PROCESS SYSTEMS ENGINEERING IN WATER QUALITY CONTROL

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INNOVA-MED Course on
Innovative Processes and Practices for
Wastewater Treatment and Re-use

8-11 Oct. 2007, Ankara University

Outline

• What is Process Systems Engineering?
• Modelling
• Control
  – Fuzzy
  – Artificial Neural Network
  – MPC
• Optimization
• Monitoring river water quality
Process Systems Engineering (PSE)

A combination of computer aided decision support methods in
  • Modelling
  • Simulation
  • Applied statistics
  • Design
  • Optimization
  • Control
for an essentially unlimited set of process; environmental, business and public policy systems

Acceptance by 1st Int Symp. in Kyoto, '82

Problems that may be solved by PSE ?!

• WWTPs need to be operated continuously despite large perturbations in
  • Pollution load
  • Flow
  Constraints on effluent become tighter each year
  • Eur. Directive 91/271 Urban Wastewater
• Many plants are either controlled manually or NOT operated!
• ‘Data mining’
  Abundant exp. data that need to be interpreted
NOT AN EASY TASK !!!

• Complex plants with processes of different nature (chemical, biological, mechanical)
• Complicated dynamics (time constants within a very extensive range)
• Varying objectives
• Frequently changing disturbances
• Some information essential for the operation cannot be quantified (smell, color, microbiological quality)
• Measurement problems (unreliable sensors, vague info)

Controlled variables
• Dissolved oxygen conc.
• Ammonia & nitrate conc.
• MLSS concentration
• $\Delta$ (BOD)

Manipulated variables
• Aeration rate
• Dilution rate
• Internal recycle flow rate
• Sludge recycle rate
• External carbon dosing
Suggested control strategies

• Simple feedback controller (usually PI)
• Fuzzy/neural network controller
• Model based controller
• …

Evaluation on the same basis important

⇒ COST Simulation Benchmark

COST Actions 624 & 682
(Vrecko et al. Wat. Sci. & Tech. 2002)

MODELLING

...the first step
**ACTIVATED SLUDGE MODEL No. 3**

(Gujer et al. 1999)

Correction for defects in ASM No.1
- Storage of readily biodegradable substrate
- Less dominating importance of hydrolysis
- Separation of conversion processes for heterotrophs and autotrophs in aerobic and anoxic state
- Alkalinity correction in nitrification rate

- 13 components (soluble and particulate)
- 12 processes

---

**ASM-3 CONVERSION PROCESSES**

**Autotrophic bacteria**

- $S_{NH}$
- Growth
- $X_A$
- Endogenous respiration
- $S_O$
- $S_{O_2}$

**Heterotrophic bacteria**

- $X_{SO}$
- Hydrolysis
- $S_O$
- Storage
- $X_{STO}$
- Growth
- $X_{SO}$
- $X_{O_2}$
- Endogenous respiration
- $X_{SO}$
1 - Hydrolysis
2 - Aerobic storage of readily biodegradable substrate
3 - Anoxic storage of readily biodegradable substrate
4 - Aerobic growth of heterotrophs
5 - Anoxic growth of heterotrophs
6 - Aerobic endogenous respiration of biomass
7 - Anoxic endogenous respiration of biomass
8 - Aerobic endogenous respiration of storage products
9 - Anoxic endogenous respiration of storage products
10 - Aerobic growth of autotrophs
11 - Aerobic endogenous respiration of autotrophs
12 - Anoxic endogenous respiration of autotrophs

ASM-3 Soluble Components (S)

- $S_O$ : Dissolved oxygen
- $S_I$ : Inert soluble organic material
- $S_S$ : Readily biodegradable organic substrates
- $S_{NH}$ : Ammonium and ammonia nitr.
- $S_{N2}$ : Dinitrogen
- $S_{NO}$ : Nitrate ve nitrite nitrogen
- $S_{HCO}$ : Alkalinity of wastewater
ASM-3 Particulate Components (X)

- \( X_I \) : Inert particulate organic material
- \( X_S \) : Slowly biodegradable substrates
- \( X_H \) : Heterotrophic organisms
- \( X_{STO} \) : Cell internal storage product of heterotrophic organisms
- \( X_A \) : Nitrifying autotrophic organisms
- \( X_{TS} \) : Total suspended solids

REATIONS

**Oxidation and Synthesis** (Heterotrophs):

\[
\text{COHNS} + O_2 + \text{nutrients} \rightarrow \text{CO}_2 + \text{NH}_3 + \text{C}_5\text{H}_7\text{O}_2\text{N}
\]

**Endogenous respiration:**

\[
\text{C}_5\text{H}_7\text{O}_2\text{N} + 5 \text{O}_2 \rightarrow 5 \text{CO}_2 + 2\text{H}_2\text{O} + \text{NH}_3 + \text{energy}
\]
NITROGEN REMOVAL

