PROCESS SYSTEMS ENGINEERING IN WATER QUALITY CONTROL

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***INNOVA-MED Course** on*
Innovative Processes and Practices for WastewaterTreatment and Re-use

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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 interpereted

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
- Δ (BOD)

Manipulated variables

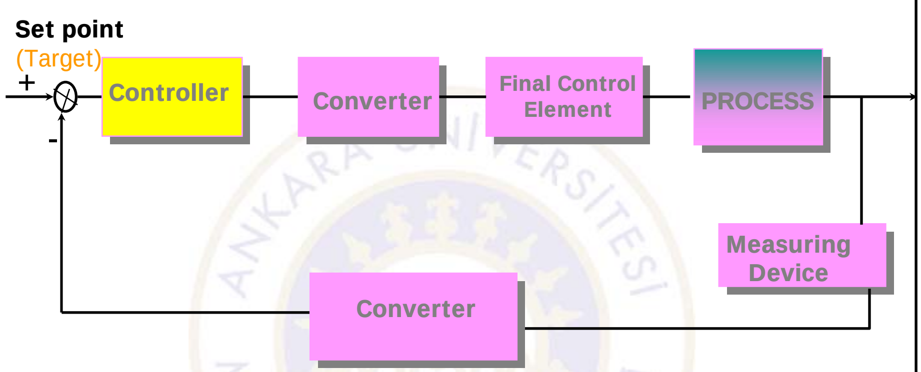
- Aeration rate
- Dilution rate
- Internal recycle flow rate
- Sludge recycle rate
- External carbon dosing

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

- ASM1
- ASM2d
- ASM3
- COST Benchmark
- …

IWA

ACTIVATED SLUDGE MODEL No. 3

(Gujer *et al.* 1999)

Correction for defects in ASM No.1

☑ Storage of readily biodegradable substrate

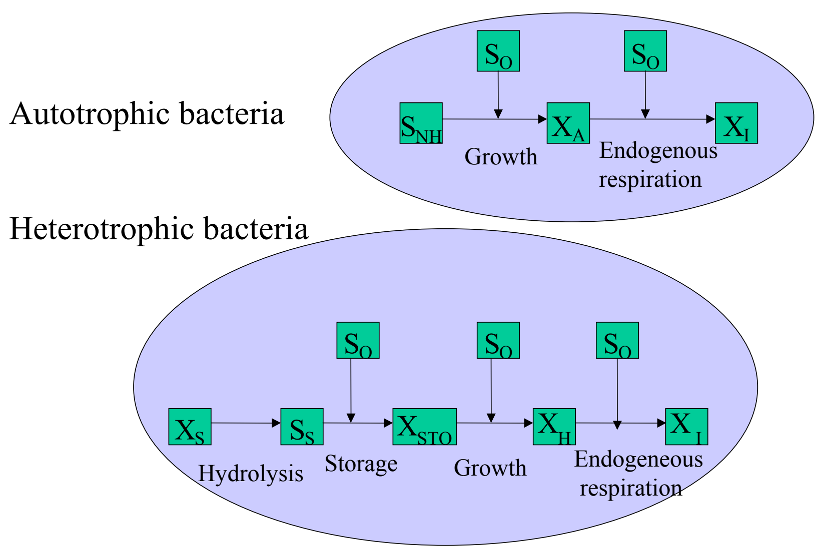
☑ Less dominating importance of hydrolysis

☑ 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



1 - Hydrolysis
2 - Aerobic storage of readily biodegredable substrate
3 - Anoxic storage of readily biodeg. 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 endo. respiration of storage products
9 - Anoxic endo. respiration of storage products
10 -Aerobic growth of autotrophics
11 -Aerobic endog. 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 : Nitrifiying autotrophic organisms
X_{TS} : Total suspended solids

REACTIONS

Oxidation and Synthesis (Heterotrophs) :

$COHNS + O_2 + \text{nutrients} \rightarrow CO_2 + NH_3 + C_5H_7O_2N$

Endogenous respiration:

$C_5H_7O_2N + 5\ O_2 \rightarrow 5\ CO_2 + 2H_2O + NH_3 + \text{energy}$

NITROGEN REMOVAL

NITRIFICATION: (*Autotrophic bacteria*)

<u>Equation for ***Nitrosomonas*** </u>:

$$55\ NH_4^{-} + 76\ O_2 + 109\ HCO_3^{-} \rightarrow C_5H_7O_2N + 54\ NO_2^{-} + 57\ H_2O + 104\ H_2CO_3$$

<u>Equation for ***Nitrospira***</u>**:**

$$400\ NO_2^{-} + NH_4^{+} + 4\ H_2CO_3 + HCO_3^{-} + 195\ O_2 \rightarrow C_5H_7O_2N + 3\ H_2O + 400\ NO_3^{-}$$

DENITRIFICATION (*Heterotrophic bacteria*) **:**

$$NO_3^{-} \rightarrow NO_2^{-} \rightarrow NO \rightarrow N_2O \rightarrow N_2$$

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):

$$\frac{dX_i^{at}}{dt} = \frac{Q_{in}X_i^{in} + Q_{rs}X_i^{rs} - (Q_{in} + Q_{rs})X_i^{at}}{V_{at}} + R_i + k_L a(S_O^{sat} - S_O^{at})$$

STATE VARIABLES

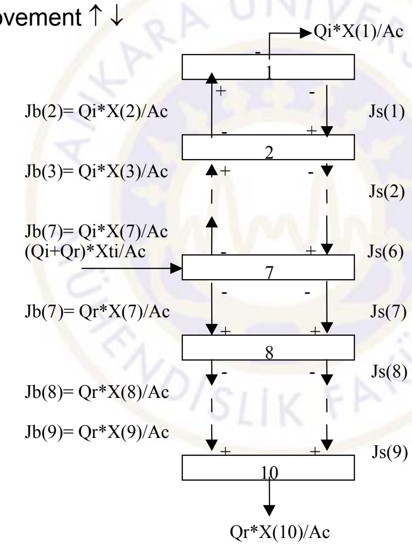
73 dimensional vector

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

10 -Layer Settling Model

Bulk movement ↑↓

↓ Gravity settling



- Kynch (1951) flux theory
- Total flux = Bulk flux + gravity
  - Bulk flux (Jb) = $Q/Ac * X_{ss}$
  - Gravity flux (Js) = $vs * X_{ss}$
- Cylindirical geometry
- No reaction
- No concentration changes in radial direction

SETTLING VELOCITY MODEL (Takacs)

$$v_S(j) = v_0 e^{-r_h X_j^*} - v_0 e^{-r_p X_j^*}$$

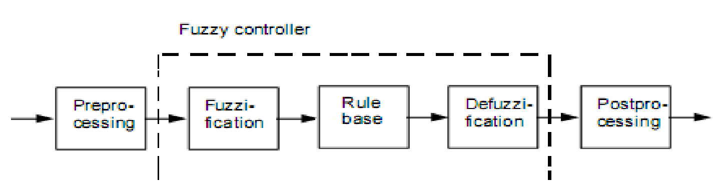
- v_S : settling velocity at layer j
- v_0 : maximum settling velocity
- r_h : settling parameter characteristic of hindered settling zone
- r_p : settling parameter characteristic of low solid concentration
- X_j^* : concentration difference between layer j and min. attainable

CONTROL

FUZZY CONTROL

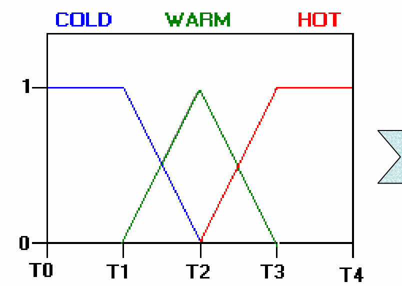
- Fuzzy logic: ''computing with words rather than numbers''
- Sentences based on empirical rules

Expert experience important



A set of ‘linguistic’ descriptors are established

(very high, high, low, true, false, OK)



Membership Function

Control rule, R:

If(

(BOD is Y_1) and (MLSS is Y_2) and (DO is Y_3) and (N-NH3 is Y_4)

then

(Ofeed is U_1) and (R_sludge is U_2)

Contribution of a control rule to the final control action:

$$\sigma_k = \min\{\mu^k_1(\mathrm{BOD}), \mu^k_2(\mathrm{MLSS}), \mu^k_3(\mathrm{DO}), \mu^k_3(\mathrm{N\text{-}NH3})\}$$

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

Membership function of the jth controller output:

$$\sigma_k = \max\{\sigma_1 \nu^j_1(\mathrm{Ofeed}), \sigma_2 \nu^j_2(\mathrm{R\_sludge})\}$$

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 accapetable generic knowledge base for WWTP control:

50 rules

(27 for stabilizing BOD, 11 for nitrification, 12 for denitrification

Detailed examples can be found in

- Müller et. al. *Water Research,* 1997.
- Manesis et. al. *Artif. Intelligence in Engineering* 1998.

