Available online at www.joac.info

ISSN: 2278-1862

Journal of Applicable Chemistry

2015, 4(2): 355-449

(International Peer Reviewed Journal)

Focused information Reviews (Foc.Inf.Rev., FIR)

OmniMetrics

Part II: Applications of neural networks (Ma_NN) in Environmetrics#

K. Ramakrishna[1], R. Sambasiva Rao[2*]

1. Department of Chemistry, Gitam Institute of Science, Gitam University, Visakhapatnam, 530 017, **INDIA**
2. School of Chemistry, Andhra University, Visakhapatnam 530 003, **INDIA**

Email: karipeddirk@gmail.com, rsr.chem@gmail.com

Accepted on 18thMarch2015

(Dedicated to Dr. Y Anjaneyulu, Professor& Director, Trent Lott Geospatial & Visualisation Research Center, Jackson State University, Jackson MS)

ABSTRACT

What the environment and system now are,in fact, a result of yotta_consequences of hexa-micro_processes and peta-macro_processes over, of course,finite (13.7 billion years) time in 5% of universe. The known chemical, biological and meteorological micro processes and their interaction are non-stationary and densely networked. Thus, even in twenty first century, the phenomenon poses a hurdle to model from first principles. Mathematical neural networks (Ma_NNs), data driven suite of algorithms are a subset of nature inspired approaches (Eman)which brought renaissance in computational environmental science during the last quarter century.

Particulate matter (PM10, PM5 and PM2.5), also concerned with health hazards, ishard to model in air. The complexity arises due to variability of meteorological factors and topographic influences. Different species of PM10 in Italy was modelled with Elman-NN. RBF and SLP were successful in forecasting PM2.5. The performance of mechanistic models for NO_x *is poor, while MLP was successful. Operational intricacies of surrounding industries affect* SO_2 *emission in addition to metrological scenario. NNs yielded better results compared to statistical approach.* NH_3, SO_2 *and aerosols are modelled successfully with SLP. Aerosols, containing different metal species and particles originating from road dust, industrial/biogenic emission, are classifiedforminor particles by ART-2a-NN. The maximum emission of* NH_3 *from manure storage is modelled with NNs and the number of inputs is less compared to Michaelis-Menten model. Here, mechanistic models are inadequate while MLR fails. Electronic nose, developed for pollen detection uses NNs. Compared to PCA, NNs achieved subtle distinction of major classes. Further, they enabled partial resolution of even classes.*

Part was presented at Int. Conf. on Frontiers in ChemicalResearch (2008Dec), Mangalore University, Mangalore.

The ground water quality with rain-water infiltration and extraction of knowledge from use of ground water/land was modelled withSOM-NN. NNs performed better than ARIMA in hydrology and management

of flood/watershed. A complex urban and rural water resource management with 1200 subsystems and 100,000 variables necessitated the use of NNs and fuzzy inferencesystem (FIS). The turbidity and color of treated drinking water was predicted with NNs. Transportable NN model was developed for annual water supply. The optimum amount of alum in drinking water treatment plants (DWTPs) in Australia is estimated with NNs. Employing NNs, Chlorcast models residual chlorine in drinking water tank and distribution system in Sanite-Foy with success in real time.

In effluent of waste water treatment plant (WWTP), MLP estimates the concentration of nitrogen as ammonia better than activated sludge model (ASM-1). Recurrent NN is used in modelling and control of combined sewer systems (CSS) in WWTP, Washington. The activation/deactivation of pumps in WWTP (which were earlier managed by human operators)are planned through NNs,. A plant in Taiwan uses a multi-objective control strategy involving NN, fuzzy logic and genetic algorithm (GA). Two single layer perceptron (SLP-) NNs in sequence are used in WWTP operation, one to control the plant and the other to monitor critical parameters. BOD and SS in treatment plant in different locations are studied as NN time series models.

The soil surface, a heterogeneous medium of chemicals, is the terrain platform for life of animals and humans. The composition and quality of soil is also at stake due to anthropogenic and non-anthropogenic reasons. The increase in concentrations of pollutants in sub- and deep- surface of soil is mainly due to drainage of domestic/ untreated industrial wastes. The distribution over wider surface is a consequence of streams, floods, riverine flows etc. The model independent paradigm, neural networks, is a versatile tools to predict the coming up scenario and has been used to implement control measures in keeping health of soil to derive quality foods, medicinal plants and edible weeds etc.

Keywords: Particular matter (PMx), Water sources, Potable water, Pollution, Waste_ water_treatment_plant, Environmetrics, Neural networks, Persistent organic pollutants, Pristine environ ment, Oil spills, rain fall, floods, ground water, soil, Environmental protection agency.

II. Environmetrics
Contents

I. Air (1-7)

1. Particulate Matter (PMx)
2. NO_x, SO_x, H2S etc
3. PCBs
4. Aerosols
5. Persistent organic pollutants (POPs)
6. Engineered nanomaterials
7. Personalized air monitoring move

II. Water (8- 11)

8. Water resources
    8. 1 Long term forecast
    8.2 Water resources and management:
        ⇨ Rainfall
        ⇨ Streams and storms
        ⇨ Rivers
        ⇨ Floods and droughts
        ⇨ Flood management
        ⇨ Ecological imbalance restoration
        ⇨ Ground water level

    8.3 Marine environment
        ↴ Rain over oceans
        ⮥ Ocean wave models
        ⇨ Sea surface wind speed
        ♦ Salinity Oceans
        Color of oceans
        Chlorophyll-a
        Cyclone forecast

9. Quality of water
    9.1 Drinking water through treatment
        – Residual aluminum
        – Residual Cl2 :
    9.2 Domestic Water consumption

10. Pollution of water bodies
    Discharge standards
        Ground water contamination
        Fecal pollution of water resources
        Marine pollution
            ⮥ Oil spill

11 Waste water (WW) Treatment

    WWTP
    Combined sewer systems (CSS)

INTRODUCTION

In 1970's US-EPA introduced pollution standard index (PSI), which is broadly employed as AQI (Air quality index), US-EPA-1999. The governmental agencies promoting environmental health in different countries are in chart A1-1[44]. Another committed focus of these elite bodies is not only to pass skills down the ladder up to maintenance stations, but to share experience, expertise and professionalism. These promote innovations in the cutting edge technologies, core science and achieve best global air-water-soil Eco balance in the coming millennium. The immediate fringe benefit is avoiding the ill-effects of pollutants on human health and on terrestrial/marine natural evolving resources. Eco system is a broad term and made up of many mega processes in natural phenomena and man-made activities. The nature and intensity of deposition of pollutant materials on a glass is a good indicator.

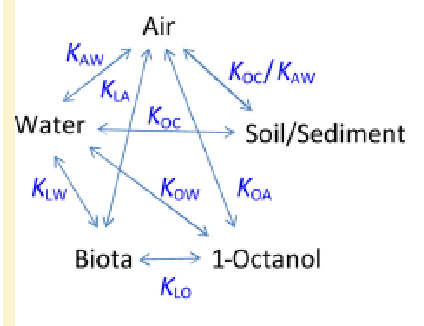
Environmental science is broad with prospecting technologies. It is a binary-, ternary-, quaternary-hybridization of several matured disciplines (Appendix 1). Metrics, on one side, is simply a measurement. At highest level, it is conglomeration of mathematics, statistics, nature-inspired algorithms at the core and software and hardware for implementation. Thus environmetrics is fusion of two paradigms viz. environmental science/technology and metrics. The mechanics is environmental processes are first translated into physical model followed by matching with standard mathematical tasks. Depending upon data structure and goal, the solution methods are selected (Appendix 2 and appendix 3). The solution and multi-dimensional graphic display is through high performance computational and visualization software. The hardware choice is dependent on required accuracy, speed, data size and most important is interpolating grids. The applications of NNs in air, water, soil pollution monitoring, abatement and futuristic planning schedules are reviewed [001-398]. Earlier, the chemistry/ polluting aspects of ozone and their impact on human health are detailed [297] and some typical applications of SOM_NN, Rec_NN, RBF_NN, MLP_NN and ART_NN in environmetrics were covered [296 and references 303 to 308 therein].

Pollution cycle in air, water and soil and their interfaces

Chart 1(a) Models-environment	
	AIR
CMAQ	Community Multiscale Air Quality Multiple pollutants at multiple scales
NWP	Numerical weather prediction
WRF	Weather Research and Forecasting
AERMOD	A steady-state plume air dispersion
EPA PMF Positive Matrix Factorization 3.0	Receptor model Constrained weighted least squares approach Ambient measurements and estimated uncertainties in those measurements to infer emission source
Unmix 6.0	Receptor model Uses ambient measurements to determine the number of source types and their impacts at a monitoring site
Fused Discrete Air Quality Surfaces	Space-time hierachical Bayesian model Daily O3 and PM2.5 predictive surfaces.
Models-Water	
WASP7 Water Quality Analysis Simulation Program	Conventional Pollutants (Nitrogen, Phosphorus, Dissolved Oxygen, BOD, Sediment Oxygen Demand, Algae, Periphyton), Organic Chemicals, Metals, Mercury, Pathogens, Temperature
EPD-RIV1	Hydraulic and water quality simulations .
QUAL2K	River and stream water quality model
AQUATOX	Predicts the fate of pollutants, rganic chemicals, effects on fish, invertebrates, aquatic plants.
Models-Waste water	
WATER9	Wastewater treatment model Analytical expressions for estimating air emissions of individual waste constituents in wastewater collection, storage, treatment, and disposal facilities

The experimental partition coefficients of volatile methylsiloxanes (VMS) are useful to predict distribution, transport and decay in environment [203].Volatilemethylsiloxanes (VMS, VOCs) found extensive industrial and personal care products. During WWTP, they are partitioned between air and sludge. A portion of sludge enters soil through application of biosolids[203]. The inter molecular forces between water molecules in interfaces (air-soil, metal surfaces, proteins, cells etc.) even at ambient conditions are significantly different (chart 1) from the bulk water and impart unique physico-chemical, mechanical, bio-physical characteristics as a result of varying structure and dynamics. These phenomena have shape many life processes, engineering products and scientific theories. The pursuit in the case of nanomaterial is at the stage of breaking the proverbial tip of the iceberg and is marching into vent able zoo of 2D- materials.

Chart 1b: Interfaces



Courtesy of Ref [203]

Partitioning coefficients	Abb.
Air/water	KAW
Octanol/water	KOW
lipid/water	KLW
Octanol/air	KOA
Soil organic carbon/ Water	KOC
Biological medium/fluid	KBioFl

I. Air (1-7)

The large thermal power plant, ferries, cruise ships and individual commuting are major sources of air pollution. The objective of air monitoring remains same viz. detecting/determining and forecasting contaminants/their degradation products in real time as accurately as (AAA) possible in spacio-temporal domain in small time intervals over small grid space. This oscillating goal has a point focus of possible clean air in as many terrine/marine pockets as possible. Fulfillment of all the objectives of NAAQS (National Ambient Air Quality Standards) compliance monitoring is a formidable reality. Yet, in near future many are achievable with evolution of sensor technology and information processing/ dissipation and inter-disciplinary tight object oriented collaboration. Although, in principle continuous pollutant monitoring is accepted and is in practice in major urban centers, calibration period and equipment failure are major factors for missing values.

The environmental conflicting issues are a complex interaction of local as well as global phenomena and their detection/resolution/remedial measures in a special dynamics are interwoven complicated interdependent micro-processes. Regression, NN models or ESs are fast but fail when the pattern changes overtime. Since NNs are data driven, generalization of model is valid only for the features embedded in the data. For example, the best predictive NN for 24-hour range, say at Santiago cannot be applied for 1-hour ahead prediction even at the same location. The others instance of failure is Cohen model, a successful predictive NN model is transferred to another location where different environmental conditions or pollution sources prevail [187].The data at multiple locations with different prediction objectives cannot be trained with a hierarchical architecture with meta rules rather than with a single huge [174] network for reliable end results in modeling and prediction.

The tools in operation on sight in environment monitoring required complex input and not only computational resources but expertise (EPA) – MODEL 5 (Bartzis, 1995). Montanari et al.[327] reported NNs in land use conflict in the harbour area (Civitavecchia) of the Rome. From a study of 27cases, it is inferred that environment-led policy is a safe approach to resolve the conflict. Kalapandidas reported a case based reasoning (CBR) system. It makes use of similar previous incidence to classify the expected levels of maximum concentration in prediction.There is a continuous addition of new cases and thus functions better in long term modeling at the same site and also imbibing the changing patterns at other places if there is provision.

The pollution index is generally expressed as integers, which are easily understood by the public. Jiang [44]used a NN model using the air pollution index and meteorological data. The values for PM_{10}, SO_2 and NOx are correlated to an extent of 0.60, 0.69 and 0.63 for the data between 17 September 2002 and 20 may 2003. Wang et al.[367] proposed a novel two stage data driven modeling strategy to compensate the uncertainties in emission and meteorological data (Alg. 1).

Alg. 1: Multilevel hybrid algorithm for compensation of uncertainties in emission and meteorological variables	
Phase I	Development of NN and SVM forecast models Data: Historical values of exogenous meteorological variables
Phase II	Residual information in previous step is calculated Forecasting model is expanded by taylor's infinite series The magnitude of forecast value is refined

NNs in meta modeling of air quality prediction: Deterministic air quality models find potential application in prediction of spacio-temporal regime by regulatory authorities for policy development locally. However, model errors perturb forecast and Wahid et al.[24] proposed meta-modelling approach with NNs (chart 2).

Chart 2: Prediction of spatial pollutant distribution with NN	
Dispersion model	
Spatially-distributed pollutant (ozone)	Fn(X) grid coordinates, topographical information, solar radiation pollutant's precursor emission)
Phase I	Air Pollution Model and Chemical Transport Model (TAPM–CTM) -- Photochemical dispersion model Input–output data correlation with ambient measurements RBF_NN
Phase II	Testing Ozone concentrations Sydney basin, Australia
Phase III	**Application** Real time ozone concentrations
	Inference RBF_NN >> TAPM–CTM model only

1. Particulate Matter (PMx)

Particulate matter, of different sizes, has adverse effects on human health causing lower respiratory problems in children and damage of upper respiratory track in aged individuals. An increase of (24 hours average) of 10 µg/m^3 of PM10 increases 1% mortality per day due to all causes. The ill effects of PM2.5 include hospitalization due to cardio respiratory disturbance and more alarmingly increase in mortality

[54]. In the current regulations, total quantity of PM is considered in warning pollution level. But, in depth studies reveal the need to correlate the ill effects on health with specific chemical elements, the concentration of each of the species in metabolism/excretion/accumulation and interaction [42]. The sources of particle for sampling are from incinerators, smelters, power plants, motor vehicles and soil. Back trajectory analysis has been in vogue. Thus, the analysis of air borne particles is equally important as gaseous pollutants. The chemical composition and size of PM are used to detect forest fire episodes. Owega [43][2004] reported the need for the refinement of the TEOM and TOFMS. LAMS (Laser Ablation Mass Spectrometer, Alg. 2b) is a real time/on-line instrument,which measures accurately aerodynamic diameter and chemical complex species of a single particle. This paves way to improve the identification (with certainty) of new episode occurrences. But, it requires accumulation of large number of mass spectra, especially during known incidences. The disadvantages are that a source emits different types of particles and many sources emit a common particle. The soft and data driven models for forecast of variation of PM are extensive.

PM10:A pre-emergency day is that when 24 hour moving average of PM10 exceeds WHO prescribed limit (of 240 $\mu g/m^3$) [49].The anthropogenic prime sources for this particle pollutant are combustion, industries and vehicular traffic. The consequence is dust from road (PM10) and black smoke of exhausts of diesel vehicle remains suspended for several hours in the air. The sources responsible for generation of PM10 are complex including meteorological factors, topographic influences of terrain, emission sources, particle characteristics like density, shape and hygroscopic characteristics. PM10 consists of several species of different concentrations. For instance, the particle size of suspended PM in aerosol is typical. The processes are also of diverse nature and the distribution in space and time is influenced by several factors viz. wind speed, surface temperature/pressure, humidity, dew point temperature etc. It is difficult to predict PM10 compared to NO_2 in urban areas [45], butimproves by including climatic (lagged PM_{10}, weather classification information, opacity, and discomfort index) and Non-climatic factors (traffic levels and indices of heavy/low traffic conditions). The fact is that variables with non-linear relation with response apparently exhibit low linear correlation [171]. Thus, inclusion of weather variables that are not linearly correlated sometimes drastically improves predictive capability.

Correlation between factors for PM10:There is a high cross correlation among topographical, traffic, meteorological and air quality variables. PCA gives linear combination of these factors, which are (independent) orthogonal with the advantage retaining maximum variance in the data. The advantage of this method is its reduction of substantial auto correlation that is present in the data. Cheng et al.[239]showed ensemble averaging method is better than MM5, WRF models in pollution events in China. The combination of ensemble with CMAQ for simulating PM10 excelled MM5–CMAQ and WRF–CMAQ (chart 3).Antanasijević et al. [369]reported two year ahead forecast (chart 4)of PM10 with NNs employing data form 26 EU countries during 1999-2006.Nyhan et al.[294] applied NNs to predict minute ventilation and masses deposited in the lung in urban commuting cyclists. The information in table 1 summarizes typical results.