NITRIFICATION: *(Autotrophic bacteria)*

Equation for *Nitrosomonas*:

\[
55 \text{ NH}_4^- + 76 \text{ O}_2 + 109 \text{ HCO}_3^- \rightarrow C_5\text{H}_7\text{O}_2\text{N} + 54 \text{ NO}_2^- + 57 \text{ H}_2\text{O} + 104 \text{ H}_2\text{CO}_3
\]

Equation for *Nitrospira*:

\[
400 \text{ NO}_2^- + \text{NH}_4^+ + 4 \text{ H}_2\text{CO}_3 + \text{HCO}_3^- + 195 \text{ O}_2 \rightarrow C_5\text{H}_7\text{O}_2\text{N} + 3 \text{ H}_2\text{O} + 400 \text{ NO}_3^-
\]

DENITRIFICATION *(Heterotrophic bacteria)*:

\[
\text{NO}_3^- \rightarrow \text{NO}_2^- \rightarrow \text{NO} \rightarrow \text{N}_2\text{O} \rightarrow \text{N}_2
\]

MASS BALANCES AROUND ACTIVATED SLUDGE SYSTEM

For non-aerated periods:

\[
\frac{dX_{i}^{at}}{dt} = \frac{Q_{in}X_{i}^{in} + Q_{rs}X_{i}^{rs} - (Q_{in} + Q_{rs})X_{i}^{at}}{V_{at}} + R_i
\]

\(i\): components of ASM 3 \(X_{i}^{rs}\) from settling model

For aerated periods (dissolved oxygen incorporated):

\[
\frac{dX_{i}^{at}}{dt} = \frac{Q_{in}X_{i}^{in} + Q_{rs}X_{i}^{rs} - (Q_{in} + Q_{rs})X_{i}^{at}}{V_{at}} + R_i + k_{i}a(S_{O}^{sat} - S_{O}^{at})
\]
STATE VARIABLES

73 dimensional vector

- 13 \( \rightarrow \) Concentrations of ASM-3 components in aeration tank
  - 7 solubles
  - 6 particulates
- 60 \( \rightarrow \) Concentrations of particulate components of ASM3 for each layer in settler

10 -Layer Settling Model

\[ \text{Bulk flux (Jb)} = \frac{Q}{A_c} \times X_{ss} \]
\[ \text{Gravity flux (Js)} = v_s \times X_{ss} \]

Kynch (1951) flux theory
Total flux = Bulk flux + gravity
Bulk flux: \( (J_b) = \frac{Q}{A_c} \times X_{ss} \)
Gravity flux: \( (J_s) = v_s \times X_{ss} \)
Cylindrical geometry
No reaction
No concentration changes in radial direction
SETTLING VELOCITY MODEL (Takacs)

\[ v_S(j) = v_0 e^{-r_h X_j^*} - v_0 e^{-r_p X_j^*} \]

- \( v_S \): settling velocity at layer \( j \)
- \( v_0 \): maximum settling velocity
- \( r_h \): settling parameter characteristic of hindered settling zone
- \( r_p \): settling parameter characteristic of low solid concentration
- \( X_j^* \): concentration difference between layer \( j \) and min. attainable

CONTROL

- Fuzzy logic: "computing with words rather than numbers"
- Sentences based on empirical rules
  Expert experience important
A set of ‘linguistic’ descriptors are established
(very high, high, low, true, false, OK)

Control rule, R:
If
( BOD is Y₁) and (MLSS is Y₂) and (DO is Y₃) and (N-NH₃ is Y₄)
then
( Ofeed is U₁) and (R_sludge is U₂)

Membership Function

Contribution of a control rule to the final control action:

\[ \sigma_k = \min\{\mu_{k1}(BOD), \mu_{k2}(MLSS), \mu_{k3}(DO), \mu_{k4}(N-NH3)\} \]

Values of membership functions corresponding to
the process outputs are computed from this array

Membership function of the jth controller output:

\[ \sigma_k = \max\{\sigma_1 v_j(Ofeed), \sigma_2 v_j(R_{sludge})\} \]

Engineering values of the controller outputs (for driving actuators) are
obtained from defuzzification of the output membership functions
(via ‘Center of Gravity’ or ‘Mean of Maximum’ methods)

An acceptable generic knowledge base for WWTP control:

50 rules
(27 for stabilizing BOD, 11 for nitrification, 12 for denitrification)

Detailed examples can be found in
ARTIFICIAL NEURAL NETWORKS

Attempt to simulate the brain
key properties of biological neurons can be
simulated to replicate the human LEARNING
procedure

AREAS OF APPLICATION
- Robotics
- Process control
- Product design
- Operations planning
- Quality control
- Real time modelling
- Adaptive control
- Pattern recognition

![Diagram of neural network](image)

- Neuron ➔ Activation Function
- Dendrites ➔ Net Input Function
- Cell body ➔ Transfer Function
- Axon ➔ Artificial Neuron Output
- Synapses ➔ Weights
"TRAINING"

- Adjusting connection strengths
  - Initialize as a blank state with random weights
  - Excite with input
  - Produce an output and compare with measured output
  - Adjust the weights so that new output will be closer

"TESTING"

- Once training is complete, testing the performance with a new set of data
- If performance is good on the novel set of data, then LEARNING has occurred...

