Modeling of Bioprocess Systems with specific reference to Wastewater Treatment: Challenges, Myths and R&D directions

By

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OVERVIEW

- Brief introduction about bioprocess systems (WWT, biodegradation, bioremediation, Bioaccumulation, fermentation)

- Introduction to modeling- concept

- Beginners (Your) understanding (on the basis of Maths, PMS-Leuben, NMCP etc.): Apologies! I am not underestimating you (because I too was in the same boat some time back- still now- I have reached A, B and C only and want to learn D to Z-

  Hopefully! God willing! may be in my next birth I will finish this task).

  (Generally, the students simulate only and do not optimize)

  In the PMS subject, you have just conceptualized the model.

- Challenges: data, lack of technical knowhow esp. because of interdisciplinary nature, lack of mathematical concepts, lack of technical knowhow , understanding of various underlying processes

Contd.

Complex non linearity and dynamic nature of real life field problems, lack of coordination, gaps between sciences and engineering, capacity building (limited and flawed)

- Myths: nomenclature (software, algorithms, program, package, model and modeling)
- Types: (Simulation and Optimization; Lumped and distributed; analytical and numerical; conceptual, black box, statistical, hybrid, DSS)

Contd.

- Example of a river water quality modeling and waste-load allocation modeling
- Suggestions
- Summary and Conclusions
- Acknowledgements

INTRODUCTION

Bioprocess Systems

- WWT
- Biodegradation
- Bioremediation
- Sludge digestion
- Bioaccumulation
- Fermentation

INTRODUCTION

INTRODUCTION-Model

- Adjective: ideal, exemplary, and perfect (Model schools).
- Nouns: Small, representation, prototype, example, and replica (school level).
- Verbs: Pose, mimic.
- Mathematical Model: Representation of a physical phenomenon/ Process in terms of mathematical equation.-This is what we want to learn.

- Model: An assembly of concepts in the form of one or more mathematical equations that approximate the behavior of natural system or phenomena.
- Computer code or program: The assembly of algorithms describing the phenomena the codified numerical solution methods and data control that can be executed beginning with the acceptance of data and instruction regarding processing, interpretation, and analysis of the specified data and any other data that resides within the code, to the reporting and delivery of the results of computerized analysis.
- Package /software (user friendly form of program that can run on different operating systems) – Most of you use this for your M.Tech/PhD

NEED FOR A MODEL

- To predict present and future behavior of a system.
- For establishing and evaluating alternative scenarios for an engineering problem.
- To solve complex real life engineering problems
- Real Time Operation and Control of Engineering Systems

Application softwares (not models)

- Railway/Air Ticketing (Reservation)
- Registration of students/ERPs
- Examination result management systems
- Election results (GENESIS for reporting)
- Counseling for various exams (SEE/JEE/AIEEE/CPMT etc.)

Then what are the models

Models

- Monsoon forecasting (16 parameters earlier, now General circulation model)
- Water Quality (QUAL2E/WASP/STREAM/QUAL2K/
- Rainfall-runoff models (SWM/KWM/HEC-RAS/SHE)

EXAMPLES (APPLICATIONS)

- CIVIL: Water Pollution- BOD/DO Model, Rainfall-runoff model, Analysis of structure, Contaminant transport
- MECHANICAL: Stress-Strain, Fluid flow, head loss, Navier Stokes equation, heat and mass transfer
- CHEMICAL: Hoop stress, Design of Pressure vessel, Gas generation in oil/gas fields, Design of ammonia reactor

Beginners understanding

- Beginners (Your) understanding (on the basis of Maths, PMS-Leuben, NMCP etc.):

Mathematics

PMS

NMCP

Biology

Chemistry

- You/we study all these in isolation
- Don’t realize the importance of Mathematics, NMCP (I too didn’t until I was doing my Ph.D)
- You/we look for shortcuts
- At the most, you/we do simulation only (using a readily available software) and validate with experimental observations/field data or vice-versa

- Most of you/we simulate only and not optimize (even when we do it, its very simple- carried out using different combinations of experiments/at the maximum RSM).
- Apologies! I am not understanding you (because I too was in the same boat some time back- still now- I have reached A, B and C only and want to learn D to Z- hopefully! God willing, may be in my next birth I will finish this task).

CHALLENGES

Story of the village with sightless people/inhabitants and Elephant

Modeling is combination of:

- Physics
- Chemistry
- Mathematics
- Biology
- Computer Science,
- Respective Engineering

- Lack of data (our possessive nature of not sharing data with others)- incidents from my own M.Tech and PhD studies-RTI
- No support from organizations dealing with data collection
- lack of technical knowhow esp. because of interdisciplinary nature of modeling
- lack of mathematical concepts,
- lack of technical knowhow
-

- Mathematician knows only solution of equation
- Absence of computer languages (C++-?; Matlab, GAMS, Oracle)-?
- Because of above, we cannot carry out numerical computation
- Limited time.

Data required for modeling

- Initial Conditions
- Boundary Conditions
- Data for Calibration
- Data for Validation

Joke by Steven Chapra

Problems in India (about correct data collection)- ex. BOD/DO in river, Discharge in rivers

At the end of this presentation, I'll ask you as to what I am?
-Physicist, Chemist, Mathematician, Biologists, Engineer or none.

Steps in modeling

- a) Conceptualization
- b) Formulation of equations
- c) Coding / Programming
- d) Calibration (Confirmation)
- e) Validation (Verification / Corroboration)
- f) Simulation
- g) Sensitivity Analysis (Uncertainty analysis) (Perturbation/Latin hypercube sampling technique)
- h) Scenario generation
- i) Post-audit

TYPES OF MODELS

- Mechanistic model / conceptual models (Q=AV) /physics based model (Bernoulli's equation)
- Lumped and Distributed model
- Deterministic and Stochastic models
- Analytical and Numerical models
- Static and Dynamic models
- Statistical models (Back box models)
- Simulation and Optimization models
- Investment and Operating models (long term projects)
- Deductive models (deduced from data)-statistical models
- Hybrid models (Neuro-Fuzzy; DSS, Linked models etc)

MYTHS

- Knowledge about whole modeling. People think running a software is modeling.
- It is not so.
- This is just one step of modeling
- Frequent/vague and wrong usage of software, model, package, code, program, simulation etc.
- Correct knowledge about types of models

- Difference between calibration and validation

SIMULATION AND OPTIMIZATION MODELS

SIMULATION MODEL

- A simulation model basically attempts to represent the physical functioning and consequent effects of causative factors on the prototype system by a computerized algorithm (James and Lee 1971).

OPTIMIZATION MODELS

- In many situations the number of reasonable alternatives is sufficiently large to preclude a simulation of each alternative.

- In such cases the time and/or a cost prohibits trial and error simulation, and the optimization models can be developed and applied as a means of substantially reducing the number of management alternatives and objectives being considered.

- Optimization model are aimed at development of management strategies.

OPTIMIZATION MODEL

- To plan a cost effective strategy
- Components

  Objective functions

  Constraints (Equality, in equality or non negativity, Bounds)

Optimization model (MOO)

Minimize / Maximize $f_m(r)$ $\quad m = 1, 2, - - - - - - - -, M$

Subject to

$$g_j(r) \geq 0 \,, \quad j = 1, 2, - - - - - - -, J$$

$$h_k(r) = 0 \,, \quad k = 1, 2, - - - - - - K$$

$$r_i^{(L)} \leq r_i \leq r_i^{(U)} \,, \quad i = 1, 2, - - - - - - -, n$$

A solution r is a vector of n decision variables; $r = (r_1, r_2, \ldots\ldots\ldots r_n)^T$.
Associated with this problem are J inequality and K equality constraints.
The terms $g_j(r)$ and $h_k(r)$ are called constraint functions.
The last set of constraints are called variable bounds, restricting each decision variable r_i to take a value within a lower bound, $r_i^{(L)}$ and an upper bound, $r_i^{(U)}$.

TYPES OF LINKING

- Response matrix (Transfer coefficient approach)
- Linked: Simulation-Optimization
- Embedded systems

Linked S-O model

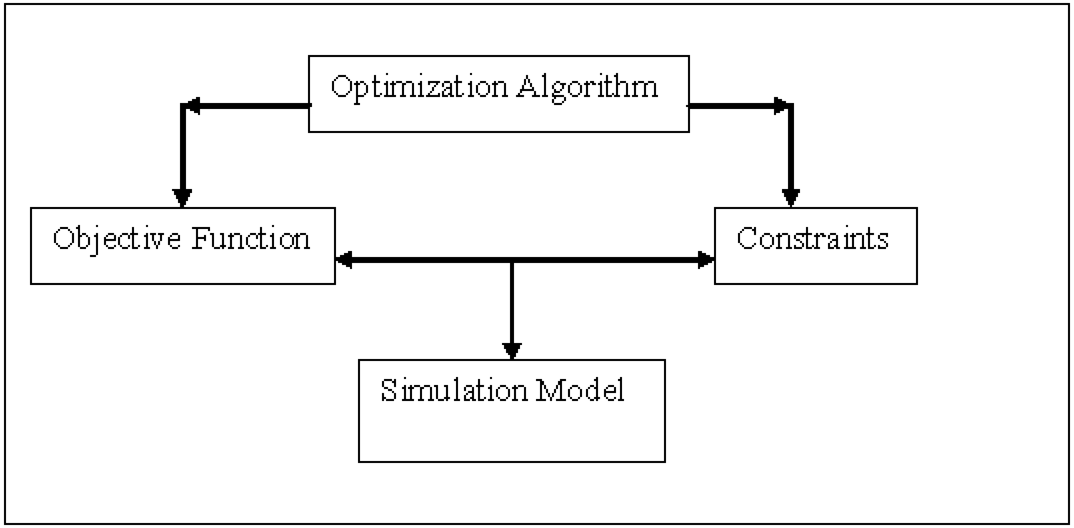
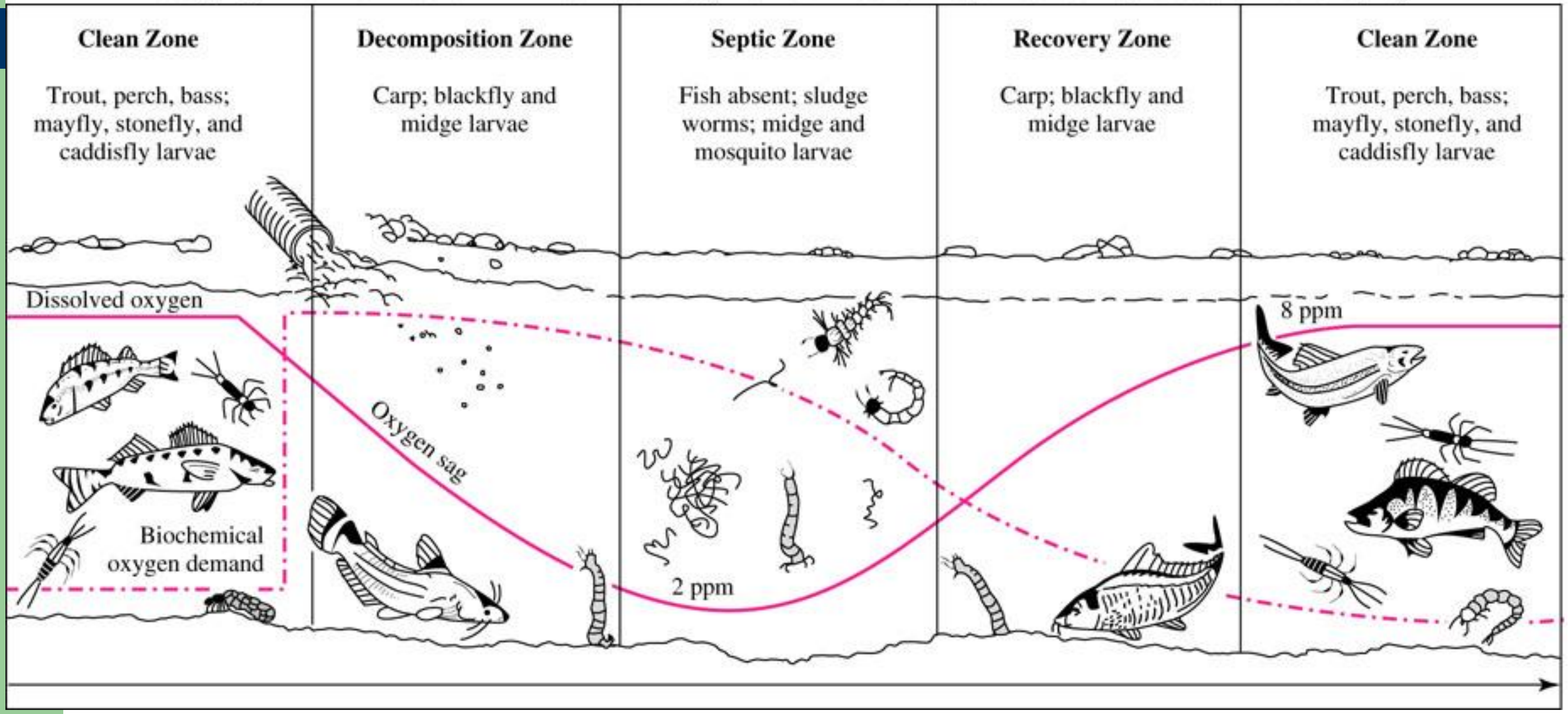


Fig 1 Linked simulation-optimization (Source: Willis and Finney 2004)

Water Quality Modeling

SIMULATION MODEL

WATER QUALITY PROCESS IN RIVER



WATER QUALITY MODEL

- A water quality model is simply a set of mathematical expressions defining the physical, biological and chemical processes that are assumed to take place in a water body (Orlob, 1992).

MASS BALANCE

- The common basis of most water quality models is the principle of continuity or mass balance.

PHENOMENON IN MASS BALANCE

- Given particular water quality constituents and the important physical, biological and chemical processes a mass balance is developed that takes into account three phenomena;
  - the inputs of constituents to the river system from outside the system. (Drains, tributary)
  - the transport of constituents through the river systems (advection, dispersion).
  - the reactions within the river system that either increase/decrease constituents concentration or mass.(Orlob, 1992).

MECHANISM IN MASS BALANCE

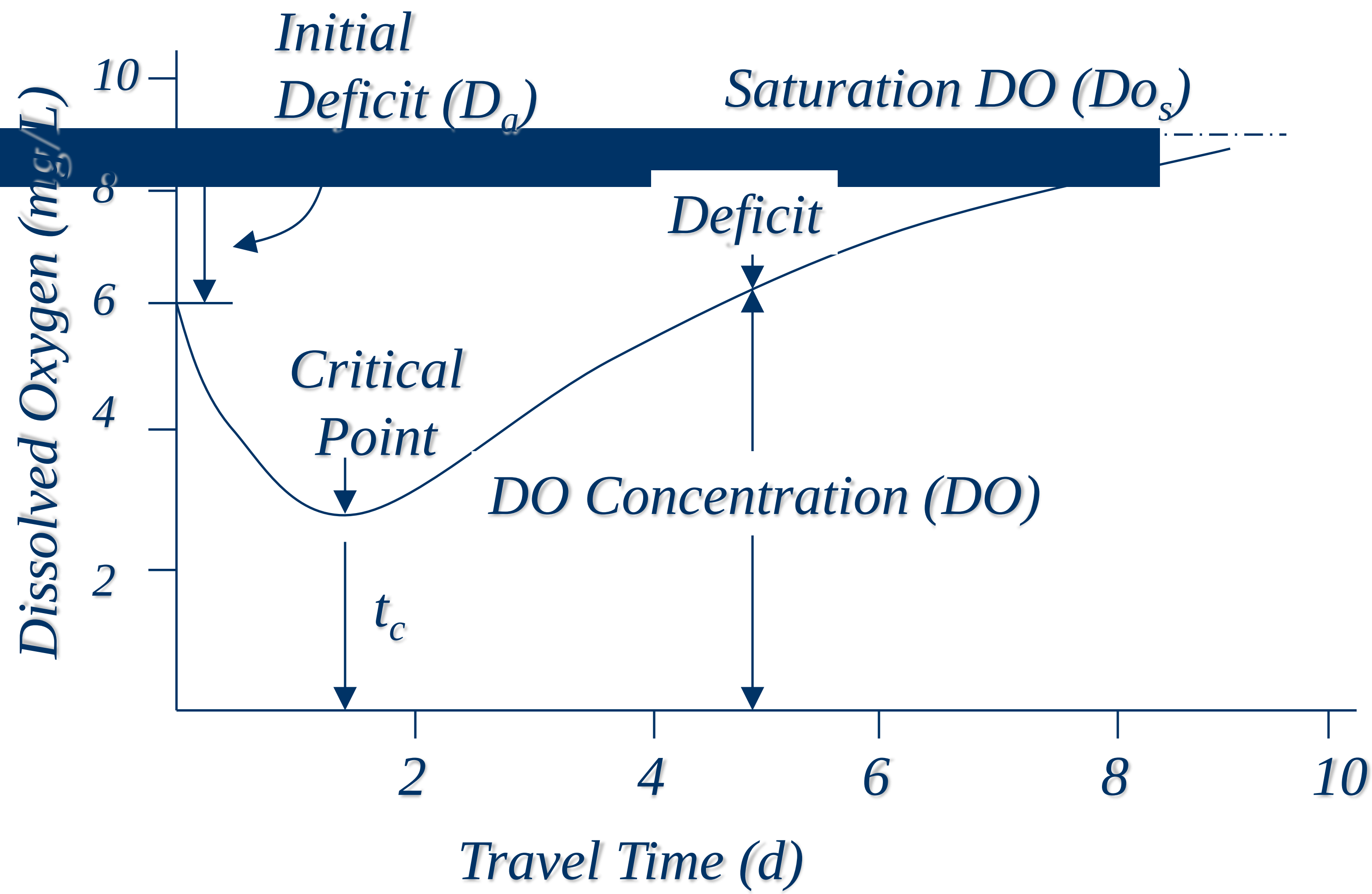
- **Inputs to river system:** In form of pollutants(usually comes from of wastewater discharges of municipal, industrial or agricultural runoff)
- **Transport of constituents :** By dispersion and/or advection(is dependent on the hydrologic and hydrodynamic characteristics of the river). Advective transport dominates river flow that results primarily from surface water runoff and groundwater inflow.
- **Biological, chemical and physical reactions:** Among the constituents**.**

ANALYTICAL MODEL

The Streeter Phelps equation (1925)- Analytical expression for oxygen balance in river. This differential equation gives the relation between the oxidation requirements for biochemical stabilization of dissolved organic matter and the replenishment of DO by mass transfer from the atmosphere.