Chart 3: performance of Ensemble_NN in PM10 and pollution episodes

Location	Meteorological models
⇨ Northern China	⇨ MM5
⇨ Time: 2006	⇨ WRF
	⇨ Ensemble_NN

Meteorological variable optimization
- ⇨ Temperature
- ⇨ Surface
- ⇨ Air pressure
- ⇨ Wind field

Performance Improvement
- ⇨ Ensemble_NN >> MM5 and the WRF
- ⇨ PM10 simulation
- ⇨ Ensemble_NN–CMAQ > 7.0% MM5–CMAQ
- ⇨ Ensemble_NN–CMAQ > 17.8% WRF–CMAQ

Chart 4: Forecast of PM10

Input	Data centers
⇨ Gross domestic product ⇨ Gross inland energy consumption ⇨ Incineration of wood	Convention on Long-range Transboundary Air Pollution

- Motorization rate
- Production of paper and paperboard
- Sawn wood production
- Production of refined copper, production of aluminum
- Production of pig iron
- production of crude steel
- preprocessing
- GA – model selection

(CLRTAP)

- EMEP Program
- Regional Air Pollution Information and Simulation (RAINS from Eurostat)
- **Location:** 26 EU countries
- **Years :** 1999 to 2006

Table 1a: Typical studies in PMx

PMx	Objective	Site	Methods	Ref
PM10	Classification 20 classes; 11,480 particles	University of California Riverside campus	ART2a	[47]
PM2.5	Day average	Elpaso (Texas) Cuydad Hyarez (Chihuahua US Mexio border	MLP RBF Persistence LS	[174]

Table 1b : Index of agreement for hourly script time series of PM10 at Toolo and Vallila [45]

Model	1996	1997	1998	1999	1996 to 1999
NNHoG	0.64	0.76	0.77	0.73	0.73
NNHeG	0.73	0.80	0.79	0.76	0.77
LIN raw	0.60	0.71	0.37	0.75	0.61
Vanilla					
NNHeG	0.70	0.71	0.75	0.77	0.73
LIN	0.64	0.66	0.47	0.75	

Alg. 2: Hybrid intelligent (Time-delay Added Evolutionary Forecasting) system for one-day-ahead forecast of PM2.5 and PM10

Phase I	GA refines Number of input nodes (time lags) Number of neurons in hidden layer Training algorithm & parameters
Phase II	Forecast for next day Objfn: min (difference between forecasting and experimental concentrations of past time series)
	Predict next day concentration Does not require exogenous information
Data	Time series at Helsinki

Table 1c: Minute ventilation levels PM10 lung deposited doses

Sixty healthy volunteers	Risk factors monitored Minute ventilation Heart rate Personal air pollution exposure Local meteorological conditions GPS acquired cycling speed Road topography Obj: predicting minute ventilation Model : NN

Table 1d: Correlation between predicted vs measured minute ventilation levels

	R^2
ANN	0.82
GAM	0.74
PLS	0.56
Empirical	0.36 to 0.43

Alg. 2b: Laser ablation mass spectroscopy (LAMS) [43]

Step	:	1	Aerosol particles are pre concentrated by a factor of ten (Virtual impact or and **cyclone).**
Step	:	2	The purpose of inlet of LAMS is to remove the gas surrounding the particles and also, to generate a single particle beam.

Step	:	3	Single particles of interest to He-Ne light whose paths *are separated by a known distance.*
Step	:	4	The scattered light from the particle is recorded with two photo-multipliers tubes. The time between these electronic pulses was converted into an aero dynamic equivalent diameter. This time is also crucial to determine when to fire a big sky-Nd-YAG laser (266 nm).
Step	:	5	It ablates the particle in the ion source chamber of a TOFMS
Step	:	6	When a particle is ablated, the ions are accelerated with electric fields into a field free drift tube.
Step	:	7	The ions enter a reflection, travel back through the field free drift tube and strike a micro channel plate detector. The signal from MCP is recorded by oscilloscope **(500 MHz).**

PM5:Particles with lower diameter than PM10 are smart enough to penetrate into the respiratory track of humans.

Particulate matter (PM2.5 and PM10): De Mattos Neto et al. [138] report that it is the start of intelligent prediction model (Alg.1) taking into consideration of pseudo-random walk behavior of this time series. These authorsproposed a hybrid system comprising of MLP_NN and GA (Alg. 2) for one-day ahead forecast of particulate matter (PM2.5 and PM10).

PM 2.5:The sources of PM 2.5 in urban areas are emissions from vehicle exhaust and re-suspended surface dust. The major components are carbon, $(NH_4)_2SO_4$, nitrate etc. [54,312] Prediction of PM 2.5 is a non-linear (NL) problem The short term forecasting of PM 2.5 by MLP_NN and RBF_NN [174] is better than MLP (table 2), although data set has high degree of noise. The incorporation of related meteorological variables and noise reduction improves the performance of NNs and leads to accurate prediction. However, different schemes to consider past values of time series needs investigation. In 1997, SCOS97-NARSTO (Southern California Ozone Study-North American Research Strategy for Troposphere Ozone) field campaign [47] was performed wherein intensive atmospheric measurements were made during both summer and fall. South California Air quality study (SCAQS) could do only a field study in the last decade. It concentrated on bulk analysis techniques. The abundant species of PM2.5 contain nitrate, sulphite, ammonium, organic carbon and elemental carbon [Chow 1994]. The limitation of this study was combinations of chemical species were not identified. Pastor et al. [47] focused real time single particle mass spectrometry with ATOFMAS using ART-2a.

Table 2a: PM2.5 modeling [174]

Year	PM2.5	SD	Max
2000	8.27	4.71	26.74
2001	8.87	3.54	87.44
2002	9.91	7.42	69.21

Table 2b: Input variables used in the forecast of PM2.5 [174]

Av.value	units	
PM2.5	$\mu g / m^3$	
Max(PM2.5	$\mu g / m^3$	
Temperature	^{o}F	
Humidity	%	
Wind speed	m/s	
Wind bearing		Wind direction index
Av.value :Average value during first 8hrs of the day		

Table 2c: Best model for forecast of PM2.5

Method	RMSE	R2	I#H#O#	
SLP	$1.58x10^3$		7-18-1	
RBF	1.28 $x10^3$	0.3712	7-20-1	Variance
RBF	1.32 $x10^3$	0.4611	7-21-1	0.25
RBF	1.23 $x10^3$	0.4554	7-20-1	0.50
RBF	1.23 $x10^3$	0.4451	7-16-1	0.75
RBF	1.30 $x10^3$	0.4380	7-10-1	1.5
RBF	1.27 $x10^3$	0.4143	7-10-1	3.5
Linear regression	0.27	0.3983		
Persistence	0.41	0.0806		

NN + Knowledge recovery system: Chan and Jian [324] appliedNN for mass concentration of PM2.5 and PM1.0 on a heavy traffic area in Hangzhou city. A knowledge recovery unit is used for post processing optimum NN architecture, Ws etc. Standard NNs estimate pollutant concentrations, but the numerical enigmas do not provide explicit knowledge of pollution levels in terms of factors. This hybrid system identifies significant factors with transparency circumventing the limitation of black box approach of NNs.

Method	Function
NN	Estimates air pollution levels from pollution factors
Knowledge discovery	Extracts explicit knowledge from optimized NN

Fine and coarse particles: He et al.[73] predicted of fine and coarse particles at street level in summer and winter with hybridized NNs with Chaotic_PSO and LM. The model is applied to forecast the trends of air pollution in similar meso-to mega-cities.

Fine PM and CO at road intersection: The running engines of idle vehicles during red light signals at cross roads and fast speed up when green lights are on result in drastic fluctuations as well higher emission rates of exhaust [30]. Added to it, in areas of frequent change of wind speeds and directions, the dispersion of pollutants is chaotic with a consequence of inadequacy of routine deterministic cause-effect models.

2. NO_x, SO_x, H2Setc.

In the management of local air quality, models are vital in addition to routine monitoring schedules. Before the year 2001, the predictive process of photochemical pollutants (NO_2, O_3 etc.) was based on only human expertise in Athens (Greece) as was the practice in most other cities. A fast short-term (day-to-day) prediction is the basic need. When an air pollution episode is predicted, a complex prediction method in real time (outputting the results within few hours) has to follow for the same location that may be operated in a sophisticated central place. The urban air pollution in many metropolitan cities like Los Angeles, Mexico and Athens is high. The forecasting of SO_2, NO, NO_2 (NO_x) and ozone were done with NNs [85].

NO_x:The source of NOx pollution is primarily from vehicle (cars, buses, trucks, off high way mobiles) exhausts in the form of NO. In fact, NO_2 is mainly produced from the interaction of NO with O_3[58]. Thus, the net concentration of NO_2 not only depends upon the traffic, meteorological conditions, but also on O_3 profile. The details of mechanistic models for NOx and poor performance of statistical models are reviewed. The unequivocal option is NNs, since the trend is highly non-linear and complex. Gardner [58] proposed acceptable predictive models for urban environment pollution with MLP-NNs. The model for NOx can still be improved provided the inaccuracy in the forecast of the meteorological data is diminished. Further, it is better to train meteorological data on a grid rather than at isolated points. The variables used in the best model (NN) are in table 3. Here, it is found that MLP is equivalent to MLR. The peaks in NO2 are much higher than predicted on 12, 13, 14, 8, 16, 17th and 28th of Dec 1991. NOx emission is of utmost concern in vehicle movements, and they can be reduced (table 3k).

Table 3a : Comparison of NN with MLR [58]

	NN	MLR
Err	0.91	0.90
RMSE	7.3	7.4

Table 3b: comparison of NN and linear regression with same input variables[58]

Model number	RMSE		r^2 (NN)
	MLP	LR	
1	18.2	19.3	0.47
2	78.6	97.0	0.54
3	17.9	18.7	0.4
4	77.5	95.7	0.55
5	**7.3**	**7.40**	**0.91**
6	33.8	34.3	0.92
7	17.1	17.7	0.5
8	80.2	89.5	0.62

Table 3c: Performance of NNs in comparison with LR for NO2 in Bilbao (Spain) [170]

Location	Forecast	*NO2*			
		MLP1	MLP2	LR	Persistence
Elorrieta	t+1	0.0008	0.0003	0.06	0.06
	t+4	0.08	0.125	0.34	0.43
Mazarredo	t+1	0.0005	0.0005	0.07	0.06
	t+4	0.0005	0.005	0.15	0.25
Txurdinaga	t+1	0.0001	0.0002	0.05	0.06
	t+4	0.002	0.007	0.573	0.30
Deusto	t+1	0.0002	0.0002	0.06	0.07
	t+4	0.0004	0.0005	0.17	0.26

Table 3d: Different categories of variables for O3 and NO2 in Bilbao (Spain)[170]

Meteorological	Units	Abbreviation
Wind speed	m/s	Vx
Wind direction	N_	Vy
Temperature	_C	TEM
Relative humidity	%	HUM
Pressure	kPa	PRE
Radiation	cal cm_2 h_1	RAD
Thermal gradient	_C	GRAD
Air pollution		
Ozone	mg/m3	O3
Nitrogen dioxide	mg/m3	NO2
Traffic		
Number of vehicles		NV
Occupation percentage	%	OP
Velocity	km h_1 100_1	KH

Table 3e: Predictive models of NOx with different inputs[58]

MLPx	O#	I#								
NO2	sin(h)	cos(h)	LOW	BASE	VIS	DRY	NO2	VP	WS	
NOx	sin(h)	cos(h)	LOW	BASE	VIS	DRY	NO*x*	VP	WS	s
NO2	---	---	LOW	BASE	VIS	DRY	NO2	VP	WS	Q
NOx	---	----	LOW	BASE	VIS	DRY	NO*x*	VP	WS	Q
NO2	sin(h)	cos(h)	LOW	BASE	VIS	DRY	NO2(t)	VP	WS	NO2(t1)
NOx	sin(h)	cos(h)	LOW	BASE	VIS	DRY	NO*x*(t)	VP	WS	NO*x*(t1)
NO2	sin(h)	cos(h)	LOW	BASE	VIS	DRY	NO2(t)	VP	WS	NO2(*t*24)
NOx	sin(h)	cos(h)	LOW	BASE	VIS	DRY	NO*x*(*t*)	VP	WS	NO*x*(*t*24)

Table 3f: NO2 pollution levels in Athens (Air quality operation center) [187]

		mg/m^3
Level 1	low	0–200
Level 2	medium	200–350
Level 3	high	350–500
Level 4	alarm	Over 500

Table 3g: Prediction accuracies at differen t levels by NEMO [187]

	1	2	3	4	Unable	% prediction accuracy	Number of Cases
Level 1	134	5				96.4	139
Level 2	38	22	2	3		33.8	64
Level 3		12	9	8		33.34	29
Level 4				4	4	50	8
							240

Table 3h: Input variables for prediction accuracies of NO2 pollution at different levels by NEMO[187]

1	Date	
2	Code of measurement station	
3 to 5	NO hourly concentration at 8 a.m. (measurement at 8, 9, 10 a.m)	
6	NO maximum hourly concentration after 10 a.m.	
7	Hour that the NO maximum hourly concentration occurred	
8 to 10	NO2 hourly concentration at 8 a.m. (measurement at 8, 9, 10 a.m)	
11	NO2 maximum hourly concentration after 10 a.m.	
12	Hour that the NO2 maximum hourly concentration occurred	
13	The wind before 10 a.m.	Factor deduced from
14	NMS wind forecast after 10 a.m.	forecast
15	The wind after 10 a.m.	measurement
16	Precipitation level from the observatory	measurement
17	NMS rain forecast	forecast
18	Temperature inversion	measurement
19	Solar radiation at 10 a.m.	measurement
20	NMS forecast of solar radiation after 10 a.m.	forecast
21	Solar radiation at 1 p.m.	
22	Maximum temperature of the day in degrees Celsius	
23 to 27	NMS forecast for next day's winds, precipitation, inversion, solar radiation, maximum temperature	

Table 3i Inputs to NN model of NO2 at the University of East Anglia[45]

Temporal variables (t+24)
- Weekday
- Sine of year day
- Cosine of year day
- Hour

Concentration variables (t)	
Variable	**Units**
✓ NOx	mg/m3
✓ NO2	mg/m3
✓ O3	mg/m3

Meteorological variables (t+24)

Variable	Units	Variable	Units
Pressure	kPa	Sine of direction of flow	
Temperature	K	Cosine of direction of flow	
Humidity	%	Windspeed	m/s
State of ground		Sunshine	h
Cloudiness	0–8	Albedo	
Dewpoint	K	Solar elevation	rad
Wetbulb	K	Solar radiation	W/m2
Rain	mm	Moisture parameters	
Visibility		Monin–Obukhov length	m
Weather		Temperature scale	K
Weather of previous hour		Friction velocity	m/s
Weather of previous 3 h		Turb. heat flux	W
Amount of clouds		Net radiation	W/m2
Type of clouds		Latent heat flux	W
Height of low clouds	m	Mixing height	m
Type of middle clouds		Convective velocity scale	m/s
Type of high clouds		Gradient of the potential temperature	K/m

Table 3j: Index of agreement for hourly time series of NO2 at Toolo and Vallila [45]

Model	1996	1997	1998	1999	1996-1999
NNHoG	0.85	0.86	0.87	0.89	0.87
NNHeG	0.89	0.90	0.90	0.91	0.90
NN2HeG	0.89	0.91	0.91	0.91	0.91
NN3HeG	0.89	0.91	0.92	0.92	0.91
LIN raw	0.78	0.83	0.84	0.81	0.82
DET raw			0.77	0.75	0.76
NNHeG	0.87	0.86	0.88	0.87	0.87
LIN raw	0.83	0.80	0.81	0.04	0.80
DET raw			0.70	0.68	0.69

Ho	Homosedastic	He	Heterosedastic
G	Gaussian	2 or 3	Two or three component mixtures of hetero sedastic noise

Table 3k: Reduction of NO_x emission

- Exhaust gas recirculation alternate fuels
- Turbo charging,
- Different mode of combustion.

SO_x:The level of SO_2[51] has been continuously decreasing in most of the western industrialized countries, while there is a noticeable increase in the developing nations and Eastern Europe[52]. Local pollution levels of SO2 are however, a consequence of typical variation of meteorological/topographical conditions and operational details of surrounding industries. The sources of this [51] classic air pollutant are combustion of fossil fuels, power generation industry, traffic and heating. The ill effects of SO2 include chronic bronchitis and low birth rates. The maximum SO2 at noon is due to indiscernible cumulative effect of all sources and meteorological conditions. Perez [51] opines that the pollutant concentration of the previous day(s) is crucial for SO_2, NO and NO_2. Hence, it cannot be pinpointed to a single source to take up preventive measure during working days. Thus, modeling SO2 is multifaceted and there appears to be no single simple modelling approach [182] for prediction of trend of SO2 at a specific location. Several statistical methods have been tried, but neuro-fuzzy-NN, Wavelet analyzers are found to be promising techniques (table 4).

Table 4a: Ranking of models based on classical statistics and advanced performance measures[182]

	RMSE	MAE	r		FA%	SI%	Auc		SP%	SR%		Bias	d
High	WAG	ANN	ANN		ANN	ANN	ANN		ANN	ANN		MNN	ANN
	MNN	WAG	WAG		MNN	WAG	WAG		WAG	MNN		PER	WAG
	-	GAM	GAM		NFU	GAM	GAM		GAM	NFU		LPH	MNN
	-	LPH	MNN		-	MNN	MNN		MNN	-		-	GAM

	-	MNN	NFU		-	NFU	LIN		NFU	-		-	-
	-	PER	-		-	-	-		-	-		-	-
Medium	NFU	-	-		WAG	-	PER		-	WAG		ANN	ANN
	GAM	-	-		GAM	-			-	GAM		WAG	-

Table 4b: Validity of NN models for different time intervals [85]

SO2 (RMSE)		Period (years)				TSP(RMSE)	
Tr	Te	Tr		Te		Tr	Te
		From	To	From	To		
18	18	1996	1997	1997	1998	20	19
19	19	1996	1998	1998	1999	21	20
20	19	1996	1999	1999	2000	21	19
19	17	1996	2000	2000	2001	20	18
Samples of SO2	Tr : 601	Te : 151					

Table 4c: Prediction performance of NN models for different time intervals[85]

SO2 NP : 151				Period (years)		TSP NP : 151			
RMSE (ug/m3	IA	Success	FP	From	To	RMSE (ug/m^3)	IA	Success	FP
38	0.47	113	38	1997	1998	52	0.69	105	46
26	0.53	125	26	1998	1999	53	0.58	103	48
21	0.71	132	19	1999	2000	39	0.53	112	39
19	0.82	136	15	2000	2001	30	0.78	121	30

Table 4d: Comparison of NNs with persistence model in prediction of SO2[51]

#hour ahead prediction	SLP	Lin NN	Persistence
4	0.34	0.39	0.65
12	0.41	0.42	0.57
16	0.89	0.88	1.69
24	0.45	0.45	0.57

Table 4e: Comparision of NN with nonlinear regression for SO2 in different locations[186]

Location	Model	RMS		corr	
		Tr	Pred	Tr	Pred
Industrial	NN	0.10	0.59	0.89	0.68
	NLR	0.40	0.62	0.64	0.57
Commercial	NN	0.10	0.53	0.80	0.72
	NLR	0.25	0.47	0.59	0.52
Residential	NN	0.10	0.46	0.95	0.63
	NLR	0.34	0.35	0.61	0.48

$$Y_{t+1} = a_1 * Y_t + a_2 * (W_t + k * a_3)^{-a_4} + a_5 * (T_{t+1} + a_6)^{-a7} + a_8 * (R_{t+1} + a_9)^{-a10} + e_t$$

Y :	Log of SO2		
W:	Wind speed	R :	Relative humidity
T:	Temperature	E:	White noise

z_t :	z at t[th] time instant	z_{t+1}:	z at t+1[th] time instant
a	Regression coefficients		

Adaptive neuro-fuzzy system (Table 4) is used to estimate and predict the air pollution levels in Zonguldak on daily basis. The impact of meteorological factors on the levels of SO2, TSP is studied. The performance is greater than 70%.