- Actually an optimization problem
  - Backpropagation
  - Quickpropagation
  - Levenberg-Marquardt

Performans functions: MeanSE, SumSE, Root MeanSE
SOME EXAMPLES OF ANN MODELLING FOR WWTPs

- Chen et al. *J. Envir. Engng*. 2001
  - Neural fuzzy modelling & **CONTROLLER**
  - Applied to a plant in Taiwan

  - Data from ASM2d
  - 45 neurons in hidden layer
  - Poor generalization (testing) capability…

  - Influent dist. generator + mechanistic model
  - Prediction on ammonia, BOD and TSSs good
  - COD and total nitrogen less satisfactory
  - ANN reduced simulation time by a factor of 36

**AN ARTIFICIAL NEURAL NETWORK MODEL FOR THE EFFECTS OF CHICKEN MANURE ON GROUND WATER**

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- Department of Chemical Engineering, Hitit University, Corum, Turkey
- Provincial Directorship of Health, Corum, Turkey
- Department of Chemical Engineering, Inonu University, Malatya, Turkey
- Department of Chemical Engineering, Ankara University, Ankara, Turkey
The problem?

- ~ 400 chicken farms in the province of Corum

  *(an important source of ground water pollution in the area)*

- Manure transferred by means of pressurized water to the manure pool
  penetrates into the ground water by
  - runoff
  - flooding
  - diffusion

- Farms get water supply from 20 to 90 m deep wells

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How to predict degree of pollution for major pollutant constituents in ground water wells?

- Identification of an input-output relationship between involved variables based on the field measurements

- Artificial Neural Networks (ANN) are powerful tools that have the abilities to recognize underlying complex relationships from ‘input–output’ data only
Motivation

Poultry manure could be a major source of ground water pollution in the areas where broiler industry is located

► extensive effects,
    when the farms use nearby ground water as their fresh water supply

Prediction of the extent of this pollution via

► rigorous mathematical diffusion modeling
► experimental data evaluation

bears importance

In this work...

Effects of chicken manure on ground water was investigated by artificial neural network modeling

✓ An ANN model was developed for predicting the total coliform in the ground water well in poultry farms

➢ Back-propagation algorithm was applied to training and testing the network

➢ Levenberg Marquardt algorithm was used for optimization

The model holds promise for use in future in order to predict the degree of ground water pollution from nearby chicken farms
Experimental

20 chicken farms were picked from the area
-- chicken population of 10,000 to 40,000
-- manure quantity between 2.4 - 7.0 tons/day

Geographical coordinates, types, design capacity, operation capacity of the farms were recorded &
- geographic features of the land
- depth of well
- distance to the Derincay river
- ways and capacity of manure stocking
- number of chicken
- feeding type

were followed during a period of 8 months at 5 different times

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Chicken Farm 6</th>
<th>Chicken Farm 7</th>
<th>Chicken Farm 8</th>
<th>Chicken Farm 9</th>
<th>Chicken Farm 10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coord. N</td>
<td>40° 33' 43.41&quot;</td>
<td>40° 33' 46.00&quot;</td>
<td>40° 33' 45.01&quot;</td>
<td>40° 33' 51.11&quot;</td>
<td>41° 05' 39.56&quot;</td>
</tr>
<tr>
<td>Coord. E</td>
<td>34° 53' 11.01&quot;</td>
<td>34° 52' 59.54&quot;</td>
<td>34° 52' 47.77&quot;</td>
<td>34° 51' 19.91&quot;</td>
<td>34° 55' 02.12&quot;</td>
</tr>
<tr>
<td>Capacity (chicken)</td>
<td>10,000</td>
<td>10,000</td>
<td>10,000</td>
<td>28,000</td>
<td>10,000</td>
</tr>
<tr>
<td>Water well depth (m)</td>
<td>20</td>
<td>32</td>
<td>90</td>
<td>32</td>
<td>30</td>
</tr>
<tr>
<td>Distance from Derinçay (m)</td>
<td>3,000</td>
<td>2,000</td>
<td>3,000</td>
<td>1,200</td>
<td>800</td>
</tr>
<tr>
<td>Method of waste Storage</td>
<td>Hole</td>
<td>Hole</td>
<td>Hole</td>
<td>Hole</td>
<td>Hole</td>
</tr>
<tr>
<td>Amount of waste (ton/day)</td>
<td>2</td>
<td>2.4</td>
<td>2</td>
<td>5.6</td>
<td>2</td>
</tr>
</tbody>
</table>