Contd.

Typical DO sag curve



Simulation models for River water quality management

- A simulation model attempts to represent the physical functioning and consequent effects of causative factors (cause-effect) on the prototype system by a computerized algorithm (James and Lee 1971).

- In the context of river water quality, simulation models indicate the values of water quality variables given the flow, the quantity and quality of the waste loadings, and the extent of measures designed to reduce waste discharges or to increase the waste assimilation capacity of the receiving river systems (Loucks 1976)

WATER QUALITY SIMULATION MODEL

-

QUAL 2E (Brown and Barnwell, 1987)

- One dimensional steady state, Numerical model.
- one dimensional advective-dispersive mass transport and reaction equation.
- It can simulate 15 water quality parameters.

GOVERNING EQUATIONS OF QUAL2E

$$\frac{\partial C}{\partial t} = \frac{\partial\left(A_x D_l \dfrac{\partial C}{\partial x}\right)}{A_x \partial x} - \frac{\partial\left(A_x \bar{u} C\right)}{A_x \partial x} \frac{dC}{dt} + \frac{s}{V}$$

Where,

x= distance

t= time

C = concentration

A_x = cross sectional area

D_L =Dispersion coefficient

Water Quality Simulation using QUAL2E

- Conceptual Representation of a River System
- Hydraulic Routing of River Flow
- Initial and Boundary Conditions
- Rate constants
- Calibration and Validation
- Simulation under baseline (existing) condition
- WQ simulation under various scenarios
- Sensitivity analysis

Hydraulic routing of river

- $V = a\,Q^{b}$
- $h = c\,Q^{d}$
- w = eQf
- a.c.e = 1
- b+d+f = 1

Initial and Boundary Conditions

- IC: data specified to define the water quality condition at the beginning of the simulation period (McCutcheon 1989).

  BOD, DO, flow

- Set of data that describe the mass and energy that enters the model domain (subset of the stream segment being simulated).- point loads and their quality, background flow, and concentration

Rate constants

- a) Deoxygenation constant (K1)
- b) Reaeration constant (K2)
- c) BOD settling rate (K3)
- d) Sediment/benthic oxygen demand (K4)

CALIBRATION OF QUAL2E

Calibration is accomplished by adjustment of model coefficient during successive/ iterative model runs, until optimum goodness of fit between predicted and observed data is achieved.

VALIDATION

- Only the variables are changed. The parameters are not changed.

OPTIMIZATION MODEL

Multiobjective optimization

Minimize/Maximize $f_m(r) \quad m = 1, 2, - - - - - - —, M$

Subject to

$$g_i(r) \geq 0 \;, \quad j = 1, 2, - - - - - - -, J$$

$$h_k(r) = 0, \quad k = 1, 2, - - - - - - K$$

$$r_i^{(L)} \leq r_i \leq r_i^{(U)} \;, \quad i = 1, 2, - - - - - - -, n$$

Least cost model (LCM)

$$Minimize\ F_1 = \sum_{i=1}^{NS} C_i(r_i)$$

Subject to

Water quality improvement constraints

$$\sum_{i=1}^{N_j} \phi_{ij} r_i \geq b_j \qquad \forall\ i, = 1, 2, \ldots\ldots, N_j$$

$$\forall\ j = 1, 2,\ \ldots\ldots\ldots, m$$

Inequality constraints

$$r_i^{(L)} \leq r_i \leq r_i^{(U)}, \qquad \forall\ i = 1, 2, ------, NS$$

Cost Assimilative capacity model (CAM)

$$Minimize\ F_1 = \sum_{i=1}^{NS} C_i(r_i)$$

$$Maximize\ \ F_3 = \sum_{j=1}^{m} A_j \qquad \forall\ \ j = 1, 2, \ldots\ldots\ldots\ldots, m$$

Subject to

$$\sum_{i=1}^{N_j} \phi_{ij} r_i \geq b_j \qquad \forall\ i, = 1, 2, \ldots\ldots, N_j$$

$$A_j = W_i\,(1 - r_i\,) \qquad \forall\ i = 1,2, \ldots\ldots\ldots\ldots, NS$$

$$r_i^{\ (L)} \leq r_i \leq r_i^{\ (U)}\ , \qquad \forall\ i = 1, 2, ------, NS$$

$$A_j \geq 0 \qquad \forall\ \ j = 1,2, \ldots\ldots\ldots\ldots, m$$

$$\phi_{i1} W_1 (1-r_1) + \phi_{i2} W_2 (1-r_2) + \ldots\ldots\ldots + \phi_{ij} W_i (1-r_{NS}) \leq y b_j \quad \ldots\ldots\ldots\ldots\ldots\ldots (1a)$$

or

$$\phi_{i1} W_1 r_1 + \phi_{i2} W_2 r_2 + \phi_{i3} W_3 r_3 + \ldots\ldots\ldots\ldots\ldots\ldots + \phi_{ij} W_i r_{NS} \geq S_j \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (1b)$$

where

$$S_j = \phi_{i1} W_1 + \phi_{i2} W_2 + \phi_{i3} W_3 + \ldots\ldots\ldots\ldots\ldots\ldots + \phi_{ij} W_i \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (1c)$$

Equation 1b states that the supply of dissolved oxygen created by treatment and flow augmentation must exceed that demanded by the gross wasteloads.

TRANSFER COEFFICIENTS FOR WQ RESPONSE

The transfer coefficient describes the effect of a unit change in waste treatment at a particular discharge point on the quality parameter at another point. Using these transfer coefficients, any desired quality improvement goal in a stream can be specified.

If it is desired to have an improvement of bj mg/l of dissolved oxygen at point j on the stream, then we require

$$\phi_{i1}x_1 + \phi_{12}x_2 + ----------- + a_{ij}x_i \leq b_i$$

and bj is the change in deficit (note: positive bj implies increasing deficits; the aij as defined are negative).

$$\phi_{11}x_1 + \phi_{12}x_2 + \phi_{13}x_3 + \phi_{14}x_4 \leq b$$

$$\phi_{21}x_1 + \phi_{22}x_2 + \phi_{23}x_3 + \phi_{24}x_4 \leq b$$

$$\phi_{31}x_1 + \phi_{32}x_2 + \phi_{33}x_3 + \phi_{34}x_4 \leq b$$

$$\phi_{41}x_1 + \phi_{32}x_2 + \phi_{33}x_3 + \phi_{34}x_4 \leq b$$

APPLICATION OF MODELS

DESCRIPTION OF THE STUDY AREA

- Delhi Stretch of River Yamuna.

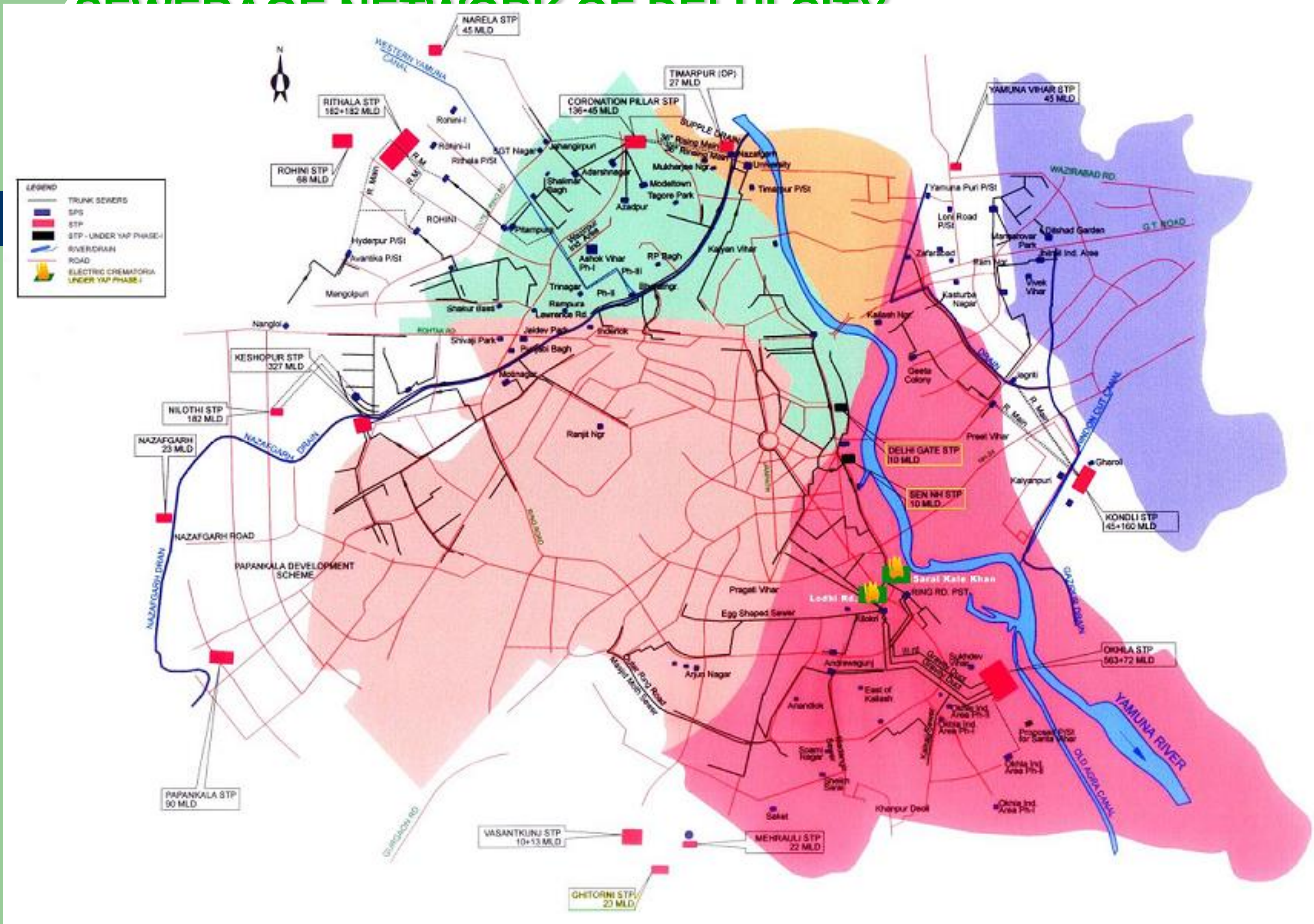
-

22 Kms stretch from Wazirabad barrage to Okhla barrage.

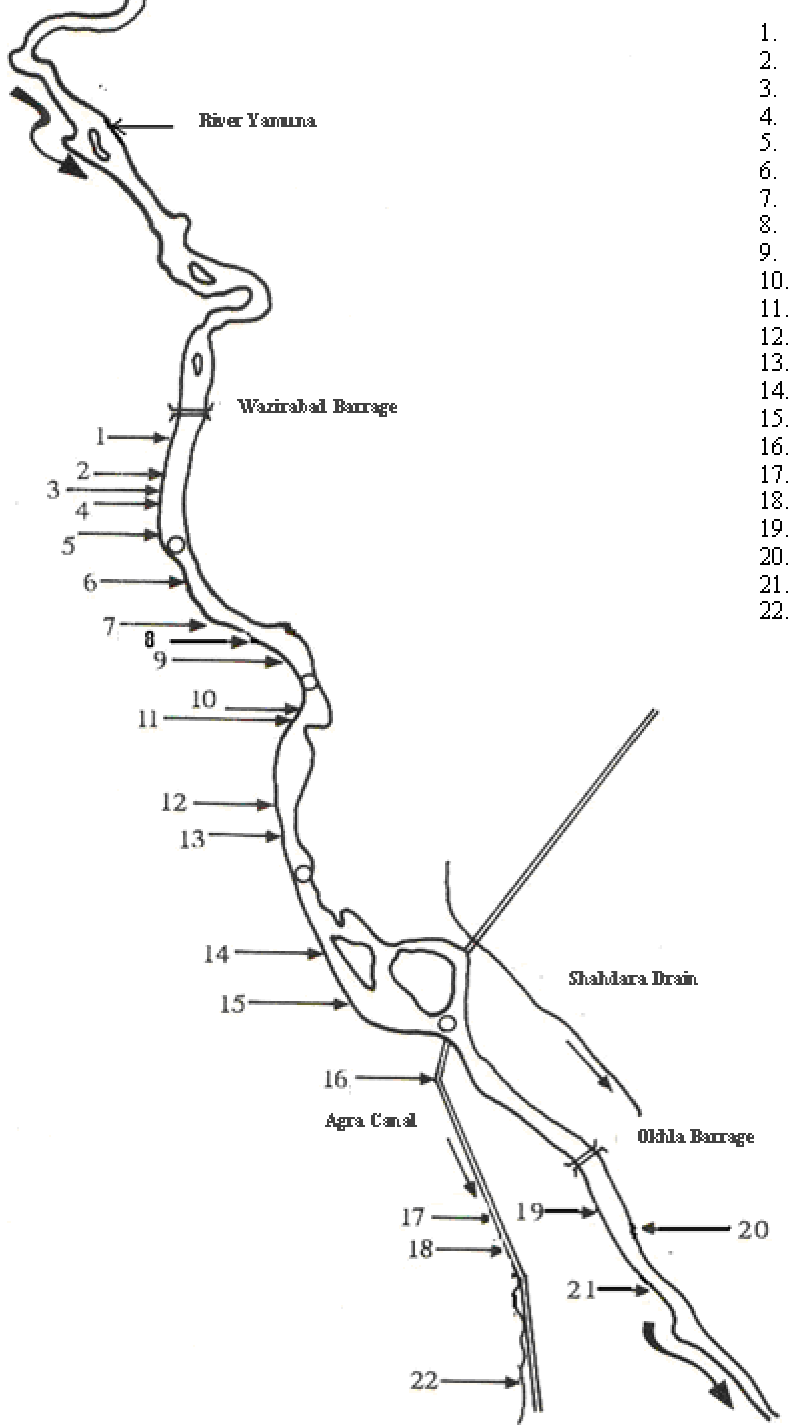
- All 15 drains discharging into this stretch considered.

- This 2% long stretch contributes 80% of the total pollution load.

SEWERAGE NETWORK OF DELHI CITY



(Source: Yamuna Action Plan Website)



1. Najafgarh Drain
2. Magazine Road
3. Sweeper Colony Drain
4. Kyber Pass Drain
5. Metcalf House Drain
6. Morigate Drain
7. Tonga Stand Drain
8. Moat Drain
9. Civil Mill Drain
10. Delhi Gate Drain
11. Sen Nursing Home Drain
12. Drain No-12A
13. Drain No-14A
14. Barapulla Drain
15. Maharani Bagh Drain
16. Kalkaji Drain
17. Sarita Vihar Bridge Drain
18. Sarita Vihar Drain
19. LPG Bottling Plant Drain
20. Shahdara Drain
21. Tuglakabad Drain
22. Tehkhand Drain

Use based classification of surface water in India

Class	pH	DO (mg/l), minimum	BOD (mg/l) max.	Total coliform (in MPN/100 ml), maximum
A	6.5-8.5	6	2	50
B	6.5-8.5	5	3	500
C	6.9	4	3	5000
D	6.5-8.5	4	-	-
E	6.5-8.5	-	-	-

Legend: Water use Classes

A- Drinking water source without conventional treatment but after disinfection

B- Outdoor bathing (organized).

C- Drinking water source with conventional treatment and disinfection

D- Propagation of wildlife and fisheries

E- Irrigation, industrial cooling, controlled waste disposal

SIMULATION MODEL

Conceptual Representation of a River System

- 16 reaches system (uniform hydraulic characteristics)
- Each reach sub divided into equal computational element of 0.3 km.
- Headwater element; Standard element; Element just upstream of a junction; Junction element; Last element in system; Input element; and Withdrawal element.