ARTIFICIAL NEURAL NETWORKS

- Attempt to simulate the brain

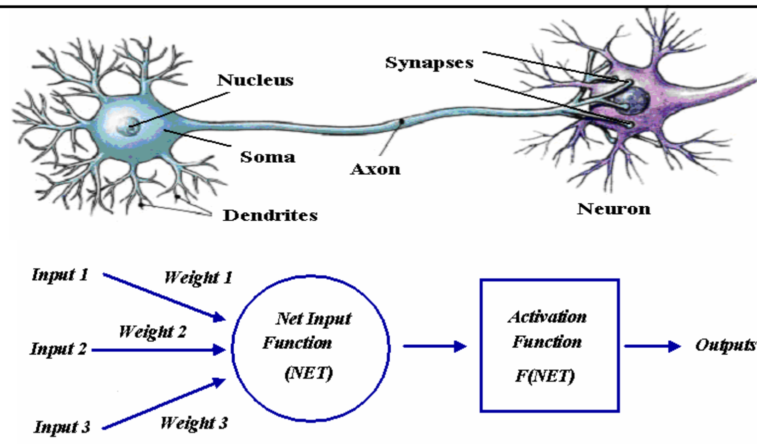
key properties of biological neurons can be simulated to replicate the human LEARNING procedure

AREAS OF APPLICATION

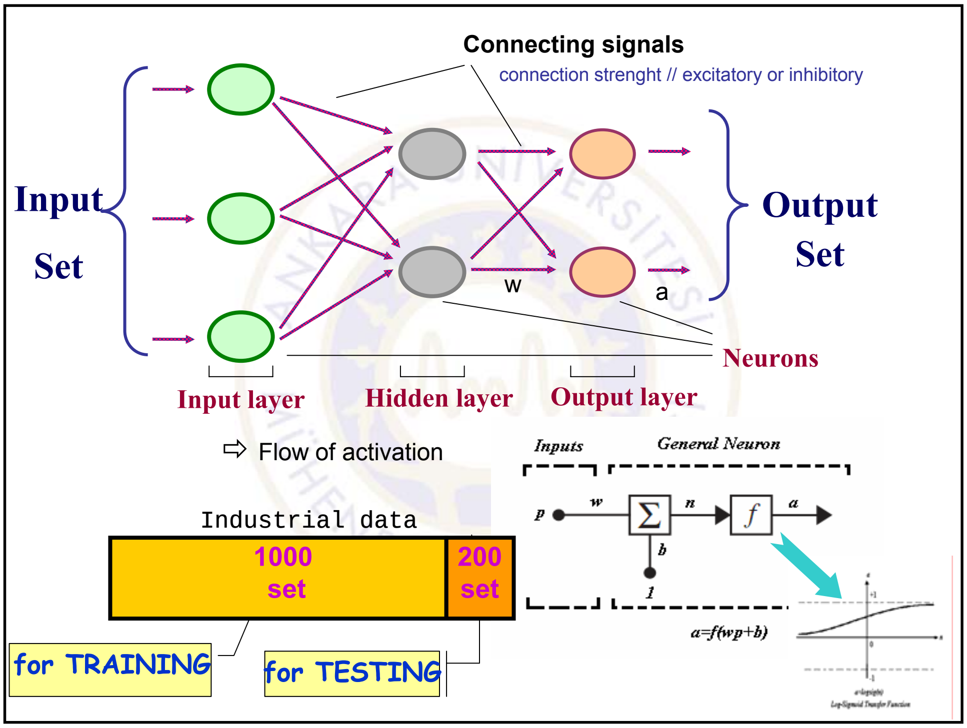
- Robotics
- Process control
- Product design
- Operations planning
- Quality control
- Real time modelling
- Adaptive control
- Pattern recognition

Biological neuron

Artificial neuron



Neuron	→ Activation Function
Dendrites	→ Net Input Function
Cell body	→ Transfer Function
Axon	→ Artificial Neuron Output
Synapses	→ Weights



"TRAINING"

- Adjusting connection strenghts

  - *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*

Backpropagation cycle

"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

- Ko et al. *Int. Workshop on Soft Computing*… Provo, Utah, 2003
  - Data from ASM2d
  - 45 neurons in hidden layer
  - → Poor generalization (testing) capability…

- Raduly et al. *Environmental Modelling and Software,* 2007
  - 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

→ Mostly modelling… ANNs require expertise!...

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

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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

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 <u>importance</u>

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
- *w*ays and capacity of manure stocking
- number of chicken
- feeding type

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

Parameters	Chicken Farm 6	Chicken Farm 7	Chicken Farm 8	Chicken Farm 9	Chicken Farm 10
Coord. N	40° 33' 43.41"	40° 33' 46.00"	40° 33' 45.01"	40° 32' 45.84"	40° 32' 29.56"
Coord. E	34° 53' 11.01"	34° 52' 59.54"	34° 52' 47.77"	34° 51' 18.91"	34° 55' 02.12"
Capacity (chicken)	10 000	10 000	10 000	28 000	10 000
Water well depth (m)	20	32	90	32	30
Distance from Derinçay (m)	3 000	2 000	3 000	1 200	800
Method of waste Storage	Hole	Hole	Hole	Hole	Hole
Amount of waste (ton/day)	2	2,4	2	5,6	2




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

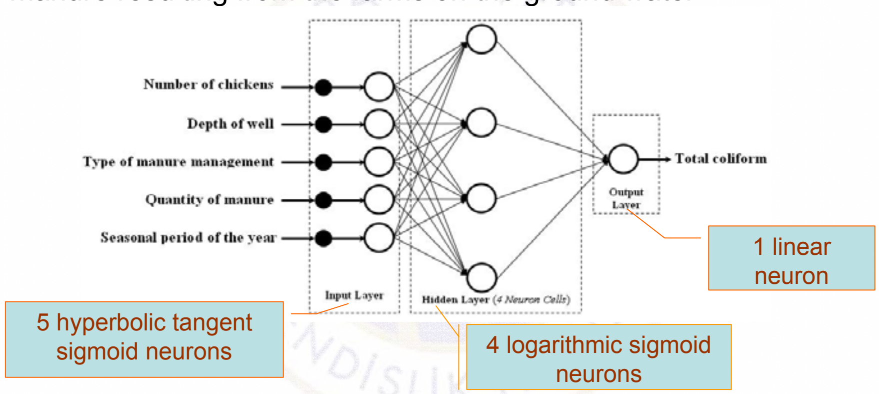
Parameters	Chicken Farm – 1			
Sampling date	22.11.2005	07.03.2006	05.04.2006	10.04.2006
Ammonia, N (mg/L)	4,68	3,32	1,5	2,62
Nitrite, N (mg/L)	0,024	0,015	0,027	0,009
Nitrate, N (mg/L)	1,6	3,2	1,9	1,0
Phosphate, (mg/L)	1,53	0,91	1,07	0,8
pH	7,9	7,78	7,68	6,96
Conductivity, (μS/cm)	2,49	2,17	2,21	1,989
Salinity, (‰)	1,5	1,3	1,3	1,2
Total dissolved solid, (mg/L)	1447	1248	1263	1140
Turbidity, (FTU)	0	0	0	1
Total hardness (mg/L $CaCO_3$)	142	142	142	142
Total coliform (MPN/100 mL)	93	240	240	240

The analysis results were in the range of

- 0.5 - 5.2 mg NO_3-N/ L
- 0.02 - 3.90 mg NH_3-N/L
- 0.51 - 1.89 mg total PO_4/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

Inputs
- 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

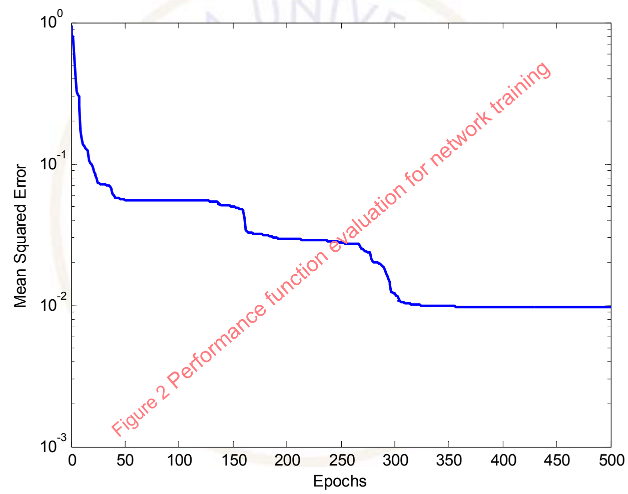
- Out of 80 data set, 60 were used for training & 20 for testing
- Performance function :

$$\Sigma\,(\text{ANN output} - \text{Laboratory analysis results})^2$$

- 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

Progress of a typical training session for proposed network structure

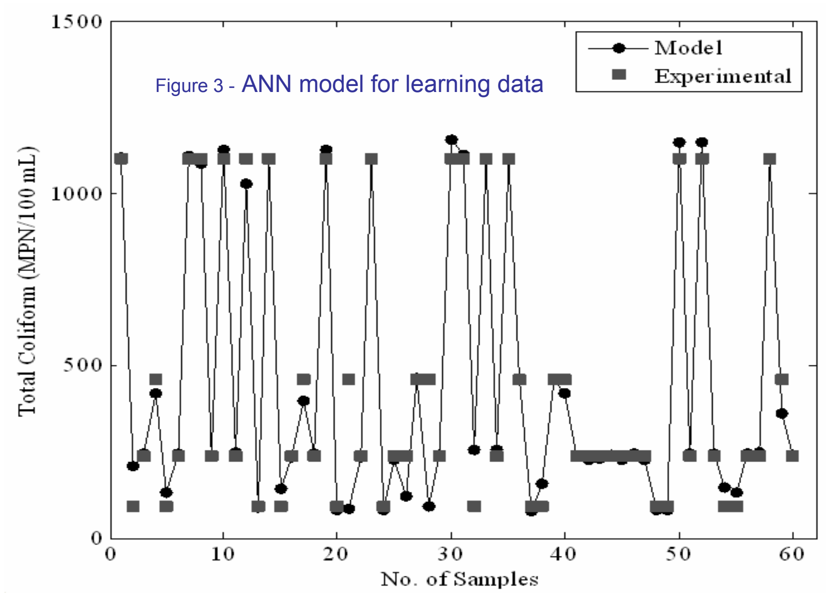


Performance function (MSE) value is calculated about 0.01 for 500 epochs

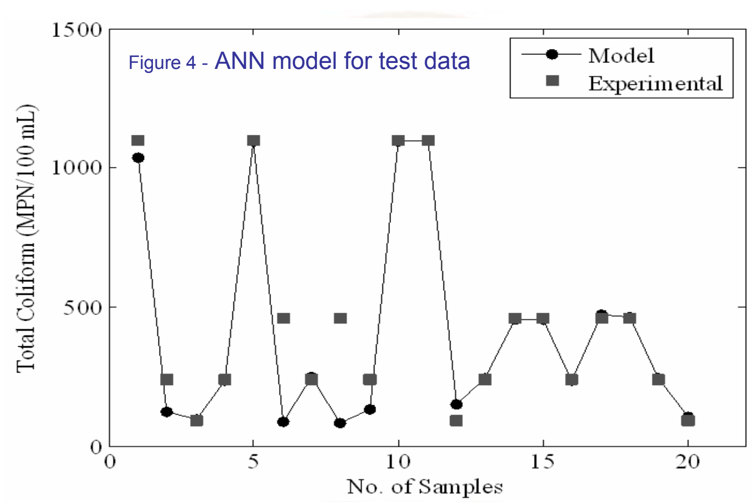
RESULTS

- 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



Testing results



The network model captures the general trend in the output

► Two statistical performance criteria for assesment;

- MAPE (Mean Absolute Percent Error)
- R (Correlation Coefficient)