Characteristics of some of chicken farms
Water samples were taken from the wells for measurements of:
- pH
- electrical conductivity
- salinity
- total dissolved solid
- turbidity
- nitrite nitrogen
- nitrate nitrogen
- ammonia nitrogen
- organic nitrogen
- total phosphor
- total hardness
- total coliform

Experimental results for Farm - 1

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Chicken Farm – 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sampling date</td>
<td>22.11.2005</td>
</tr>
<tr>
<td>Ammonia, N (mg/L)</td>
<td>4.68</td>
</tr>
<tr>
<td>Nitrite, N (mg/L)</td>
<td>0.024</td>
</tr>
<tr>
<td>Nitrate, N (mg/L)</td>
<td>1.6</td>
</tr>
<tr>
<td>Phosphate, (mg/L)</td>
<td>1.53</td>
</tr>
<tr>
<td>pH</td>
<td>7.9</td>
</tr>
<tr>
<td>Conductivity, (µS/cm)</td>
<td>2.49</td>
</tr>
<tr>
<td>Salinity, (%)</td>
<td>1.5</td>
</tr>
<tr>
<td>Total dissolved solid, (mg/L)</td>
<td>1447</td>
</tr>
<tr>
<td>Turbidity, (FTU)</td>
<td>0</td>
</tr>
<tr>
<td>Total hardness, (mg/L CaCO₃)</td>
<td>142</td>
</tr>
<tr>
<td>Total coliform, (MPN/100 mL)</td>
<td>93</td>
</tr>
</tbody>
</table>
The analysis results were in the range of

- 0.5 - 5.2 mg NO3-N/L
- 0.02 - 3.90 mg NH3-N/L
- 0.51 - 1.89 mg total PO4/L
- 481 - 1852 mg/L total dissolved solids
- 93 - 1100 MPN/100 mL total coliform

**Modelling Procedure**

- ANN model was constructed by using the experimental observations as the input set in order to identify the possible effects of chicken manure resulting from the farms on the ground water.

  - Training → Levenberg - Marquardt method
  - Training accuracy, # of secret layers, # of neurons in the hidden layer, # of iterations → trial and error
Input data and the output data

- number of chickens in the farm considered,
- depth of well where the measurements were taken
- type of manure management
- quantity of manure
- seasonal period of the year

Output
- total coliform

were normalized and de-normalized before and after the actual application in the network

- Out of 80 data set, 60 were used for training & 20 for testing

- Performance function:
  \[ \sum (\text{ANN output} - \text{Laboratory analysis results})^2 \]

- Network was trained for 500 epochs

- Computation was performed in MATLAB 7.0 environment
  A MATLAB script was written, which loaded the data file, trained and validated the network and saved the model architecture
The model developed in this study aims at assessing the effects of chicken manure on the level of pollution in ground water.

Thus the model was created by considering the total coliform concentration in the chicken manure on ground water as the output variable.
Training results

Figure 3 - ANN model for learning data

Testing results

Figure 4 - ANN model for test data

The network model captures the general trend in the output
Two statistical performance criteria for assessment:
- MAPE (Mean Absolute Percent Error)
- R (Correlation Coefficient)

<table>
<thead>
<tr>
<th></th>
<th>Training</th>
<th>Testing</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAPE</td>
<td>0.072 %</td>
<td>0.387 %</td>
</tr>
<tr>
<td>Correlation Coefficient</td>
<td>0.98</td>
<td>0.95</td>
</tr>
</tbody>
</table>

As magnitudes of both errors were quite small for prediction of total coliform, this was considered as an indication of a reliably performing model.

CONCLUSIONS

Developed ANN model predicts the possible amount of total coliform in the ground water well in poultry farms, when:
- number of chickens
- depth of well
- management type of manure pool
- quantity of manure and
- month of the year are given

Encouraged by the results, the model is expected to be of use in future for predicting the degree of ground water pollution from nearby chicken farms.
MODEL PREDICTIVE CONTROL

• At time $k$, solve the open-loop optimal control problem on-line with $x_0 = x(k)$
• Apply the optimal input moves $u(k) = u_0$
• Obtain new measurements, update the state and solve the OLOCP at time $k+1$ with $x_0 = x(k+1)$
• Continue this at each sample time

Implicitly defines the feedback law $u(k) = h(x(k))$

From our studies:

**MPC of a WWTP**

**Consider a simple model** (Nijari et. al. 1999, Caraman et. al. 2007).
**Assumptions**

Steady-state regime
\( (Fin = Fout = F, \ D = F/V) \)

Recycled sludge : \( rF \)

Sludge removal : \( \beta F \)