Table 4f: Variation of RMSE for SO_2 with input in ANFIS [85]

Input set	Training error (RMSE)	Average test error (RMSE)	AP	Atmospheric pressure
AP, RH, WS, SR, P, T, SO2,j_1 or TSPj_1	18	18	RH	Relative humidity
WS, RH, T, (SO2j_1 or (TSPj_1	19	21	WS	Wind speed
AP, RH, WS, SR, P, T	25	32	SR	Solar radiation
AP, RH, WS, SR, P	30	38	P	Precipitation
			T	Temperature
			(SO2j1 (TSPj1	Previous day's SO2 concentration
			(TSPj1	Previous day's s TSP concentration

Table 4g: Forecast of Pollutants with Elman NN in Italy [37]

Station	Units	RMSE							
		Belgio	Boccadifalco	Castelnuovo	Di Blasi	Giulio Cesare	Indipendenza	Torrelunga	Unita` d'Italia
SO2	$\mu g\, m^{-3}$	3.13	0.58	3.5	4.14	2.61	2.4	2.31	3.12
CO	$mg\, m^{-3}$	0.65	0.13	0.29	0.39	0.36	0.29	0.29	0.50
NO2	$\mu g\, m^{-3}$	32.09	7.02	5.23	6.37	4.89	4.5	5.23	8.46
O3	$\mu g\, m^{-3}$	---	---	4.99	4.44	----	---	---	
PM10	$\mu g\, m^{-3}$	6.47	--	6.43	5.33	7.44	4.53	----	

Volcanic air pollution

The continual eruption of Mount Kilauea/ Hawaiian Islandsoutbursts SO_2 and sulphates.Their interaction with oxygen and water vapor forms Vog, a source of air pollution in this area.Perez [33] found NN and frequency model capture central tendency, but poor in predicting extreme events(chart 5).

Chart 5: Vog models in Hawaii

	Models
Location: west, south and southeast coasts of Hawaii	ॐ Regression ॐ NN ॐ Frequency

SO2	Freq >NN
SO_4^{--}	NN >Freq

+ Models capture general tendency
- Poor to predict extreme events
- Irregular outliers

H2S:The biogas is produced from anaerobic digestion of municipal sewage sludge, organic wastes from industries, households and farms. The major application of biogas is in heat and power generators apart from the routine use as a cooking fuel. The presence of H_2S, NH_3 and X_2 (halogens) in the biogas and non-methane organic compounds reduce the lifetime of fuel cells to a greater extent[175](table 5). Further, the information on the toxicity is inadequate. Thus, the detection, reduction and complete avoiding of the trace quantities are essential in producing biogas of requisite quality and here, NNs played a role.

The mechanistic models for the emission of NH_3 from manure storage using volume and surface area as inputs are proposed. However, extension of the model to the field study is much more complex and the results are not astounding. A model including the inputs from atmospheric transfer and soil processes,did not succeed. It is reconciled due to unaccounted variation of manure patches, droplets and pH, which are not easily predictable in the process. Thus, mechanistic models are not adaptable for emission of NH_3 in the field studies in real time. The emission of NH_3 from manure was modeled with MLR and it was observed that the regression is time dependent. To circumvent the limitation, MLR model for different time periods (0 to 6, 7 to 12, 13 to 24 hrs and 1 to 6 days) was proposed consisting of linear profiles.The emission of $NH_3$is fitted with two parameters. The accumulated ammonia emission value for 227 data sets is fitted with Michaelis-Menten equation with a overall R^2 value of 0.94. However, Emax and kn = a/b depend upon experimental conditions. This restricts the use of linear and non-linear regressions. Thus, data driven models are preferable and NN is a prospecting tool.

Table 5: NN modeling of H_2S

(a) Input for predicting H2S t+1 [175]

- Sulfate loading rate
- H2S in biogas ppm NH3 in biogas ppm
- Total sulfides in reactor
- Biogas-productivity
- pH
- Organic loading rate

(b) : Architecture of NN for the prediction of H2S[175]

Architecture	I#-5-1	I#-7-1
Transfer functions	Tansig	Purelin
Number of training data	100	131
Number of validated data	35	27
O#	Hydrogen sulfide in biogas [ppm] t+1	
O#	Ammonia in biogas [ppm] t+1	

(c): Training strategy of NN for the prediction of H2S[175]

Train function	Traing dm
Learning rate	0.001
Train epochs	5000
Performance goal	0.02
Minimum performance gradient	$1*10^{-8}$
Momentum constant	0.9
Maximum performance inc	1.04
Alg. batch gradient descent with momentum algorithm	

NH_3: NN requires less number of input variables compared to Michaelis-Menten model to calculate K_m and $E_{max.}$ The quality can definitely be improved with more data points and advances in NN(table 6). The amount of nitrogen available in the long term and NH_3 emitted during manure application on the fields was modeled by NNs, which predicts a part of effect of NH_3 on environment[52].

Table 6(a): Input for predicting NH3 t+1[175]

	Units
Nitrogen loading rate	G N m^{-3} d^{-1}
Ammonia in reactor	mg N-NH3 l^{-1}
Ammonium in reactor	mg N-NH4
Total inorganic nitrogen in reactor	mg N-NH4
Biogas-productivity	m^3 Biogas m^{-3} d^{-1}
pH	
Organic loading rate	kg CODm^{-3} d^{-1}

Table 6(b) Input (X) in NH3 models [52]

Dry matter (% total matter)	Minimum temperature (°C) 1st day & 2nd day
pH-value	Maximum temperature (°C) 1st day & 2nd day
Ammonium concentration (kg Nm^{-3})	Precipitation (mm) 1st day & 2nd day
Ammonium applied (g Nm^{-2})	Wind speed (m s^{-1}) 1st day & 2nd day
Vegetation type 1=bare soil 2=grass 3=shoots land 4=residue	Irradiation, daily sum (Whm^{-2}) 1st day & 2nd day

Table 6(c) : Input to NN model of NH3 emission[52]

Minimum temperature	°C	pH-value	
Maximum temperature	°C	Ammonium concentration	kg N m^{-3}
Irradiation, daily sum	Whm^{-2}	Ammonium applied	g N m^{-2}
Windspeed	m s^{-1}	Dry matter	% total matter
Vegetation type	1=bare soil 2=grassland 3=shoots 4=residue	Precipitation	mm

Ćirović et al.[214] used NNs for routing light delivery vehicleswith data driven NN approach (chart 6d).

Chart 6d: Route design of environmentally friendly and un-friendly vehicles with NNs

Phase I	NN model for route calculation for EFV and EUFV
	Performance test
Phase II	Modified Clark–Wright algorithm
Testing model	Centre of Belgrade
Model input	Monitoring data at 40 automatic measuring stations for the air quality (SEA, 2012)

Chart 7: Tropospheric ozone models for Tabriz

Input	Models
Temperature, Solar radiation Dew point temperature wind speed	MLR NNs Gene expression programming AR type chaos theory ARIMA
Data August 2010 to March 2011 Hourly data	
Inference MLR,NN, GEP < AR	

Input	Model
Logistics operating costs Environmental parameters (exhaust emissions and noise)	NN Trn : SAA Environment noise Logistics operating costs

Chart 8: PCB-11 in consumer goods

PCB-11 levels	Materials
0.27 to 86 ppb Location: 26 countries five continents	Magazines Advertisements Maps Postcards Brochures Napkins Garments

Ozone:The models viz.LDF (linear discriminant function), QDF (quadratic discriminant function), MLR, MLR-BP_NN, RBF_NN are compared to forecast possible shifts in the prediction of ozone in Houston from a 12 year (1990 to 2002) period from daily air quality data collected by Texas commission on environmental quality. This is an extensive comparative study while the earlier studies used ARIMA.Khatibi et al. [284]reported Tropospheric ozone(chart 7) models for Tabriz with auto regressive, regressive and NN type models.

Some of the recent applications of NNs include pollution studies in Annaba, Algeria [63], volcanic smog (vog) in Hawaiian islands [35], prediction of tropospheric ozone concentrations in Dilovasi, Turkey [124], particulate matter from satellite and ground based observations [370], forecasting PM10[33, 369] in Thessaloniki and Helsinki [372,139], metropolitan areas [198], PM2.5 [324], evolution of haze, SO2, NO2 [32], classification of SO2 pollutant concentrations in Salamanca, Mexico [32, 28], fungal spores [306] and detection of atmospheric perturbation[140], The determination of diffusion coefficients of pure compounds in air [76], dew points of acidic combustion gases (SO3, SO2, NO2,HCl and HBr)[133], regional air quality modeling [239] and cooperative 3D-air quality [341] are also benefited by data driven neural network models.

3. PCBs

PCB-11: The non-Aroclor congener (3,3′-dichlorobiphenyl) of DCP had been a byproduct inadvertently generated since early 1970s in the manufacture of organic pigments. The scale was in ppb (parts-per-billion) in different printed materials, but recently found even in air, water, sediment and biota. Lohani et al.[255] found that the sources of high levels of PCB 11 measured in environment are plausibly due to pigments (chart 8). Toxic Substances Control Act (TSCA) stipulates a maximum average of 125 ppm and at this rate the maximum allowed is of the order 42 kg y^{-1}. But, the amount of outflows and sequestration of PCB 11 in Delaware River Basin is in the range of 30 and 280 kg y^{-1} sounding an alarming scenario.

PCB Effects on health: The PCB exposure at prenatal stage was as a consequence of mother eating Lake Michigan sports fish contaminated with this toxic pollutant. Around 234 children were born with low birth weight. If PCB were transmitted further with breast feeding, it has a pronounced effect on cognitive functioning.

Breast milk toxicity:Kowalski et al.[378] studied toxicity of breast milk with PCB for new born in Brazil using Kohonen NNs (chart 9). The typical factors found are industries, proximity to a polluted river, type of milk (colostrum, foremilk and hindmilk) and also number of past pregnancies.

4. Aerosols

Exposure to ambient aerosols is unavoidable and the best is to reduce the exposure time. It requires not only accurate measurement techniques, but also robust predictive models for aerosols and its constituents. Motor vehicle exhaust, road dust, industrial/biogenic emission [12] and other species are the prime sources of the dangerous pollutant particles in the aerosols. Metals in aerosols are of varying sizes and exist as different species. Thus, metal markers are good indicators to identify the major sources of primary urban aerosol particles [42]. The specific relationship between ambient aerosol and adverse health effects are not fully well understood/established, although, the effects of chemical elements have been hypothesized. Bulk compositions are essential to design pollution control strategies and study relationships between ambient aerosols and human diseases. Aerosol time of flight MS (ATOF-MS) instrument was developed in 1994 which measures size and composition of individual aerosol particles in real time. Only 12 samples were used in multivariate calibration (MVC) model to predict bulk chemical composition. The advantage was not clear because of small size of the data. The disadvantage of this method is that it doesn't give quantitative estimation of species, although it outputs total concentration. The morbidity data is correlated with the size and distribution of particles in the atmosphere. The increase in number of vehicles, depletion of petroleum resource leads to diesel engines as an alternative. The ways and means of reducing emission rates will continue until exhaust reduces to zero level.

ART-2a is used to classify the minor components of the aerosol particles. The data is from **RSMS III**, a laser ablation time-of-flight-MS, which simultaneously detects positive/negative ions. NNs take care of non-linearity introduced by measurement errors (response, concentration), experimental equations and assumptions on the accuracy of calculation model. Zhao and Hopke [12] used ART-NNs and PLSR to estimate bulk aerosol composition from ATOFMS data. The predictions for 1996 were reasonably good based on 1995 data set. This three layer NN model [51] can be made operational for Santiago. After training the data set for other stations, the model will result as an efficient SO_2 predictive tool.

Aerosols_microbial: Dueker et al.[210] found Actinobacteria and Proteobacteria in bacterial aerosols at Newtown Creek (NTC). It is reported as the first study of community composition and local deposition of bacterial aerosols in public waterway (chart 10) and Superfund site with a high dense population located in New York.

Chart 9: Toxicity of breast milk due to PCBs

Location	
Brazil South Southeast Northeast North	Twelve PCB Analysis: SPME-GC-ECD Model Kohonen_NN

Chart 10(a): Monitoring parameters

- Sewage
- Hydrocarbons
- Heavy metals
- Industrial waste

Bacteria

- Aerosol
- Distributions
- Concentrations
- Size
- Fallout rates
- Community composition

- Gravitational settling
- Surface interceptioninhalation

Chart 10(b) Superfund site (NTC)

Input

- High volumes of untreated sewage input via a combined sewer system
- Exposed to
  - Over 140 years of industrial waste dumping
  - Ongoing oil seepage
    - Largest underground oil spills
      - Greenpoint Oil Spill, approximately 1.7×10^6 gallons of underground oil)

Bacteria in sewage → water → air → humans through inhalation

It is reported that bacteria (pathogens) are viable for aerosolization from terrestrial and aquatic surfaces. The aerosols travel even thousands of kilometers spatially before coming back to ground. The sources of the bacteria (pathogens) are generally disposal of untreated sewage into local waterbodies, rivers, estuarine and coastal systems. The fresh water sewage with human pathogens remains in a dense stratified surface area. The bubbles release them in to air forming aerosols. Onshore winds transport the material along with water and deposits on the terrain surface. In the near-shore inhabitation places, coarse aerosols contain even more hazardous larger particles (PMx).

The prediction of emission levels inLPG-Diesel Dual Fuel Engine [135,340] with ANFIS and emissions of a biodiesel fuel [29] of NN are successful.

5. Persistent organic pollutants (POPs)

They are semi-volatitle compounds with moderate vapor pressure. POPs discharged in the lower latitude tropical/subtropical countries (Australia, Botswana, China, Hong Kong, India, Japan, South Korea, etc.) even locally, reach polar and pristine (remained in a pure state or clean from dirt or decay by human activity) environmental regions through long-range atmospheric transport (LRAT or global fractionation and condensation) and persist long. Thus, xenobiotic persistent organic pollutants are ubiquitous in the environment. Hence, a less error prone data and robust knowledge is the need of the hour to estimate toxicological adversities upon generations of biota as well as human race. It is interesting to compute the time for POPs to fall below threshold limits, if the emissions are cut off in totality [206]. As a partial answer, long term (exceeding a decade) continuous monitoring programs are in operation. The different types of trends are in chart 11c.Advanced technologies in water wastewater treatment minimize the release of environmental POPs.Choi et al. [213]simulated concentrations of range of compounds in different in warm temperate environment using a regional contaminant fate model, CoZMo-POP and a generic bell-shaped emission profile. The ranges of partition and degradation characteristics are same as those for POPs (chart 11).

Chart 11(a): Effect of POPs on regional and global pollution

Sampling ⇨ Passive air samplers XAD resin ⇨ Location Karachi, coastal city Lahore, agricultural region	<table><tr><td>Pollutant</td><td>ng/PAS</td></tr><tr><td>Heptachlor</td><td>10−26</td></tr><tr><td>HCHs</td><td>33−65</td></tr><tr><td>DDTs</td><td>63−92,</td></tr><tr><td>Endosulfan</td><td>39−101</td></tr><tr><td>PCBs</td><td>48−61.</td></tr></table>
− High Lindane, Endosulfan Ongoing use in agricultural fields − DDTs Older dumps Secondary sources	− Agricultural/industrial waste through river − Streams in to Arabian Sea − Weathered POPs → regional/global maritime pollution

Chart 11(b):Hazardousenvironmentalhormones

- Organochlorine pesticides (OCPs)
- Polychlorinated biphenyls (PCBs)

Agricultureal yield enhancers

Herbicides, fungicides, Plasticizers, polystyrenes,

Chart 11(c) :Trends in concentration with emission and reversibility

Trend	Reversibility
Concentrations rise and drop in concert with emissions	Fast
Concentrations rise and drop with emissions Maximum in concentrations considerably delayed relative to maximum in emissions	Slow
Concentrations rise But do not drop in response to emission reductions	No
Concentrations rise and initially drop in response to emission reductions But stabilize at a constant level or decline at much slower rates	Partial

Chart 11(d):Models for uptake of chemicals by plant from polluted soils

- Root uptake,
- Shoot uptake

	▶ Via root, ▶ Via soil-air ▶ From deposited soil

EPA-pesticide datasets

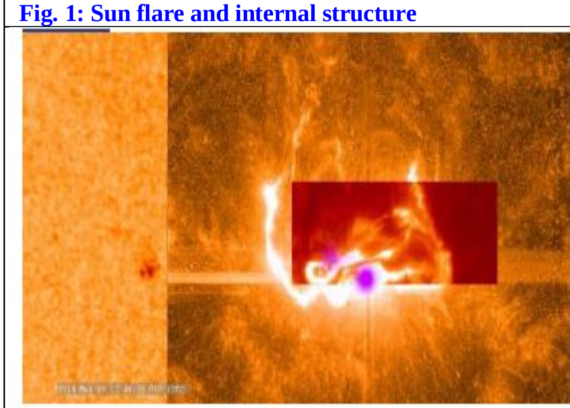
Chlordane Pesticide Dataset (EPA): This dataset containing 2,400 enantiomer-specific measurements for five pairs of chlordane enantiomers were compiled by EPA from peer reviewed published results.

Pesticide Dataset (EPA): The chemical information (structures, chemical names, identification numbers, pesticide class [insecticide, herbicide, and fungicide]) for 1,700 pesticides is available in a spreadsheet format with twenty fields.

Environmental hormones: These are natural/ xenobiotic (synthetic) chemicals (resembling endocrine hormones) released into environment (chart 11b). When they reach ground or inhaled, disrupt hormonal activity resulting in many reproductive health hazards. The endocrine-disrupting compounds (EDCs) are xenobiotic chemicals interfering with theendocrine systems of mammals and lower animals. Each toxicant is present below a toxic level. But, one is exposed to numerous agonists and antagonists which perturb several steroid-dependent signaling pathways with a cumulative effect. Vinclozolin, a fungicide,is also endocrine disruptors producing epigeneticchanges in the genome without altering DNA sequence.These endocrine disrupting chemicals act as estrogens, antiestrogens or antiandrogens and thus alter reproduction in a variety of organisms. In fact, the exposures during early development of fetes have consequences on adult stages and the effects are transgenerationally transmitted.