	Training	Testing
MAPE	0.072 %	0.387 %
Correlation Coefficient	0.98	0.95

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

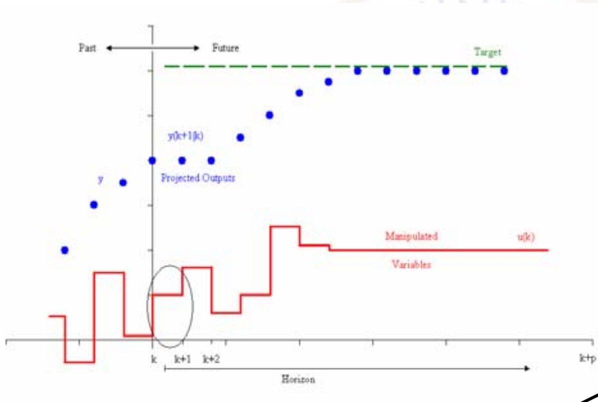
► Developed ANN model predicts the possible amount of total coliform in the ground water well in poultry farms, when

- 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



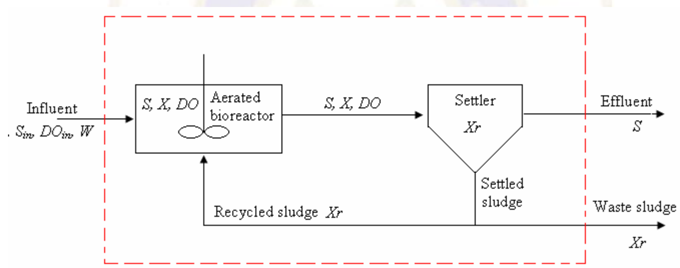
- At time k, solve the open-loop optimal control problem **on-line with $x_0=x(k)$**
- Apply the optimal input moves $u(k)=u_0$
- Obtain new measurements, update the state and solve the OLOCP at time $k+1$ with $x_0=x(k+1)$
- Continue this at each sample time

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

From our studies:

MPC of a WWTP

Consider a simple model (Nijjari et. al. 1999, Caraman et. al. 2007).



<u>Assumptions</u>

Steady-state regime

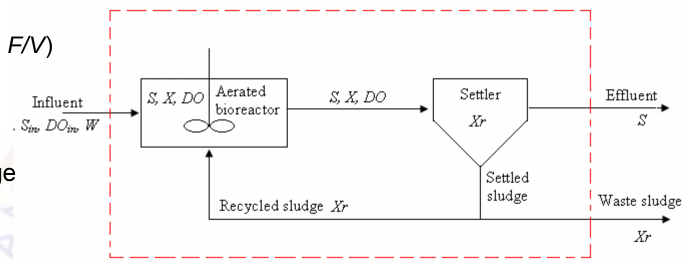
(*Fin = Fout = F, D = F/V*)

Recycled sludge : *r F;*

Sludge removal : β *F*

No substrate or DO

in the recycled sludge



$$\frac{dX(t)}{dt} = \mu X - D(1+r)X + rDX_r$$

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

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

$$\frac{dX_r(t)}{dt} = D(1+r)X - D(\beta + r)X_r$$

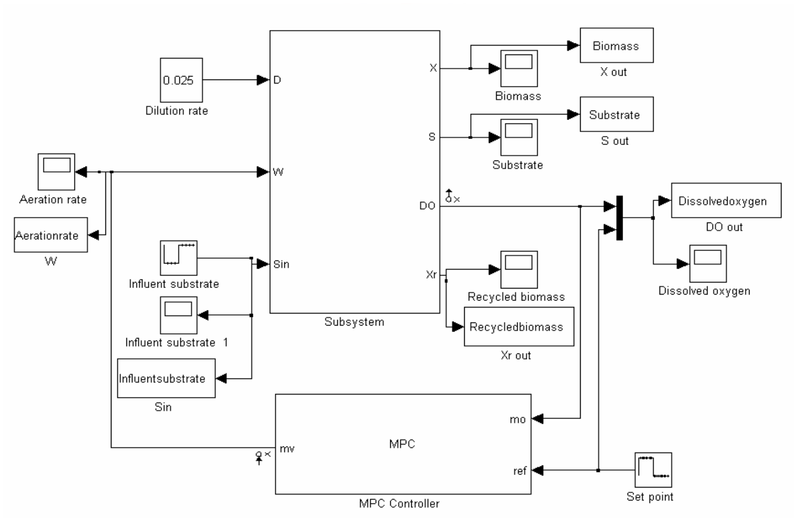
$$\mu(t) = \mu_{\max}\frac{S}{k_s + S}\frac{[DO]}{K_{DO} + [DO]}$$

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, =10mg/l
D	: dilution rate *(assumed constant here)*
S_{in} and $[DO]_{in}$	: substrate and dissolved oxygen concentrations in the influent
Y	: biomass yield factor
M	: biomass growth rate
μ_{max}	: maximum specific growth rate
k_S and K_D	: saturation constants
α	: oxygen transfer rate
W	: aeration rate
K_0	: model constant
r and β	: ratio of recycled and waste flow to the influent

Kinetic parameters: Y = 0.65; α= 0.018; K_{DO} = 2 mg/l; K_0 = 0.5;
μ_{max} = 0.15 mg/l; k_S = 100 mg/l; r = 0.6

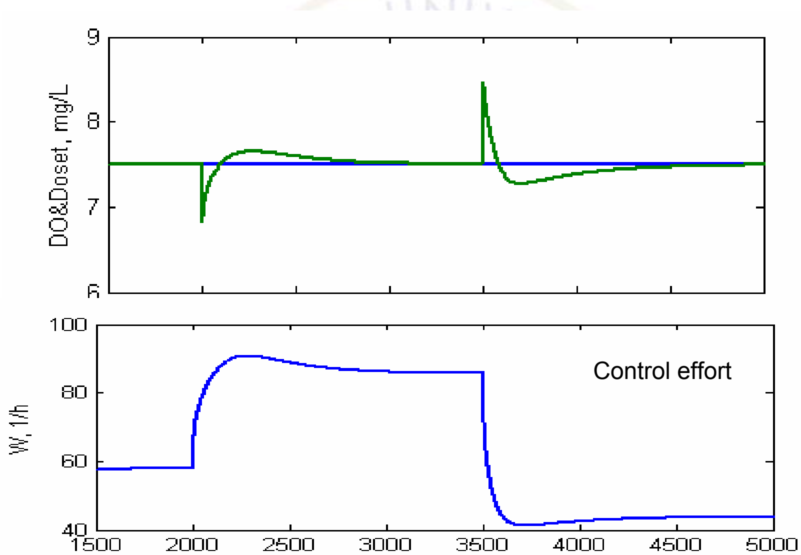
NMPC simulation block diagram in MATLAB

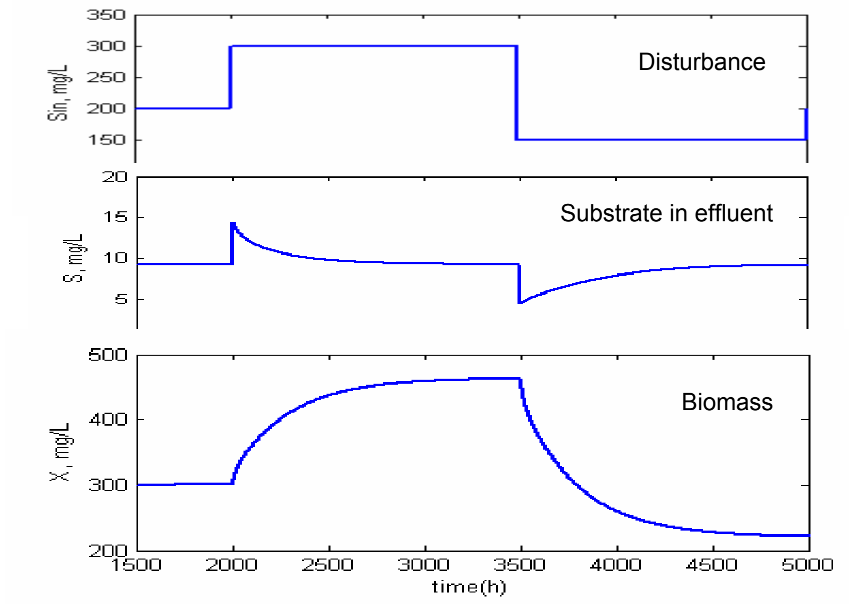


Controlled variable: DO concentration, Manipulated variable: Aeration rate
Prediction horizon : 5 Control horizon:1

Disturbance rejection

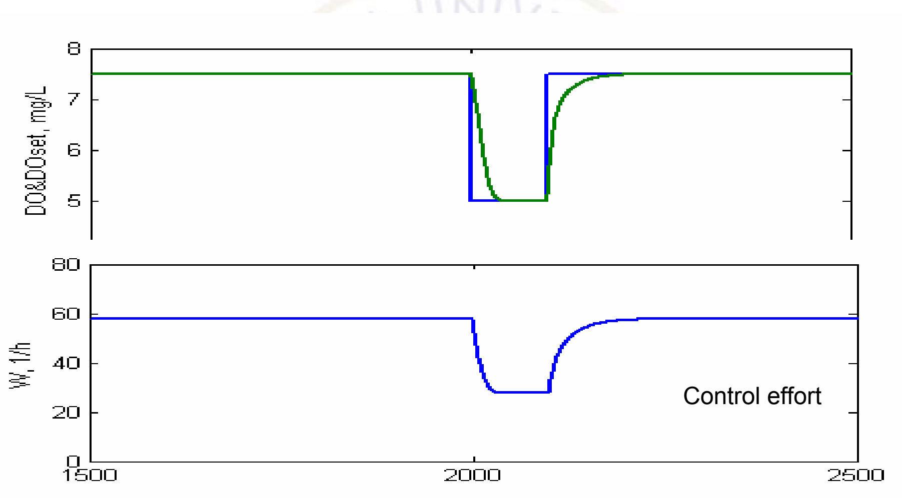
DO_{set} = 7.5 mg/l, constant; S_{in} changes in time



