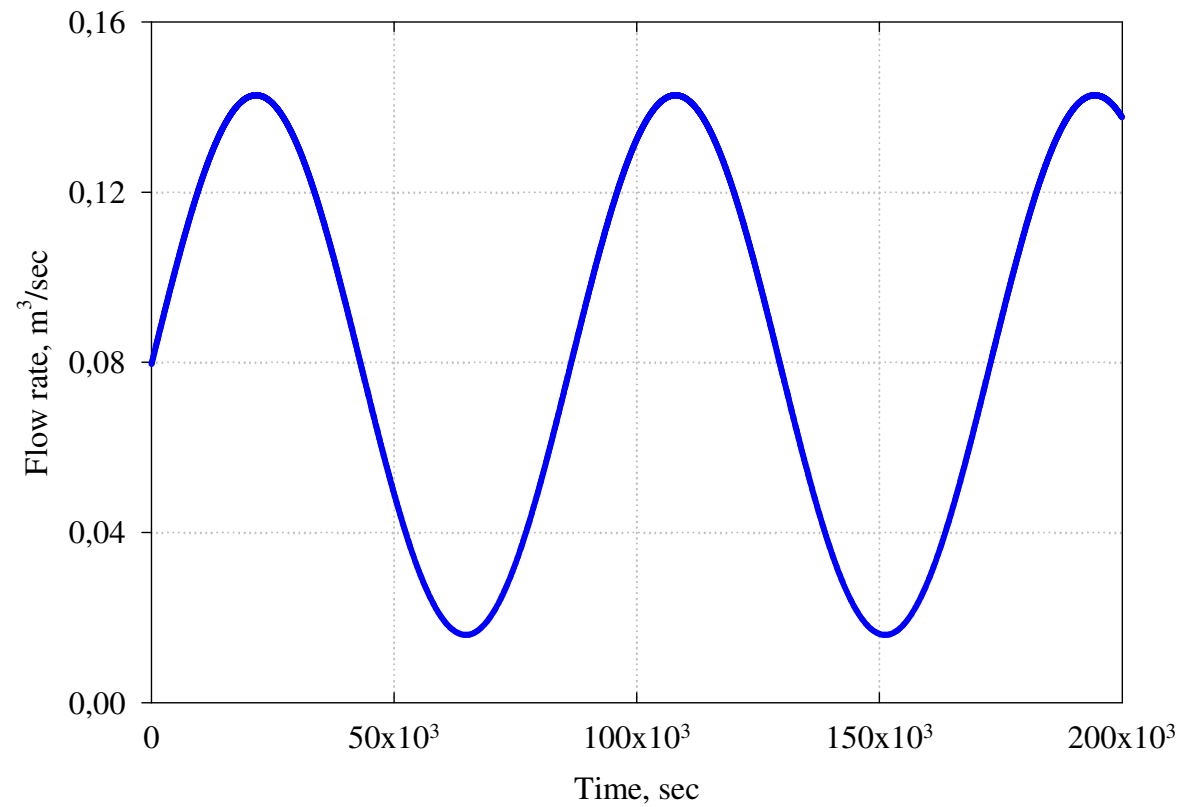
Reactor Number	Process Gain, K_{gain}	τ (m)	Delay (D) (m)
50	0.061785	32	73
100	0.062154	19	80
200	0.0622	10	85
300	0.062153	7	87

Reactor Number	Process Gain, K_{gain}	τ (m)	Delay (D) (m)
50	0.062066	29	74
100	0.062247	16	81
150	0.062231	8	86

Reactor Number	Process Gain, K_{gain}	τ (m)	Delay (D) (m)
50	0.062314	22	79
90	0.062267	7	87