No substrate or DO in the recycled sludge

\[
\frac{dX(t)}{dt} = \mu X - D(1+r)X + rDXr
\]

\[
\frac{dS(s)}{dt} = \frac{-\mu}{Y} X - D(1+r)S + DS_{in}
\]

\[
\frac{d[DO](t)}{dt} = -K_o \frac{\mu}{Y} X - D(1+r)[DO] + \alpha W ([DO]_{max} - [DO]) + D[DO]_{in}
\]

\[
\frac{dXr(t)}{dt} = D(1+r)X - D(\beta + r)Xr
\]

\[
\mu(t) = \mu_{max} \frac{S}{K_s + S \ K_{DO} + [DO]}
\]

Where

- \( X(t) \): biomass in the bioreactor
- \( S(t) \): substrate
- \([DO](t)\): dissolved oxygen
- \( X_r(t) \): biomass in the settler
- \([DO]_{max} \): maximum dissolved oxygen, \( =10 \text{mg/l} \)
- \( D \): dilution rate \( \text{(assumed constant here)} \)
- \( S_{in} \) and \([DO]_{in} \): substrate and dissolved oxygen concentrations in the influent
- \( Y \): biomass yield factor
- \( M \): biomass growth rate
- \( \mu_{max} \): maximum specific growth rate
- \( k_s \) and \( K_D \): saturation constants
- \( \alpha \): oxygen transfer rate
- \( W \): aeration rate
- \( K_0 \): model constant
- \( r \) and \( \beta \): ratio of recycled and waste flow to the influent

**Kinetic parameters**:
\( Y = 0.65; \ \alpha = 0.018; \ K_{DO} = 2 \text{ mg/l}; \ K_0 = 0.5; \)
\( \mu_{max} = 0.15 \text{ mg/l}; \ k_s = 100 \text{ mg/l}; \ r = 0.6 \)
NMPC simulation block diagram in MATLAB

Controlled variable: DO concentration, Manipulated variable: Aeration rate
Prediction horizon: 5, Control horizon: 1

Disturbance rejection

$DO_{set} = 7.5 \text{ mg/l, constant; } S_{in} \text{ changes in time}$
Set point tracking
DO$_{\text{set}}$ from 7.5 to 5 for 100 hours; $S_{\text{in}} = 200$ mg/l
Set point & Disturbance together

What happens to substrate & biomass in the effluent?
Some Recent Control Studies

  ASM2d with SIMBA software
  NMPC and direct model reference adaptive controller for nutrient and P removal

  COST benchmark model
  MPC on two simulated case

• Caraman et al. *Int. J. of Computers, Communications and Control, 2007.*

  Sewer system + WWTP + River model
  (KOSIB – ASM1 – SWMM5 combined in SIMBA5)
  Multiobjective optimization by genetic algorithm
  → Max DO & Min NH₃ in river, Min energy for piping & aeration

![Diagram](Storm tank - 1st clarifier - AS Reactor - 2nd clarifier)

COST benchmark model
5 compartment (1 anoxic, 4 aerobic)
Manip. var.: External C flow rate
DO set point
$K_L$ a (oxygen transfer rate)

- $O_2$ PI control
- Nitrate & ammonia PI control
- Nitrate PI & ammonia FF-PI control
- MPC

Overall aim: reduction in operating cost
MPC effective in high influent loads

**Operational map for $O_2$ PI control**

...importance of optimization

---

Operating costs
Max. effluent total nitrogen conc.
Max. effluent ammonia conc.
(dash–dotted)
Min. OC

Stare et. al. 2007
Br dys et al. *Control Engng. Practice, 2007*

- Integrated ‘WWTP + sewer’ system
- 3 control layers:
  - Supervisory (coordinates & schedules, selects control strat.)
  - ‘Optimizing’ (LONG (w)/ MEDIUM (h)/ SHORT (m) term control duties) with ‘soft switching’ in between
  - Follow-up (Lower level controllers, hardware maneuv., PIDs)
- Applied to WWT system in Kartuzy, Poland

**INTEGRATED PROCESS SYSTEMS ENGINEERING APPROACH**
ALTERNATING AEROBIC ANOXIC SYSTEMS AND THEIR OPTIMIZATION IN ACTIVATED SLUDGE SYSTEMS

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Ridvan BERBER

Ankara University
Faculty of Engineering
Chemical Engineering Department
TURKEY

CHISA 2004, Prague, 25 August 2004

ACTIVATED SLUDGE SYSTEM
SCOPE

Alternating Aerobic-Anoxic (AAA) systems (carbon and nitrogen removal)
Main operational cost is due to energy used by the aeration equipment (operated consecutively as nonaerated/aerated manner)
Energy optimization is sought by minimizing the aerated fraction of total operation time

A non-trivial dynamic optimization problem

STEPS OF THE STUDY

Selection of
- Activated sludge model (ASM-3)
- Settler model (Vitasovic, 10 layers)
  - Settling velocity model (Takacs)
Mass balances; a general dynamic model for activated sludge system
Simulation for start-up period
Optimal aeration profile for normal operation period
START-UP SIMULATION