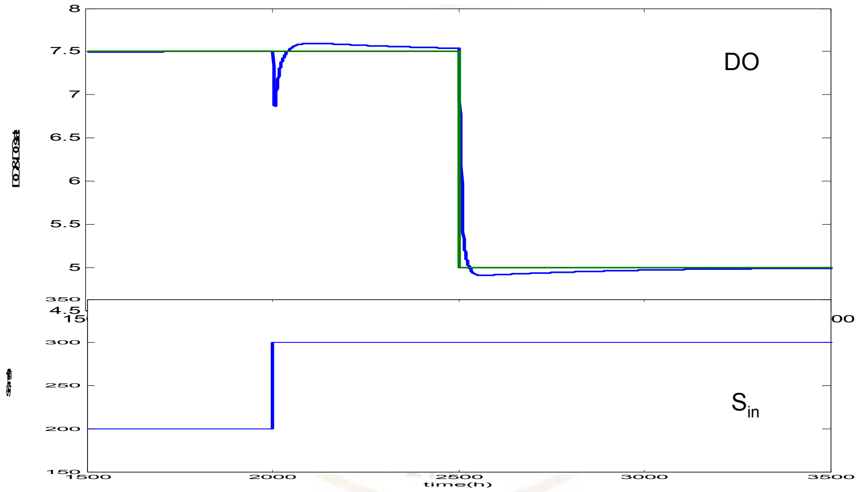


Set point tracking

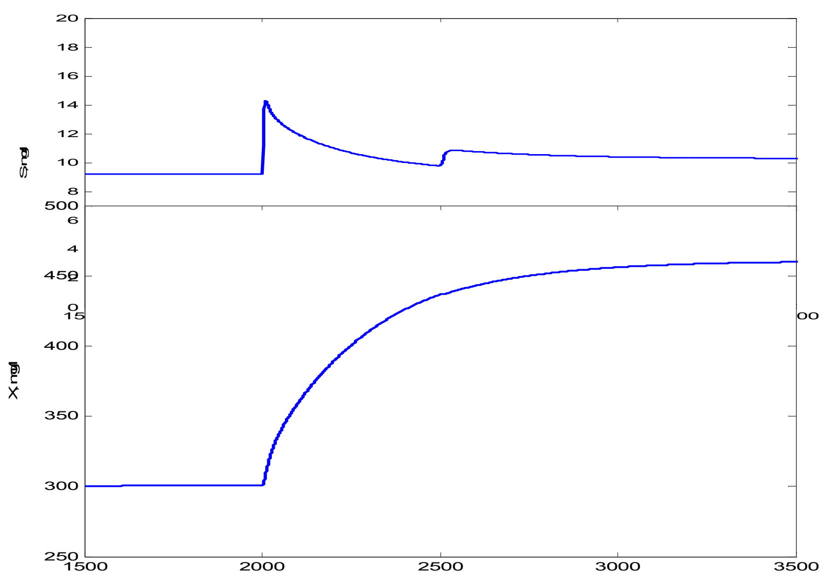
DO_{set} from 7.5 to 5 for 100 hours; S_{in} = 200 mg/l



Set point & Disturbance together



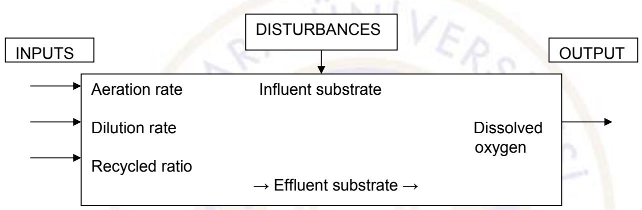
What happens to substrate & biomass in the effluent ?



Some Recent Control Studies

- Chotkowski et al. *Int. J. Systems Sci.* 2005.
  - ASM2d with SIMBA software
  - NMPC and direct model reference adaptive controller for nutrient and P removal
- Holenda et. al. *Comp. & Chem. Eng.* 2007.
  - COST benchmark model
  - MPC on two simulated case

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



- Fu et al. *Envir. Mod. Soft.* 2007.
  - Sewer system + WWTP + River model
  - (KOSIB – ASM1 – SWMM5 combined in SIMBA5)
  - Multiobjective optimization by genetic algorithm
  - → Max DO & Min NH_3 in river, Min energy for piping & aeration

Storm tank - 1st clarifier - AS Reactor - 2nd clarifier

Stare et al. *Water Research* 2007.

COST benchmark model

5 compartment (1 anoxic, 4 aerobic)

Manip. var. : External C flow rate

DO set point

K_La (oxygen transfer rate)

O_2 PI control

Nitrate & ammonia PI control

Nitrate PI & ammonia FF-PI control

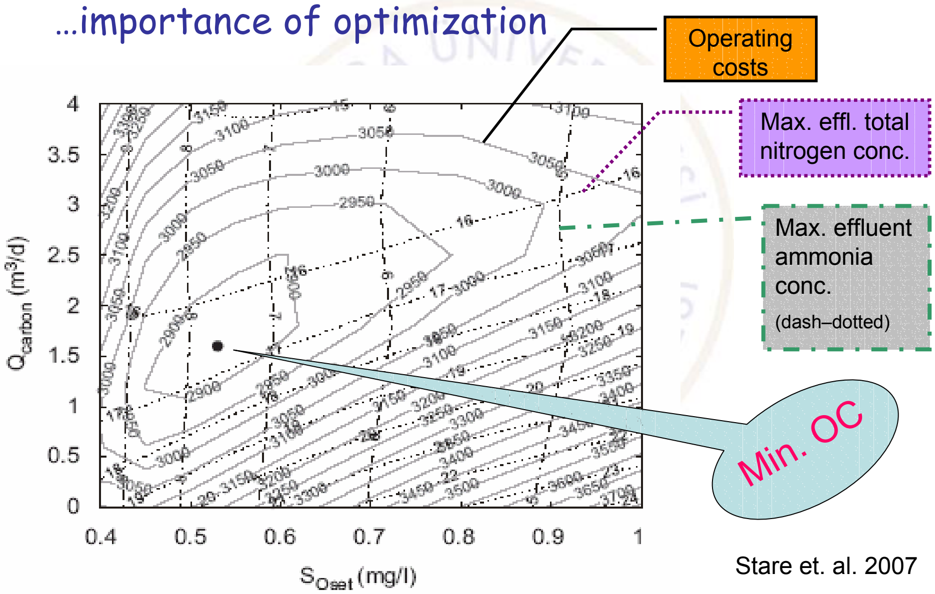
MPC

Overall aim: reduction in operating cost

MPC effective in high influent loads

Operational map for O_2 PI control

...importance of optimization

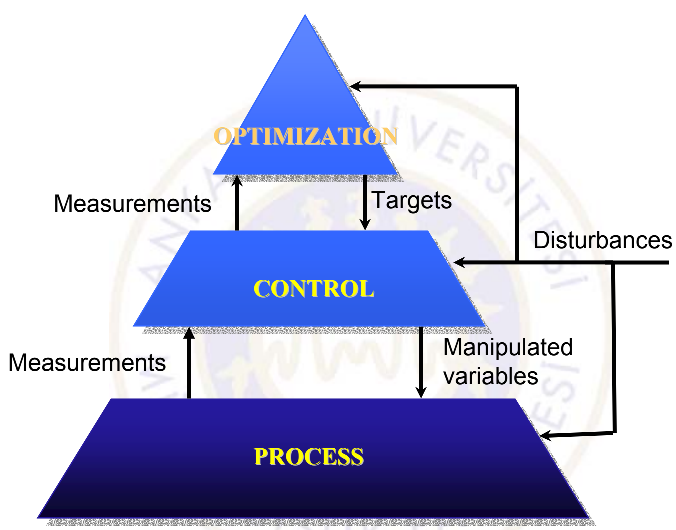


Stare et. al. 2007

Brdys 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

NOT in the sense of
INTEGRATED ENGINEERING
i.e. providing set points...



INTEGRATED PROCESS SYSTEMS ENGINEERING APPROACH

ALTERNATING AEROBIC ANOXIC SYSTEMS AND THEIR OPTIMIZATION IN ACTIVATED SLUDGE SYSTEMS

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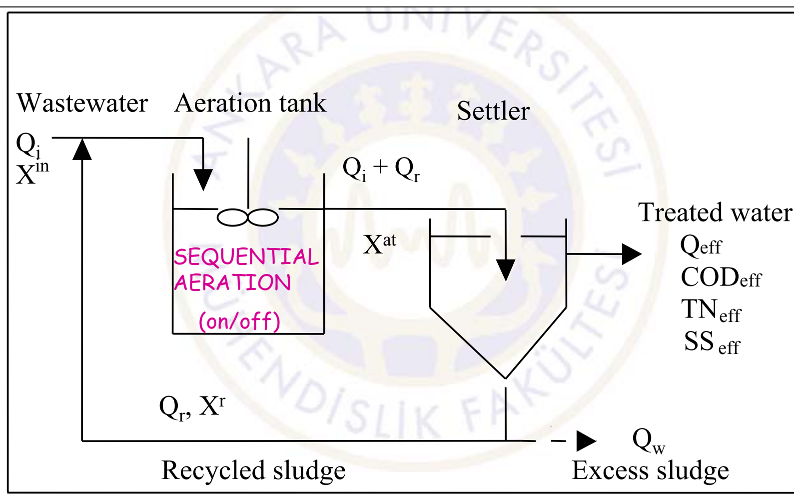
Ridvan BERBER

Ankara University
Faculty of Engineering
Chemical Engineering Department
TURKEY

CHISA 2004, Prague, 25 August 2004

AAA
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

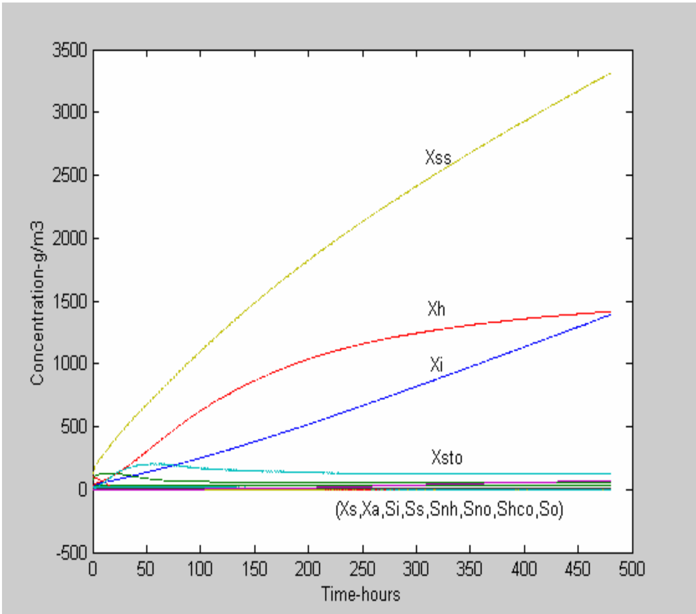
- Selection of
  - **Activated sludge model** (ASM-3)
  - **Settler model** (Vitasovic, 10 layers)
    - ***Settling velocity model*** *(Takacs)*
- Mass balances; a general dynamic model for activated sludge system
- Simulation for start-up period
- Optimal aeration profile for normal operation period

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



Heteotr organ.