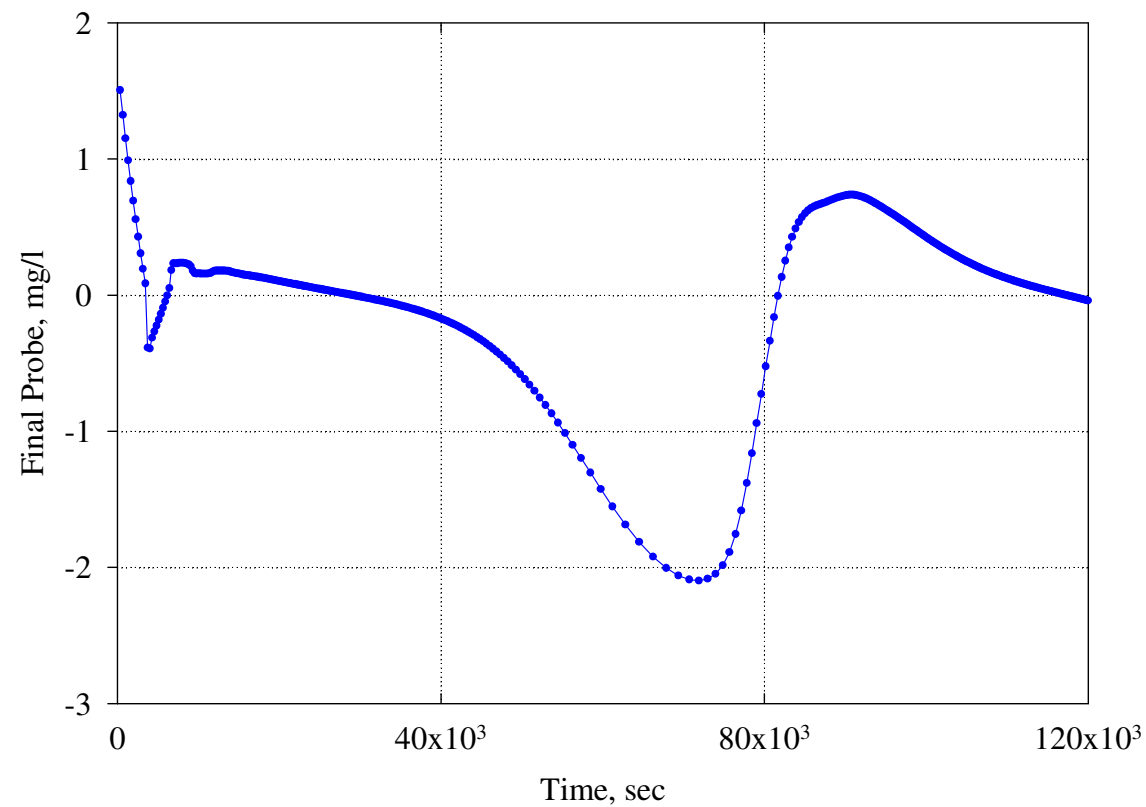
Flow rate of the wastewater

Assumed sinusoidal change in the flow rate of wastewater over time



Closed loop simulation result

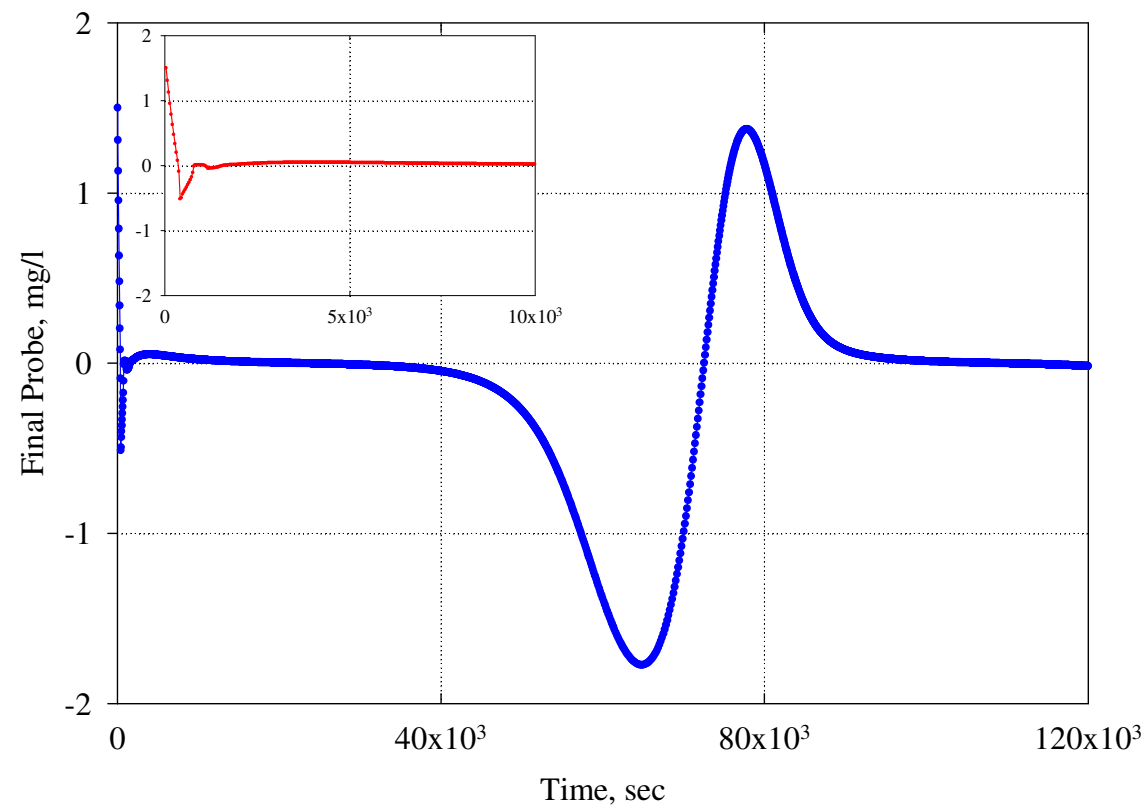
The closed loop performance is poor