Solar radiation forecasting: The insular feature is a hurdle in solar (Fig.1, chart 12) forecasting. The one-day-ahead-forecast (with a 1 h temporal resolution) of global horizontal irradiance (GHI) from weather research and forecasting (WRF) model is biased. Lauret, et al.[134] proposed NN as a post-processing method in the forecast of (WRF) model for solar radiation at mesoscale numerical weather prediction (NWP). The data used is from ground station and bias error analysis was performed by NN, which picks up relevant inputs. Here, specific model output statistics (MOS) is employed in the frame of a solar PV forecasting project that takes place in La Reunion Island, a French oversea territory located in the Indian Ocean.

Fig. 1: Sun flare and internal structure

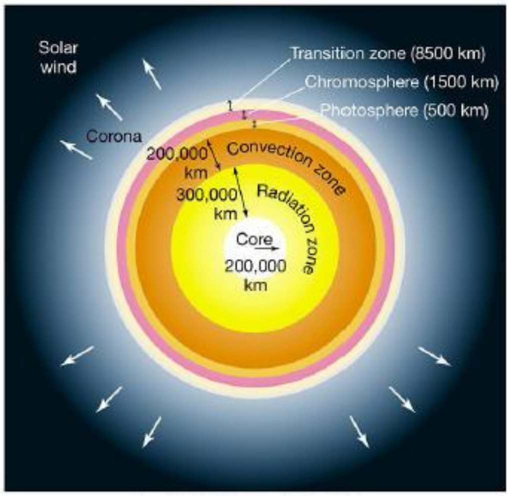


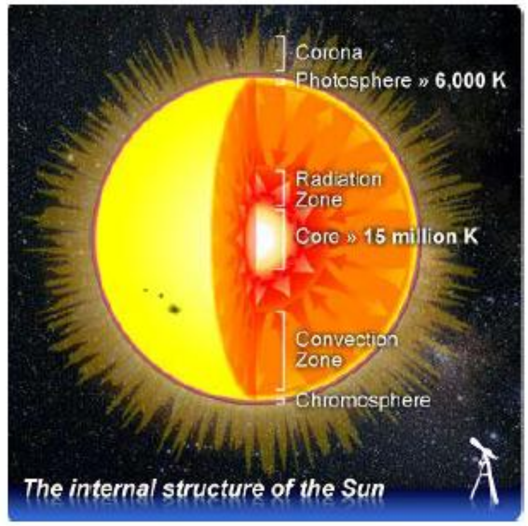
Sun flare (Courtesy of NASA report)

Chart 12: Facts and figure of Sun

	G2 star
Diameter	1,390,000 km
Composition	70% hydrogen
	28% helium
Mass	1.989e30kg
Temperature_ Surface	5,800 ^{o}k

Sun_Core	
Temperature	15.6 million ^{o}k
Pressure	250 billion atmospheres
Density	>150 * (water_density = 1)





6. Engineered nanomaterials

The sparkling utility of nanomaterials from medical applications to consumer products increased their production on exponential scale. The literature reports on cytotoxicity and genotoxicity of carbon-nanotubes, nano_Ag, nano_TiO2 on human lung, dermal, and visceral cells warrant preventive care.

Nanotechnology: It is a comprehensive tool making use of science, engineering, and technology at nanoscale (approximately 1 to 100 nano (10^{-7}) meters) for applications in industry, medicine, cosmetics with almost unattained characteristics in the last century materialistic world.

Nanomaterial contamination of natural environment: The complicated wastewater matrix promotes transformation of nanomaterials into different species. These various forms remain in sludge, effluent and further transported in landfill or incineration operations. Thus, wastewater treatment plants (WWTPs) are one source of nano species into natural environment including aerosols. Some of the NP compounds are very reactive in natural environment and many chemical, physical and biological transformation of differing toxicities result. Thus, extrapolation of laboratory data (for example pristine ENMs) to in vivo is erroneous and lead to mysterious conclusions. Further, their contamination in water, soil and air comprehensively demand a complete picture of toxicity to eco-systems.

Nanomaterial exposure to humans: The humans are invariably exposed to engineering nanomaterials (chart 13) at manufacturing units and transportation. The inhalation through aerosols is the second route for human exposure.

SToxR of nanomaterials: Thecytotoxicity and genotoxicity of nanoAg, nano zerovalent iron, nanoTiO2 and nanoCeO2 (0.1 to20 mg/L) from sequencing batch reactors were studied for A549 human lung epithelial cells.

Chart 13: Nanomaterials and environment

Nanotechnology
Materials of 1-100nm size
▶ Synthesis
▶ Measurement
▶ Property

Abbreviation	Expanded form	Abbreviation
NP	NanoParticles	NanoPart
MNP	MetalNanoParticles	MetNanoPart
fMNP	Functionalized MNP	fMetNanoPart
fAuNP	Functionalized gold nano particles	fAuNanoPart
ENM	Engineering nano materials	EngNanoMat

- Toxicity
- SXR
- Modeling
- Informatics

Factors affecting lifecycle of nanomaterials

- Environmental
- Ecological
- Technological
- Economic
- Sociopolitical

Abbreviation	Expanded form
CQC_nano	Computational quantum chemistry of nano materials
SXR_nano	SXR for nano materials
NN_nano	Neural network models for nano materials

X	Nano_X
Atom	Nano_Au; Nano_Ag
Molecule	Nano_H_2O; Nano_NaCl;
Material	Nano_graphite Nano_fenofibrate

NanoMat_informatics

- Data
  - Nanotechnology processes
  - Materials
- Data cycle
  - Collection
  - Organization
  - Validatation
  - Storing
  - Sharing
  - Model

Nanoinformatics → rational decision tools

- Stardized data
- Analysis tools
  - Quantitative qualitative data
  - Toxicity
  - Environment
    - Transport
    - Fate

Uncertainities

- Data
- Modeling
- Toxicity metrics
- Prediction acceptance levels
  - false positives
  - false negatives

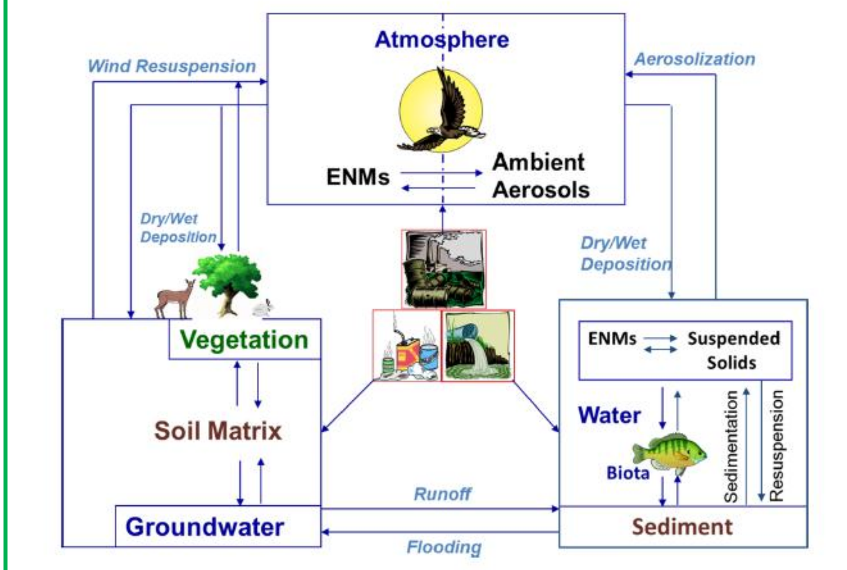
- Prediction
- Experimenta l
- Achievement

Toxicity-Metrics

- In vitro
- In vivo
  - HT Exp.
  - LT Exp.
- In silico
  - Mechanistic
  - Conceptual
  - First principles
- SXR_nano

Computational_Nano_Science

- Critical tools
- Simulations
- Computations
- Predictive modeling
- Nano
  - Materials
  - Devices
  - Systems



Transport of nanomaterials in environment(**Courtesy of Ref 1**)

Monitoring metal ions pollutants:Wilson et al.[377] reported an automatic monitoring system for binary/ ternary polluting metal ions using biosorption principle and NN modeling (chart 14).

Chart 14: Metal ion monitoring by bio sorption and NN models

Biosorption system	Monitoring Instrument
Fixed-bed column filled with wine industry waste grape stalks	computer FIP ET based array of 9 flow-through ion-selective electrodes
Ion mixtures	**Computations**
Binary Cu2$^+$/ Pb2+ (Cu2$^+$/ Zn2$^+$) Ternary (Cu2$^+$/ Pb2$^+$/ Zn2$^+$) (Cu2$^+$/ Zn2$^+$/ Cd2$^+$)	Fourier Transform FIA peaks Model NN Input --selected coefficients

FIP : Flow-injection potentiometry
ET : Electronic tongue detection

Chart 15: Prediction of air pressure in slurry shield tunneling

ENN Predictor Controller PSO Lrn	Test data Yangtze river_bed metro tunnel project, Wuhan, China.

Chart 16: MLP_NN prediction of traffic-generated noise levels

Input	Y
Total vehicle volume/hour % heavy vehicles Average speed of vehicle	Leq L10
Expt Field measurements	Model MLP_NN (BP) TrnAlg: LM Regression

L10: Ten Percentile exceeded sound level
Leq: Equivalent continuous sound level in dB (A)

Pollution with lead (Pb) metal: Czech et al.[132] found that MLP_NN (Statistica 9.0)predicts that lead in animal tissues and organs correlates excellently with measured values in locations in surroundings (100 km^2 around) of a lead–zinc ore mining and processing plant ('Boleslaw') at Bukowno in southern Poland. The goal was to monitor the transfer of lead in the soil–plant–animal system from different features of soil and plants and extent of pollution.

Air chamber pressure

Zhou et al.[71] found enhanced face stability in slurry shield tunneling using Elman NN both for control and prediction of air chamber pressure (chart 15).

Noise pollution prediction on highways: In India, the highway traffic is typical in a variety of two- wheelers with exponential growth in their numbers. The overall poor maintenance of heterogeneous vehicles, non-adherence of traffic norms and high pitch continuous horn blowing for longer time intervals worsen the extent of noise pollution scenario. Kumar et al.[383] predicted traffic-born noise levels on highway with MLP_NN (chart 16) with success.

Pollen complexes: Air borne pollen causes allergy [59] in human beings. The material was collected on a tape and manual inspection under a microscope was earlier practice. The limitations of the method are requirement of skilled technicians, long time and non-feasibility of continuous monitoring. *NN* could predict*Artemisia and Phleum but not Betula.* It demands an improvement in gas sensors employed and advances in NN methodology is required. Pollen is distinguished from other air borne particles now with an electronic nose. It consists of a gas sensor array, pyrolysis unit and NNs. The samples used are, dust from windows near the traffic zone, ordinary soil and pollen/ diesel/ petrol soot. The gases evolved, after heating at 250K in a specially designed furnace, are analysed by electronic nose. PCA although divides the classes, it could not resolve the groups within pollen. NN not only improved the major classes, but also resulted in partial resolution of groups within the classes. Kalman [59] suggests an ionization chamber and electro filter for sampling and heating in the experimental front.

Pollution at filling stations: Benzene is carcinogenic and the maximum limit stipulated by European community by the year 2010 is $5\,\mu g/m^3$. The exposure of employees involved in filling operations/miscellaneous tasks including cash collection is a matter of prime concern. The amount of benzene in urban and rural filling stations is monitored and a separate NN is trained for each group of workers. Passive sampling resulted in a maximum of 27 $\mu g/m^3$ integrated over two weeks for the employees. The seasonal variation is significant and there is a variation of 20% between summer and winter. This study suggests for the improvements of the infrastructure of the gasoline station including up gradation of vapor recovery systems.

Statistical models function in cause and effect framework. Ozone conducive meteorological conditions are well known now. The photochemical smog is very high during summer. It is due to the high temperature, high insulation, high stability, low mixing heights and low mid-day relative humidity. Many of the ozone episodes occur when the listed conditions prevail

Pollution due to insecticide residuals: From 1950s onwards, more than ten million tons of lindane (γ-HCH being active isomer) were used as insecticide. The three isomers (α-, β- and γ-) have the potential to travel long distances (chart 17). They are persistent in the environment and also bioaccumulate in organisms resulting in adverse toxic effects. However, in 1990s, production of HCH was abandoned and in 2009 Stockholm convention on persistent organic pollutants (POP), no exemptions were sanctioned even for ongoing production. Wo□hrnschimmel et al.[211] reported a global model for its fate and transport over the period 1950 to 2050. This has a goal of noting alarming levels even in remote locations with estimated emissions in near future.

Chart 17:Uncertainties with model for concentrations of α- and β-HCH

- Errors in expected long-term changes in climate → perturbs current forecast of climate temperatures and precipitation during the 21st century
- Emission inventory fails to identify past hotspots → Local high discrepancies between observed and model ouputs
- Unrecognized emissions in Northern Russia → underestimation of oceanic concentrations in the Bering and Chukchi Seas
- Underestimation of oceanic concentrations → uncertainity in predictions of the sea-ice effect on atmospheric levels
- Uncertainties of input parameters in environmental and chemical model

7. Personalized air monitoring move

Like personalized medicine dreamt a decade ago,personalized air monitoring systems now appear in advanced countries to augment better health care by reducing long exposures to high transient air pollution (chart 18). The per capita increase of asthma and other bronchial diseases can be intercepted with next generation finer-grained PMx personal air monitoring systems.Snyder et al. [207] from EPA,US elaborated the state of air monitoring programs and future directions in increasing the accuracy and involvement of public in sharing the knowledge for a better informed society to meet challenges and comply with the benefits of e-governance in bringing down pollution and its ill effects. Some of fine and coarse PM has wider spatial and longer temporal distribution compared to secondary pollutants viz. ozone and particulate sulphates. Further, the concentrations of NO2, CO, HAPs, ultrafine(< 0.1 μm) PMs differ within tens to hundreds of meters along highway side if downwind blows with high rate.

Chart 18: State-of-art-of air-monitoring systems and future gadgets

AirNOW (EPA) program
- High quality mobile air pollution sensors
- physiological sensors and location (GPS),
- health indicators (e.g., heart rate, blood oxygen levels)
- a person's exposure
- Internet technology
- + high information
- states, industry,
- Federal, State

Data collection
- Small
- Lowercost
- Mass-produced sensors

Organizations	Information dissipation
Government	Government
Industry	www
Researchers	Research Databases

Goal
- Forecast
- Monitoring
- Compliance
- Trends
- Research
- Enforcement

PM sensors
- Light scattering
- Light absorption
- Direct particle mass
- directly by changes in frequency of an oscillating sensor
  - indirectly based by light scattering using a
  - proportionality constant that relates the scattered light to a
  - defined (e.g., <2.5 µm) aerodynamic diameter

Basic components of sensors
- Sensor element responding to varying pollutant species; mass in a given volume of sampled air
- Transducer → converts responses to electrical signals;
- Data storage / link to a communication device
  - Microradio transmitter or cell phone
- Power source
  - Battery or energy harvesting like solar power

Technical and experimental challenges in Air monitoring
- Robust sensors
- High quality data,
- Integration from multiple sensors
- visualization
- Rigorous evaluations of sensors,
- Data of poor or unknown
- Quality → wrong decisions.
- More harmful than no data

Current air pollutants measurements (U.S.)
- regulated under EPA's NAAQS (http://www.epa.gov/air/criteria.html),
- PM chemicals
- fine coarse
- hazardous
- benzene, toluene, xylene
- emitted directly into air
- CO, NO, NO2, and certain

Basic principles of commercial gas sensors

Interactions between the sensing gas phase pollutant

Sensor	Gas monitored				
Electrochemical cell	CO	NOx	O_3	---	VOC
Metal oxide semiconductor	CO	NOx	O_3	---	VOC

Measure absorption of light

Non-dispersive IR 4.26 mum	CO_2	---	---
UV 254nm	CO_2	---	---
Visible	CO_2	O_3	---
Chemiluminescence	---	---	NO_2

II. Water (8-11)

8. Water resources

Long term (20, 50, 100 years) ahead forecasts (of even low accuracy) of climatic conditions, resources of river basins, population, health hazards and natural catastrophic events are of critical value to plan a sustained progress of society.

8.1 Long term forecast

Forecast of Climate by 2100: Inspite of intense research to forecast climatic conditions by 2100, the picture is still misty. But, at the secondary level, stream water/ atmospheric/ sea surface temperature, rain fall, pollutant concentration level of ground level, global warming and its consequences are vital for aquatic life and human comfort/ health/ life span etc.Piotrowski et al. [96] studied the impact of Levenberg_Marquardt and nature-inspired methods in training NN models (chart 19) to forecast temperature of Biala Tarnowska river (a natural stream) in southern Poland. The prominent prediction errors are related to freezing and melting processes in river during winter in the mountainous catchment.

Chart 19: TrnAlgs of NN of NN models of stream water
ॐ PSO
ॐ Evol Strategies
ॐ Direct search
ॐ 22 Metaheuristics
ॐ LM

Precipitation during 2070-2099 in New Zealand: NNs are used to derive the changes of site of and temperature characteristics over New Zealand. These models are used to obtain the changes of mean monthly precipitation from circulation variables projected in a transient climate change experiment performed by Hadley Centre Global climate model. The results are predicted for a far off period 2070-2099.

Conditional density estimation network (CondDensEstNN): It is a probabilistic extension of MLP. Cannon [101]used this model to forecastprecipitation downscaling, extreme value analysis in hydrology, wind retrievals from satellites and air quality (Alg.3). The software is developed in R programming language and applied for suspended sediment concentrations and discharge data in Fraser River at Hope, British Columbia, Canada.

Alg. 3. CondDensEstNN (R-package)
✚ Estimation of parameters of a specified PDF of predictors with conditional distribution
✚ Flexible model for the mean, the variance, exceedance probabilities, prediction intervals, etc

Streamflow: Su et al.[346] used MLP_NN to predict streamflow in the Songhuajiang River basin, an agricultural land in China. It is a noteworthy forecast study for the next forty years (chart 20).

Streamflow and discharge: Araghinejad et al. [286] applied ensemble_NN (Alg. 4) to forecast peak discharge of red river (Cannada) and stream flow of Zayandeh-rud (Iran) with better results compared to classical approaches (chart 21).

River discharge: Zeng et al. [347] performed a long term (forty years ahead) discharge forecast of river (Yangtze) discharge with NNs (chart 22). The prediction is possible by global climate model extrapolation of climate.