- With assumed constant aeration profile
  (0.9 hrs non-aerated / 1.8 hrs aerated)
  for 20 days $k_{l,a} : 4.5 \, h^{-1}$

- Increase microorganism concentration
- Improve settling
- Determine initial values of state variables

ASM-3 variables during start-up

![Graph showing ASM-3 variables over time]
**ASM-3 Soluble Components (S)**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_O$</td>
<td>Dissolved oxygen</td>
</tr>
<tr>
<td>$S_I$</td>
<td>Inert soluble organic material</td>
</tr>
<tr>
<td>$S_S$</td>
<td>Readily biodegradable organic substrates</td>
</tr>
<tr>
<td>$S_{NH}$</td>
<td>Ammonium and ammonia nitr.</td>
</tr>
<tr>
<td>$S_{N2}$</td>
<td>Dinitrogen</td>
</tr>
<tr>
<td>$S_{NO}$</td>
<td>Nitrate &amp; nitrite nitrogen</td>
</tr>
<tr>
<td>$S_{HCO}$</td>
<td>Alkalinity of wastewater</td>
</tr>
</tbody>
</table>

**ASM-3 Particulate Components (X)**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_I$</td>
<td>Inert particulate organic material</td>
</tr>
<tr>
<td>$X_S$</td>
<td>Slowly biodegradable substrates</td>
</tr>
<tr>
<td>$X_H$</td>
<td>Heterotrophic organisms</td>
</tr>
<tr>
<td>$X_{STO}$</td>
<td>Cell internal storage product of heterotrophic organisms</td>
</tr>
<tr>
<td>$X_A$</td>
<td>Nitrifiying autotrophic organisms</td>
</tr>
<tr>
<td>$X_{TS}$</td>
<td>Total suspended solids</td>
</tr>
</tbody>
</table>
OPTIMIZATION PROBLEM

\[
\begin{align*}
\text{min} \quad & J = \sum_{k=1}^{M} b^k / \sum_{k=1}^{M} (a^k + b^k) \\
\text{s.t.} \quad & \text{mass balance equations} \\
& \frac{dX}{dt} = f^{(1)}(X) \quad \text{nonaerated periods} \\
& \frac{dX}{dt} = f^{(2)}(X) \quad \text{aerated periods}
\end{align*}
\]

HARD CONSTRAINTS

- Min. and max. lengths of non-aeration and aeration periods
- Treated water discharge standards
- Total operation time
- Dissolved oxygen concentration
EVOLUTIONARY ALGORITHM (EA)

- Darwin’s natural selection principle
- Genes: durations for non-aerated / aerated periods
- Chromosome (individual): an aeration profile
- Population: pool of aeration profiles

- Start from an initial population
- Evaluate ‘fitness value’
- Create a new generation

GENETIC OPERATORS

- SELECTION (ranking and roulette wheel)
- CROSS-OVER (mixing two individuals)
- MUTATION (creating a new individual)
- ELITISM (adding the best parent individual to the new population)

CONSTRAINTS HANDLING METHODS

- Rejection of infeasible individuals
- Penalizing infeasible individuals
EVOLUTIONARY ALGORITHM
Rejection of Infeasibles

START
Random initiation of population
NO
Genes satisfy boundaries?
YES
Replacement of genes
NO
Parent population
i=1
NO
RUN MODEL
Chromosomes satisfy constraints?
YES
Rejection
i+1
NO
Evaluate objective function
YES
Elite
i
NO
New population
GA operators
STOP

Optimal chromosome

Optimal aeration profile
(REJECTION)
Comparison of Algorithms

<table>
<thead>
<tr>
<th>Constraint handling algorithm</th>
<th>Rejection of infeasibles</th>
<th>Penalizing infeasibles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Treatment</td>
<td>Proper</td>
<td>Proper</td>
</tr>
<tr>
<td>Objective function (%)</td>
<td>55.04</td>
<td>58.07</td>
</tr>
<tr>
<td>Energy savings (relative %)</td>
<td>17.44</td>
<td>12.90</td>
</tr>
<tr>
<td>CPU time (hours)</td>
<td>68.00</td>
<td>65.36</td>
</tr>
</tbody>
</table>

ASM3 Components in Aeration Tank by optimal aeration profile
Operation results by optimal aeration profile  _1

![Graph 1]

Operation results by optimal aeration profile  _2

![Graph 2]
TREATMENT PERFORMANCE

Objective function : 58.0 %
Energy savings : 12.90 %

<table>
<thead>
<tr>
<th>Treatment parameters (g/m³)</th>
<th>Inlet flow</th>
<th>Effluent (24 hours)</th>
<th>Discharge standards</th>
</tr>
</thead>
<tbody>
<tr>
<td>COD</td>
<td>260</td>
<td>37.42</td>
<td>125</td>
</tr>
<tr>
<td>Total nitrogen</td>
<td>25</td>
<td>4.82</td>
<td>10</td>
</tr>
<tr>
<td>Total suspended solids</td>
<td>125</td>
<td>7.91</td>
<td>30</td>
</tr>
</tbody>
</table>