Schematic representation of the study stretch

Details of stream reach configuration

Reach No.	Name of the reach	Reach chainage		Total elements
		Begin (km)	End (km)	
1	Wazirabad Barrage to Najafgarh Drain	0.0	0.3	1
2	Najafgarh Drain to Magazine Road Drain	0.3	1.5	4
3	Magazine Road Drain to Sweeper Colony	1.5	1.8	1
4	Sweeper Colony Drain to Khyber Pass Drain	1.8	3.6	6
5	Khyber Pass Drain to Metcalf House Drain	3.6	4.2	2
6	Metcalf House Drain to Morigate Drain	4.2	5.7	5
7	Morigate Drain to Tonga Stand Drain	5.7	6.3	2
8	Tonga Stand Drain to Moat Drain	6.3	6.6	1
9	Moat Drain to Civil Mill Drain	6.6	7.2	2
10	Civil Mill Drain to Delhi Gate Drain	7.2	9.0	6
11	Delhi Gate Drain to Sen Nursing Home Drain	9.0	12.0	10
12	Sen Nursing Home Drain to Drain No.12A	12.0	13.5	5
13	Drain No. 12A to Drain No. 14A	13.5	14.1	2
14	Drain No. 14A to Barapulla Drain	14.1	15.6	5
15	Barapulla Drain to Maharani Bagh Drain	15.6	18.0	8
16	Maharani Bagh drain to Okhla Barrage	18.0	21.9	13

Wazirabad Barrage
0.0 Km
Qin = 1.5 m3/sec, BOD = 3 mg/l, DO = 5.5 mg/l
Najafgarh Drain (D1)
(20.68)
0.3 Km
Magazine Road Drain (D2)
(0.07)
1.5 Km
Sweeper Colony Drain (D3)
(0.13)
1.8 Km
Khyber Pass Drain (D4)
(0.13)
3.6 Km
Metcalf House Drain (D5)
[redacted]
Qudsia Bagh Drain (D6)
(0.39)
5.7 Km
Tonga Stand Drain (D7)
(0.09)
6.3 Km
Moat Drain (D8)
(0.001)
6.6 Km
Civil Mill Drain (D9)
(0.52)
7.2 Km
Delhi Gate Drain (D10)
(0.56)
9.0 Km
S.N. Home Drain (D11)
(1.01)
12.0 Km
Drain No-12A (D12)
(0.04)
13.5 Km
Drain No-14 (D13)
(0.37)
14.1 Km
Barapulla Drain (D14A)
(1.35)
15.6 Km
Maharani Bagh Drain (D15)
(0.74)
Hindon cut
(30)
Agra Canal
18.0 Km
Qout=55.671 m3/sec, BOD=17.8, DO=1.4 mg/l
Okhla Barrage
22.00 Km

DATA REQUIREMENT FOR WQSM

i.

Water quality data of various reaches and drains of the river

ii. Hydraulic (flow, velocity) and geometrical data (width, depth) of the 22 Km river stretch

iii. Elevation, latitude, longitude of the basin

iv. Rate constants

Geometric and hydraulic data of the Delhi stretch of the river Yamuna

Name of reach	Length (Km)	Width (m)	Depth (m)	Flow (Q in m^3/sec.)	Velocity (m/sec.)
R1	0.3	60	0.4	1.0	0.032
R2	1.2	83	1.1	22.97	0.25
R3	0.3	110	1.1	23.027	0.19
R4	1.8	110	1.1	23.131	0.21
R5	0.6	110	1.3	23.245	0.178
R6	1.5	100	1.3	24.187	0.186
R7	0.6	130	1.4	24.682	0.13
R8	0.3	120	1.3	24.759	0.158
R9	0.6	125	1.2	24.7591	0.165
R10	1.8	185	1.2	25.436	0.13
R11	3.0	170	1.2	27.335	0.14
R12	1.5	115	6.0	28.329	0.1
R13	0.6	120	1.8	28.519	0.132
R14	1.5	130	2.1	28.709	0.105
R15	2.4	272	3.0	30.585	0.075
R16	3.9	200	2.5	30.80	0.117

Reach No.	Velocity-discharge relation	Depth-discharge relation
1	$V = 0.0396\,Q^{0.5138}$	$h = 0.4411Q^{0.3374}$
2	$V = 0.0758\,Q^{0.3961}$	$h = 0.2852Q^{0.4215}$
3	$V = 0.0584\,Q^{0.3714}$	$h = 0.3096Q^{0.4083}$
4	$V = 0.2108Q^{0.029}$	$h = 0.1085Q^{0.7411}$
5	$V = 0.232\,Q^{0.0686}$	$h = 0.0996Q^{0.778}$
6	$V = 0.3081\,Q^{0.1571}$	$h = 0.0736Q^{0.6727}$
7	$V = 0.2215Q^{0.0622}$	$h = 0.0782\,Q^{0.8538}$
8	$V = 0.2475Q^{0.0931}$	$h = 0.0679Q^{0.796}$
9	$V = 0.25Q^{0.0955}$	$h = 0.06Q^{0.7308}$
10	$V = 0.0169Q^{0.6028}$	$h = 0.4271Q^{0.3146}$
11	$V = 0.4554\,Q^{0.3677}$	$h = 0.0498Q^{0.6146}$
12	$V = 0.0321\,Q^{0.1096}$	$h = 03732\,Q^{0.3784}$
13	$V = 0.0396\,Q^{0.5138}$	$h = 0.4411Q^{0.3374}$
14	$V = 0.0396\,Q^{0.5138}$	$h = 0.4411Q^{0.3374}$
15	$V = 0.0396\,Q^{0.5138}$	$h = 0.4411Q^{0.3374}$
16	$V = 0.0396\,Q^{0.5138}$	$h = 0.4411Q^{0.3374}$

Values of hydraulic parameters of the stream

Reach No.	Hydraulic Coefficients/Exponents for the Delhi reach			
	Velocity discharge relationship		Depth discharge relationship	
	coefficient	exponent	coefficient	Exponent
1	0.0396	0.5138	0.4411	0.3374
2	0.0758	0.3961	0.2852	0.4215
3	0.0584	0.3714	0.3096	0.4083
4	0.2108	0.029	0.1085	0.4411
5	0.232	0.0686	0.0996	0.378
6	0.3081	0.1571	0.07362	0.6727
7	0.2215	0.0622	0.0782	0.8538
8	0.2475	0.0931	0.0679	0.796
9	0.25	0.0955	0.06	0.7308
10	0.0169	0.6028	0.4271	0.3146
11	0.4554	0.3677	0.0498	0.6146
12	0.0321	0.1096	0.3732	0.3784
13	0.0396	0.5138	0.4411	0.3374
14	0.0396	0.5138	0.4411	0.3374
15	0.0396	0.5138	0.4411	0.3374
16	0.0396	0.5138	0.4411	0.3374

Values of reaction coefficients

Reach No.	BOD decay (K_1 per day)	BOD settling (K_3 per day)	SOD rate (K_4 per day)	Reaeration coefficient (K_2 per day)
1	0.31	0.9	0.5	5.75
2	0.42	0.9	0.5	1.824
3	0.23	0.9	0.5	1.603
4	0.43	0.9	0.5	1.68
5	0.55	0.9	0.5	1.0967
6	0.31	0.9	0.5	1.2
7	0.33	0.9	0.5	0.81
8	0.45	0.9	0.5	1.037
9	0.44	0.9	0.5	1.25
10	0.32	0.9	0.5	1.12
11	0.314	0.9	0.5	1.034
12	0.295	0.9	0.5	0.0342
13	0.39	0.9	0.5	0.4826
14	0.26	0.9	0.5	0.314
15	0.24	0.9	0.5	0.272
16	0.38	0.9	0.5	0.23

CALIBRATION

Point loads and withdrawals-Calibration

Name of drain	Flow (m^3/sec)	BOD (mg/l)	DO (mg/l)	Temperature (°C)	Percentage treatment
Najafgarh drain	21.97	58	0.0	28	0.0
Magazine Road drain	0.057	448	0.0	28	0.0
Sweeper Colony drain	0.104	286	0.0	28	0.0
Khyber Pass drain	0.114	92	0.0	28	0.0
Metcalf House drain	0.942	84	0.0	28	0.0
Mori Gate drain	0.495	174	0.0	28	0.0
Tonga Stand drain	0.077	84	0.0	28	0.0
Moat drain	0.0001	78	0.0	28	0.0
Civil Mill drain	0.677	134	0.0	28	0.0
Delhi Gate drain	1.899	88	0.0	28	0.0
Sen Nursing Home drain	0.994	74	0.0	31	0.0
Drain No. 12A	0.19	92	0.0	31	0.0
Drain No. 14	0.19	170	0.0	31	0.0
Barapulla drain	1.871	92	0.0	32	0.0
Maharani Bagh drain	0.224+28.00*	46	0.0	32	0.0

* - Flow through Hindon Cut

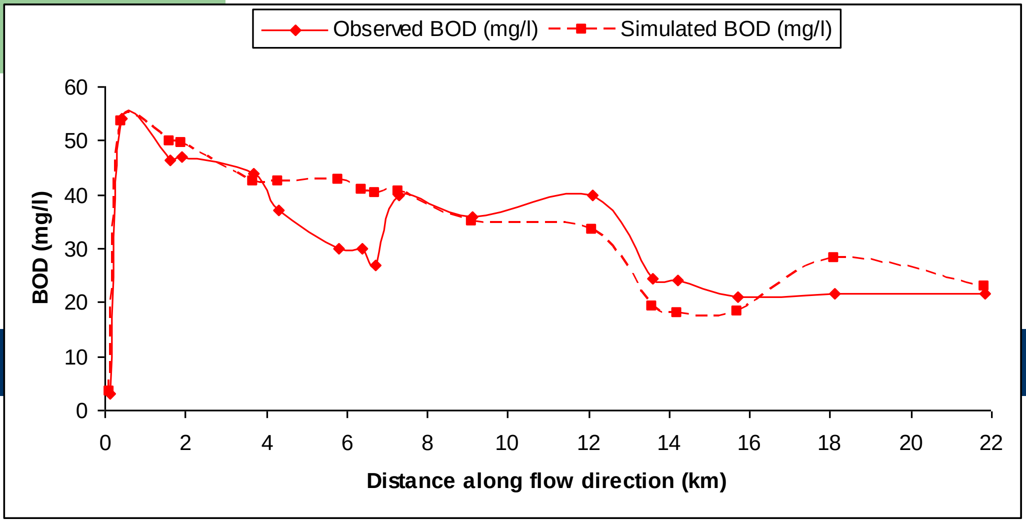


Fig 4.4a Calibration-Profiles of observed and simulated BOD

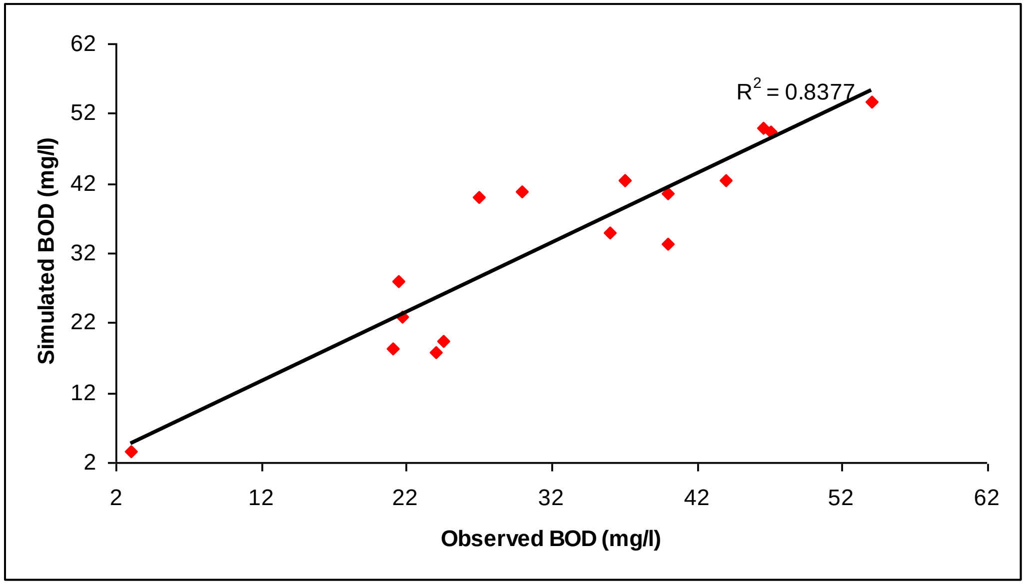


Fig 4.4b Calibration-Correlation between observed and simulated BOD

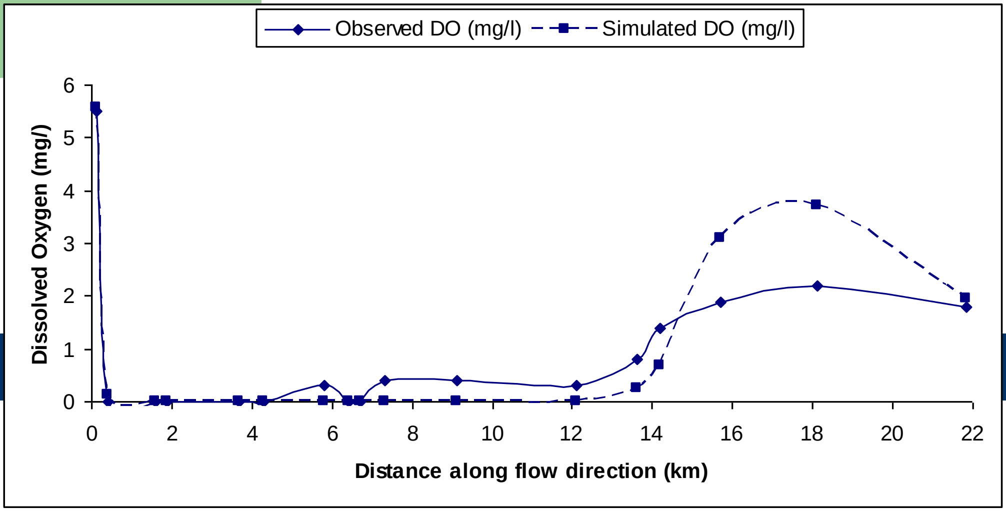


Fig 4.5a Calibration-Profile of observed and simulated DO

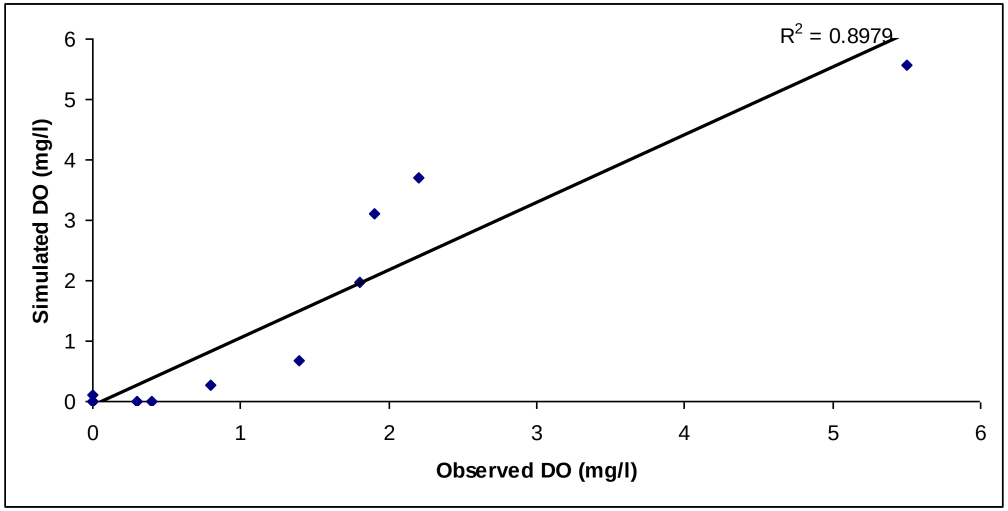


Fig 4.5b Calibration-Correlation between observed and simulated DO

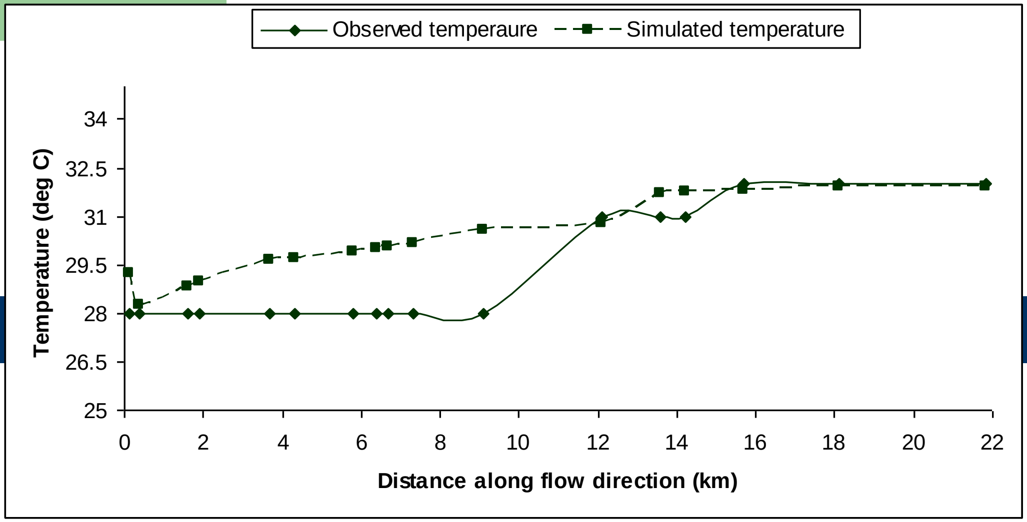


Fig 4.6a Calibration-Profile of observed and simulated temperature

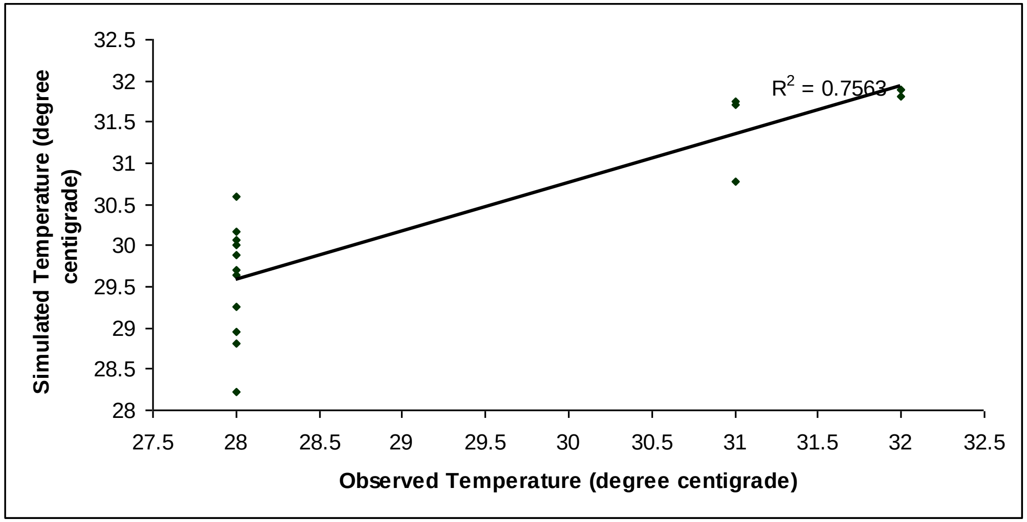


Fig 4.6b Calibration-Correlation between observed and simulated temperature

VALIDATION

Table 4.10 Point load and withdrawals for validation

Name of drain	Flow (m^3/sec)	BOD (mg/l)	DO (mg/l)	Temperature (C)	Percentage treatment
Najafgarh drain	25.709	40	0.0	28	0.0
[redacted]					0.0
Sweeper Colony drain	0.053	180	0.0	28	0.0
Khber Pass drain	0.15	100	0.0	28	0.0
Metcalf House drain	0.287	60	0.0	28	0.0
Mori Gate drain	0.387	60	0.0	28	0.0
Tonga Stand drain	0.143	40	0.0	28	0.0
Moat drain	0.058	50	0.0	28	0.0
Civil Mill drain	0.557	190	0.0	28	0.0
Delhi Gate drain	1.328	100	0.0	28	0.0
Sen Nursing Home drain	1.765	300	0.0	31	0.0
Drain No. 12Ar	0.044	60	0.0	31	0.0
Drain No. 14	0.34	40	0.0	31	0.0
Barapulla drain	0.541	60	0.0	32	0.0
Maharani Bagh drain	0.176+28.00*	40	1.5	32	0.0