Chart 20: Forecast of precipitation and streamflow in Songhuajiang River basin during 2011–2050

Three scenarios
- Climate conditions of ECHAM5/MPI-OM
- Ensemble mean of CMIP5 models

Inference : Precipitation and streamflow

- Seasonal / inter-annual tendencies differ if emission scenario changes
- Inter-decadal changes are not obvious

Chart 21: Forecast of river stage with ensemble NNs

peak discharge during floods	Red River, Canada
seasonal streamflow	Zayandeh-rud, Iran
	NN kNN
ensemble ANNs > probabilistic forecast	

Alg. 4: Ensemble of NNs

Step 1: Create individual ensemble members
Step 2: Combination of outputs of the ensemble members
Method: probabilistic approach using k-nearest neighbor regression
Output

Chart 22: Long term (2050) forecast of Yangtze river discharge

Data	Model
Precipitation, Temperature, River discharge Period : 1961 to 2000	NN Forecast climate Global climate model ECHAM5/MPI-OM. Forecast (2011-2050) discharge Yangtze River basin Datong hydrological stations

Inferences of forecast

River discharge _ time interval	Trend
Annual	No obvious trends
Decadal	Small
Seasonal	Different trends during 2011–2050
Four seasons	Ratios of river discharges within a year tend to change

Chart 23: NN prediction for Habitat suitability modelling for mayflies

Location: Flanders (Belgium)

	(presences)	mayflies
samples	4289	

- Trn : 66%
- Test : Ten fold CV

Factors
- physical–chemical water characteristics,
- dominant land use type
- structural parameters

Samples with mayflies	Samples without mayflies
Lakes O2 Forests	Ammonium nitrite Kjeldahl nitrogen total phosphorous Orthophosphate BOD, COD, pH Conductivity Industrial areas

Models
- Logistic regression
- SVM
  NN
- Random forest
- Classfiication trees

Prediction

Year	mayflies prevalence %
1990s	20 to 40,
Last decade	same
	Forecast
2015	46
2027	72 by

Performance percent correctly classified instances kappa-statistics	

Short term forecast

Prediction of mayflies (Ephemeroptera) in the next decades in Belgium: Lock and Goethals [123] predicted with ensemble of NN, SVM etc. that mayflies (Ephemeroptera) in Flanders (Belgium) will increase to 46% by 2015 and to 72% by 2027 (chart 23).

Absorption in natural waters by 2022: Chen et al.[351] predicted total absorption (a(λ)) and backscattering (bb(λ)) coefficients of natural waters in the years 2015, 2022 (chart 24) by neural network-based semi-analytical algorithm (NNSAA) and the initial values are based on quasi-analytical algorithm.

Chart 24: Forecast of absorption coefficient of natural waters by 2022

	NNSAA	QAA
Yellow Sea and China East Sea	$R2 > 0.82$ MRE = 20.6–35.5%	$R2 < 0.73$ MRE = 32.2–69.6%
Global 1922 climatological seasonal mean	1923 July 2002 to September a : 443 bb: 555	

Information bits

If	equatorial oceans
Then	a(443) value in the surface water in the equatorial Pacific > equatorial Atlantic in the upwelling region & integrate a(443) in the Atlantic >> tropical gyre areas

8.2 Water resources and management

The water catchment information with minimum/ maximum values and uncertainties in consumption for various purposes along with desired quality measure indices are prime factors in water management.

Precipitation: Li et al.[262] compared efficiency of four precipitation **products** in estimation of hydrological research over Yangtze River basin (chart 25).

Chart 25a: High resolution multisensory precipitation products

TRMM Multisatellite Precipitation Analysis TMPA research	3B42 V7
(Near) real-time	3B42 RT
Climate Prediction Center MORPHing t	CMORPH
Precipitation Estimation from Remotely Sensed Information using NNs	PERSI_NN

Gauge data

Location:	Yangtze River
Time period:	April 2008 to March 2012
Temporal scales:	Year to day

Chart 25b: Intercomparision of four high resolution sensors		
RMSE Probability of Detection daily scale	3B42 V7	Not always superior to CMORPH
Near real-time datasets	3B42 RT	Overestimates annual rainfall over the basin
	CMORPH and PERSI_NN	Underestimate it.
Upper Yangtze	3B42 RT dataset	Positive bias (>1 mm day−1)
	CMORPH dataset	Negative bias (−0.2 to −1 mm day−1)
Seasonal scales	CMORPH	Exhibits negative bias during cold periods.
gauge data	CC(CMORPH, data)	Highest
	CC(3B42 RT, data)	More scattered
PDFs	3B42 V7 3B42 RT	Retrieve PDFs in high-intensity events

Daily forecast:Yu et al.[263] proposed two hybrid algorithms combining fuzzy_NN with discrete and continuous wavelet transforms for long term precipitation, evaporation and river stage data (chart 26).

Chart 26: Long term forecast of river TS data

Data
- One station
  - Daily precipitation
  - Evaporation
- Two stations
  - river stage

CWT	TLT	Poor performances
DWT	SLT	Effective

Forecast-practical utility
TLT >> SLT

CWT Cont.WT:	Continuous Wavelet Transform
DWT Discr.W:	Discrete Wavelet Transform
LT:	Long term
SLT:	Seeming
TLT:	True
TS:	Time series

DWT-Fuz.NN	TLT		Weaken DWT advantages
	River stage signals	Short term periodicities zero value data	Significant advantage
Inference **Prediction of hydro-meteorological TLT signal** DWT-NF >> [component; other hyrid] models			

Chart 27: Long-term spring rainfall prediction			
X Lagged El nino Southern oscillation Indian ocean dipole		**Performance measures** MSE, MAE, CC Willmott index of agreement	
Generalisation			
Victoria	CC		
	MLR	NN	
East	−0.99 to −0.90	0.42–0.93;	
West	0.68–0.85	0.58–0.97	
Inference NN_LM >> [MLR, large scale climate models]			

Chart 28: Seasonal rainfall forecast in Queensland, Australia using Pacific Oscillation parameter	
X Climate indices	y Rainfall forecast [continuous variable]
Model NN	Performance measures RMSE, MAE, CC

Rainfall

Mekanik et al.[260] reported NN trained with LM algorithm predicts long-termspring rainfall with higher generalization ability compared to MLR and climate models of large scale (chart 27).

Forecast of rainfall in Queensland, Australia:Abbot and Marohasy [61]employed inter-decadal Pacific Oscillation for forecast of rainfall. This index was never used earlier in official seasonal forecasts for Queensland. Most of earlier studies were confined to statistical models. The results at three geographically different areas were compared with POAMA (Predictive Ocean Atmosphere Model for Australia)(chart 28). POAMA is a General Circulation Model currently in use in official seasonal rainfall forecasts.

Thunderstorms and rain:Manzato[67] proposed a NN model to predict occurrence and intensity of thunderstorms and rain in Venezia Giulia, Italy from sound, light and meteorological data (chart 29).

Chart 29: Forecast of thunderstorm and rainfall	
Location : Plain of the Friuli Venezia Giulia,Italy	
Input Sounding Lightning strikes Mesonet station Rain Wind	**Training** 1995–2002 : April to Nov **Test** [2003 to] 2004

Phase	model	Output
I	NN_classification	convective activity
If convective activity Thenregression_ ANN		
II	NN_regression	Thunderstormintensity forecasting

Rainfall retrieval: Wei [321 identified influential factors viz. brightness temperatures of 19, 22, 37 and 85 GHz for retrieval of rainfall. The results of Bayesian networks (BN) and BN hybridized with scattering index (SI)/ polarization corrected temperature (PCT) are compared with SI, SI_SVR and MLP_NN (chart 30).

Rainfall and runoff (TS) forecast: Farajzadeh et al.[398] forecasted monthly rain fall in Urmia lake basin for the period 2012-2017 with NN and ARIMA models(chart 31). The correlation coefficient and RMS are 0.62 and 12.43mm. Urmia lake basin, located in northwestern Iran, is the second largest saline lake in the world. The water level of the Urmia Lake has been decreased from 1997 as a cumulation of consequences of construction of dams, climate changes and mismanagement of water resources. The result was emergence of thousands of hectares of salty land with ecological imbalance. Soil moisture is critical geo-physical parameter playing a key role in absorption and runoff of rain.

Hourly run off:Tayfur et al.[256] predicted hourly run off at small catchment areas with generalized regression_NN in Italy from measurements of soil moisture and rainfall (chart 32).

The drastic seasonal changes render the prediction of runoff of Annapolis River catchment a hard task to model. Piotrowski and Napiorkowski [283] found that NNs with hybrid training using DE with Local/ Global Neighbors, LM excels other EAs in forecast of runoff river(chart 33).

Chart 30: identification of rainfall intensity

Data	Model
Location: Tanshui river basin, Taiwan meteorological data Period: 2000–2012 ; typhoons :71 Instrument :Special Sensor Microwave/Imager (SSM/I) of the National Oceanic and Atmospheric Administration (NOAA) Response : seven passive microwave brightness temperatures, Obj : detect rain rates	Bayesian networks + polarization corrected temperature (PCT) + scattering index (SI) methods Learning Alg Tabu search Simulated annealing Genetic algorithm

Expert opinion

- BN identifies influential factors in rainfall retrieval and causal relationships
- BN + [PCT, SI] >> [SI-SVR] [MLP_NN] if heavy/ torrential downpouring rainfall

Chart 31: Multiple-models

NN ARIMA	Test period : 2012-2017
Predictive uncertainties	R = 0.62 RMS = 12.43 mm

Chart 32: Forecast of hourly run off

Input Rainfall + soil moisture Depth 10, 20, 40 cm	Trn : October 2002–March 2003 Predict: anuary–April 2004
Output Discharge	**Sub-catchments of Tiber river** Colorso : 13 km^2 Niccone : 137 km^2
Model	**Performance**

	Generalized regression_NN	R^2 :0.87 Nash–Sutcliffe efficiency: 0.86

Chart 33: Forecast of rainfall-runoff

River : Annapolis River catchment
daily rainfall–runoff

Seasonal changes

- Runoff
- Rapid floods
- Dry summers
- Severe winters with snowfall
- Snow melting
- Frequent freeze and thaw
- Presence of river ice

Tr. Alg.Model.Evolution (Tame)

- **Differential Evolution (DE)**
  - Distributed DE + Explorative–Exploitative Population Families
  - DE + Self-Adaptive
  - DE + Global and Local Neighbors
  - DE + Grouping
  - JADE
- **PSO**
  - Comprehensive Learning Particle Swarm Optimization
  - Efficient Population Utilization Strategy Particle Swarm Optimization
- **Levenberg–Marquardt** algorithm

Levenberg–Marquardt alg

- Speed
- Trapped in poor local optimum
  - **Remedy:** Multi-start approach

Chart 34 : Forecast of runoff Annapolis River, Nova Scotia, Canada

- Differential Evolution
- Global and Local Neighborhood
- Trailing
  - Levenberg–Marquardt
  - Evolutionary Computation

Table 7: Explanatory variables of predictive model for stream nitrogen concentration [397]

Input variables	
Forest	FOR
Agriculture	AGR
Urban	URB
Wetland	WET
Other categories	OTH
Animal unit density	ANI
Average annual precipitation	PRE
Annual stream flow	FLO.
OTH	Difference between total watershed area and the four other areas
Output variables	
Mean Inorganic nitrogen concentration	INC
Total nitrogen concentration	TNC

Table 7(b) : Performance of NN in prediction of stream N2 with input variables

Data	**Average CC for five sets of data**	
	Total nitrogen	**Inorganic nitrogen**
Tr	0.861	0.845
Te	0.845	0.832

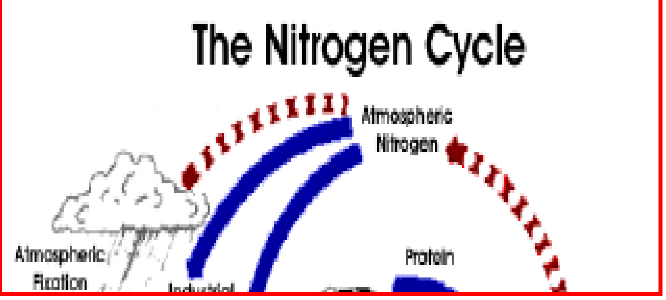


Table 7(c): Comparison of NN stream N2 with FAS at different sites [397]				
Site	MSE		CC	
	NN	FAS	NN	FAS
Duifpolder local control	0.0003	0.028	0.999	0.913
Woudse Droogmakerij Local control	0.065	0.959	0.179	0.918
Woudse Droogmakerij Centralized control	0.021	0.986	--	--

Courtesy from Olery et al (1997)

Product-Units_NN: The first hidden layer consists of neurons where inputs are raised to exponential weights. In the other layer, summation function is used for the neurons. Although, it is difficult to train unbounded weights, acceptable results are found for weights in the interval [−1, 1]. Piotrowski and Napiorkowski[4] applied ProdUnitNN to forecast runoff of Annapolis River, Nova Scotia, Canada with success(chart 34).

NNs have been proven with better prospects in imputation of missing data inrainfall around Luvuvhu river catchment [333], air pollutant prediction,streamflow in the Shire river basin, Malawi [335] anddaily flow rates of Middle Firat catchment [136].

⇨ Stream water:

The streams and natural rivers consist of a main channel and flood plains. Rainfall-/stream-/river- flow models have a function in flood mitigation measures, construction of hydraulic structures, and prediction load of sediment and water resource management of arid inland zones. The nitrogen concentration in streams is through non-point source pollution at the watershed level. The concentration has been found to increase in USA and Europe. Denitrification process is used when high nitrogen concentration is found. The control requires the origin and distribution of N2 in stream water. The spacio temporal patterns are complex. Lek [397] predicted the export of nutrients (inorganic and total N2) in stream water versus the parameters of watershed drainage area and its environment(table 7). The patterns are non-linear or with non-monotonous trends. The maximum contaminant level stipulated by US-EPA for NO_3-N is 10 mg/lt. WASMOD is nitrogen-modeling software, which accepts the description of nitrogen discharge as a function of soil relief, land use and climate. Performance of radial basis and MLP_NN (trained with LM) in predicting daily watershed runoff is better than that with MLR.Zounemat-Kermani et al.[25] reported NNs are superior to MLR in one-day ahead forecast of stream flows in Alabama, USA (chart 35).

Chart 35: Prediction of one day ahead stream flows

MLR MLP_NN RBF_NN	Location Cahaba River, Alabama Residual analysis RMSE, MAE CC K-fold CV
Test	Performance
Mann-Whitney	statistical significance (measured median - predicted median)
Levene's	Differences in variances

Statistic	MLP_NN (LM)	MLR
Average (MAE)	100-18	100
Ave(RMS)	100-21	100

	RMSE m^3/s		
Prediction	RBF_NN		MLP_NN (LM)
Highest flow rate rangeduring flood	26.8	<<	40.2
Watershed runoff	19.2	>>	18.8

Chart 36: Monthly streamflow forecast
Data

Chart 36(b) Chemical composition of synthetic storm water	
Solution of deionized water → autoclaved	
Concentration	Major ions

six monthly streamflow sets two successive gauging stations	
Phase I: SLP_NN Phase II: Input(s) and output records were decomposed into sub-time series components using wavelet transform. Phase III: Wavelet_NN for each sub-time series	
Performance RMSE Nash–Sutcliffe efficiency	**Inference** LGP >> WANN

mM	
5.1	NaCl
0.75	CaCl2
0.075 mM	of MgCl2
0.33	Na2SO4
1	NaHCO3
0.072	NaNO3
0.072	NH4Cl
0.016	Na2HPO4
Ionic strength	20 mM
pH range	[6.9 to 7.2]
pH adjusted with 0.1 N NaOH or 0.1 N HCl	

Stream flow prediction: Mehr et al.[265] found linear GP is better than wavelet_NN in the prediction of monthly streamflow (chart 36). Mehr et al.[98] found that Linear_genetic_Programming performs better than NNs (MLP_, RBF_ and GR_) in successive-station monthly streamflow prediction for two gauging stations on Çoruh River. RMS and Turkey Nash–Sutcliffe measure are considered for performance comparison.

NN + ABC:Kisiet al.[282] reported a hybrid NN with artificial bee colony (ABC) algorithm to estimate a daily stream flow and river carried suspended sediment concentrations at Rio Valenciano and Quebrada Blanca Stations. The logarithm transformed data were also used as input to the model and the hybrid model was better than neural differential evolution, adaptive neuro-fuzzy and rating curve.

⇨ Stormwater

The storm water originates during precipitation and snow/ice melt events. It soaks into the soil (infiltrate), held on the surface and evaporate or runoff. Finally, it end up in nearby streams, rivers, or other water bodies (surface water). It contains a myriad of contaminants including suspended solids, nutrients, heavy metals, hydrocarbons, and pathogens.

⇨ Rivers

For successful water resources management, the key factors are accurate/precise measurements, shrewd analysis, trustworthy future plans for irrigation, energy generation and drinking water. The Water Resource Data mining (WR_DM) is interlinked with climate changes, land utilization and pollution. The land ocean coupling is understood from river flow involving processes based on land-atmosphere characteristics. Albostan et al. [136] found NNs are superior to MLR in predicting daily rainfall data at a station not included in training from four stations on Murat River. Cole et al. [259] successfully predicted daily mean temperature in Delaware River over a wide range of conditions with GLScos, ANN, and HFM models (Chart 37, table 8). It serves as a basis to manage thermal releases in regulated river systems.

Chart 37:Prediction of temperature of Delaware River

Input

Weather station

- Climate data
- Solar radiation
- Wind speed

U.S. Geological survey gages

- Temperature
- Hydrologic data

Location

- Upper Delaware River (USA)

(1-, 3-, 5-) day ahead forecast_success

- Baseline-modified prime index of agreement

Data	years
Trn	2008 to 2011
Test	2012

Performance

- RMSE
- Nash Sutcliffe efficiency
- percent bias
- Index of agreement statistics

Models

- Gen.LS
- Cosine trend
- ARIMA
- NN
- Mechanistic Heat Flux
  - Basis: Energy gain and loss

Table 8: predicted daily mean river temperature

Statistic	ARIMA	All models
RMSE	0.57	0.58–1.311
NSE	0.99	0.99–0.97
d	--	0.98–0.99

River flow: Nayak et al.[269] investigated conceptual and Wavelet_NN models for river flow from the results of rainfall_runoff relationships in Malaprabha basin in India (chart 38). The results show that the loosely coupled sequential hybrid model consisting of wavelets transforms and NNs excelled simple NNs and also popular NAM (North American Mesoscale) model. Badrzadeh et al.[270] proposed a hybrid NN model for m-day ahead forecast of Harvey river flow with higher accuracy compared to component models(chart 39). He et al.[257] found SVM excels NN and ANFIS in the forecast of river flow in semiarid mountain regions of China (chart 40). Lohani et al. [255] introduced a concept of rare and frequent hydrological situations in fuzzy models. Threshold subtractive clustering based Takagi Sugeno (TSC-T–S) fuzzy inference system is used to predict low to medium (frequent events) as well as high to very high flows (rare events) in upper Narmada basin, India (chart 41). Antanasijević et al. [254] reported generalized regression NN to forecast dissolved oxygen in river Danube with good modeling practices (chart 42). Sirdari et al.[233] found that NN (accuracy: 97%) is better than genetic programming (93%) in modeling bedload transport of small rivers in Malaysia (chart 43). Kim et al.[126] found that a tight coupling of phase wise refinement of knowledge and evolutionary optimization of parameters of multivariate models of riverine water increased the quality by more than 50% compared to MLR and NNs(chart 44).