OVERALL EVALUATION

… holds promise for

- Nitrogen removal with no additional investment cost in existing plants
- Easy design and low investment cost for new plants
- Easy operation, and energy savings
OPTIMIZATION BY SQP

Saziye Balku, Mehmet Yüceer & Ridvan Berber
Ankara University Faculty of Engineering

Based on “control vector parameterization”

- Choose initial values for $a^k$ and $b^k$, $k = 1, \ldots, M$
- Initialize state variables
- Integrate aerated and non-aerated models forward in time starting from end of previous one
- Evaluate the objective function
- Solve nonlinear quadratic problem by SQP algorithm

Performed in MATLAB® 6.0 environment

Optimum Aeration Profile

![Graph showing the optimum aeration profile with time intervals and periods]
CHARACTERISTICS OF TREATED WATER

OVERALL EVALUATION

Objective function : 0.479
Energy savings : % 28.1
compared to the arbitrary aeration

<table>
<thead>
<tr>
<th>Treatment Parameters (g / m³)</th>
<th>Inlet flow</th>
<th>Effluent</th>
<th>Discharge standards</th>
</tr>
</thead>
<tbody>
<tr>
<td>COD</td>
<td>260</td>
<td>33.7</td>
<td>125</td>
</tr>
<tr>
<td>Total nitrogen</td>
<td>25</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Total suspended solids</td>
<td>125</td>
<td>0.17</td>
<td>30</td>
</tr>
</tbody>
</table>
MONITORING RIVER WATER QUALITY: Modelling & Calibration Through Optimum Parameter Estimation

Mehmet Yuceer
Ridvan Berber

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Faculty of Engineering
Ankara University, Turkey

Motivation

Water quality models require a large number of parameters to define functional relationships.

Since prior information on parameter values is limited, they are commonly defined by fitting the model to observed data.

Estimation of parameters, which is still practiced by trial-and-error approaches (i.e. manually), is the focal point.
State of the art in river water quality modeling by Rauch et al. (1998) indicated 2 out of 10 offer limited parameter estimation capability.

Mullighan et al. (1998) noted practitioners often resorted to manual trial-and-error curve fitting.

 Generally accepted software: EPA’s QUAL2E (Brown and Barnwell, 1987)

However, few practical problems such as the issue of parameter estimation is missing...

What we have done...

We have suggested a dynamic simulation and parameter estimation strategy so that the heavy burden of finding reaction rate coefficients was overcome (Karadurmus & Berber, 2004 a).

Modeling: segment of river between sampling stations was assumed as ‘a CSTR’

Later extended to ‘series of CSTRs’ approach & a MATLAB-based user-interactive software was developed for easy implementation (Berber et al. 2004 b,c).

⇒ RSDS (River Stream Dynamics and Simulation)
Dynamic Model

Serially connected CSTRs are assumed to represent the behavior of river stream.

Each reactor forms a computational element and is connected sequentially to the similar elements upstream and downstream such as shown in Figure 1.

Assumptions employed for model development:

- Well mixing in cross sections of the river
- Constant stream flow & channel cross section
- Constant chemical and biological reaction rates within the computational element.

[ Similar to QUAL2E (Brown & Barnwell 1987) ]
The model was constituted from dynamic mass balances for

- different forms of nitrogen (organic, ammonia, nitrite, nitrate)
- phosphorus (organic and dissolved)
- biological oxygen demand
- dissolved oxygen
- coliforms
- chloride
- algae

for each computational element

- 11 state variables

Just as an example;

Ammonia nitrogen:

\[
\frac{dN_1}{dt} = \beta_3 \cdot N_4 - \beta_1 \cdot N_1 + \frac{\sigma_3}{d} - F_1 \cdot \alpha_1 \cdot \mu \cdot A + (N_1^0 - N_1) \cdot \frac{Q}{V}
\]

where \( F_1 \) is given by Brown & Barnwell (1987)

\[
F_1 = \frac{P_N \cdot N_1}{P_N \cdot N_1 + (1 - P_N) \cdot N_3}
\]
Organic phosphorus;

\[
\frac{dP_i}{dt} = \alpha_2 \cdot \rho \cdot A - \beta_4 \cdot P_i - \sigma_3 \cdot P_i + (P_i^0 - P_i) \cdot \frac{Q}{V}
\]

Carbonaceous BOD;

\[
\frac{dL}{dt} = -K_1 \cdot L - K_3 \cdot L + (L^0 - L) \cdot \frac{Q}{V}
\]

Physical, chemical and biological reactions and interactions that might occur in the stream have all been considered.