$$K_{gain} = 0.06155, \text{ reactor num.} = 500, \tau = 10, t = 0.5, D = 85.$$

Closed loop simulation result

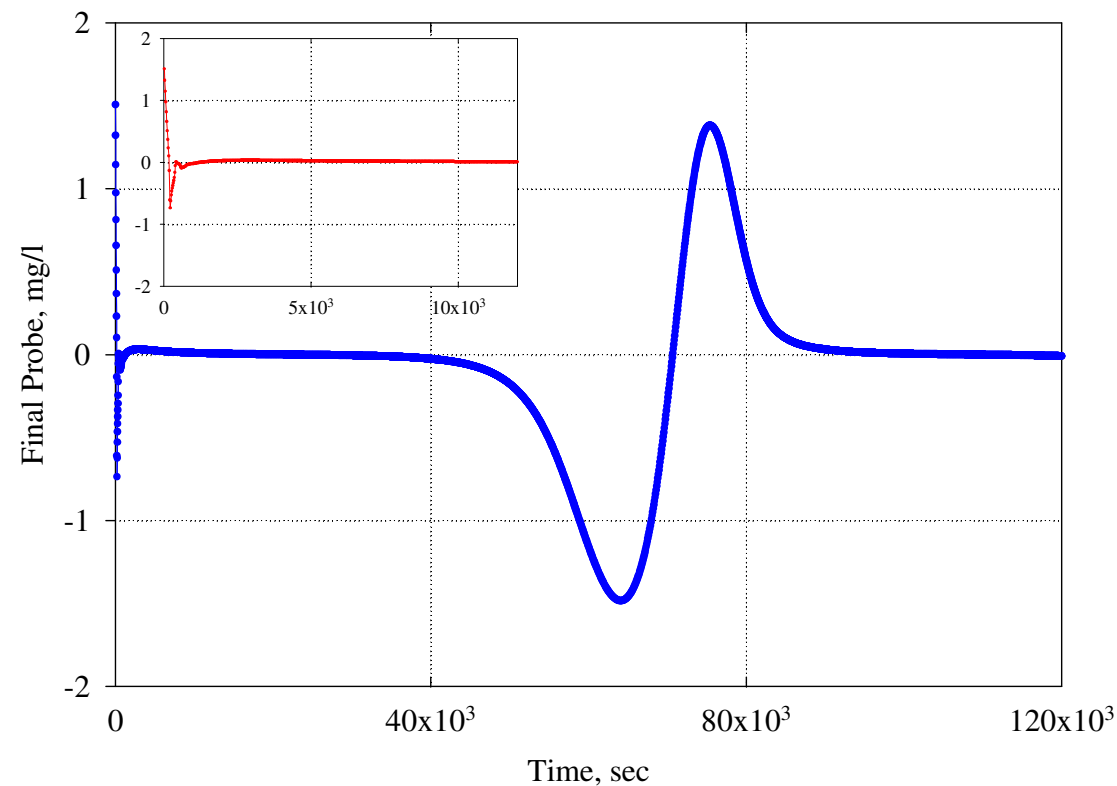
The performance is improved because the deviation values of the final probe measurements are close to zero