Inert. part. org. mat.

Cell int. storage products

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 & 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	: Nitrifiying autotrophic organisms
X_{TS}	: Total suspended solids

OPTIMIZATION PROBLEM

min $J = \sum_{k=1}^{M} b^k / \sum_{k=1}^{M} (a^k + b^k)$

s.t. mass balance equations

$\frac{dX}{dt} = f^{(1)}(X)$ nonaerated periods

$\frac{dX}{dt} = f^{(2)}(X)$ aerated periods

Soft constraints

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

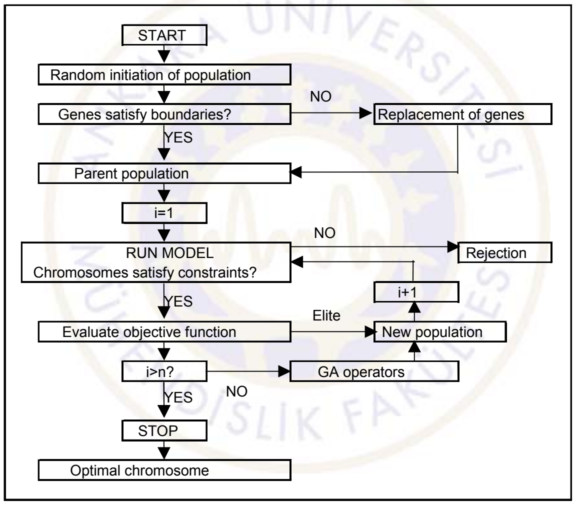
GENETIC OPERATORS

- 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)*

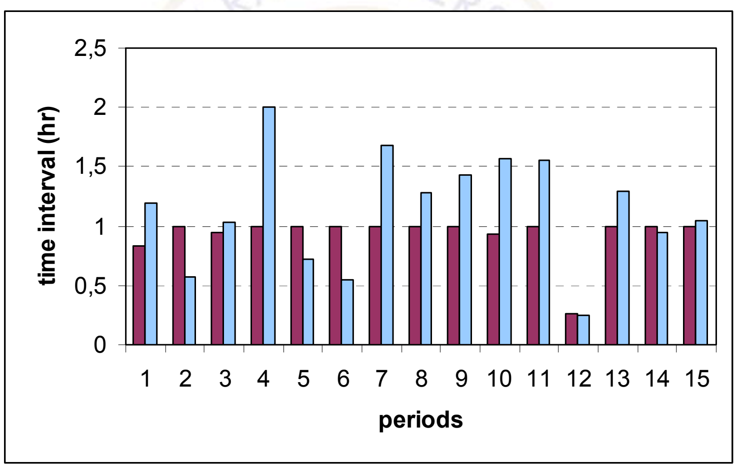
CONSTRAINTS HANDLING METHODS

- Rejection of infeasible individuals
- Penalizing infeasible individuals

EVOLUTIONARY ALGORITHM
Rejection of Infeasibles



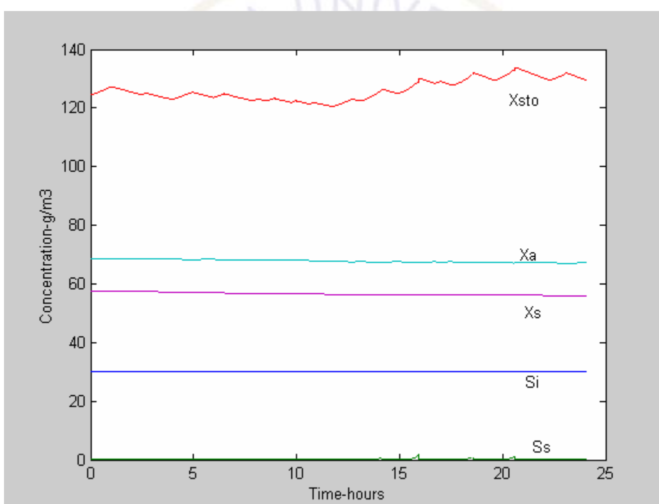
Optimal aeration profile
(REJECTION)



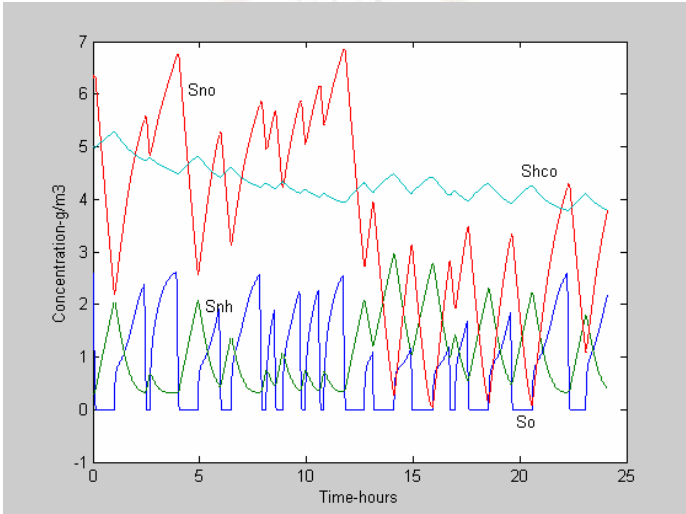
Comparison of Algorithms

Constraint handling algorithm	**Rejection of infeasibles**	**Penalizing infeasibles**
Treatment	Proper	Proper
Objective function (%)	55.04	58.07
Energy savings (relative %)	17.44	12.90
CPU time (hours)	68.00	65.36

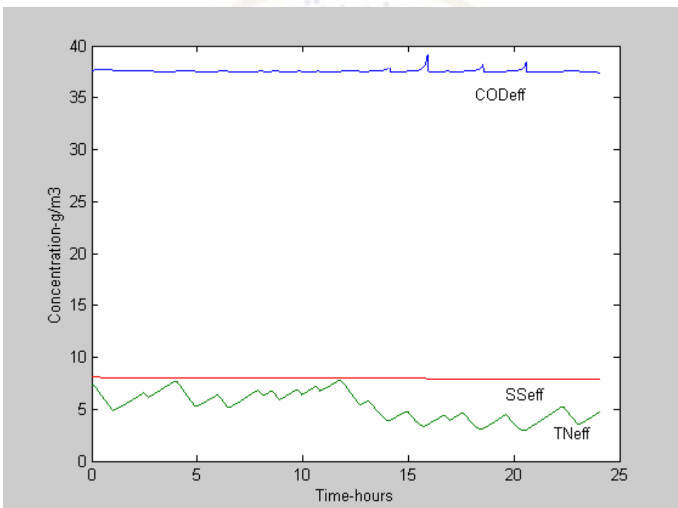
ASM3 Components in Aeration Tank by optimal aeration profile



Operation results by optimal aeration profile _1



Operation results by optimal aeration profile _2



TREATMENT PERFORMANCE

Objective function : 58.0 %

Energy savings : 12.90 %

Treatment parameters (g/m^3)	Inlet flow	Effluent (24 hours)	Discharge standards
COD	260	37.42	125
Total nitrogen	25	4.82	10
Total suspended solids	125	7.91	30

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

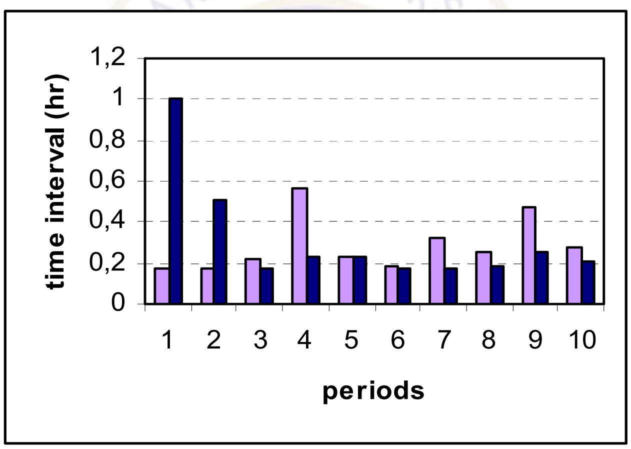
Saziye Balku, Mehmet Yüceer &
Ridvan Berber
Ankara University Faculty of Engineering

Based on "control vector parameterization"

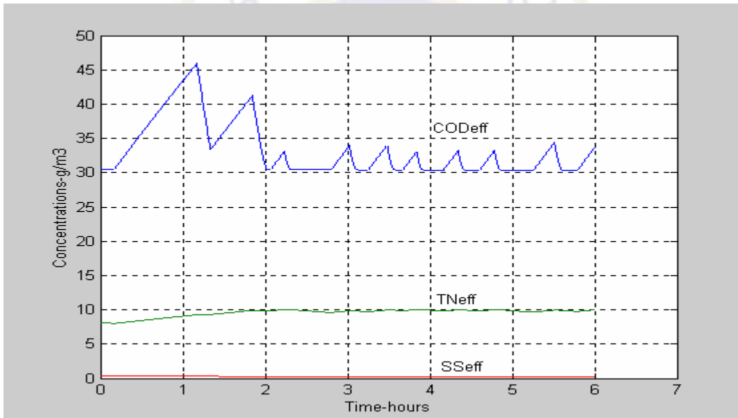
- Choose initial values for a^k and b^k, k = 1,....M
- Initialize state variables
- Integrate aerated and non-aerated models forward in time starting from end of previous one
- Evaluate the objective function
- Solve nonlinear quadratic problem by SQP algorithm

Performed in MATLAB® 6.0 environment

Optimum Aeration Profile



CHARACTERISTICS OF TREATED WATER



OVERALL EVALUATION

Objective function : 0.479

Energy savings : % 28.1

compared to the arbitrary aeration

Treatment Parameters (g / m^3)	Inlet flow	Effluent	Discharge standards
COD	260	33.7	125
Total nitrogen	25	10	10
Total suspended solids	125	0.17	30

MONITORING RIVER WATER QUALITY :
Modelling & Calibration Through Optimum Parameter Estimation

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Motivation

Water quality models require 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

Mulligan *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...