*- Flow through Hindon Cut Canal

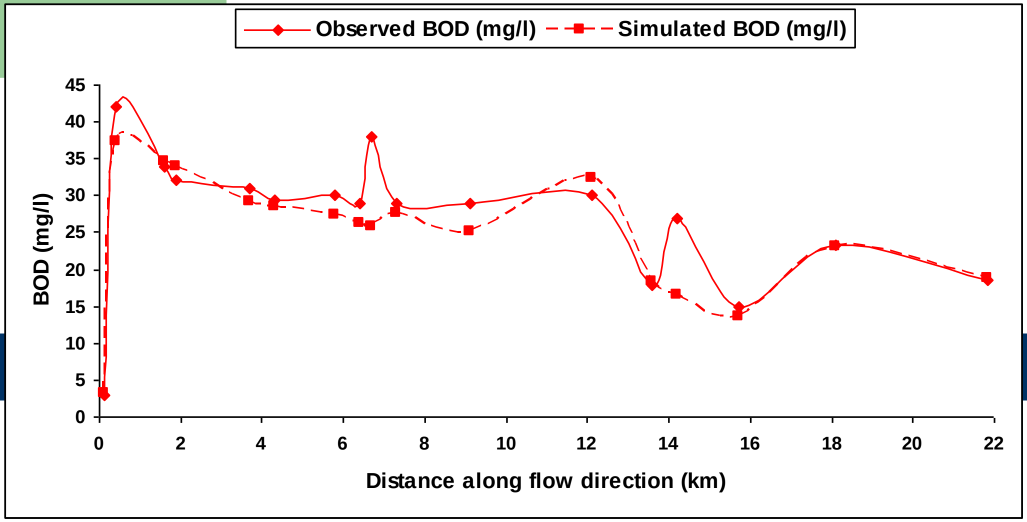


Fig 4.7a Validation–Profile of observed and simulated BOD

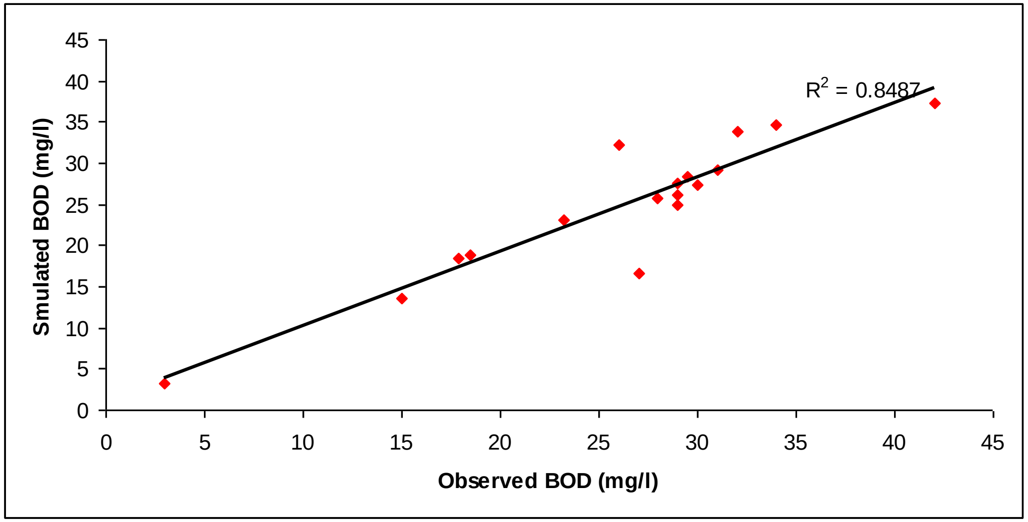


Fig 4.7b Validation–Correlation between observed vs. simulated BOD

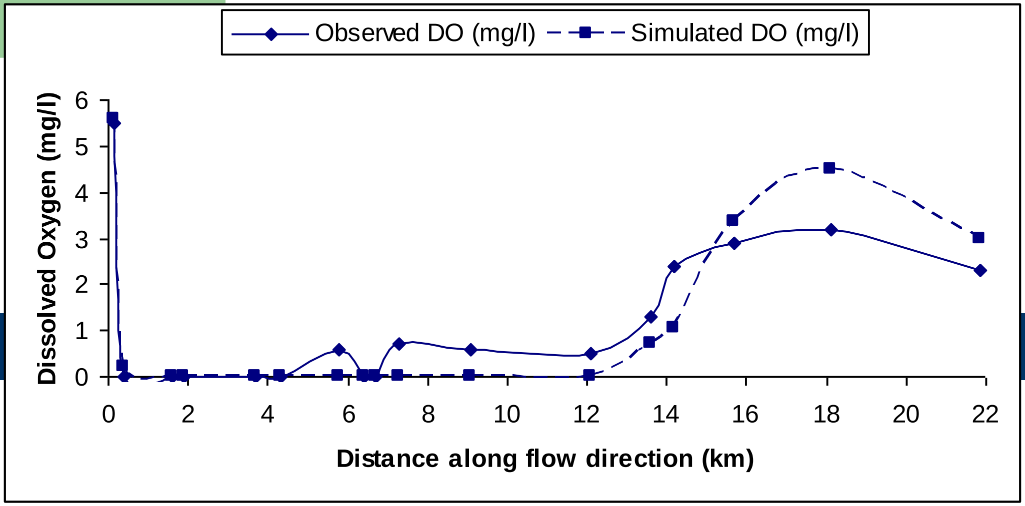


Fig 4.8a Validation–Profile of observed and simulated DO

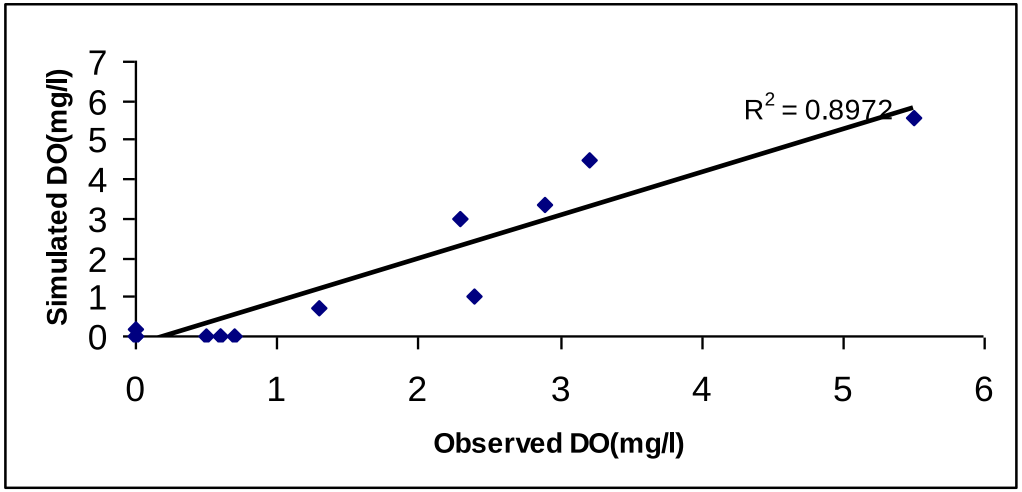


Fig 4.8b Validation–Correlation between observed vs. simulated DO

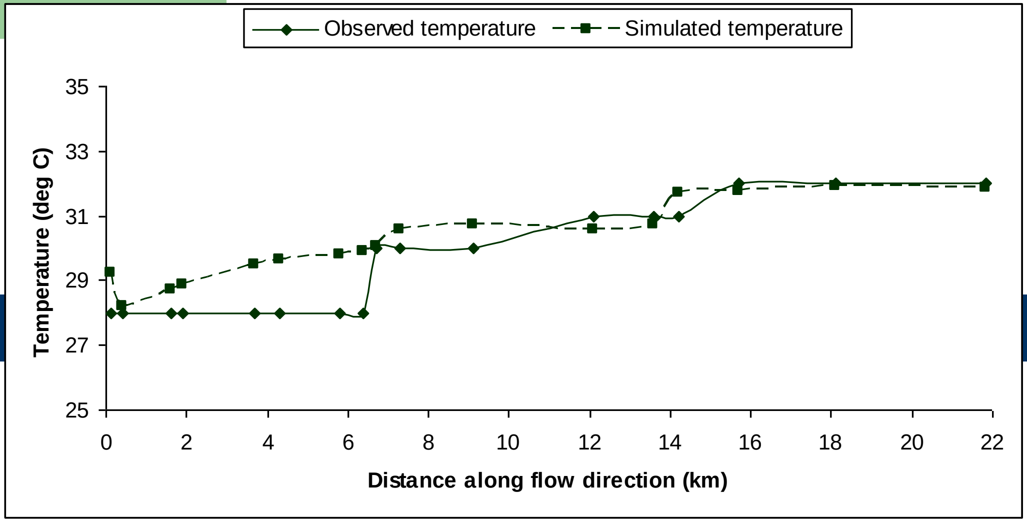


Fig 4.9a Validation–Profile of observed and simulated temperature

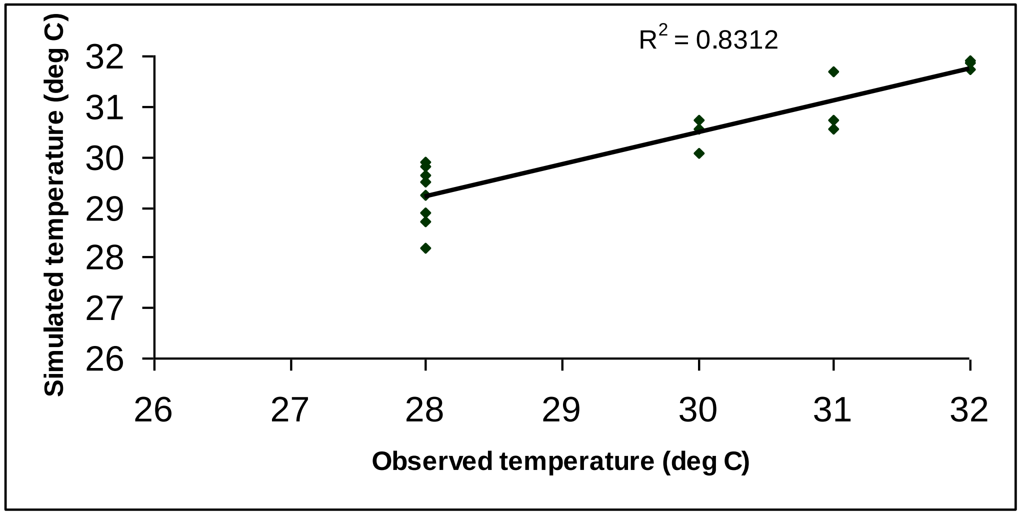


Fig 4.9b Validation–Correlation between observed and simulated temperature

Summary of performance indices

Parameters	Calibration		Validation	
	Coefficient of correlation	Index of agreement	Coefficient of Correlation	Index of agreement
BOD	0.8377	0.8428	0.8487	0.7123
DO	0.8979	0.9761	0.8972	0.9544
Temperature	0.7463	0.818	0.8312	0.9352

BASE LINE CONDITION

Water quality simulation under baseline condition

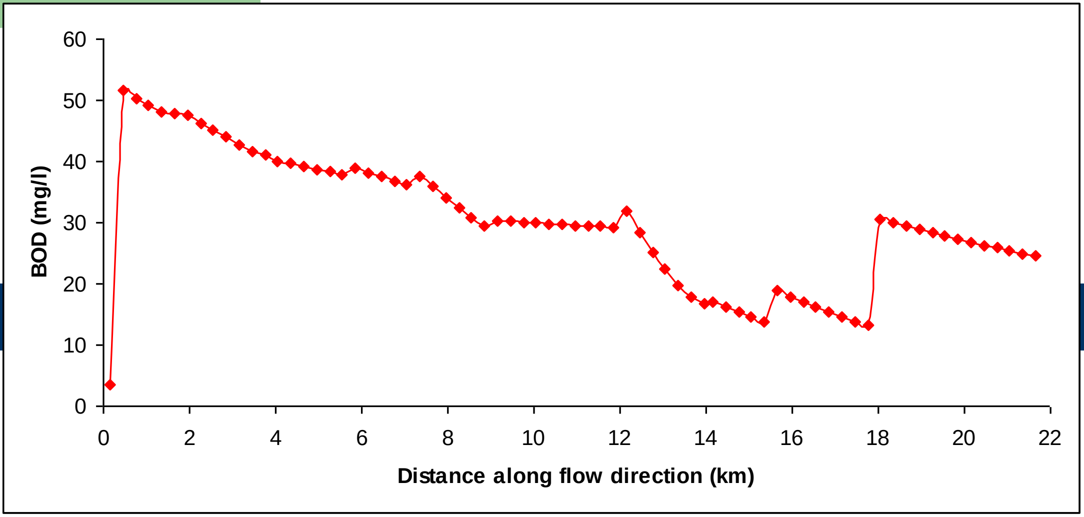


Fig 4.10a Variation of BOD under baseline condition

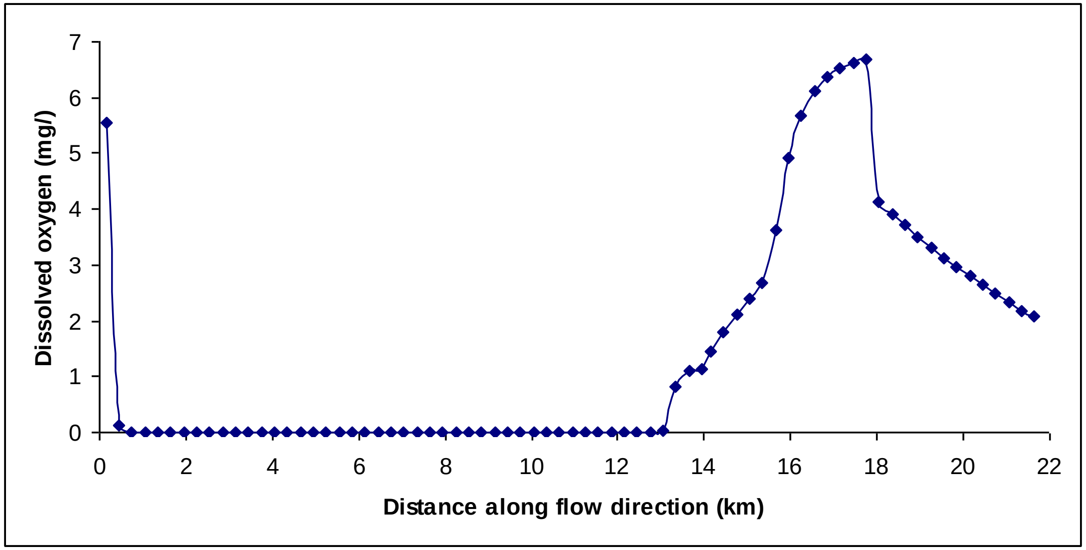


Fig 4.10b Variation of DO under baseline condition

Water quality under baseline conditions

Reach No.	BOD Range (mg/l)	DO Range (mg/l)	Reach No.	BOD Range (mg/l)	DO Range (mg/l)
R-1	3.45	5.56	R-9	36.15-36.76	0.0-0.0
R-2	48.12-51.51	0.0-0.14	R-10	29.45-37.7	0.0-0.0
R-3	47.89	0.0-0.0	R-11	29.32-30.29	0.0-0.0
R-4	41.65-47.54	0.0-0.0	R-12	19.8-31.95	0.0-0.83
R-5	40.12-41.07	0.0-0.0	R-13	16.68-17.96	1.09-1.15
R-6	37.95-39.63	0.0-0.0	R-14	13.84-17.04	1.45-2.69
R-7	38.06-38.87	0.0-0.0	R-15	13.28-18.83	3.63-6.67
R-8	37.47	0.0-0.0	R-16	24.58-30.41	2.07-4.13