Chart 38: Rainfall-runoff model for Malaprabha basin

Model

I. Phase
- Rainfall-runoff

II. Phase II
- River flow

Wavelet_NN modeling

Stage	Input	Model	Output
I	**Daily data** Rainfall Discharge Evaporation **Time period** 1980 to 2000	Wavelet transform	Decomposed sub series
II	Decomposed sub-series	NN	Calibration Performance Nash–

Chart 40: River flow forecast in semiarid mountain regions in China

Models	Performance
NN SVM ANFIS	RMSE, CC Nash–Sutcliffe efficiency coefficient Mean absolute relative error

Inference

SVM > [ANN; ANFIS]

Chart 41: Threshold subtractive clustering based Takagi Sugeno (TSC-T–S)-FIS for river flow prediction

Data: Hourly rainfall	Preprocessing
River flow Location Upper Narmada basin,	Rainfall–runoff data classified into frequent and rare events

			Sutcliffe efficiency coefficient
			RMS

Inference for flow duration curve

Wavelet_NN >> [NN; NAM]

Central India	
Models	Performance measures
SOM_NN TSC-T–S fuzzy model	RMSE, CC Peak % threshold statistics

Chart 39: Multi-step-ahead forecast of river flow

m-day ahead forecast m : [1, 2, 3, 4,5]	Harvey River Western Australia		Daubechies and Symlet wavelets	→	decomposes river flow time series to different levels

Model	Training		Ws
wavelet neuro-fuzzy model	LM	→	optimum number of fuzzy rules
NN	Subtractive clustering method		

Chart 42: Dissolved oxygen Forecast in Danube River

Objectives

- Optimum data normalization
  - Monte Carlo
  - Min–max
  - Median
  - Z-score
  - Sigmoid /tanh
- Input selection techniques
  - Variance inflation factor
  - Correlation analysis
  - Genetic algorithm
- Uncertainty analysis
  - Input variables
  - Model

Input	
water quality variables	19
# sites	17
Sampling	9 years monthly

Best results of GRNN

- Normalization
  - Min–max
- Input selection
  - CC(DO, X)

Inferences

- CC(measured vs. predicted) DO : 0.85
- distribution (model results) ≏ distribution (experimental data)
- Influence of variables on model
  Temp > pH > HCO_3^- > SO_4^{2-} > NO_3-N

Chart 43: NN modeling of bedload transport of small rivers in Malaysia

small rivers in Malaysia	y
X ▶ flow discharge ▶ water depth ▶ water surface slope ▶ surface grain diameter (d50)	Estimate bedload transport

Chart 44: Tight integration of KB refinement and Evol optimization

Iterate

Knowledge refinement
New case studies
Evolutionary Alg.
- Optimise MV_ model-parameters such that
  - Values are within range &
  - Consistent with ecological a priori knowledge

End Iterate

Limitatons of complicated Env models (save EPA, US models)
- Poor prediction and reality
- Inaccurate/ out-of-range parameters
- Non-accountability of rare nonlinearities.

GreyNNs in river stage forecast: Alvisi and Franchini [334]introduced grey number theory into NN modeling of river stage forecast(chart 45). They found that even when data is uncertain, Grey_NN is better than Bayesian_NN. The parameters of NN are represented by grey numbers and output is an interval (not a crisp floating point value) unlike in all types of NNs.

NN + SVR: Chih-Chiang Wei[142] et al. reported NN and SVR are better than MLR to forecast river stages during typhoons in Tanshui River Basin in Taiwan (chart 46)

Chart 45: Grey_NNs in river stage prediction

- Crisp forecasts derivable from output of grey_NN
- Output_ bands of grey_NN narrower than Bayesian_NN
  - % of observed values are same

band : [envelope of the intervals]

Chart 46: NN prediction of river stage during typhoons

- Tanshui River Basin,Taiwan
- Hydrological datahourly
- Period : 1996–2007.
- 50 historical typhoon events
- Forecast : [1 h to 4 h]

Inference

[NN, SVR] > MLR

Models

- Lazy learning models
  - Locally weighted regression
  - *k*-nearest neighbor
- Eager learning
  - MLR
  - SVR
  - NN

Temperature of river water: DeWeber and Wagner[253] brought out neural network ensemble for prediction of mean daily temperature of river water in eastern U.S. (chart 47).The model could predict mean daily water temperature in 197,402 individual streams in the warm season (May–October) of 2010 endorsing its generalizability for newer streams under different environments.

Chart 47: Ensemble of NNs in prediction of mean daily temperature of river water

Predictor categories
- Climatic
- Landform
- Land cover attributes

Data	RMSE °C
1980 to 2009 Trn : 886	1.91
Test 2010	1.93
Validation 96 sites	1.82

Influential predictors
- Mean daily air temperature
- Prior 7 day mean air temperature
- Network catchment area

Predictors with negative effects
- Forest land cover
  - Riparian
  - catchment

DO in Surma river: Masrur Ahmed [288] predicted dissolved oxygen with MLP_NN and RBF_NN models by measuring BOD and COD in the Surma River, Bangladesh for a three year period (table 9a).

Rapid changes in river flow: In Taiwan, typhoons and intensive storms resulting in rapid and short term high river flows pose a threat to the quality of water and plight of ecosystem. This necessitates the monitoring/estimation of daily water quality rather than conventional monthly/quarterly schedules. Chang et al.[245] found NARMAX_REC_NN modeling using hydrological data successfully estimated ammonia nitrogen, an indicator of water quality. Further, the model detects peak values during the critical period (September–April) for pollution (chart 48).

Chart 48: NN model for Ammonia nitrogen in Taiwan river	Chart 48(b) Typical input factors for river water quality[163]
Hydrological Input factors Discharge Days w/o discharge Water temperature Rainfal Model : NARX_RecNN CC 0.926 RMSE 0.386	%DO % Dissolved Oxygen Cond Conductivity e Lab Meter DO Dissolved Oxygen DOC Dissolved Non-Purgeable Organic C DRP Dissolved Reactive Phosphorus Ecoli Escherichia Coliforms e MF MFC/ NA-MUG FC Faecal Coliforms e MF MFC FS Faecal Streptococci e MF HardT Hardness Total HCO3 Bicarbonate HPC Heterotrophic Plate Count 35"C

Cruise in river: Lu and Liu [23] simulated and tested a hybrid (fuzzy_NN and ACO) model based controller for vessel cruise on a river (chart 49).

Chart 49: Simulation and cruising vessel on a river with hybridized NN

Function	Algorithm
Optimal sailing line Short sailing time	ACO
Tidal current, river current vessel velocity Position of the coordinate	searching pattern of ACO
Tracking error	switching law
Compensation of uncertain nonlinear factors	FNN controller
Estimation of vessel velocity	identifier
Tuning of parameters	Adaptive law from Lyapunov function
Compensation uncertainties of tidal current River current	Robust controller
Simulation & practical cruising Vessel on a river	Model test

Chart 50: Long-term (6 and 12 months ahead) forecasting of Standard Precipitation Index drought

Location	Models
Awash River Basin in Ethiopia Performance RMSE, MAE, R2 Persistence measure	ARIMA NN SVR wavelet +NN wavelet + SVR Preprocessing wavelet

The data driven robust NNs have been found superior to other model driven procedures in water quality index for Kinta River (Malaysia) [305],also other rivers [339,394], precipitation over complex mountainous terrain [5], water flow [99], discharge routing of Kizilirmak river in Turkey [284], spatial distribution of macro invertebrates under flow regulation in the Lijiang river [125], estuary water stage [2], river stage forecasting with uncertainty [334], flood evaluation river mapping from MODIS images [3], monthly reservoir inflow forecasting [278], prediction of daily and hourly multi-time-step ahead intermittent reservoir inflow of Koyna river watershed in Maharashtra, [279], steel pipe pile in Arkansas river [107], daily suspended sediment in river [224], eco system health by richness of native fish Júcar River Basin District [371], blind fish [113], river discharges at Yichang and Datong hydrological stations under three greenhouse gas emission scenarios from 2011 to 2050 in the Yangtze River [347], runoff at Annapolis River, Nova Scotia, Canada [4], catchment [271], prediction of discharge in straight compound open channel flow [221], monthly stream flow forecasting[280], total nitrogen concentration on monthly basis in streams [240], forecasting river flow rate from the Melen Watershed of Turkey Western Black Sea region [275], estimation of monthly river flow in arid inland basin of Northwest China [276], monthly river flow forecasting [277], river flow forecasting [283], riverbed grain-size distribution [272], dissolved oxygen in a riverine [118], riverine fish diversity [266], longitudinal dispersion coefficients in rivers [217] prediction of river temperatures [274], sediment load of river systems (Mississippi, Missouri and Rio Grande) in USA [9], soil acid sulfate mapping in Sirppujoki River catchment area, south-western Finland [247], Soil water dynamics [287], spatial distribution of soil heavy metals in Huizhou City [344], suspended sediment concentrations in Fraser River at Hope, British Columbia, Canada [101], suspended sediment modeling [281], prediction of daily sediment (suspended) load in rivers [373], predicting sediment yield in the Nagwa agricultural watershed in Jharkhand, India [8], prediction of upstream and downstream station sediment data [273], river suspended sediment estimation [103], suspended daily load in Doiraj River, Iran [268], chemical pollution in sediments in estuary of Nerbioi-Ibaizabal River (Bilbao, Basque Country), discharge-suspended sediment relationships [282], longitudinal velocity in open channel junctions [222], water resource, SST [345] and sediment classification [114].

⇨ Floods and droughts

The floods in River Nile destroy houses, crops, roads and basic infrastructure causing people to migrate to other regions. Elsafi [10] predicted flooding at Dongola Station for Nile (Blue Nile, White Nile, Main Nile) and Atbara rivers using the data between the period 1965 and 2003. A wavelet NN along with parallel GA is proposed to simulate and predict floods in arid areas in China. The model was compared with Xinanjiang hydrological model. The success of the NN is in that the simulated runoff is strongly related to the rainfall with four time steps lag and the observed runoff with three step lag. The wavelet TF models have strong nonlinear trends. GA overcomes local optima often encountered in BP training. The parallel version drastically (82%) reduces CPU time. Belayneh et al.[258] found that NN or SVR with wavelet pre-processing is an adequate model for 6 and 12-month ahead forecast of drought index for a river basin in Ethiopia (chart 50).

Alternate floods and droughts: These irregular cyclic phenomena occur in Southwest China over a large karst plateau (Yun–Gui Plateau) [349] as a consequence of total water storage anomalies for the last three decades (chart 51).

Chart 51a: Hind-cast of total water storage anomalies (TWSA, Tot.Wat.Store.Anomal.) in Yun–Gui Plateau, China

- Data Gravity Recovery Climate Experiment (GRACE) satellite
- Model : NN

River	R^2
upper Mekong	0.91
Pearl	0.83
Wujiang basins	[0.76 0.57]

Chart 51a: Flood and drought cycle

Years	TWSA
1980s	Fairly stable
1990s	Increasing trend @5.9 ± 0.5 mm/a
1990 July to 1991	Extreme flooding
>2000	Drastic fluctuation

Severe spring Droughts	2003 to 2006
Most extreme Spring drought	2010

2008	Severe flooding

⇨ Flood management

Forecasting the extreme values rather than a normal one of discharge in a river is crucial to manage floods and droughts. Experimental monitoring is hazardous and is to be planned fast at the time of catastrophe. The incidents are untold and thus spread over a long period of time. Hence, the activity is costly. The long practiced rating curve is a cause and effect functional relationship between measured discharge and water level. ARIMA is inadequate as the phenomenon is complex [326]. Thus, the routine hydrological models often fail especially to predict run offs or the extreme (very high or very low) values [173]. Further, results are not convincing even in gazed catchment areas for short-term and long-term management. However, neural networks a machine-learning paradigm supersedes in performance in hydrology, watershed and flood management. Bhattacharya [326] compared the results of NN, rating curve and M5 model tree. The combined urban and rural water system management prevents flooding water, scarcity and quality of drinking water. The system is multifarious and dynamic in time. For example, a typical large water system consists of 1200 subsystems, 1500 regulating structures in 12 time steps. The data for optimization consists of 100K variables, 100K constraints and 350K non-zero data points [385]. AQUARIUS is a software package, which builds deterministic models for water quality and quantity in urban and rural areas. Lobbrecht [385] employed NNs and fuzzy adaptive system to control the operation of water management with acceptable accuracies. The machine learning technique is used for flood prevention.Juma et al.[220] found that SLP excels MLR in predicting discharge coefficient (Cd) for a hollow semi-circular crested weirs (table 9), which are small overflow dams. They are used to alter/raise water flow upstream and regulate spill water downstream watercourses and rivers. Tayyebi and Pijanowski [231] found NNs are superior to CART and MARS in modeling land use change in South-Eastern Wisconsin (SEWI) and Muskegon River Watershed (MRW), Michigan (chart 52).

Table 9(a): Prediction of DO with MLP_NNand RBF_NN

Dataset	MSE	E	R
Test	0.465	0.905	0.904
validation	1.009	0.966	0.963

E: coefficient of efficiency

Table 9(b): NN model of Q(t) as a function of artificial precipitation for three years [385]

Site	MSE		cc	
	NN	FAS	NN	FAS
Duifpolder local Control	0003	0.028	0.999	0.913
Woudse Droogmakerij Local control	0.065	0.179	0.959	0.918
Woudse Droogmakerij Centralized control	0.021	--	0.986	--

Table 9(c): Comparision of models applied to AQUARIUS control[385]

Site	Average water level (m+MSL)		
	Control with	Intelligent control with	
	AQUARIUS	ANN	FAS
Duifpolder	3.16 * 0.104	3.15 0.085	3.14 0.099
Woudse Droogmakerij	4.56* 0.034	4.60 0.029	4.59 0.028
Woudse Droogmakerij	4.56 ** 0.035	4.55 0.048	--

** : central control *: local control

Table 9(d): SLP_NN for discharge coefficient estimation

	MSE	R
SLP 2-10-1	0.0011	0.91
	SLP >> MLR	

Table 9(e): comparison of RMSE for water level discharge models and prediction accuracies[326]

Model	RMSE		%Ve data with prediction error		
	Tr	Ve	>5%	>10%	>20%
Model tree	92.0	69.7	20.3	1.6	0.2
ANN	90.5	70.5	21.4	3.1	0.3
Conventional rating	143.3	111.2	42.4	11.8	1.9

Chlorophyll-a

Cho et al.[310] reported the influential factors to predict chlorophyll-a (chart 52a) and consequently abundance of algae in a water reservoir behind the dam on the river using NNs. Muñoz-Mas et al.[148] studied microhabitat suitability for adult brown trout (Salmo trutta L.) with prob_NNs in Iberian rivers.

Effect on habitat: Fukuda et al.[122] used NN, CART etc. to find spatial heterogeneity of habitat in small agricultural canals of Japan. This information based on quantity and quality of medaka (Oryzias latipes) is pivotal in conservation and restoration to increase biodiversity (chart 53).

Chart 52a: NNs to predict Chl-a in man-made Lake Juam

Automatic monitoring data	Weather data
Water temperature pH Dissolved oxygen Electric conductivity Total organic carbon Chl-a Total nitrogen Total phosphorus	Precipitation Temperature Insolation Duration of sunshine
TimeSeriesData Trn: 2008–2010 Test : 2011	Hydrologic data Water level Discharges Inflows

Chart 52(b)Land use classes

- Agriculture
- Forest
- Urban

Chart 52(c): Land use change models

USA	Time interval
South-Eastern Wisconsin (SEWI)	1990–2000
Muskegon River Watershed Michigan	1978–1998

Chart 52(d): Inferences

- Forest gain close to current forests
- Agriculture gain closer to agriculture and forest patches
- Influence of elevation is high onurbanization
- No effect in SEWI

Chart 53: Models for spatial heterogeneity of habitat

Input	Models
water depth flow velocity **Species** Japanese medaka (Oryzias latipes),	CART NN SVM Xx

Model	Function
2D hydrodynamic Basis: Information entropy	Instream special habitat conditions
Coupled ecohydraulics	Quantification Habitat quality & spatial heterogeneity → Differences in canals Earthen Concrete-lined

Chart 54: NN model for respiration rates of global krill

Oceanographic conditions with depth	Basal variables
Temperature Light Oxygen availability Latitude Day of the year # daylight hours	oxygen consumption Temperature Body mass Depth

Chart 55: SLP_NN for conservation of biodiversity

- Area : yangtze river basin
- 2.143 million km^2, (20% of china's territory)

- Biodiversity
- Habitats of 627 indicator species

- Planning tool,
- Marxan,
- Output: Optimal set of planning units,

- Models
- Priority ranking analysis with SLP_NN(6-12-1 BP)
- Hierarchical cluster analysis → classifications of human disturbances

Chart 56: Simulating groundwater flow Kathajodi–Surua Inter-basin of Odisha

Data for MODFLOW model

Calibration	Period :	February2004 to May 2006
	Frequency :	Weekly
Validation	June 2006 to May 2007	

Simulation

Groundwater levels	18 observation wells

NN model

Weekly rainfall, evaporation River stage Water level in drain Pumping rate of tube wells Groundwater levels at previous time step	Trn: 122 Test : 52

Week_ahead Prediction

groundwater levels	18 observation wells

Chart 57: Imputation of missing data

Data	Location
Rainfall	Luvuvhu River Catchment
RBF_NN Par_opt : Shuffled Complex Evolution	ObjFn : RMSE

	NSE	% Bias
Calibration	[0.55 to 0.85]	[−2 to 23]
validation	[0.49 to 0.75]	[2 to 19]

NSE:Nash–Sutcliffe Efficiency

SOM+ART: Park [364]reported a two level classification approachwith SOM and ART to understand the multivariate ecological data. This hierarchical clustering process is used to study the variations in communities of macro invertebrate in stream eco systems. Ab initio understanding of ecological model is beyond the present realm of understanding. Fuzzy inference system (FIS) introduces experts' heuristic/empirical as well as traditional skills from practitioners' knowledge.