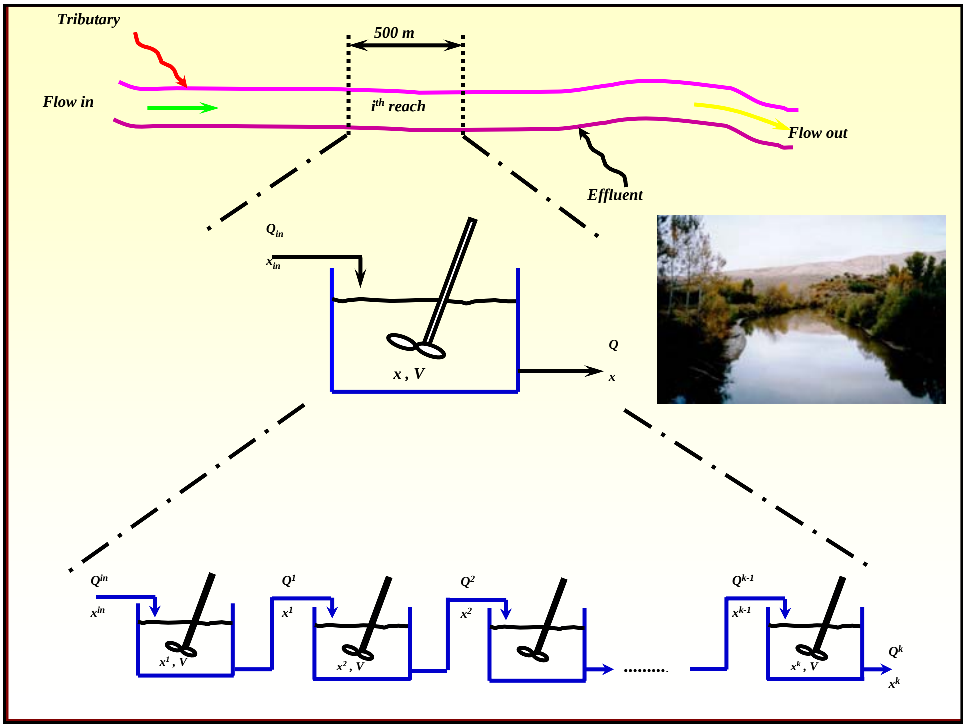
What we have done...

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:

$$\frac{dN_1}{dt} = \beta_3 \cdot \mathrm{N}_4 - \beta_1 \cdot \mathrm{N}_1 + \frac{\sigma_3}{\mathrm{d}} - \mathrm{F}_1 \cdot \alpha_1 \cdot \mu \cdot \mathrm{A} + (\mathrm{N}_1^0 - \mathrm{N}_1).\frac{\mathrm{Q}}{\mathrm{V}}$$

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

$$F_1 = \frac{P_N.N_1}{P_N \cdot N_1 + (1-P_N).N_3}$$

Organic phosphorus;

$$\frac{dP_1}{dt} = \alpha_2 . \rho . A - \beta_4 . P_1 - \sigma_5 . P_1 + (P_1^0 - P_1) . \frac{Q}{V}$$

Carbonaceous BOD;

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

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

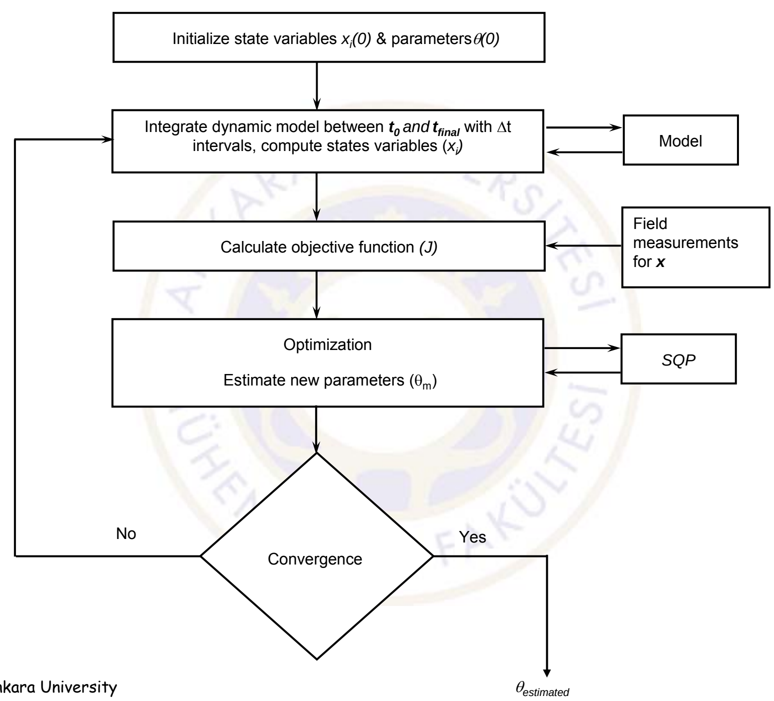
Obj. function

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

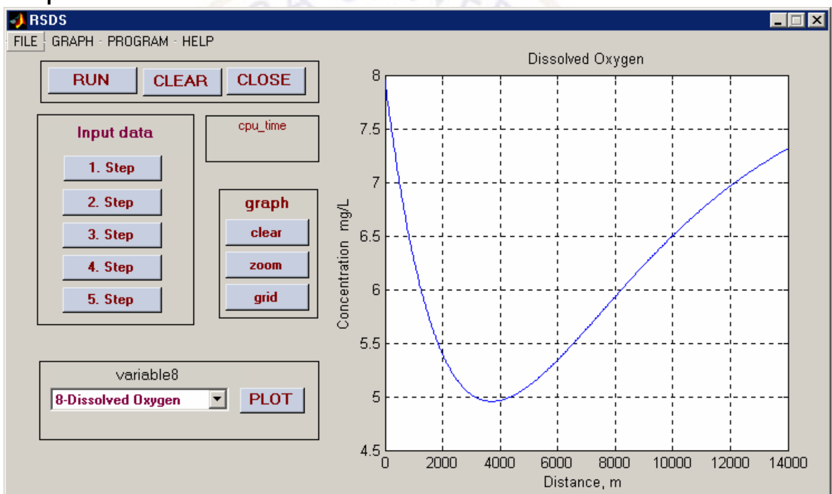
where

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.



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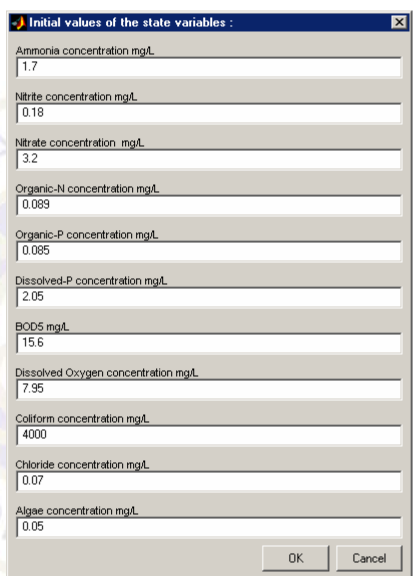
Another view from the GUI



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Dynamic Sampling and Analysis

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

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Field data was collected for two cases:

❶ 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

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❷ Observation and data collection
for a 36 kms section of the river

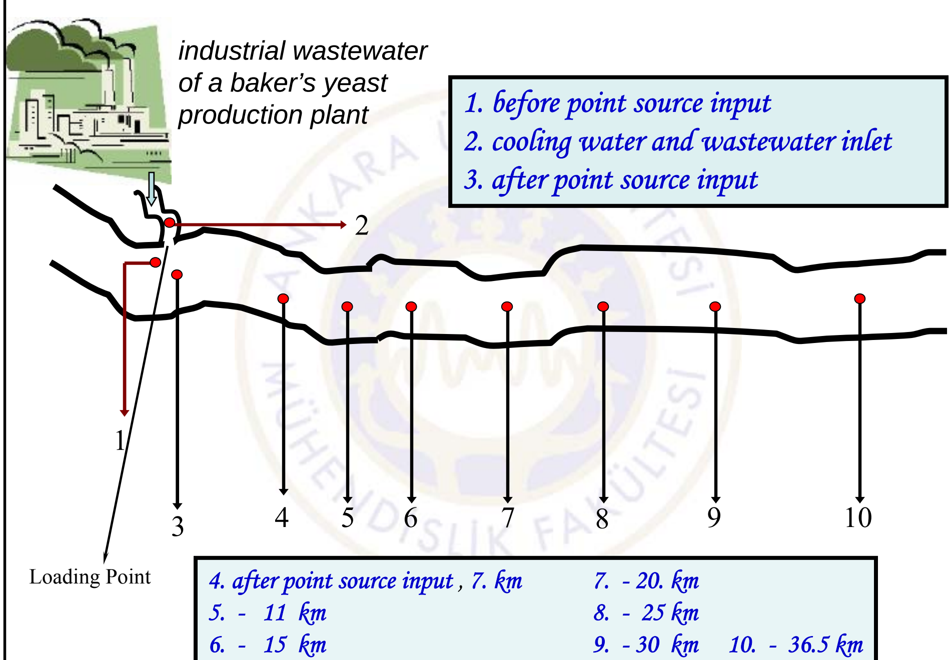
⇨ MODEL VERIFICATION & COMPARISON TO QUAL2E

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)

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

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

%AAD=Σ((|experimental value - calculated value|) x100/experimental value)/no. of measurements)

(Thorlaksen *et al.* 2003)