SCENARIO GENERATION

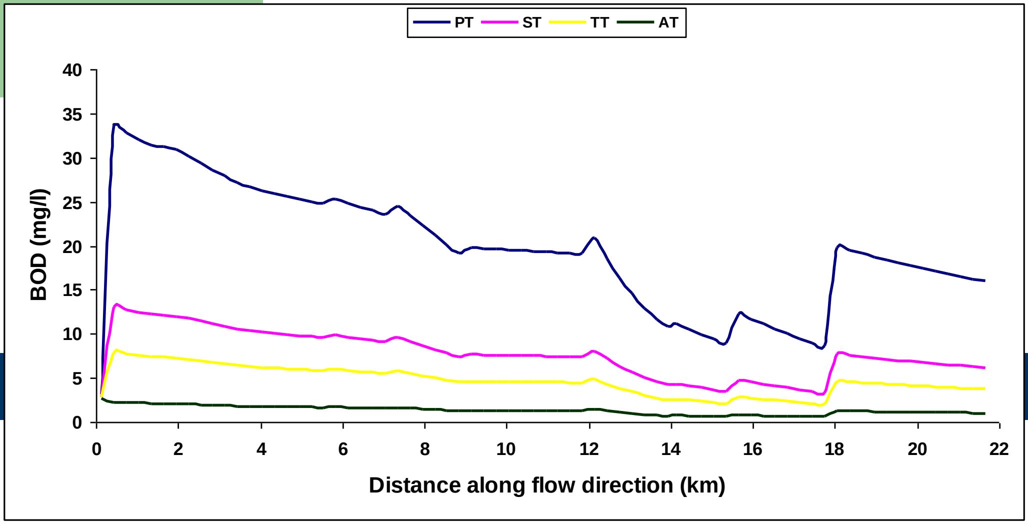


Fig. 5.1a Variation of BOD with varying treatment levels (Case A)

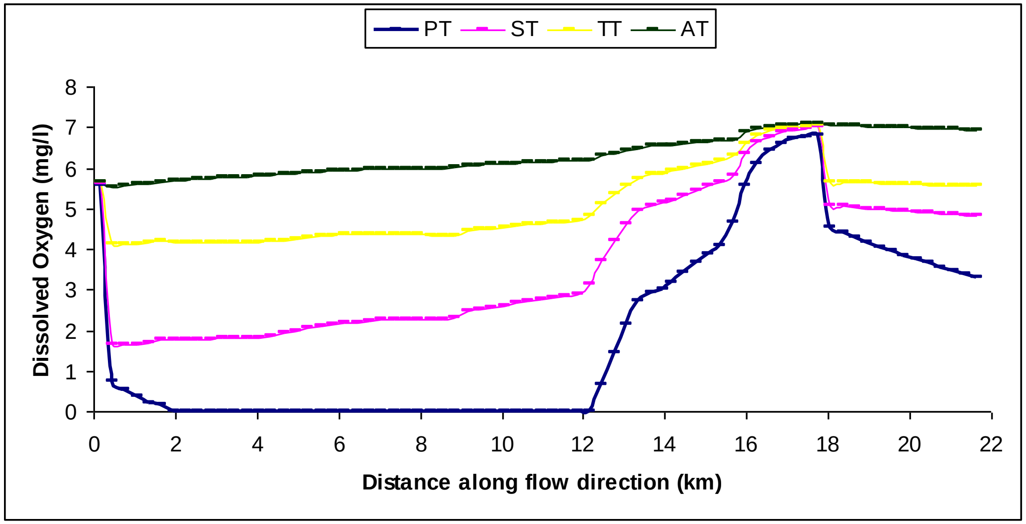


Fig. 5.1b Variation of DO with varying treatment levels (Case A)

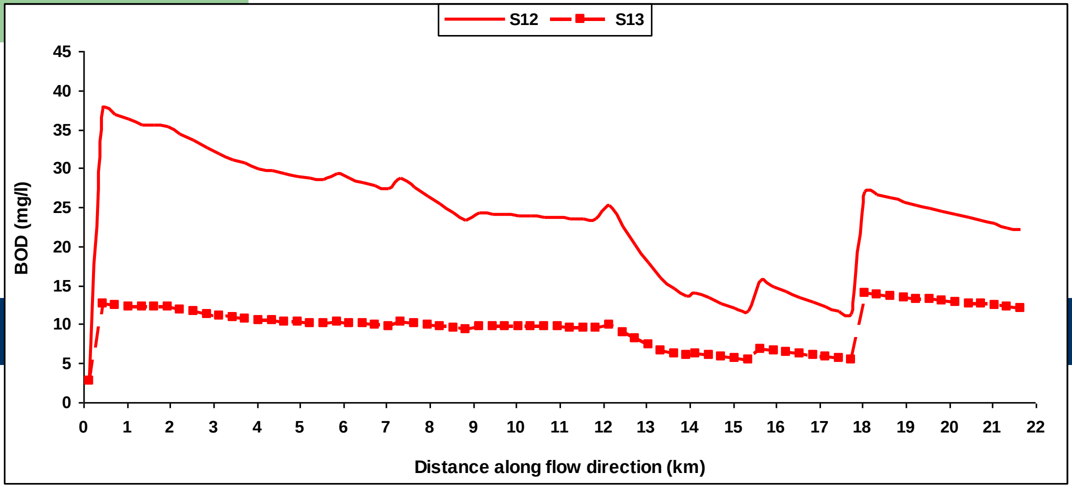


Fig 5.4a Variation of BOD with varying flow augmentation (Case A)

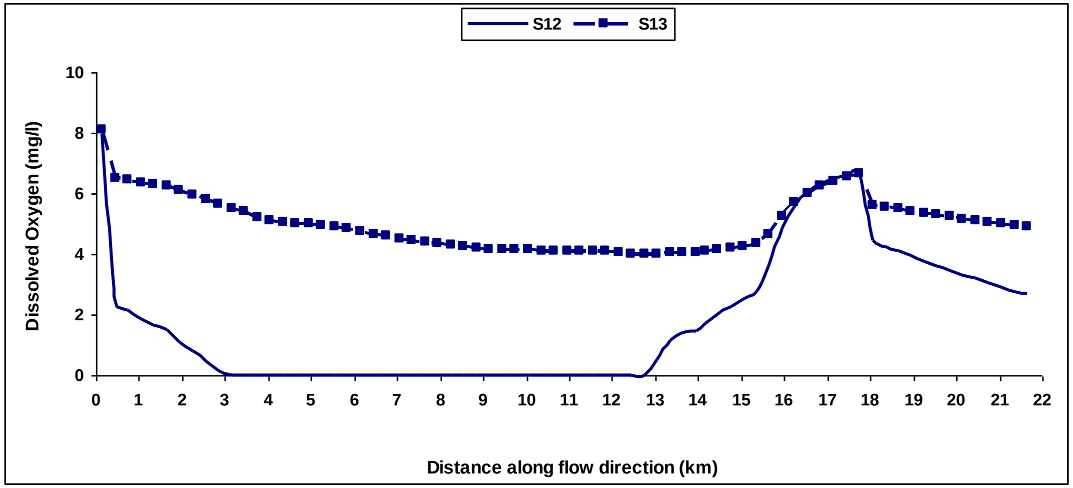


Fig 5.4b Variation of DO with varying Flow augmentation (Case A)

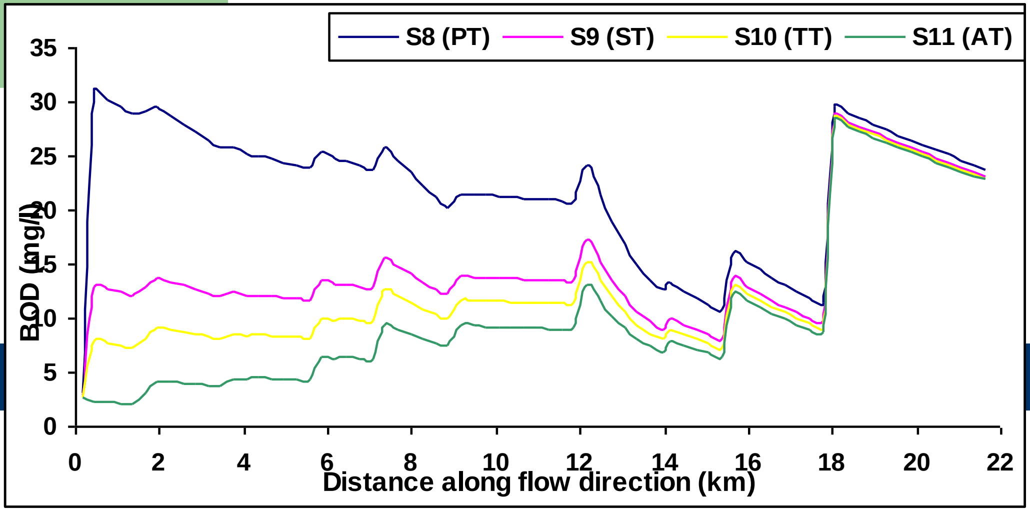


Fig 5.3a Variation of BOD with varying treatment to Najafgarh drain

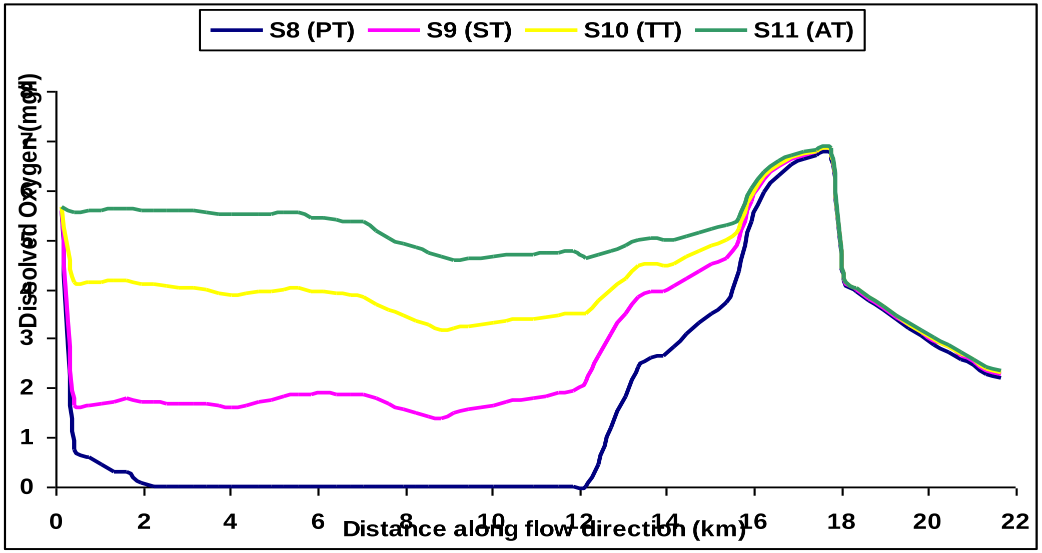


Fig 5.3b Variation of DO with varying treatment to Najafgarh drain

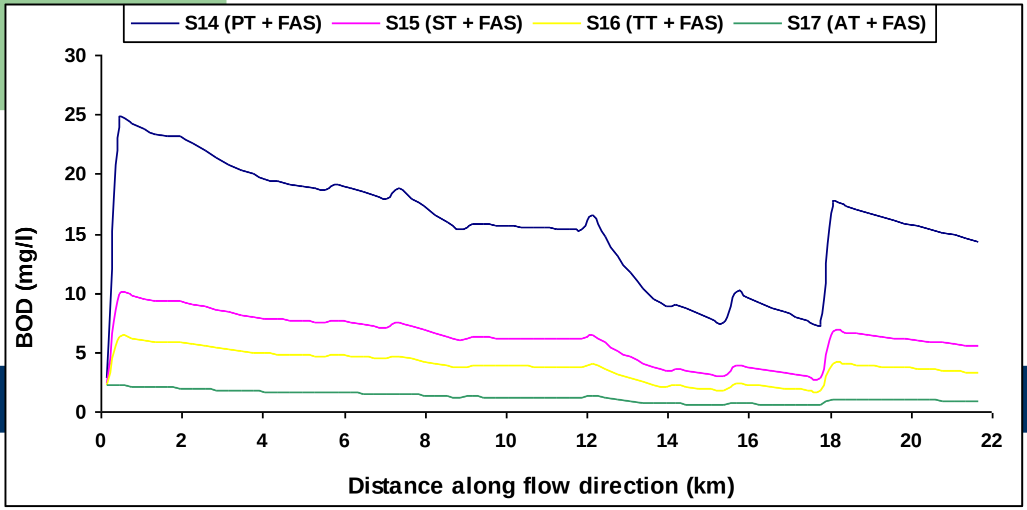


Fig. 5.5a Variation of BOD with varying treatment levels and statutory flow augmentation (Case A)

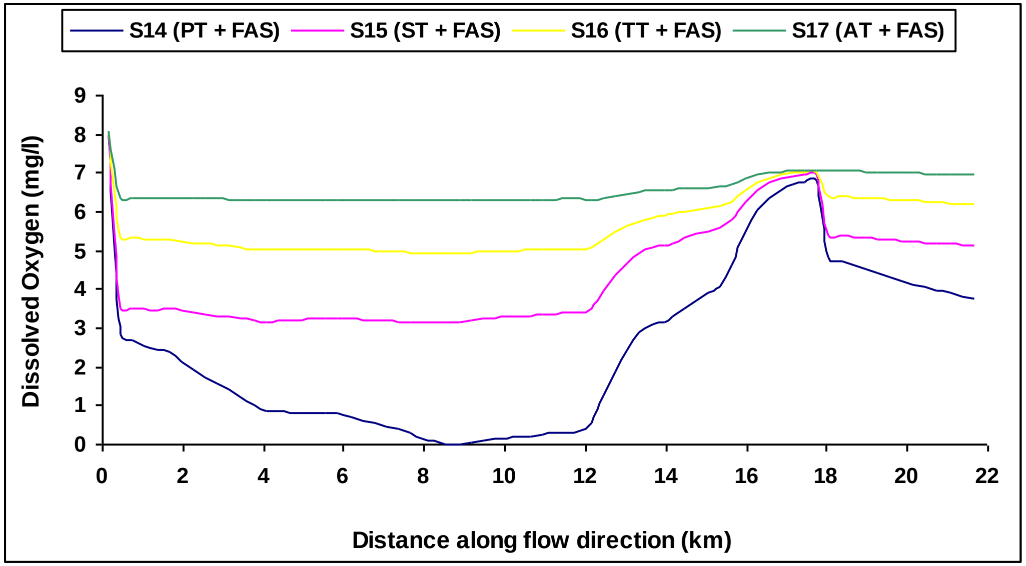


Fig. 5.5b Variation of DO with varying treatment levels and statutory flow augmentation (Case A)

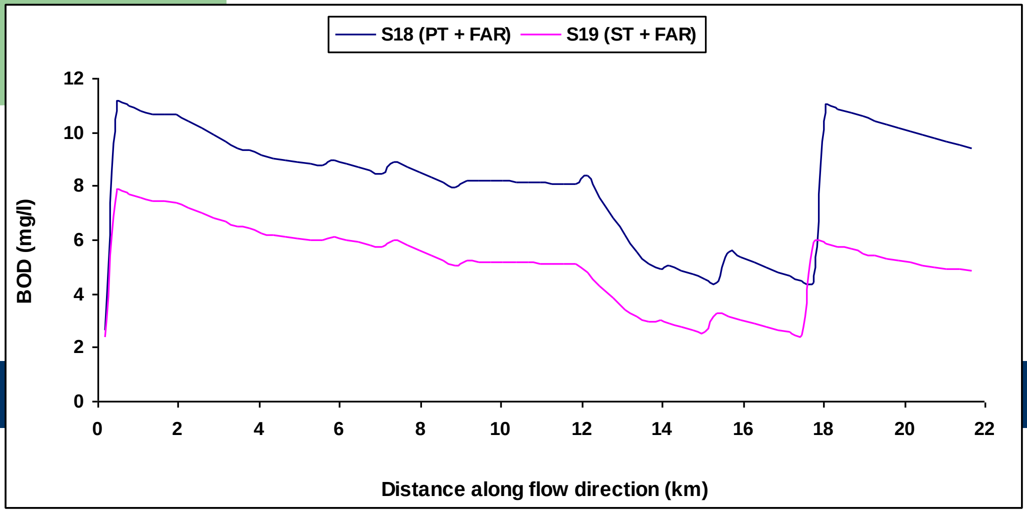


Fig 5.6a Variation of BOD with varying treatment levels and corresponding requisite flow augmentation (Case A)