Respiration of krill: Tremblay et al.[127]studied respiration rate with seasonality ofAntarctic krill, North Pacific krill Euphausia Pacifica (chart 54). NN model for a global krill respiration has a correlation of 0.78 indicating a decrease in respiration with increasing LAT and decreasing DLh.The standard respiration rates with MLR and general additive model accounting seasonal effects showed that in mid-June metabolic activity was minimum while it is at maximum in late December.

- **Ecological imbalance restoration**

Ecological engineering designs of river banks with concrete structure: The construction of concrete banks along rivers associated with human development has become a serious problem in Taiwan. Most ecosystems used by amphibians are lakes and stream banks, yet no related design solutions to accommodate the needs of amphibians. The need to develop the relevant design specification considering protection of the amphibian is imperative. Chuang and Chang [117] simulated climbing ability of Swinhoe's Frog with NNs with good concurrence of experimental data. These results are critical in ecological engineering designs of river banks in any region. Zhang et al.[246] used results of SLP_NN and defined 17 biodiversity priority areas containing 33,200 units (approximating to of 0.83 million km^2 area) in Yangtze River Basin, China (chart 55). It is based on experts' knowledge, mountain boundary data and irreplaceability of units in the model. There is protection of 56% of 32 types of rare forest ecosystem in these areas.

- Ground water level

Mohanty et al.[267found NN results are better than those of simulation model (MODFLOW) for weekly forecast of ground water level in 18 wells in Kathajodi–Surua Inter-basin of Odisha, India (Chart 56).

- **Missing data and imputation**

It is not uncommon that most datasets is riddled with missing values, questionable quality especially in low budget situations. The hydrological modeling, water resources planning and management are not an exception. But, the primary requirement of reliable information is primary data of good quality for long duration over shorter grid intervals with state-of-art-sampling, analytical methods and processing algorithms. Mawale et al.[335] reported that SOM_NN is promising tool to impute missing values of rainfall and stream flow in Shire River basin in Malawi. Nkuna and Odiyo [333] proposed RBF_NN imputation method to fill missing data in rain fall based on neighboring stations measurements. It is satisfactory (chart 57) for hydrological modeling as well as planning and management of water resources.

8.3 Marine environment

Around 70% of earth surface is covered with (oceanic) water bodies. The atmosphere above and earth crust below is its environment apart from distinctly diverse flora and fauna, living organisms, and energy and mineral resources. The main constituent water has miraculous physic-chemical-biological characteristics in all its three phases and in nano- to macro assemblies of pure compound and in association with organic and inorganic species and in interfaces. This marine component as a whole is an important sub-category of global eco-system. During last few decades, a large number of different kinds of wastes are discharged into oceans/seas indiscriminately.

- Rain over oceans

Ghosh et al.[350] applied NNs in detection and estimation of extent of rain (precipitation) over the global oceans from Oceansat-II scatterometer data (chart 58). NNs are used in identification of rain/no_rain and quantitative measure of extent of rain. The prediction of instantaneous/ 3-day/ monthly/ seasonal rain rates and probability distribution of monthly values of scatterometer agree well with AMSR-E data.

Chart 58: Satellite data for prediction of rainfall over global oceans

Detection of rain	Oceansat-II overpasses
Oceansat-II scatterometer ○ Radar back scattering coefficient and ○ Brightness temperature measurements from Rain sensitive parameters Weather prediction NN model	Rain/no_rain prediction Tropical Rainfall Measuring Mission (TRMM) Advanced Microwave Scanning Radiometer for Earth Observation Satellite (EOS) (AMSR-E)

Chart 58b: Quantitative estimation of rain by NN

Region	I	II	III	IV	V
Geographic	(25°N–25°S)	(15°N–45°N)	(35°N–70°N)	(15°S–45°S)	(35°S–70°S)
Rain %	93	87	90	79	85
No_rain %	97	87	86	84	86
Rain ($mm\ h^{-1}$)	45	25	25	45	20
RMS error of instantaneous rain	1.86	0.69	0.47	0.56	0.46

Ocean wave models

The phenomenon of wave transmission through floating breakwaters by considering all the boundary conditions is difficult to model. One of the reasons is vagueness of values of variables, complicated interactions and also their effect on breakwater. This being so, the entire ocean system is responsible of rain cycle, temperature equilibrium and typhoons /tsunamis. It is similar to other mega complicated systems viz. solar system, human brain, life, origin of universe and beginning of life. Puscasu [336] proposed Neural Network Interaction Approximations (NNIA) in third generation ocean wave models resulting in noteworthy improvements (chart 59).

Chart 59: NNs in third-generation ocean wave models

Wavewatch III model	Datasets
Robust NNIA Speed_of_ model NNIA > 2 * DIA NNIA > 200 * (- Web-Resio Tracy,exact method) Emulates exact nonlinear interaction for single- and multi-modal wave spectra	Test scenarios Idealistic Real **Accuracy_ NNIA** Configuration dependent **Future scope** Emulation- practical Time consuming exact nonlinear interactions Fast, high accuracy

wind-wave spectra $\xrightarrow{\text{Direct mapping}}$ Exact nonlinear interactions

Sea surface wind speed

Sea surface wind speed is calculated fromAdvanced Microwave Sounding Radiometer 2 (AMSR2) data. In the first algorithm, brightness temperature at higher frequency over the oceans is simulated by numerical procedures and subsequent inversion with NNs. The second procedure is based on low frequency channels. These values are highly correlated with estimates of MetOp-A scatterometer ASCAT for low and moderate wind speeds. The study area [352] is at platform weather stations in the North Sea and Norwegian Sea even for high wind events.

- Salinity Oceans

The measurement of salinity in large scale in open ocean environments from space has been a long term practice. But, this is not used for estimation in coastal regions. Geiger et al.[110] compiled~2 million salinity records from four regional research vessels and analysed for prediction of salinity in Mid-Atlantic coastal region and estuaries (chart 60). Gueye et al.[97] reported an inverse model with SOM_NN to estimate vertical salinity profiles(chart 60b) in tropical Atlantic Ocean only from input of surface characteristics. It is considered as a classification task. The tidal levels and fresh water discharge effects are influential factors for many human activities in estuarine waters.

Chart 60: NN prediction of salinity in Mid-Atlantic coastal ocean and estuaries

Salinity is critical for circulation patterns, river plumes, transport ecosystem	Corr ([spectral shape of water-leaving radiance, sea surface temperature] versus in_situ_salinity) = Very high

# records	~ 2 million salinity
Regional research Vessels	Four
Period (years)	2003–2008

Data	
~9 thousand salinity records MODIS-Aqua data.	High matching

Predictive_NNs for salinity

Mid-Atlantic coastal region	Estuaries Hudson, Delaware Chesapeake

	Range of RMS_errors (psu)	
NN model	**1.40**	**2.29**
Null model	4.87	10.08
Natural range	**0**	**32**

Chart 60b: SOM_NN to predict vertical salinity in tropical Atlantic ocean

Input	Performance
Latitude Sea surface salinity	+ CC >0.95 + SOM_NN >> [in situ data ; classical_ model]

− Inadequate model for high time-space variable areas
Reason: Limited available dataset in spacio-temporal domain

The salinity of near-surface coastal and estuarine waters changes drastically in spacio-temporal regime and an accurate quantitative data is an absolute need for probing into ecological processes. The satellite remote sensing is a sought after method. But, sensors and algorithms available to monitor open ocean salinity are not adequate [359] for coastlines high resolution applications. Liu et al. [95] reported random forest (RandForest) model was better than MLP_NN, CART etc. to predict SSS (sea surface salinity)in coastal waters making use of in situ as well as remotely sensed data (chart 61).

Chart 61: Prediction of sea surface salinity (SSS)

	Hong Kong Sea, China
Data In situ measurements Optical remotely sensed data from China's HJ-1	**Models for SSS = fn (X;)** MLR MLP_NN (BP)

satellite	CART

X	
SST pH	Total inorganic nitrogen (TIN) Chl-a

Color of oceans

Remote sensing data has unique features like wide range, synchronization and high spatial resolution. This data is useful to monitor the color of waterand to assess the water quality parameters of oceanic, coastal and inland waters. In the estimation of color of oceans from satellite data, the primary pre-processing required is filtering (removal) of atmospheric signal. The black pixel assumption valid for phytoplankton dominatedwaters is generally employed. But, turbid water violates this heuristic. Goyens et al.[354] compared the performance of four algorithmsviz. standard NIR from NASA, NIR similarity spectrum, NIR-SWIR, NN. These results are instrumental in improving retrieval of leaving radiance (Lw(λ)) in water from satellite images. Ioannou et al.[355] retrieved inherent optical properties (IOP) of Phytoplankton and non- Phytoplankton in ocean water with NN modeling from remote sensing satellite data (chart 62). In another step, chlorophyll concentrations were calculated more nearer to measured ones than in earlier similar high tech ventures. Orzepowski et al.[7] studied the efficiency of MLP_NN (chart 63) in retrieving diffuse attenuation coefficient for down welling spectral irradiance ((Kd at landa=490)) using field measurements of global oceanic and coastal waters.

Chart 62: Prediction of Phytoplankton characteristics and chlorophyll concentration with NNs using remote sensing satellite data in multiple-sequential-steps

Input (X)	Model	Output
Wavelength 412, 443, 488, 531, 547, 667 nm	NN	In-water particulate backscattering (bbp), phytoplankton (aph) Non-phytoplankton (adg) absorption coefficients at 443 nm.
Non-phytoplankton absorption coefficient (adg) at 443 nm		dissolved (ag) particulate (adm)
Data set (NOMAD) Rrs	NASA bio-Optical Marine Algorithm NN model	retrieve IOP at 443 nm Res (measured NOMAD and retrieved IOP values): Very low
Input IOP related Rrs values	NN	chlorophyll concentration [Chl]
Inference Accuracy_[Chl] >> MODIS OC3 algorithm ; >> without_IOP in input		Satellite MODIS (or similar satellite) Probe: water remote sensing reflectances (Rrs)

Chart 63: Diffuse attenuation coefficient	
Datasets	Models
NASA bio-optical marine algorithm dataset (NOMAD) Eastern China Seas dataset	Lee's quasi-analytical algorithm-based semi-analytical model, Wang's switching model, Chen's semi-analytical model, Jamet's neural network model, MBPNN

Instrument(MODIS)	
NASA Moderate 5420 Resolution Imaging Spectroradiometer ()	
Atmospheric effect removal	Near-infrared band-based and shortwave infrared band-based combined models

Inferences
MLP_NN >>other models
28% uncertainty in estimating Kd(490) from the MODIS data

Neural network modeling is used in ocean color [338,358], color of European seas[357], tropical cyclone track forecasting [62], ocean wave energy in Atlantic/ Pacific Oceans, [329], wave transmission prediction [330], wave forecasting in East-coast of India [331], forecasting ocean wave height [328], oceanic total alkalinity estimation [289], surface salinity in the Chesapeake Bay [359], prediction of two unnamed seamounts in the Arabian sea [232], prediction of bathymetry from satellite altimeter [232], sea level in Darwin Harbor [100] and prediction of marine beach water daily quality in Hong Kong [251].

Chlorophyll-a

Coad et al.[149] proposed successful predictive models for Chlorophyll-a concentrations with NNs. The accuracy decreases with one-, three- and seven day-ahead predictions(chart 64). A further step in near real time sourced data from telemetered monitoring buoys, automated systems and results of mixing predictive model enhanced the efficacy of proactive algal bloom managerial strategies. Awad [121] estimated concentration of chlorophyll-a from Hyperion satellite hyperspectral images using FF_NN data driven model (chart 65).

Palmer et al.[348] performed an intensive study of algorithms for retrieval of chlorophyll-a (chl-a) in the highly turbid and productive waters of Lake Balaton, Hungaryby MERIS (MEdium Resolution Imaging Spectrometer)data of 10 years. Sentinel-3 Ocean and Land Colour Instrument (OLCI) will be used in the phase of the study.

Fluorescence Line Height Maximum Chlorophyll Index	Good
NN	Less accurate

Chart 64: Prediction Chlorophyll-a concentrations

Monitoring schedule (15 min intervals) ⇨ Chlorophyll-a, ⇨ Temperature (water and air) ⇨ Salinity ⇨ Photosynthetically available radiation	▶ One, three and seven days in advance ▶ Daily mean, 10th and 90th percentile Model NN

Chart 65: Factors affecting Quality of coastal sea water

- Turbid river inputs
- Open sea flushing
- Different pollution sources
- environmental disasters manmade
  - Oil spill
  - Continuous discharge
    - Chemical
    - Solid wastes.

Factors for cyclone track

- Wind pressure
- SST
- Air temperature
- Ocean currents
- Earth's rotational force coriolis force

Chart 66: Multiphase modeling of time series

Method	Function
NARX	Identification of wave-structure interaction system
Multi-tone harmonic probing method	Linear and quadratic frequency response functions
Quadratic Volterra series	Prediction of time series of response

The content of chlorophyll a in coastal waters of Galician rias (NW Spain) from MERIS full resolution data [361] and in optically complex waters (rias Baixas, NW Spain) [360] were investigated with NNs. The origin of green macroalga [87], macro invertebrate image databases retrieval [108] and dispersal of a pelagic species [131] drew attention with data driven NNs.

Marine structure

Kim[22] applied NARMAX based quadratic Volterra seriesto predictdynamic response of a slender marine structure (chart 66).

Cyclone forecast

In accurate forecast of cyclone, a combination of global as well as basin specific techniques is used to minimize economic toll and no-loss–of-human life. The dissimilarity of geographical and climatological profiles of various cyclone formation basins are hurdles for a single forecast system.

9. Quality of water

Water quality analysis, stipulations and their indicators vary with purpose and standards of the concerned authority/governess. Concentrating on recent trends, multivariate statistics, time series analysis and neuralnetworks are sought after tools in number crunching to bring out information and action course by agencies. Liu et al.[307] applied hybrid SVR with real coded GA in forecasting water quality in aquatic factories of YiXing, in China (chart 67). López-Lineros et al.[252] validated an automatic detection of incorrect records and retaining quality control stipulations for ten-minute river stage data using non-linear_ autoregressive_NN (NonLin-AR-NN). The detection efficacy was ascertained by injecting noise of different magnitude. The hybrid NN detected more than 90% of altered records, while long practiced conventional tests detected only around 13% for high noise. Further, nonLin-AR-NNhas consistent efficiency even at intermediate/ lower error ratios, while earlier test could detect up to 6% of erroneous data. Olawoyin et al.[215] used SOM_NN to probe into water, soil and sediment quality in petrochemical regions of NigerDelta (Nigeria) (chart 68).

Knowledge extraction by rough sets in water quality (TDS) analysis: The vagueness and inherent uncertainties in water contamination/pollution poses a threat to reach the desired accuracy. Karami et al.[109] used rough sets, variable consistency dominance-based tool, to derive knowledge in TDS (chart 69) in Latyan Watershed, north of Tehran, Iran.

Chart 67: Prediction of water quality in aquatic factories of YiXing, in China

Real-valued GA	Optimal SVR parameters
SVR	Input : optimal parameters

Inference

[SVR + GA_realValue] >> SVR or MLP_NN_BP

Chart 68 : SOM_NN for quality of water, soil and sediment in into petrochemical areas of Nigeria

- Goals
- Identification of pollution sources
- Similarities in quality of samples

Model

SOM_NN

X

- Chemical,
- Ecotoxicological
- Toxicokinetic
- Physical

	#Samples
Water	11
soil	38
sediment	54

Location

Niger Delta, Nigeria

4 areas

Table 10: Quantitative estimation of phycocyanin in potable water sources with NNs

Model	(R^2) Location	
	CIN	SA
PLS_NN	0.92	0.09
TBM	0.77	0.94
NN	0.86	0.95

Spectra (Expt & simulated)
- RRS
- ESA/Sentinel-3/ OLCI
- EO-1/Hyperion spectra

- NP : 363
- #field surveys: 24

\

RRS	Remote Sensing Reflectance Spectra
OLCI	Ocean And Land Color Instrument
SA	South Australia
TBM	Three Band Model
CIA	central Indiana USA

Chart 69: Rough sets in rule extraction of TDS in water

X

- Precipitation
  - River water temperature
  - Runoff measured at 22 monitoring sites
  - MODIS sensor
    - 16-day NDVI
    - Land surface temperature

Time period : 2002–2007

Pre-processing

- Moving average filter
  - Decreased noise
  - Reduction in the width of the boundary region between the lower and upper approximations

Rule (If X then $$_TDS) generation

Data mining tool

VC-DRSA TDS data to the explanatory variables

extracted rules

- Effective
- Straightforward in probing into relationships between TDS & environmental factors

9.1 Drinking water

According to one estimate, one billion (884 million) people have no access to safe drinking waterworldwide. Estrogens are common in river and sometimes found even in drinking water. The scarcity of potable water and even fresh water for domestic/industrial use is multiplying with increase in world population as well as contamination of water bodies. Now, even using water once in a day has become luxury. Phycocyanin is a threat to diminution of quality potable water sources. The remote monitoring of

cynobacterial blooms in central Indiana and South Australia is of recent interest. Song et al.[234] reported (table 10) PLS_NN is better than TBM and NN through remote sensing spectral data.
Soak holes: They are drilled directly into the top of the fractured-rock. The storm water and sediment runoff from the city streets are collected into the soak holes and reaches water table through infiltration. The immediate effect in Mt.Eden aquifier cannot be predicted by conventional mathematical methods. Hong [386] studied the effect of storm water infiltration of rainfall on the ground water quality using SOM-NN. The extraction of knowledge from ground water usage, the land use patterns and geological data is performed through hierarchical Kohonen SOM-NN. The decrease in contamination of surface water of the urban streams, and increasing the recharge of the shallow aquifer are the noteworthy advantages.

Reservoirs: These are an alternative major source of drinking water in regions with insufficient ground water sources. NNs were used as innovative computational tools in water resource management in Cyprus. NN model performs better in the estimation of annual water supply with inputs -- area of the watershed, altitude, slope, average of annual and monthly rain height. Iliadis [163] proposes that this model can be applied to other countries with appropriate changes to imbibe the information about areas facing the water deficit or flood.