Criterion for quantitative evaluation

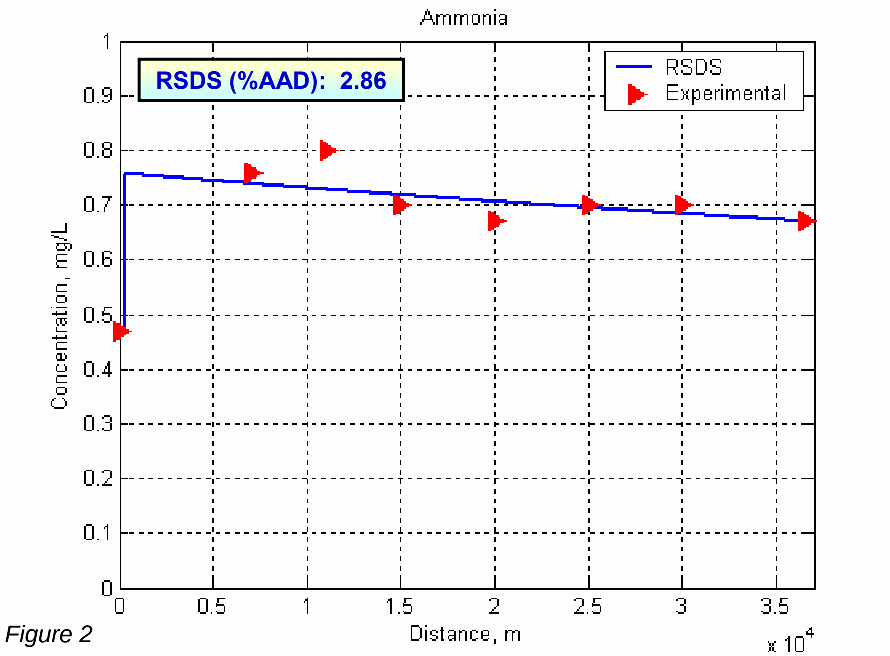


Figure 2

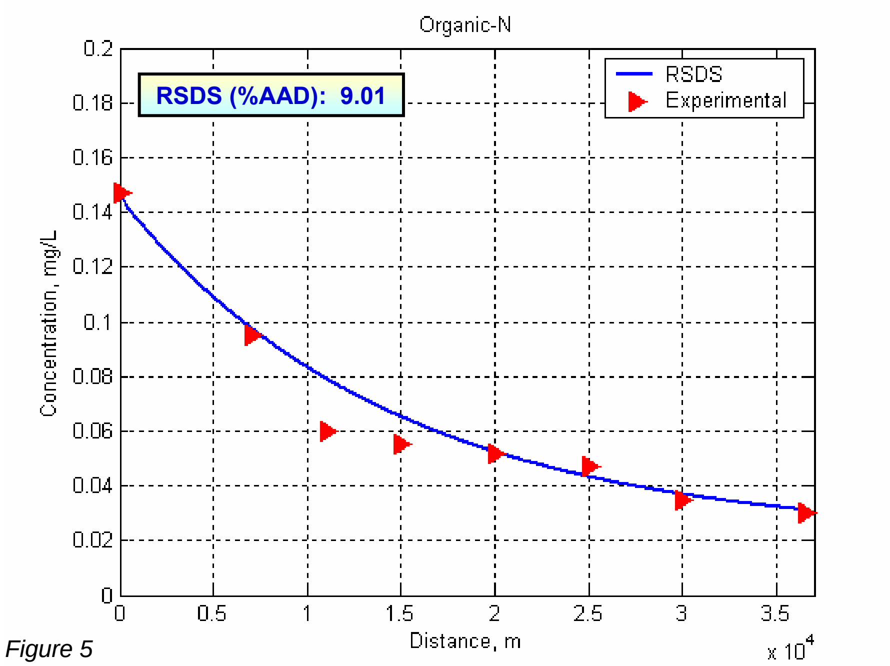


Figure 5

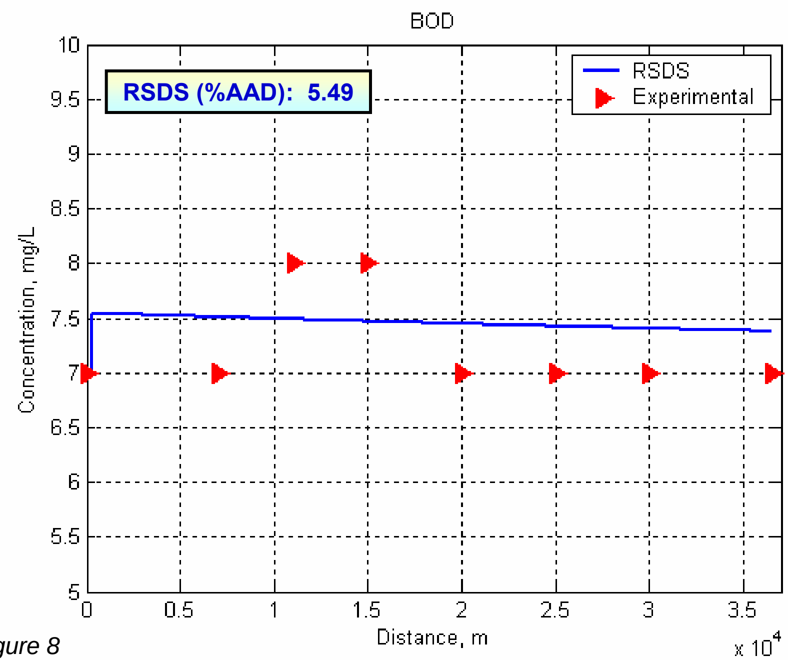


Figure 8

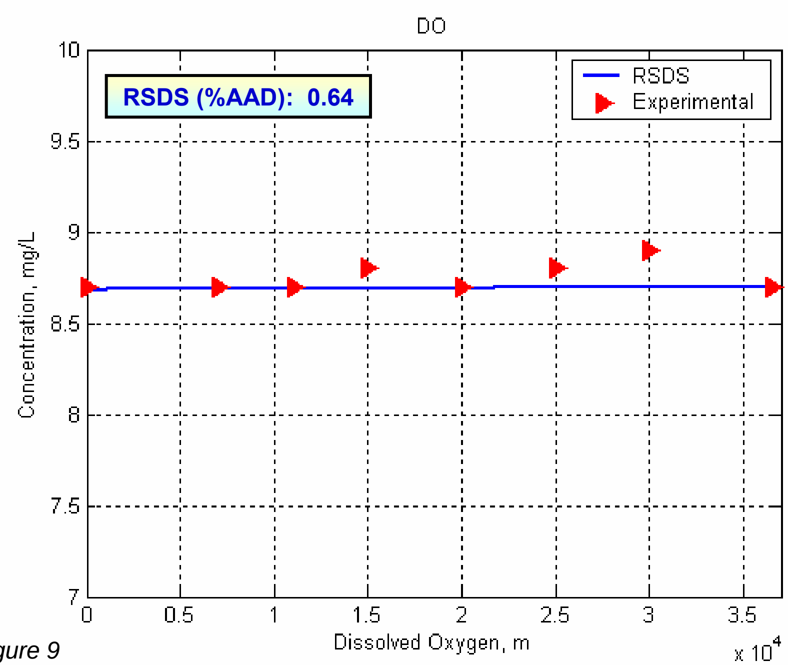


Figure 9

State Variables	RSDS (% AAD)
Ammonia Nitrogen	2.86
Nitrite Nitrogen	29.59
Nitrate Nitrogen	2.71
Organic Nitrogen	9.01
Organic Phosphorus	2.09
Dissolved Phosphorus	1.89
BOD	5.49
Dissolved Oxygen	0.64
Coliform	6.87
Chlorine	20.19
Algae	4.97

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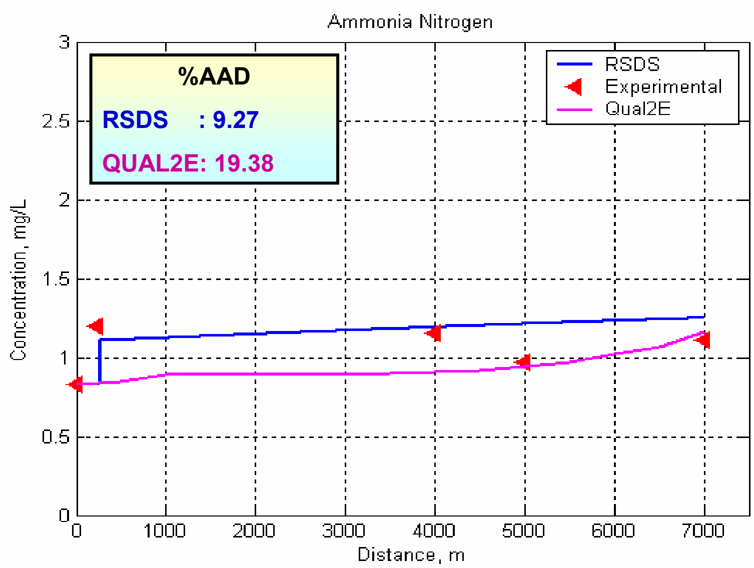
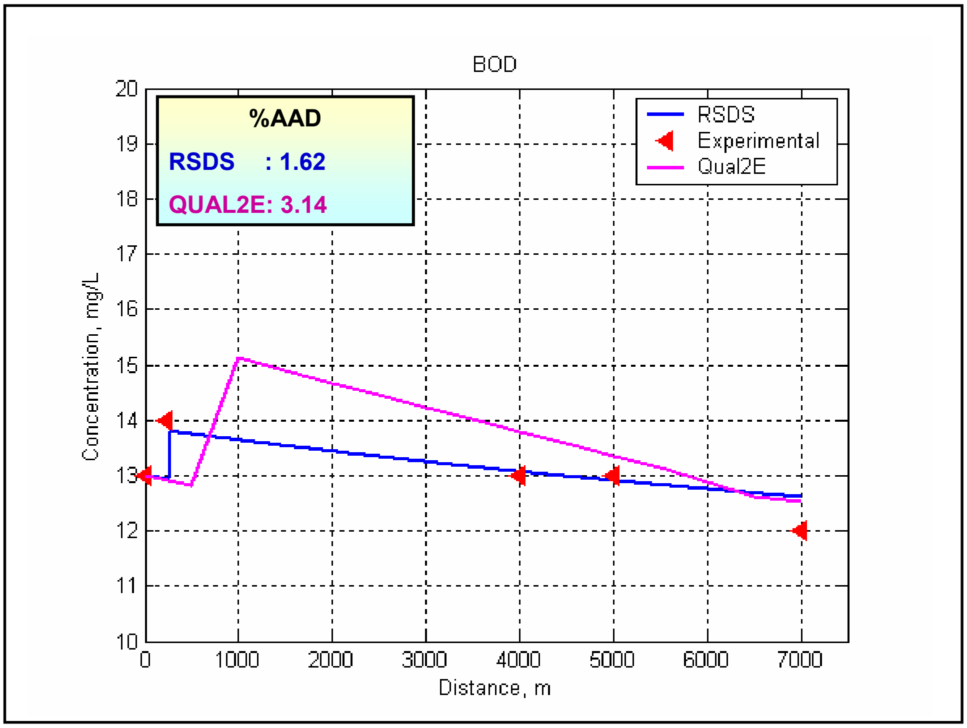
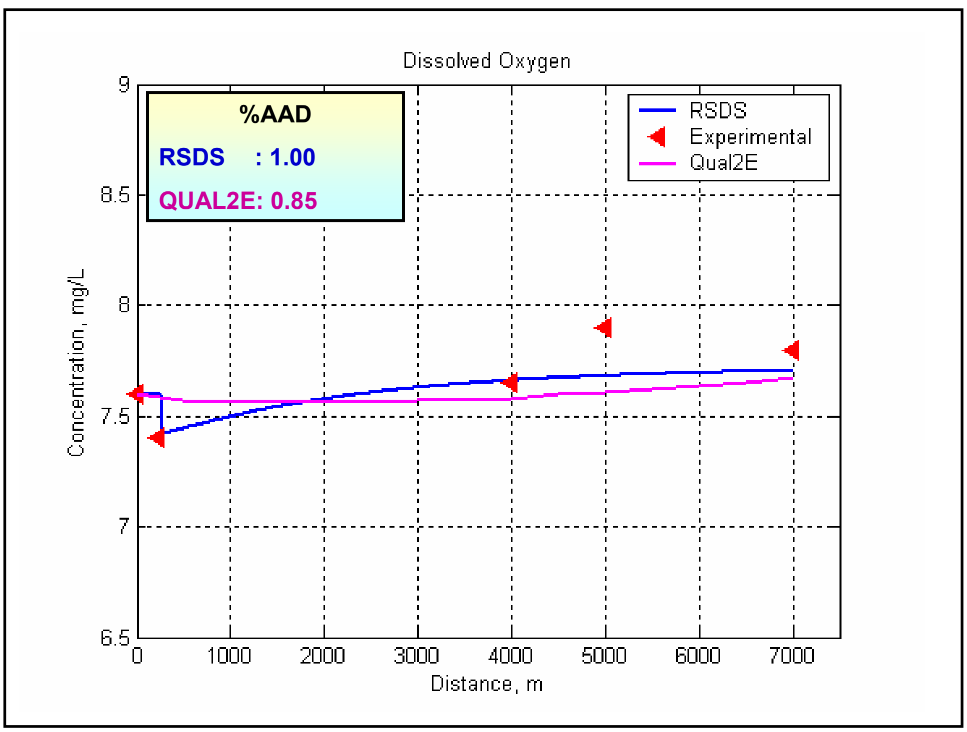
Results from COMPARISON to QUAL2E for a 7 kms section of the river *(Berber et al 2004c)*