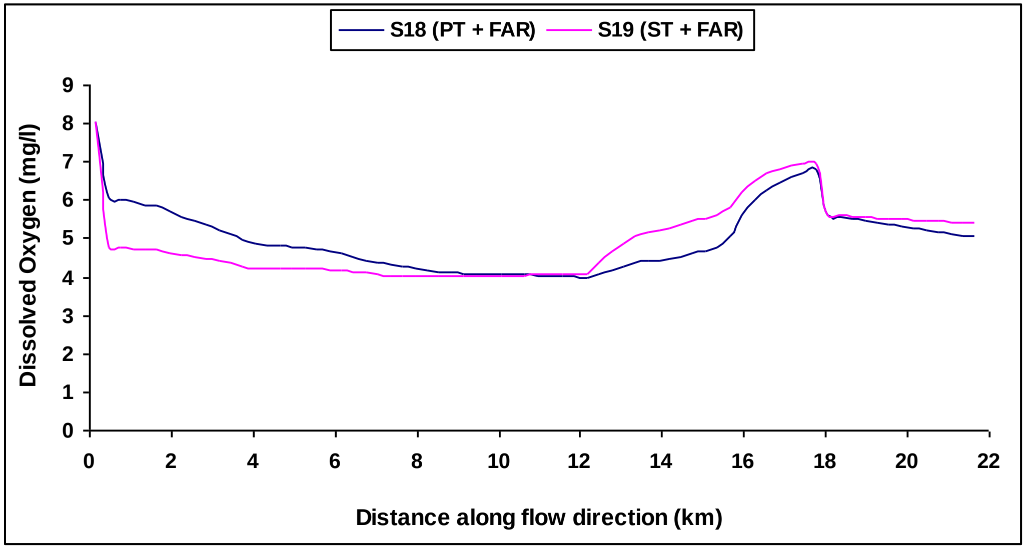


Fig 5.6b Variation of DO with varying treatment levels and corresponding requisite flow augmentation (Case A)

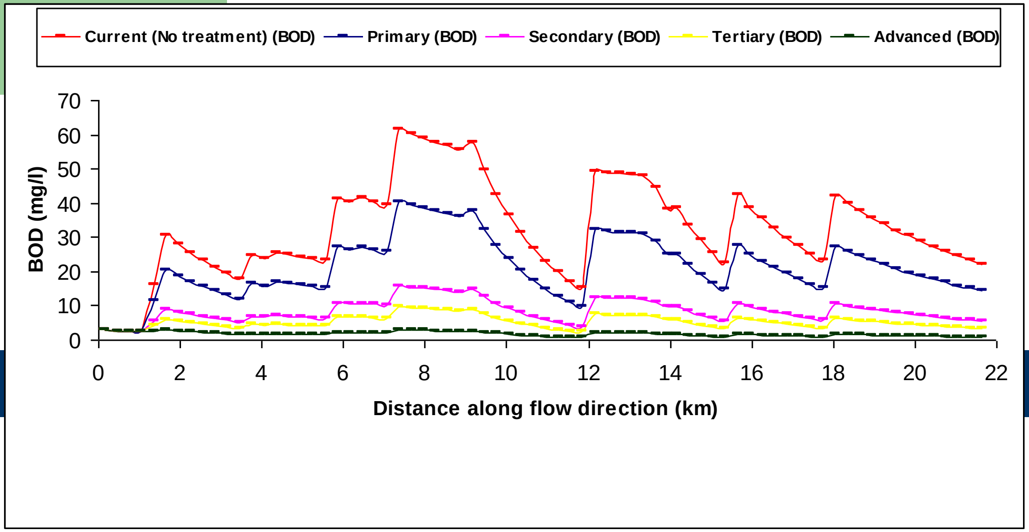


Fig 5.7a Variation of BOD with varying treatment levels (Case B)

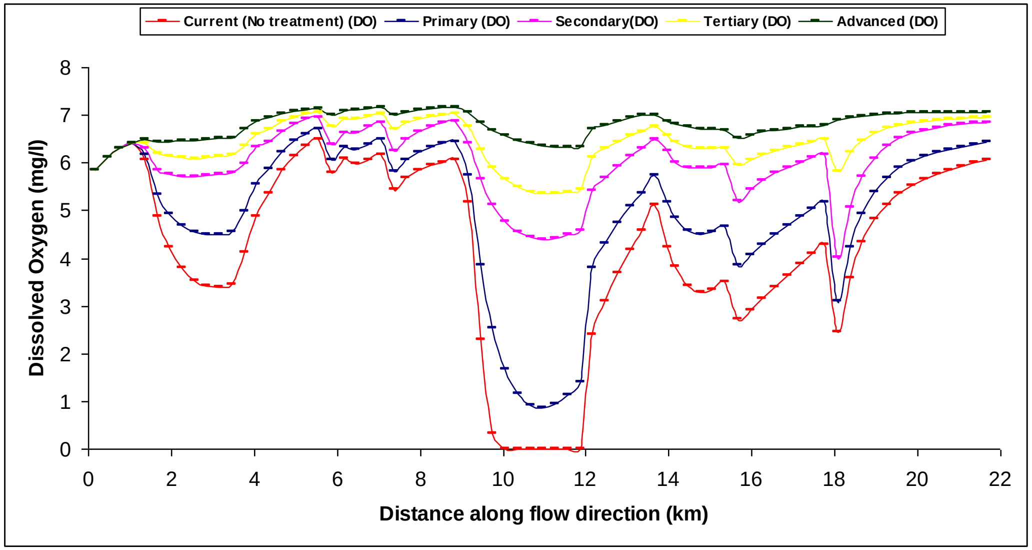


Fig 5.7b Variation of DO with varying treatment levels (Case B)

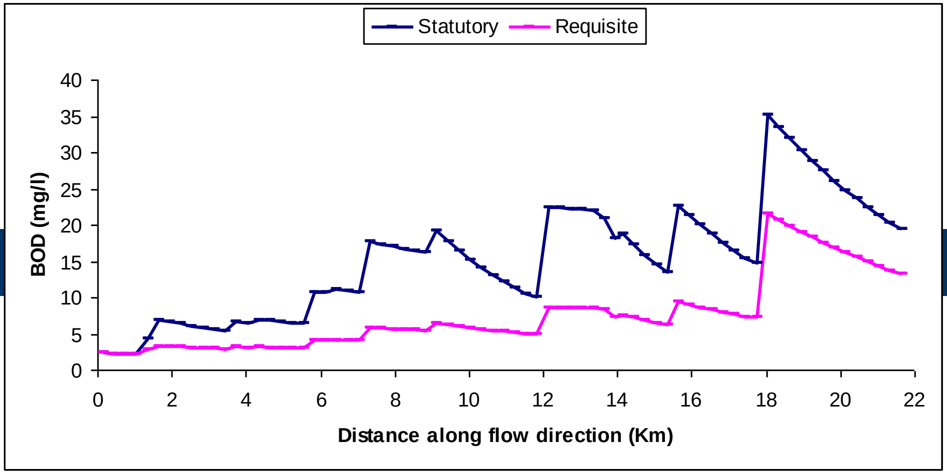


Fig 5.8a Variation of BOD with flow augmentation (Case B)

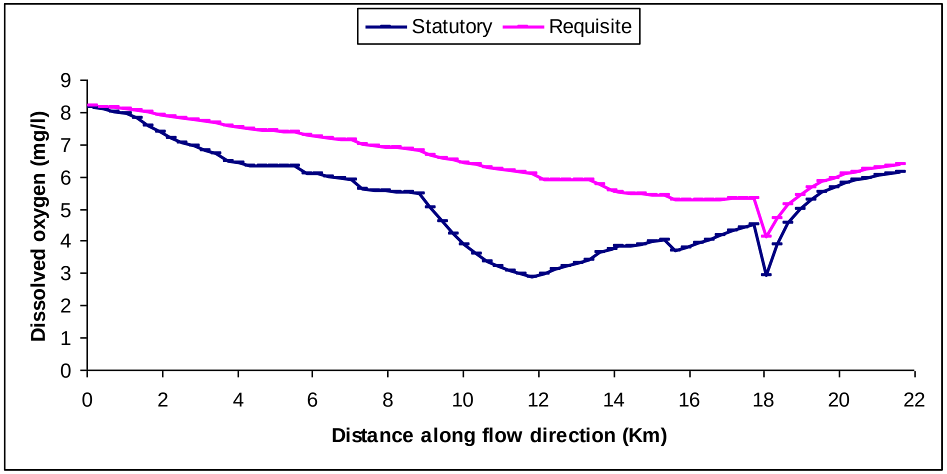


Fig 5.8b Variation of DO with flow augmentation (Case B)

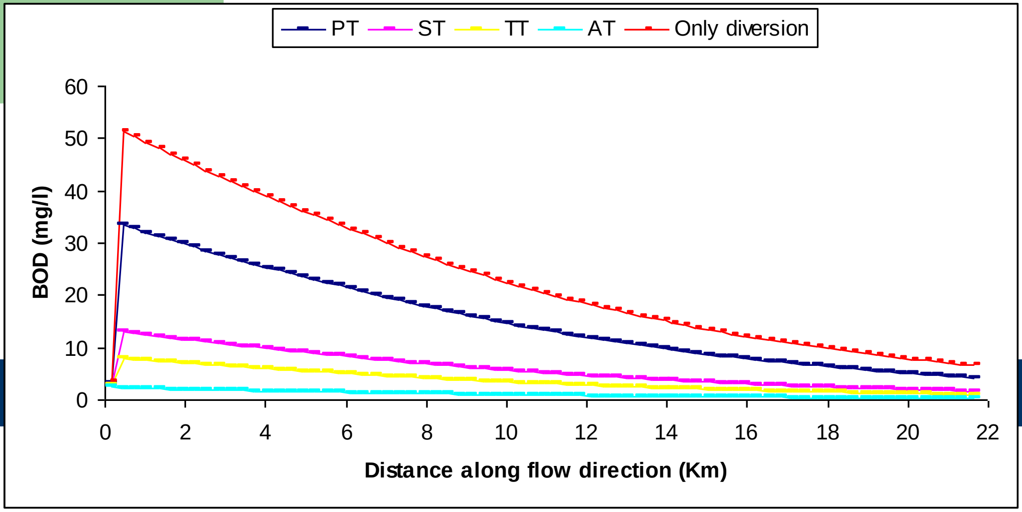


Fig 5.9a Variation of BOD with varying treatment levels (Case C)

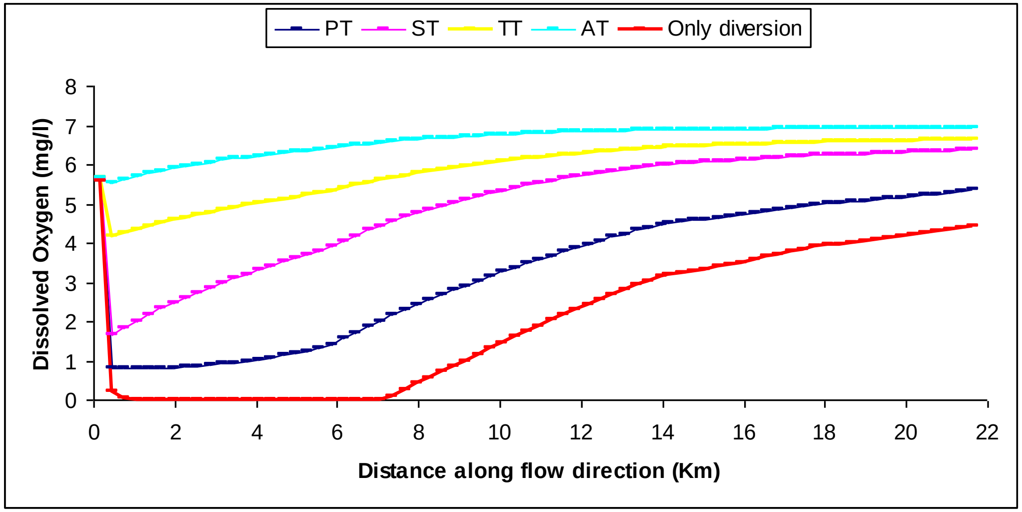


Fig 5.9b Variation of DO with varying treatment levels (Case C)

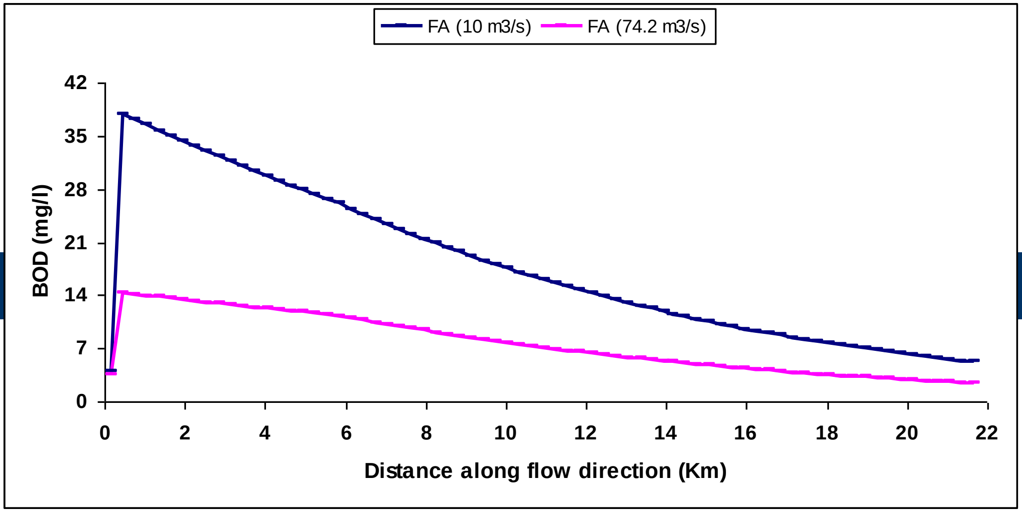


Fig 5.10a Variation of BOD with flow augmentation (Case C)

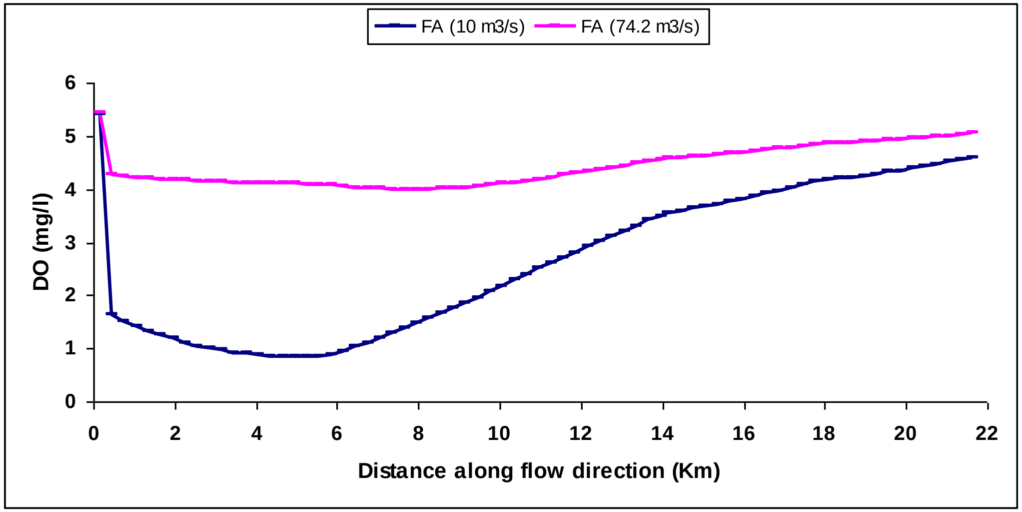


Fig 5.10b Variation of DO with flow augmentation (Case C)