$$K_{gain} = 0.06215, \text{ reactor num.} = 200, \tau = 10, t = 5, D = 85.$$

Closed loop simulation result

More improved control performance

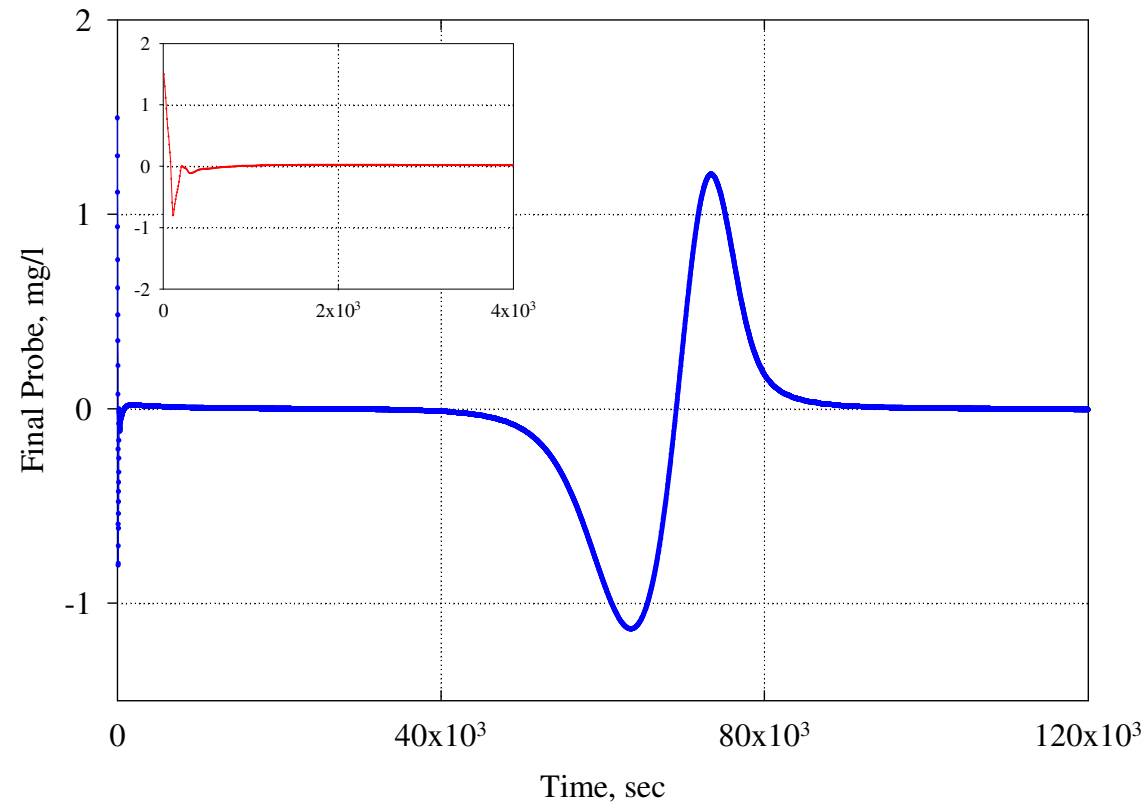


$$K_{gain} = 0.06225, \text{ reactor num.} = 100, \tau = 16, t = 10, D = 81$$

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

Acknowledgements

- Sincere appreciation to Prof. Dr. Oscar D. Crisalle and Wilbur W. Woo (M.Sc) for their excellent assistance and advices
- Thanks the Kanapaha Water Reclamation Facility and the University of Florida Wastewater Treatment Plant personnel for their help

Article

Feridun Demir, Wilbur W. Woo, 2014. Feedback control over the chlorine disinfection process at a wastewater treatment plant using a Smith predictor, a method of characteristics and odometric transformation, Journal of Environmental Chemical Engineering 2 1088–1097, <http://dx.doi.org/10.1016/j.jece.2014.04.006>