BOD
%AAD
RSDS : 1.62
QUAL2E: 3.14
RSDS
Experimental
Qual2E
Concentration, mg/L
20
19
18
17
16
15
14
13
12
11
10
0
1000
2000
3000
4000
5000
6000
7000
Distance, m

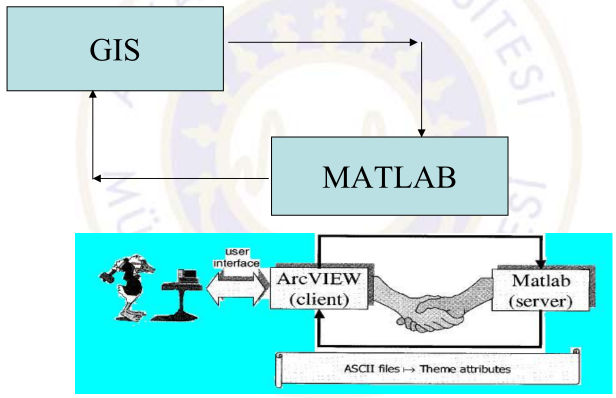

Dissolved Oxygen
%AAD
RSDS : 1.00
QUAL2E: 0.85
RSDS
Experimental
Qual2E
Concentration, mg/L
9
8.5
8
7.5
7
6.5
0
1000
2000
3000
4000
5000
6000
7000
Distance, m

State Variables	%AAD	
	RSDS	QUAL2E
Ammonia Nitrogen	9.2728	19.38
Nitrite Nitrogen	28.9094	76.40
Nitrate Nitrogen	3.6912	24.32
Organic Nitrogen	42.4853	11.80
Organic Phosphorus	9.4859	3.46
Dissolved Phosphorus	5.2614	6.92
BOD	1.6156	3.14
Dissolved Oxygen	1.0057	0.85
Coliform	7.2321	4.73
Chlorine	29.0589	23.19
Algae	0.4828	9.78

Conclusions

- Predictions from RSDS indicate good agreement with experimental data
  - ➔ 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 assesment*' easier

RSDS has been accommodated within a Geographical Information System (ArcMap)



[Yetik, K., Yüceer, M. & Berber, R. 2007 - Unpublished]

"CENTRAL RIVER MONITOING AND POLLUTION CONTROL SYSTEM"

TÜBİTAK - 105G002

Supported by TURKISH SCIETIFIC AND TECHNICAL RESEARCH COUNCIL

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Bakanlığı

Ministry of Environment & Forestry

HİTİT UNIVERSITY
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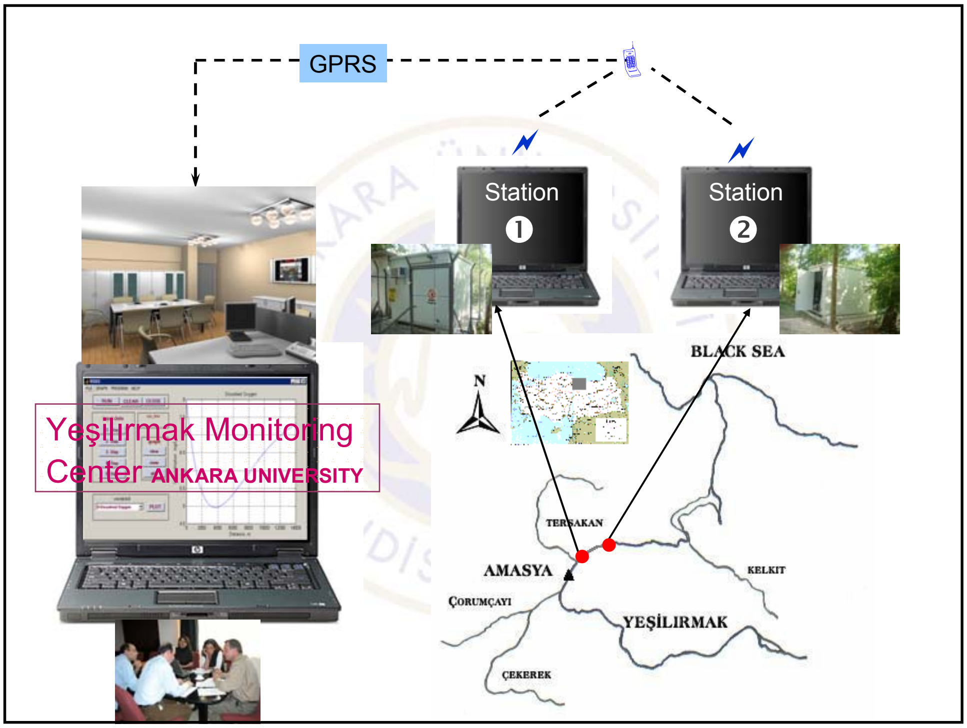
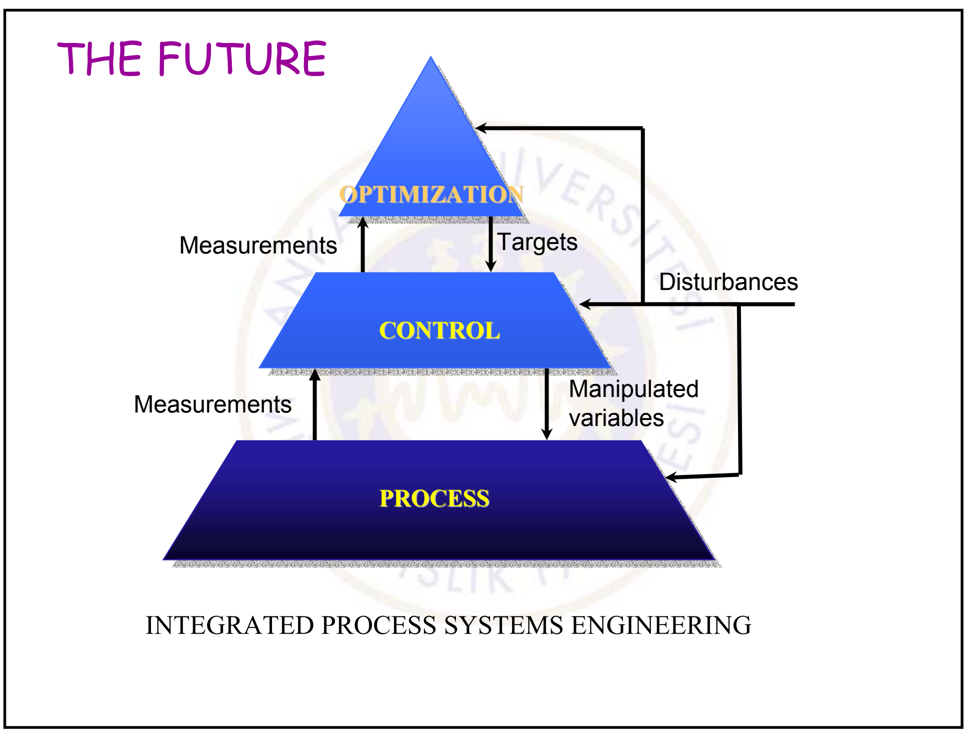
MUNICIPALITY OF AMASYA


GPRS
Station 1
Station 2
BLACK SEA
N
Yeşilırmak Monitoring Center ANKARA UNIVERSITY
TERSAKAN
AMASYA
KELKIT
ÇORUMÇAYI
YEŞİLIRMAK
ÇEKEREK


THE FUTURE
OPTIMIZATION
Measurements
Targets
Disturbances
CONTROL
Measurements
Manipulated variables
PROCESS
INTEGRATED PROCESS SYSTEMS ENGINEERING

The work and contributions by

- **Mehmet Yüceer**
- **Şaziye Balku**
- **Erdal Karadurmuş**

are acknowledged…