Sensitivity due to model parameters

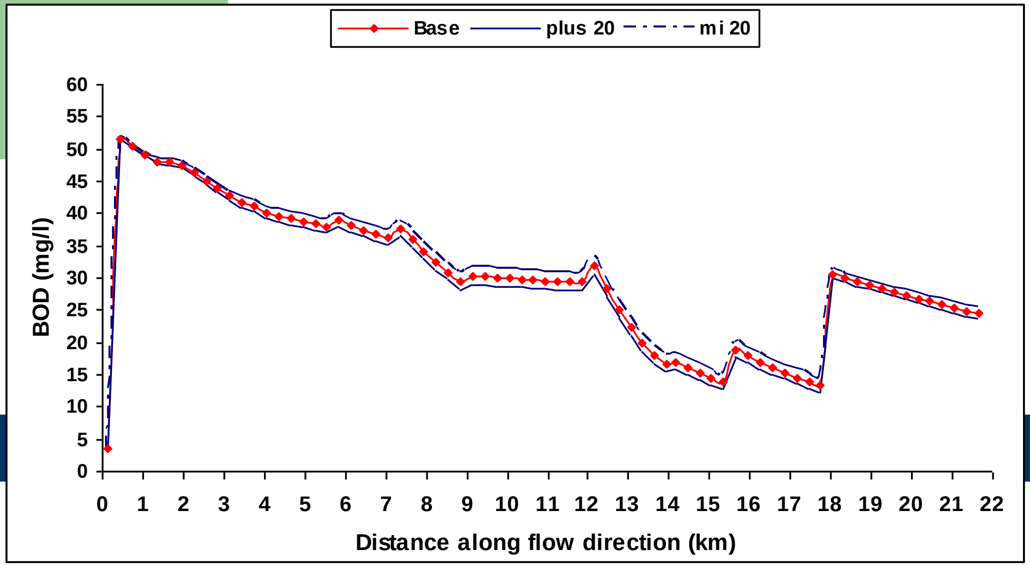


Fig 5.12a Distribution of BOD with varying K_1

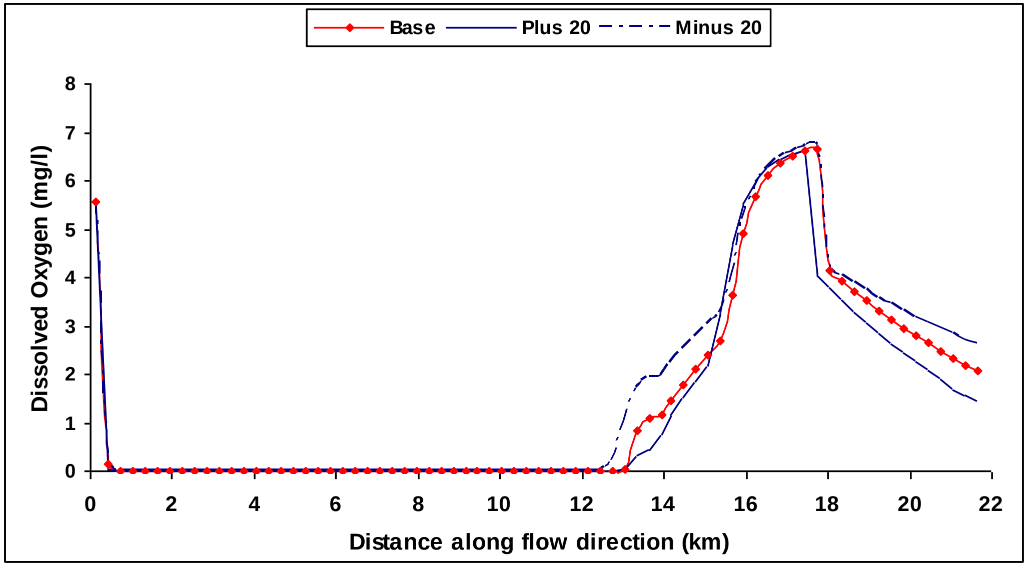


Fig 5.12b Distribution of DO with varying K_1

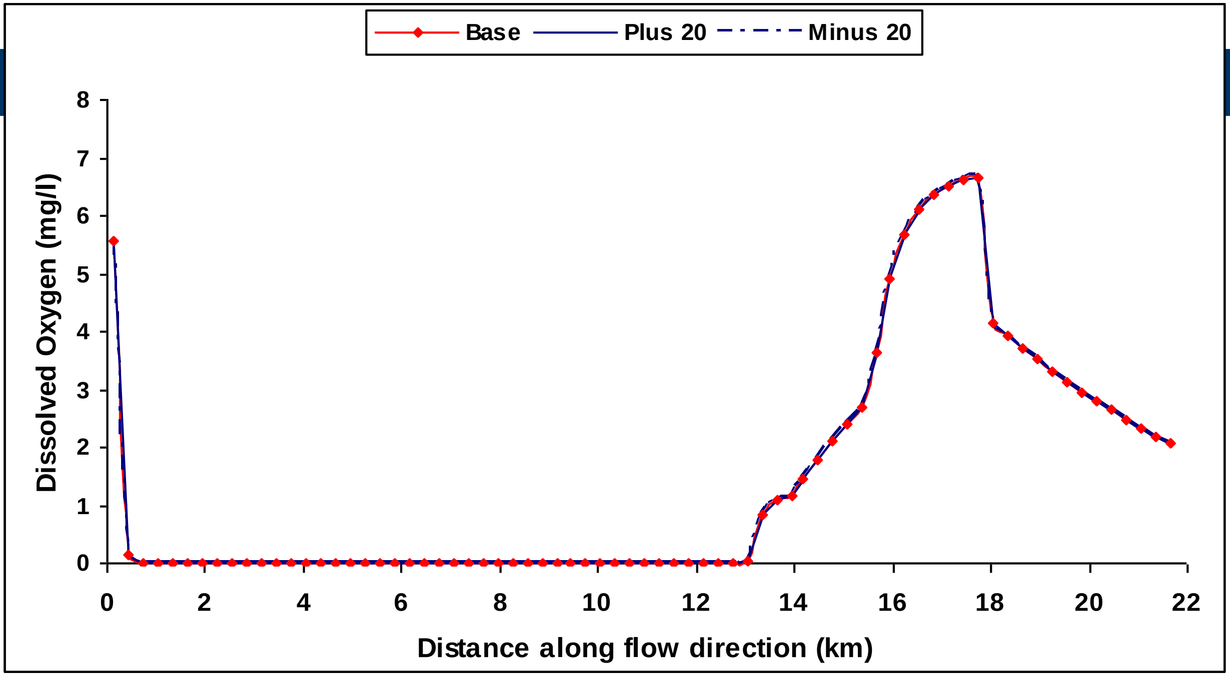


Fig 5.13 Distribution of DO with varying K_2

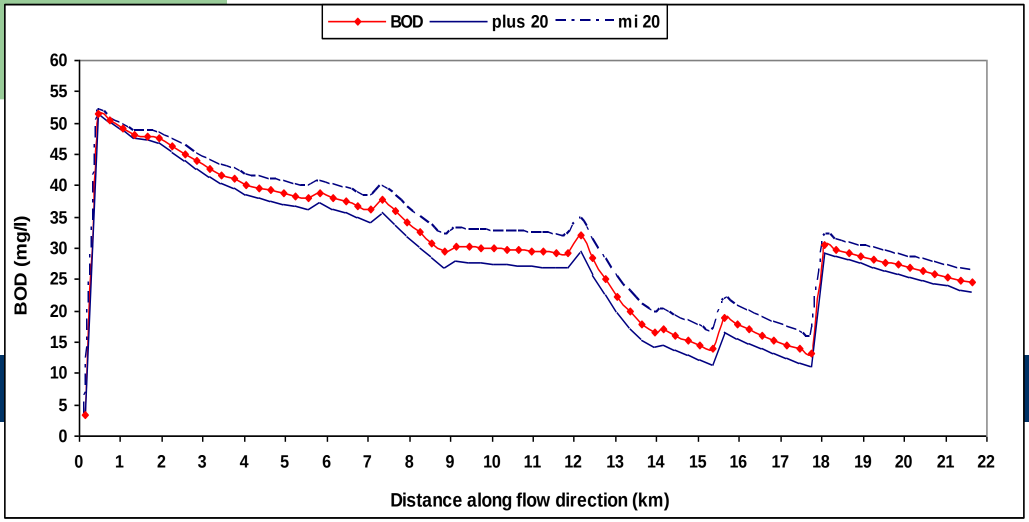


Fig 5.14a Distribution of BOD with varying K_3

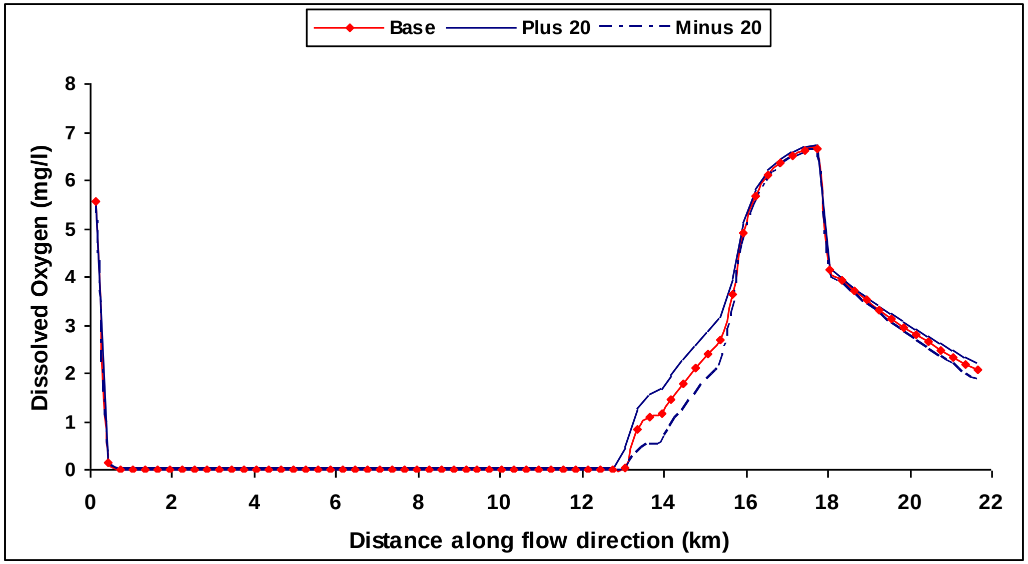


Fig 5.14b Distribution of DO with varying K_3

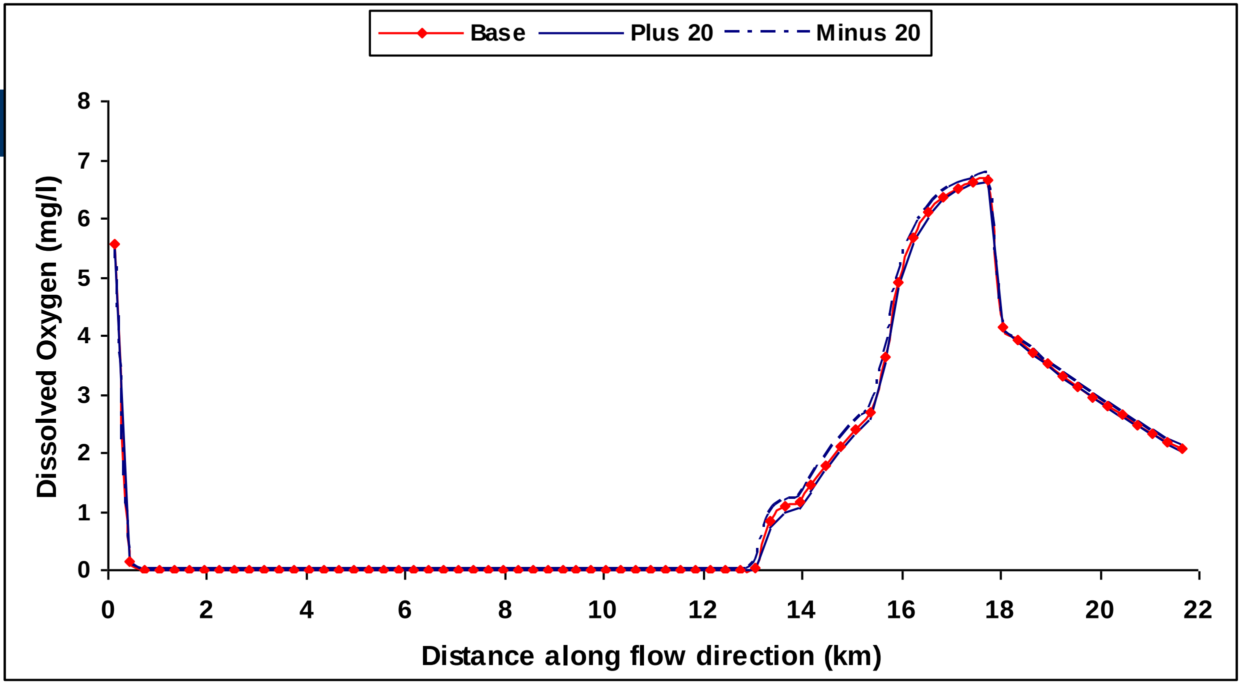


Fig 5.15 Distribution of DO with varying K_4

Application of Optimization model

Waste load allocation and its steps

- Development of cost function.
- Estimation of water quality response.
- Optimal solutions

Development of Cost functions – Data requirement

Type Capacity (MLD)

Year of construction.

Capital Cost

Capital recovery factor (4%, 20 years)

Amortized Cost

O & M Cost (per annum)

Annualized Cost (lacs per year)

Developing Cost functions for Wastewater treatment by STP.

- Cost is amortized to find the present cost of STP's (in 2005)- 105 plants.

- The O & M cost is added to amortized to obtained annual amortized cost.

- The cost is a function of percentage BOD removal by the treatment plant.

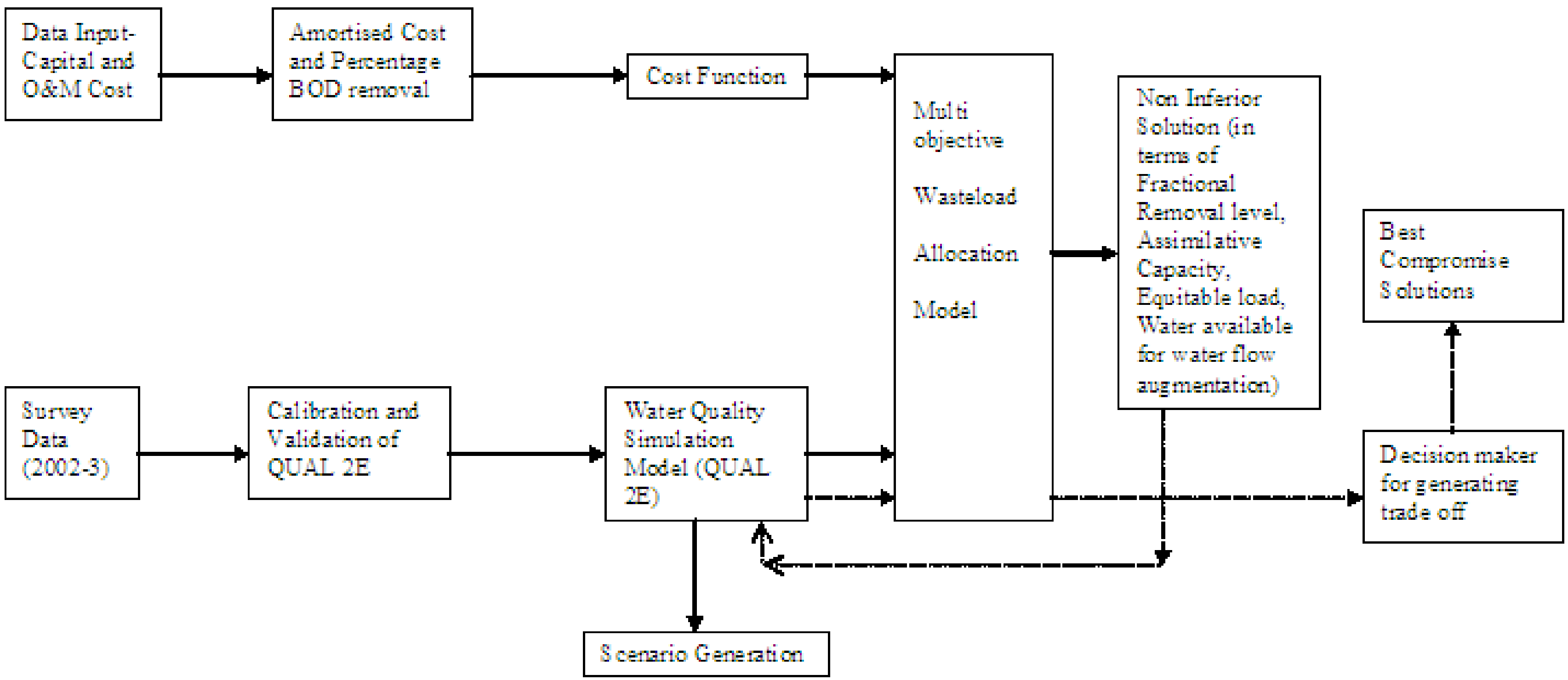


Fig. 1. Schematic sketch of Multiobjective Wasteload Allocation Framework

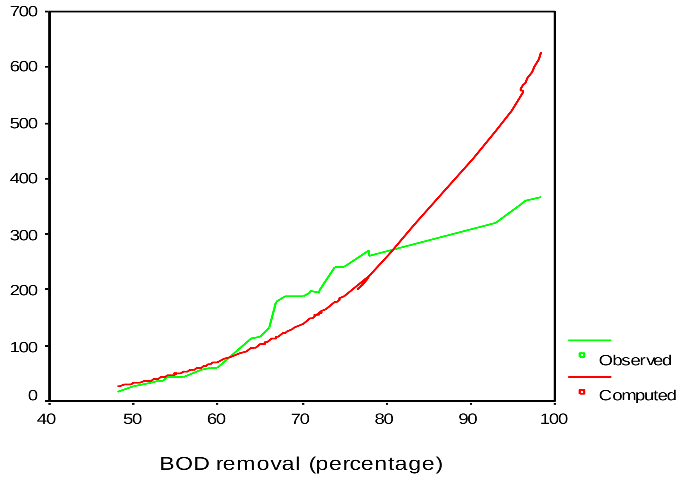


Fig 5.21a Profiles of the observed and computed cost curves for 6-20 MLD capacity

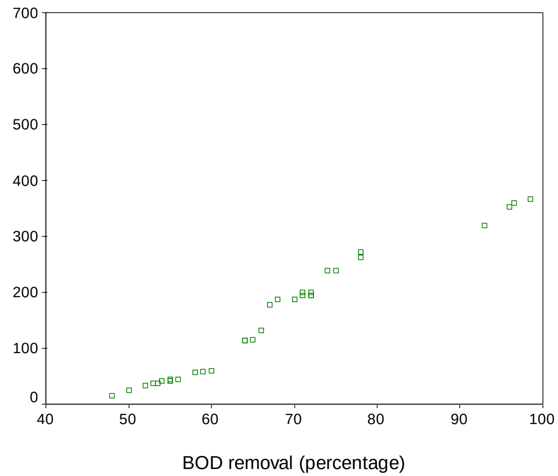


Fig 5.21b Observed BOD trend for 6-20 MLD capacity

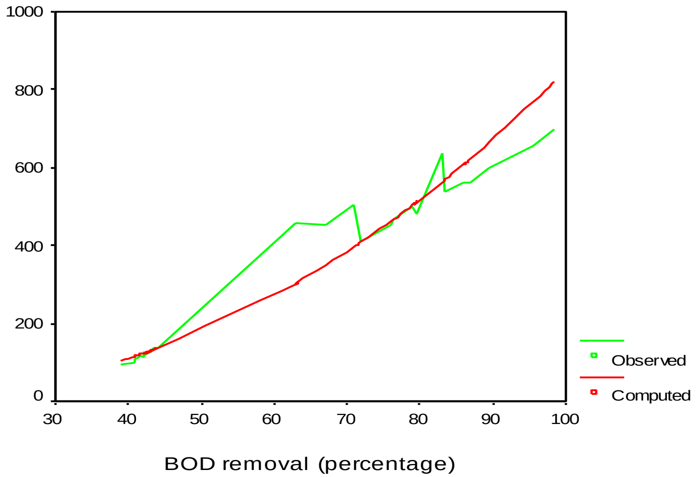


Fig 5.22a Profiles of the observed and computed cost curves for 21-35 MLD capacity

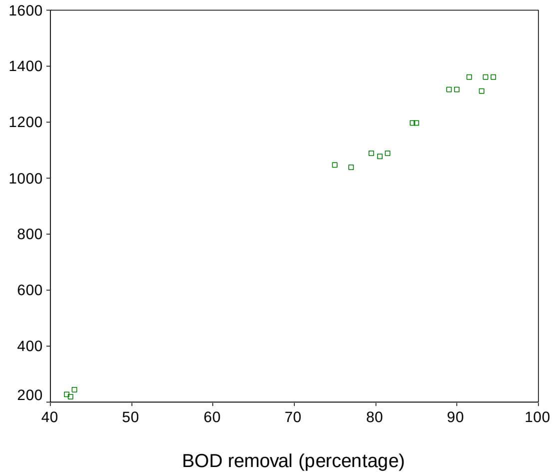


Fig 5.22b Observed BOD trend for 21-35 MLD capacity

Developed cost functions

Range of flow	Drain Nos.	Cost function (C)	R^2
0-5 MLD	D8, D12	$0.000010282\,r^{3.525}$	0.9949
6-20 MLD	D2, D3, D4, D5, D7	$0.0011654\,r^{2.7795}$	0.8882
21-35 MLD	D6, D13	$0.1548\,r^{1.8462}$	0.9399
36-50 MLD	D9, D10,	$0.4524\,r^{1.6944}$	0.7406
51-70 MLD	D15	$0.2352\,r^{1.9171}$	0.975
71-100 MLD	D11	$0.8314\,r^{1.5179}$	0.7326
$\geq$ 100	D1, D14	$0.001395\,r^{3.4277}$	0.9395

Where r : percentage of BOD removal.