Parameter estimation

Model parameters, conforming to those in QUAL2E water quality model, were estimated by

- Control vector parameterization combined with Sequential Quadratic Programming (SQP) algorithms

by minimizing the objective function & utilizing dynamic field data for state variables collected from two sampling stations.
the sum of squares of errors between the predicted and measured values for all of the state variables for a dynamic run

$$J = \sum_{i=1}^{n} \sum_{j=1}^{m} (x_{ij} - x_{d,ij})^2$$

where

- $x$ : computed value
- $x_d$ : observed value
- $n$ : total number of state variables
- $m$ : total number of observation points

Computation was done in MATLAB 6.5 environment.
A software **RSDS** (River Stream Dynamics and Simulation), coded in MATLAB™ 6.5 has been developed to implement the suggested dynamic simulation and parameter estimation technique.
Dynamic Sampling and Analysis

Study area: Yeşilirmak river around the city of Amasya in Turkey

Field data was collected for two cases:

1. Dynamic data collection for an element of 500 m
   MODEL CALIBRATION
dynamic simulation & parameter estimation

Concentrations of 10 water-quality constituents, corresponding to the state variables of the model
(indicative of the level of pollution in the river)
were determined in 30 minutes intervals either

- on-site by portable analysis systems, or
- in laboratory after careful conservation of the samples
Starting from the 2nd sampling station described above, water quality constituents were determined at various locations along a 36.5 km long section of the river.

*Just like dynamically keeping track of an element flowing at the same velocity as the main stream*

**Waste water of a baker’s yeast production plant nearby was being discharged as a continuous disturbance...**

*Its effect on the water quality downstream*
Results

Predictions from the RSDS are compared to field data for 36.5 kms section of the river after point source

Profiles of the pollution variables (BOD, DO, i.e.)

Field Observation /Model Consistency

Absolute Average Deviation (AAD)

\[
\%AAD = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{|y_{exp} - y_{cal}|}{y_{exp}} \right) * 100
\]

N: Number of measurements, \( y_{exp} \): experimental value, \( y_{cal} \): calculated value

\( \%AAD = \sum((experimental \ value - calculated \ value)) \times 100/\text{experimental \ value} / \text{no. of measurements} \)

(Thorlaksen et al. 2003)

Criterion for quantitative evaluation
Figure 8
RSDS (%AAD): 5.49

Figure 9
RSDS (%AAD): 0.64
### State Variables

<table>
<thead>
<tr>
<th>State Variables</th>
<th>RSDS (% AAD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ammonia Nitrogen</td>
<td>2.86</td>
</tr>
<tr>
<td>Nitrite Nitrogen</td>
<td>29.59</td>
</tr>
<tr>
<td>Nitrate Nitrogen</td>
<td>2.71</td>
</tr>
<tr>
<td>Organic Nitrogen</td>
<td>9.01</td>
</tr>
<tr>
<td>Organic Phosphorus</td>
<td>2.09</td>
</tr>
<tr>
<td>Dissolved Phosphorus</td>
<td>1.89</td>
</tr>
<tr>
<td>BOD</td>
<td>5.49</td>
</tr>
<tr>
<td>Dissolved Oxygen</td>
<td>0.64</td>
</tr>
<tr>
<td>Coliform</td>
<td>6.87</td>
</tr>
<tr>
<td>Chlorine</td>
<td>20.19</td>
</tr>
<tr>
<td>Algae</td>
<td>4.97</td>
</tr>
</tbody>
</table>

Results from **COMPARISON** to QUAL2E for a 7 kms section of the river *(Berber et al 2004c)*

![Graph](image.png)

**Ammonia Nitrogen**

- **%AAD**
  - RSDS: 9.27
  - QUAL2E: 19.38
### Conclusions

- Predictions from RSDS indicate good agreement with experimental data.

  - A systematic procedure suggested here provides an effective means for reliable estimation of model parameters & dynamic simulation for river basins.

  - Contributes to the efforts for predicting the extent of the effect of possible pollutant discharges in river basins.

  - Helps make 'environmental impact assessment' easier.
RSDS has been accommodated within a Geographical Information System (ArcMap)

GIS

MATLAB


“CENTRAL RIVER MONITING AND POLLUTION CONTROL SYSTEM”

TÜBİTAK - 105G002

Supported by TURKISH SCIENTIFIC AND TECHNICAL RESEARCH COUNCIL

ANKARA UNIVERSITY
FACULTY OF ENGINEERING

HİTİT UNIVERSITY
FACULTY OF ENGINEERING

MUNICIPALITY OF AMASYA

Ministry of Environment & Forestry
THE FUTURE

INTEGRATED PROCESS SYSTEMS ENGINEERING
The work and contributions by
• Mehmet Yüceer
• Şaziye Balku
• Erdal Karadurmuş
are acknowledged…