Details of cost functions for drains

Drain No.	Name of drain	Cost function
D1	Najafgarh	$C_1 = 0.001395 r_1^{3.4277}$
D2	Magazine Road	$C_2 = 0.0011654 r_2^{2.7795}$
D3	Sweeper Colony	$C_3 = 0.0011654 r_3^{2.7795}$
D4	Khyber Pass	$C_4 = 0.0011654 r_4^{2.7795}$
D5	Metcalf House	$C_5 = 0.0011654 r_5^{2.7795}$
D6	Qudsia Bagh	$C_6 = 0.1548 r_6^{1.8462}$
D7	Tonga Stand	$C_7 = 0.0011654 r_7^{2.7795}$
D8	Moat	$C_8 = 0.000010282 r_8^{3.525}$
D9	Civil Mill	$C_9 = 0.4524 r_9^{1.6944}$
D10	Delhi Gate/Power House	$C_{10} = 0.4524 r_{10}^{1.6944}$
D11	Sen Nursing Home	$C_{11} = 0.8314 r_{11}^{1.5179}$
D12	Drain No. 13	$C_{12} = 0.000010282 r_{12}^{3.525}$
D13	Drain No. 14	$C_{13} = 0.1548 r_{13}^{1.8462}$
D14	Barapulla	$C_{14} = 0.001395 r_{14}^{3.4277}$
D15	Maharani Bagh	$C_{15} = 0.2352 r_{15}^{1.9171}$

Where r and the associated subscript represents the percentage of BOD removal and the drain number, respectively.

Flow availability in the river Yamuna during August to September 2010

Date	Flow in cusecs
Aug 22nd 2010	3,24,365
September 8th 2010	607000
September 9th 2010	1,00,000
September 12th 2010	41,748
September 22nd 2010	2,56,100
September 23rd 2010	3,56,050
September 24th 2010	2,16,600
September 25th 2010	2,13,790
September 26th 2010	1,30,240
September 27th 2010	83,307
September 28th 2010	73,430
September 29th 2010	66,000
September 30th 2010	54,400
Total	25,23,030 cusecs

Transfer Coefficients

- The transfer coefficients have been obtained from the QUAL2E steady-state water quality simulation model.
- The transfer coefficients were obtained by treating the BOD inputs for each discharger, and holding all other inputs constant to calculate the marginal effect of each source, , on water quality in each downstream stretch .
- The outcome of this is a transfer coefficient .
- This process was continued and additional runs of QUAL2E simulation model taken until improvement in all the reaches was observed to the desired standard of 4 mg/l.

Sample matrix of transfer coefficients used in the least cost model.

	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16
D1	4.9	4.65	4.6	4.55	4.52	3.82	3.57	3.51	3.44	3.25	1.8	2.96	2.79	1.63	0.68
D2	0	0.98	0.85	0.34	0.32	0.58	0.57	0.57	0.55	0.48	1.42	2.93	2.75	1.61	0.68
D3	0	0	0.85	0.34	0.32	0.58	0.56	0.56	0.55	0.48	1.41	2.93	2.75	1.61	0.68
D4	0	0	0	0.34	0.32	0.58	0.56	0.56	0.55	0.48	1.41	2.93	2.75	1.61	0.68
D5	0	0	0	0	0.32	0.58	0.56	0.56	0.55	0.48	1.41	2.93	2.75	1.61	0.68
D6	0	0	0	0	0	0.58	0.57	0.56	0.56	0.48	1.41	2.93	2.75	1.61	0.68
D7	0	0	0	0	0	0	0.56	0.56	0.55	0.48	1.41	2.93	2.75	1.61	0.68
D8	0	0	0	0	0	0	0	0.56	0.55	0.48	1.41	2.93	2.75	1.61	0.68
D9	0	0	0	0	0	0	0	0	0.55	0.49	1.42	2.93	2.75	1.61	0.68
D10	0	0	0	0	0	0	0	0	0	0.48	1.42	2.93	2.75	1.61	0.68
D11	0	0	0	0	0	0	0	0	0	0	1.41	2.93	2.75	1.61	0.68
D12	0	0	0	0	0	0	0	0	0	0	0	2.93	2.75	1.61	0.68
D13	0	0	0	0	0	0	0	0	0	0	0	0	2.75	1.61	0.68
D14	0	0	0	0	0	0	0	0	0	0	0	0	0	1.61	0.68
D15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.68

Least cost model (LCM)

Minimize F_1=

$$0.001395 r_1^{3.4277} + 0.0011654 r_2^{2.7795} + 0.0011654 r_3^{2.7795} + 0.0011654 r_4^{2.7795} +$$

$$0.0011654 r_5^{2.7795} + 0.1548 r_6^{1.8462} + 0.0011654 r_7^{2.7795} + 0.000010282 r_8^{3.525} +$$

$$0.4524 r_9^{1.6944} + 0.4524 r_{10}^{1.6944} + 0.8314 r_{11}^{1.5179} + 0.000010282 r_{12}^{3.525} + 0.1548 r_{13}^{1.8462} +$$

$$0.001395 r_{14}^{3.4277} + 0.2352 r_{15}^{1.9171}$$

Subject to

a) Linear Constraints (Water quality improvement constraints)

$$-4.9 r_1 \leq -3.86$$

$$-4.65 r_1 - 0.98 r_2 \leq -4$$

$$-4.6 r_1 - 0.85 r_2 - 0.85 r_3 \leq -4$$

$$-4.56 r_1 - 0.34 r_2 - 0.34 r_3 - 0.34 r_4 \leq -4$$

$$-4.52 r_1 - 0.32 r_2 - 0.32 r_3 - 0.32 r_4 - 0.32 r_5 \leq -4$$

$$-3.82 r_1 - 0.58 r_2 - 0.58 r_3 - 0.58 r_4 - 0.58 r_5 - 0.58 r_6 \leq -4$$

$$-3.57 r_1 - 0.57 r_2 - 0.56 r_3 - 0.56 r_4 - 0.56 r_5 - 0.57 r_6 - 0.56 r_7 \leq -4$$

$$-3.51r_1 - 0.56r_2 - 0.56r_3 - 0.56r_4 - 0.56r_5 - 0.56r_6 - 0.56r_7 - 0.56r_8 \leq -4$$

$$-3.44r_1 - 0.55r_2 - 0.55r_3 - 0.55r_4 - 0.55r_5 - 0.56r_6 - 0.55r_7 - 0.55r_8 - 0.55r_9 \leq -4$$

$$-3.25r_1 - 0.48r_2 - 0.48r_3 - 0.48r_4 - 0.48r_5 - 0.48r_6 - 0.48r_7 - 0.48r_8 - 0.48r_9$$
$$-0.48r_{10} \leq -4$$

$$-1.48r_1 - 1.42r_2 - 1.41r_3 - 141r_4 - 1.41r_5 - 1.41r_6 - 1.41r_7 - 1.41r_8 - 1.42r_9 - 1.42r_{10}$$
$$-1.41r_{11} \leq -4$$

$$-2.96r_1 - 2.93r_2 - 2.93r_3 - 2.93r_4 - 2.93r_5 - 2.93r_6 - 2.93r_7 - 2.93r_8 - 2.93r_9$$
$$-2.93r_{10} - 2.93r_{11} - 2.93r_{12} \leq -2.91$$

$$-2.79r_1 - 2.75r_2 - 2.75r_3 - 2.75r_4 - 2.75r_5 - 2.75r_6 - 2.75r_7 - 2.75r_8 - 2.75r_9$$
$$-2.75r_{10} - 2.75r_{11} - 2.75r_{12} - 2.75r_{13} \leq -2.55$$

$$-1.63r_1 - 1.61r_2 - 1.61r_3 - 1.61r_4 - 1.61r_5 - 1.61r_6 - 1.61r_7 - 1.61r_8 - 1.61r_9 - 1.61r_{10}$$
$$-1.61r_{11} - 1.61r_{12} - 1.61r_{13} - 1.61r_{14} \leq -0.37$$

$$-0.68r_1 - 0.68r_2 - 0.68r_3 - 0.68r_4 - 0.68r_5 - 0.68r_6 - 0.68r_7 - 0.68r_8 - 0.68r_9$$
$$-0.68r_{10} - 0.68r_{11} - 0.68r_{12} - 0.68r_{13} - 0.68r_{14} - 0.68r_{15} \leq 0.13$$

b) Bounds

$$0.0 \leq r_i \leq 0.96 \qquad \forall i = 1, 2, \ldots\ldots\ldots\ldots, 15$$

Optimal solution for least cost model (LCM)

Drain No.	Name of the drain	BOD removal (r)
D1	Najafgarh	0.855
D2	Magazine Road	0.15
D3	Sweeper Colony	0.15
D4	Khyber Pass	0.15
D5	Metcalf House	0.15
D6	Mori Gate	0.25
D7	Tonga Stand	0.15
D8	Moat	0.15
D9	Civil Mill	0.25
D10	Delhi Gate	0.25
D11	Sen Nursing Home	0.0
D12	Drain No. 12A	0.0
D13	Drain No. 14A	0.0
D14	Barapulla	0.0
D15	Maharani Bagh	0.53
	Total cost	Rs. 660.164 million

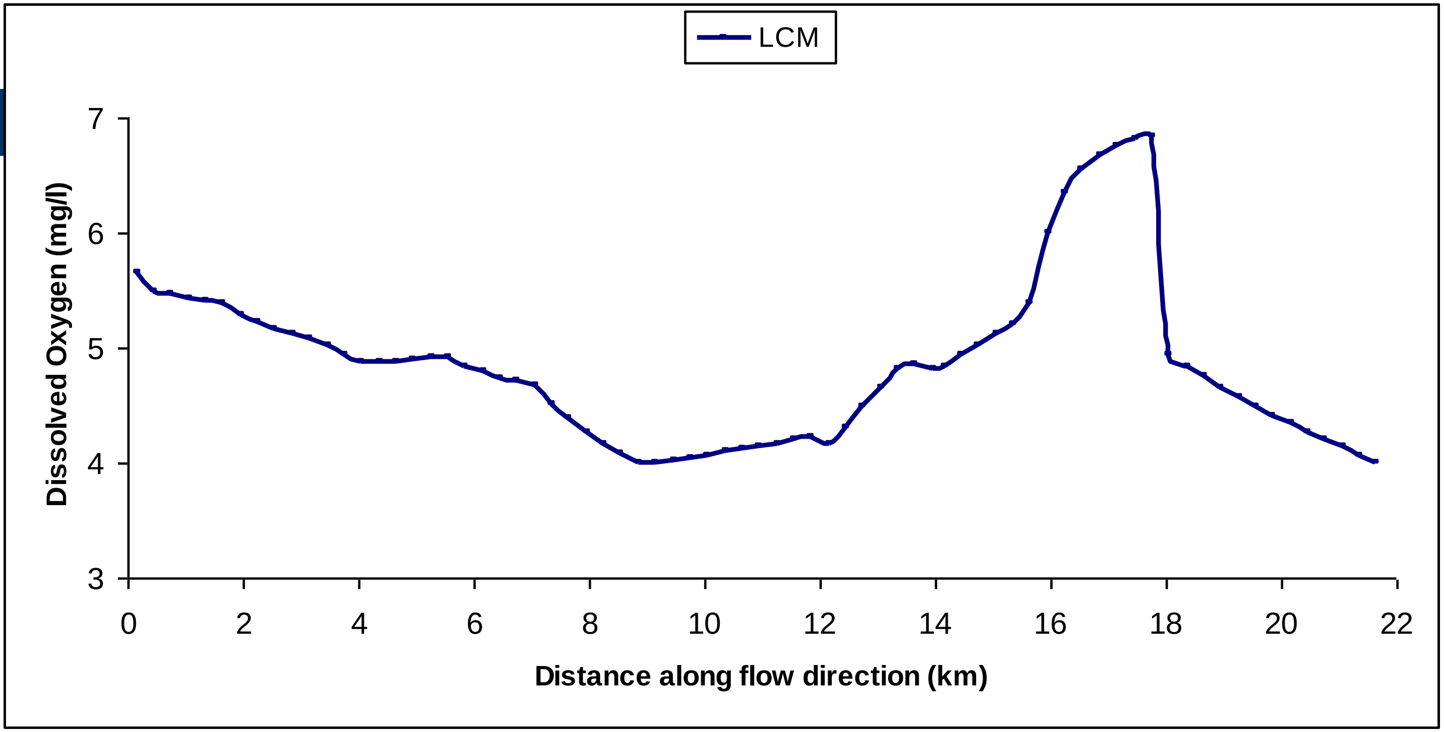


Fig 5.28 Dissolved Oxygen Profiles for Least Cost Model

Conclusions for the Modeling Application

- 1. Results of the baseline condition reveal that:

the first 13.2 km (except for the first reach of 0.3 km) is devoid of DO and the BOD ranges from 3.45 to 51.51 mg/l.

Last 8.7 km stretch has DO ranging from 0.03 to 6.67 mg/l.

Case A

- Results under Case A reveal that when wastewater treatment alone is adopted as a pollution abatement measure, the DO criterion is satisfied after tertiary treatment is applied, i.e. after 85% BOD removal.

However, the BOD criterion of 3 mg/l is not satisfied until advanced treatment is applied.

- When FA alone is adopted, it is found that the statutory flow requirement of 10 m^3/s downstream of the Wazirabad Barrage does not give any desirable results in terms of water quality.
- A total of 90 m^3/s of flow is required to satisfy the DO standard.

- When WWT is tried in combination with the statutory FA (10 m^3/s), tertiary treatment is needed for achieving the DO standard.

Contd.

- When WWT is tried in combination with FA of 57.5 and 21.6 m^3/s, the river water quality can be improved with primary and secondary treatment, respectively.

Case B

- Secondary treatment is required for all fourteen drains to meet the DO standard of 4 mg/l.
- Further, 40 m^3/s of flow is required to meet the water quality standard in terms of DO if flow augmentation is tried stand alone.

Case C

- Tertiary treatment is required to meet the DO standard. However, the BOD standard is satisfied only after advanced treatment.

- Results obtained for all the layouts reveal that Case A is the most practical in terms of water quality improvement. This is because Case B and Case C both require a minimum of tertiary treatment for water quality improvement (DO).

NEW TOOLS

NEW TOOLS

- Artificial neural network
- Genetic Algorithm – (and other EAs)
- Fuzzy Systems
- Geographical Information System
- Remote Sensing

Geographical Information System

- **GIS** is a system for capturing, storing, analyzing and managing data and associated attributes which are spatially referenced to the earth
- In a more generic sense, GIS is a tool that allows users to create interactive queries (user created searches), analyze the spatial information, edit data, maps, and present the results of all these operations

ARTIFICIAL INTELLIGENCE TOOLS

- A **genetic algorithm** (or **GA**) is a search technique used in computing to find true or approximate solutions to linear and non linear optimization.
- **Fuzzy systems**: Tool to quantify uncertainty because of Vague and imprecise concepts.
- **ANN** involves a network of simple processing elements (Neurons) which can exhibit complex global behavior, determined by the connections between the processing elements and element parameters.

DECISION SUPPORT SYSTEM

- In early 1960's MM was in embryonic stage.
- Models were more the playthings of their creators than useful tools for DM.
- Advent of PC brought revolution.
- Graphic Capability.
- Proliferation of computers and user oriented graphic interface have placed DSS at disposal of resource managers

CONCLUSIONS

- It has attempted to shed some myths, the beginners / students / researchers have, about modeling.
- It has offered some caveats, the present day engineers/decision makers become enamored with software /newly discovered tools without realizing their limitations.
- Lastly, it has emphasized the need for good quality/quantity data, technical expertise, research facility and academia-industry interaction, interdisciplinary approach, if mathematical models are to be accepted as tools for future to solve real life problems.

Bridging the Gap

Conceptual Gap between People and Planners as a result of their different perception of Community ideas

Who am I? –Engineer, Mathematician, Physicist, Chemist …

Ans. - None

Thank You Very Much