Quality of the potable water: The quality of the potable water reaching the consumer depends on multistage compound subsystems viz., quality of input water, processes in treatment plant, distribution system, chemical/microbiological deterioration [181] in the distribution pipes etc. Of the several processes, coagulation/flocculation/ sedimentation/ filtration are typical sub processes deserving attention. The practices in water treatment are governed by complicated non-linear relationship between a large number of physical, chemical, biological parameters, operational conditions and the quality of the chemicals used. Further, the processes in coagulation are multiple interwoven and are not understood rendering the development of a mechanistic/physical model extremely difficult. Thus NNs, the data driven models have been in vogue with commendable success rate. This drinking water source protection measures in operation in China after 2005 incident in Songhua River are still hampered by inadequate monitoring schedules. It is worth noting that GA-NN model predicted better even 8 h ahead of time.

9.1 Drinking water through treatment

- Residual aluminum

In order to keep the outlet from water treatment plant (WTP) [183]as clean as possible, the optimum alum and powdered activated carbon for diff183erent control actions are critical. The acceptable residual aluminum concentration in the water is 0.2 mg/lt [190]and any higher amount of Al is against the imposed laws. In coagulation, alum ($Al_2SO_4.18H_2O$) is used. If the PH is not maintained, the added alum decreases the pH resulting in removal of DOC (Dissolved Organic Carbon) [White-1997]. NN was used as a module in the process for predicting optimum concentration of alum and carbon. Jar test determines optimum alum dose [190], the disadvantage being cost and longer time(table 11). These limitations are circumvented in current drinking WTPs by inverse-process models as well as earlier ones. Since, the prediction was poor; the forecasted water quality parameters are included in the input. It is a straightforward prediction approach of optimum alum doses directly. Maier [181] employed the NN model to assist the treatment plant operators in estimating optimum alum dose [183]for WTPs in southern-Australia, which is based on improving inverse model. The model predicts treated water quality parameters from raw input --turbidity, color, residual aluminum, absorbance of UV light at 254nm, pH and alum dose. Another option is prediction of optimal alum dose from raw and analytical parameters of treated water.

Table 11: details of NN predictive model for optimum alum dose in water treatment for drinking [181]

Model	Output		Input			Architecture I-H1-H2-O	Lr rate	Momentum
M1	Turb	Col	Turb UVA-254	pH	Col	7-8-0-3	0.5	0.5
	UVA254		Alk	DOC				
M2	Resid-Al	pH	I# of M1 + UVA-254	Turb	Col	10-8-0-2	0.8	0.2
			Alum-dose					
M3	Alum-dose		I# of M1 +	Turb	Col	9-8-8-1	0.8	0.2
			UVA-254	Resid-Al				

- Residual Cl2 in drinking water

Chlorination is carried out in the final disinfection phase of a drinking water treatment system to eliminate pathogens [194]. The amount of chlorine should be sufficient to ensure microbiological stability and as low as possible not to cause odor throughout the distribution system. Residual chlorine is an efficient indicator of quality of water in the distribution system. The minimization of disinfection by-products, which are formed by the interaction of organic matter and excess residual chlorine in the treated water, is warranted [183]. Further the greater the organic matter present in the water, the higher is the chance for the formation of DBPs. The decay of residual chlorine is related to operational conditions of the treatment plant, the characteristics of pipelines in the distribution system and the quality of the input water. The chlorine content is controlled by monitoring it at strategic points in the treatment plant and distribution system. Although, online-analysis is employed, there is a time delay due to the passage of water between different points. Thus, modeling and prediction of residual chlorine in the entire cycle is of prime concern(table 12). From the forecast values of residual chlorine, the operator will adjust the dose in the treatment plant, for example, the storage tank outlet and at a point located down the stream in the pipeline [194].

Chlorcast is a decision support system with NN in the core, to model the residual chlorine in drinking water tank and water distribution system for a city(table 12). It is applied for water distribution at city of Sainte-Foy [183]based on time series model for evolved residual chlorine. The advantage of this method is generation of information useful for operator. The chlorine dosage or residual concentration at critical location can be modeled separately. Yet, the disadvantages noted are requirement of large amounts of past data, disability to explain results, bacterial regrowth due to under doses of chlorine and by-products formation [190]that are harmful to human health due to over doses.

Table 12a: Model errors of forecast model (residual chlorine –verification database) [194]

Model	*Erel* (%)	REQ
Trivial 0.089	11.3	0.122

Table 12b: Forecast models in different seasons [194]

Model	Winter		Summer	
	Erel (%)	REQ	*Erel* (%)	REQ

ARX (6 inputs)	11.5	0.130
ANN (6 inputs)	11.1	0.128
ARX (7 inputs)	9.0	0.111
ANN (7 inputs) 0.073	8.8	0.108

ARX	7.9	0.100	10.1	0.120
ANN	7.8	0.091	9.8	0.114

Table 12c: Average errors in forecast model for extreme values of residual chlorine under summer condition [194]

Values of residual chlorine at the tank outlet	ARX	NN
<Mean ± 6 S.D.	0.162	0.121
>Mean -S.D.	0.151	0.103

Table 12d: Forecast models in different seasons [194]

Model	4-inputs		6-inputs	
	***Erel* (%)**	**REQ**	***Erel* (%)**	**REQ**
Trivial	9.3	0.036		
	Winter condition			
ARX	26.3	0.090	9.1	0.037
ANN	**25.5**	**0.087**	**8.9**	**0.036**
	Summer condition			
ARX	18.8	0.098	9.0	0.055
ANN	**17.9**	**0.092**	**8.8**	**0.053**

Table 12e: Performance of Chlorcast in Treatment for drinking water (Clear water tank)[190]

Data	**#observations**	***R2***	**MAE (mg/l)**
Entire data sets	3551	0.9871	0.012
Training	2494	0.9990	0.003
Test	701	0.9603	0.032
Prediction	356	0.9551	0.032

MAE : Mean average error

Table 12f: Performance of Chlorcast in drinking water treatment (distribution network) [190]

Data	**#Observations**	***R2***	**MAEa (mg/l)**
Entire data sets	2886	0.9904	0.008
Training	2025	0.9999	0.001
Test	581	0.9710	0.024
Production	280	0.9624	0.025

9.2. Domestic Water consumption

In Kuwait, fresh water is only from desalination plants and 88% of the total consumption is in the residential houses [387]. The inputs for NN are those from best MLR model. The treatment plants of drinking water remove microorganisms and natural/anthropogenic chemicals [190].The reduction of color, odor, turbidity etc., ensures acceptability from aesthetic point of view, while removal of biological and chemical components is to safeguard the health of the consumers. A NN model was developed to predict the turbidity and color of treated water from Rossdale water plant in Edmonton, Alberta, Canada. The software employs only a single parameter, (i.e absorbance of UV light at 254nm) to control turbidity and color. The limitation of this method is that it ignores high aluminum content, responsible for Alzheimer disease. Further, it is implicated in individuals requiring renal dialysis. The water use in different countries and the variables relevant are described in table 13.

Table 13a: Water consumption in different countries

Water consumption per person per day	**Liters**
Bahrain,	526
Kuwait,	481
UAE	700
USA	744

Table 13b:Input variables to model weekly water consumption in few of residences of Kuwait [387]

I#	Name of Input variable	Model 1	Model2	Model3	Model4
X1	Income category	✖	✓	✓	✓
X2	Number of rooms	✓	✓	✓	✓
X3	Number of bath rooms	✓	✓	✓	✓
X4	Number of people residing	✓	✓	✓	✓
X5	Size of attached garden	✓	✓	Log(x5)	Log(x5)
X6	Temperature (average)	✓	✓	Log(x6)	✖
X7	Humidity (average)	✖	✖	Log(x7)	✖
X8	Transformed week-in-the-year	✖	✖	✖	✓

10. Pollution of water bodies

- Discharge standards

The discharge standards of effluents waste and gases into environment (air, water and land) are a part of keeping up the quality standards [183]of environment. This in turn produces healthy living surroundings for the inhabitants.

Urban lakes contaminated with Perfluorooctane sulfonate (PFOS): Perfluorooctane sulfonate (PFOS) is a wide spread pollutant in urban lakes worldwide. Xiao et al.[393] performed EDA of PFOS concentration in 304 fish from 28 urban lakes using GIS information. The NN model is applied to lakes in Minnesota contaminated with high levels of PFOS (chart 70). The highlights and limitations of EDA and Kriging interpolation are compared.

Chart 70: NN model for PFOS in urban lakes

☞ Preliminary classification	☞ Hierarchical cluster analysis
☞ Predictor Screening	☞ Regression tree
☞ Model : NN ☞ Test data ⇨ Minnesota ⇨ #lakes :40	Source of pollution ☞ Industries ☞ Commercial activities ☞ Vehicular traffic ☞ Surface runoff

Chart 71: SOM_NN + PCA for water toxicity in river basin

Pollutants 60 Period : 2007 and 2008	Sampling stations: 232

PCA	Influential variables trends in pollution
Kohonen_ SOM_NN	Spatial distribution of toxic risk

Water toxicity:Carafa [374] et al. reported tool for water managers in mitigating Water toxicity in a Mediterranean River Basin District using SOM_NN (chart 71). The field data on macroinvertebrate and diatom communities are correlated with NN_model predicted toxic profiles.

Arsenic pollution and its effects on human health:The increase in arsenic levels in environment is through anthropogenic activities. The species of inorganic arsenic (as As(III) or As(V)) in the ground water depend up on pH, adsorption reactions, biological activity and redox conditions. The contaminated drinking water and crops harvested are routes of ingestion causing severe ill effects on human health [293].

Health hazard due to edible mushrooms

Li et al. [77] reported SparR (structure parameter relationships) for logarithm of formation constant of macrocyclic ligands and cesium with six molecular descriptors using MLR, NN, uniform design optimized (UDO_) SVM with a correlation coefficient of 0.95 for test set. Edible mushrooms have high affinity for cesium with a consequence that humans eating those mushrooms accumulated cesium and had health disorders.

✍ Surface water pollution

The fast pace industrialization and growing population are key factors for surface water pollution events even in China in the last two decades. Burchard-Levine et al.[236] reported an early (2 h ahead) warning model topredict NH3–N, COD and TOC with GA-ANN using most sensitive input variables monitored 12 km upstream(Chart 72).

Chart 72a: GA_NN for drinking water source quality

	Sensitive Input	MSE	MPE	Regression
NH3–N,	✍ TOC, ✍ CODmn,	0.0033	6	92

Chart 72b: Quality of surface waters

Protection of ecosystems

	TP, NH3–N Turbidity				
COD	Turbidity CODmn	0.201	5	0.87	
TOC	Turbidity CODmn	0.101	2	0.94	

- Long term sustainable water supply
- Control of emissions
  - Minimize priority pollutants in surface water
- Protection of coastal seawater on an international basis → min (anthropogenic pollutants)

Aquifer quality deterioration

Other sources of contamination for aquifers, like in ground water, are residential, agricultural and industrial activities. Further the untreated wastewater or even the partially treated one decreases the quality of water [185]. Nitrate, both from point and non-point sources pollute shallow aquifers. Nitrate is lost from soils by leaching because of its high mobility. The generation of land use scenarios is an optimization task.

Ground water contamination

A number of human induced changes continuously threaten natural aquatic ecosystems. The ground water is contaminated through transportation of chemicals from industrial, commercial, residential activities as well as influences from the storm water infiltration, transport and reactions. Accidental spills, landfills, storage tanks, pipelines etc. further deteriorate its purity. Thus, decrease in the quality is due to complex and uncertain factors. When the reservoirs are near the agricultural land, the nutrients/pesticides diffuse through leaching. The chlorinated compounds in air reach surface of land as dense nonaqueous phase. It then passes through unsaturated zone under capillary and gravitational force and settles in low geological layers of low permeability resulting in long term (persistent) contamination of groundwater. On the other hand, chlorinated ethenes in the ground water volatilize and migrate by diffusion into soil surface and then into air. The thermodynamics and kinetics of the mass transport processes between unsaturated and saturated zones of sub surface dictate net fate of the chemicals [208]. One of the groundwater pollution sources is nitrate nitrogen (NO3−-N) from agricultural activities. The saturated water content (SWC), field water capacity (FWC) [88], effects of chicken manure on ground water [26] and groundwater pollution in Shandong by nitrate nitrogen [308] were investigated with NN modeling.

Fecal pollution of water resources

Fecal indicator bacteria (FIB)

The downstream water is generally contaminated with fecal indicator bacteria (FIB) rendering them for high risk to waterborne illness, if consumed as potable or during recreational exposures. LVQ_NN has been used to forecast recreational water quality using fecal indicator organisms [394] in Charles River Basin (Massachusetts, USA).

Fecal indicator bacteria (FIB)
- Enterococcus faecalis
- Escherichia coli

Microbial fecal source tracking (MST): Reischer et al.[212] reported that dominant sources of fecal pollution in mountainous karst spring catchment area of Austria were ruminant animals(chart 73). This is from a monitoring schedule of 17 months employing nested sampling design covering hydrological and pollution dynamics of the spring. E. coli is one of the FIB used in regulatory limits. But, recently fecal Bacteroidetes having host-specificity are detected by quantitative real-time PCR

Marine pollution

The transportation on seas and oceans day by day introduce marine invasive species posing a great threat for the sustenance of marine organism. The genus Physalia (Cnidaria: Siphonophora) around coastal New Zealand, were used to arrive at factors influencing a passive disperser. Of several routes of marine pollution, oil spills counts high and arise due to uncontrollability over made-made ventures themselves.

- **Oil spill**

The eco system pays a price for Oil spills (Chart 74) which indirectly affects of welfare of mankind and life of marine organism. A simulation model was developed for trajectory of oil released from pipeline leaking in the Gulf of Mexico. For synthetic-aperture-radar (SAR) observations, a Texture-Classifying Neural Network (Tex.Class_NN) was used to delineate ocean oil slicks. During the simulation, GNOME model was driven with ocean currents from NCOM (Navy Coastal Ocean Model) outputs and surface wind data measured by an NDBC (National Data Buoy Center). Wei et al.[299] employed NN classification to pin point the oil spill areas from SAR images. Based on historical data of other oil-spill episodes, MLR model was developed. Singh et al. [303] proposed a semi-automatic model for detection of oil spill with NN . The system is optimized utilizing wind and current history information for near real time offshore platform pollution making use of TerraSAR-X over the North Sea. Synthetic Aperture Radar (SAR) is an effective tool for remote sensing through satellite.

Chart 73: Monitoring parameters

- Genetic markers for fecal sources
- Microbiological
- Hydrological
- Chemo_physical

Chart 74(a): Cost of losses

Cleanup
- Socioeconomic
- Environmental

Chart 74(b): Semi-automated approach for oil spill detection

- Data: 156 TerraSAR-X images
- X: Eight feature parameters extracted from each segmented dark spot
- Classification algorithm: NN

Chart 74(c): Marine pollution due to a few oil spill accidents

2006	pipeline bombing	Lagos, Nigeria	People # Killed 270 injured 170
2010,	Drilling Platform explosion	Deepwater Horizon Gulf of Mexico	oil Leak: 1.43 million m^3 water pollution: 9900 km^2
2011	Pipeline explosion	Dalian, China	oil Leak: 1500 tons water pollution: 430 km^2
Daily production of oil:			87 million barrels globally

Schulz and Matthies et al.[301] found NN is superior to MLR in predicting litter from fishing, shipping, and tourism sources in southern North Sea even with less information. Lammoglia, [356]detected oil seepages on the ocean surface by qualitative remote characterization.

Influential factors
- Biological nature of the process.
- Variability of influent composition
- Dynamic nature

11. Waste water (WW) Treatment

- Delay of analytical results and
- Lack of on-line sensors

The prime concern is to maintain natural water systems with as high quality as possible (AHQAP). Waste water treatment before letting them into rivers helps in ensuring good quality of flora and fauna in marine/riverine environment and other water bodies. Thus, the management of wastewaters or waste solid is indispensable, but not an option. Municipal wastewater contains suspended solids, organic matter, pathogens and nutrients. Oxidation of biodegradable organics is stabilized as low energy compounds by maintaining the optimum level of microorganisms and oxygen through aerators [192]. The management of odor in waste water treatment plants (WWTP) and solid waste is complicated. The emissions from bio waste and their treatment plants are more offensive to the public. It leads to an odor impression with 50% of defined population. The laws in Germany are stringent regarding the odor acceptance.

WWTP (Waste water treatment plant)

The processes depend upon sources of wastewater, their flow rates/chemical/biological composition/processes, ambient conditions etc. The recycle rate of the settled sludge and mode of operation in different seasons and geologically diverse sites dictate the requisites parameters for real time control. The multiple objectives in this pursuit are target efficiency of process and minimum ratio of cost to throughput under dynamic loading conditions [166]. Thus, the wastewater treatment plants (WWTP) involve composite physical/biological/chemical/ processes not viable by classical modeling approaches [183]. The number of influencing factors for anaerobic digestion is large and differs with the source of the waste. The physical modeling of biogas formation involves mass transfer between gas and liquid phases. The data on mass transfer coefficients between gas and liquid phases are scarce rendering anaerobic biological treatment of wastewater is an intricate process. Further, the processes in WWTP are dynamic involving incoming water discharge, actuation and outgoing variables [192]. They are with strong non-linear distribution between I/O variables in spatio-temporal domain. Input as well as output variables are interrelated. Missing data, variable errors associated with different factors are common. The magnitude of variables in time domain is in small chunks with varying patterns. Hence the process is multifaceted and not amenable for straightforward solution. Thus, WWTP translates into inverse-hard, non-polynomial (NP)-incomplete models. The solution is not unique and the choice of best set of models from the multiple sets of solutions is also not viable. NNs had a track record of offering a solution for systems with incomplete information. But, the complicated equations are solvable with recent numerical methods using high-ended hardware systems.Thus, translation into mathematical model is not trivial.

WWTP processes→ inverse-hard, non-polynomial (NP)-incomplete models

Limitations of mechanistic models in WWTP:Mechanistic or ab initio physico-chemical-biological-meteorological principles projected on to mathematical framework results in a set of stiff differential equations. The data requirement, boundary conditions and solution procedures are not a cake walk like for a small set of ODEs in routine use [164]. Further, extensive simulations are required before arriving at even a sub optimal solution. Also, the system of equations developed for WWTP are stiff with a broad range of time constants necessitating long simulation time due to small integration steps required(table 14).The way out is to resort to surrogate mechanistic approach, where in complex mechanistic models are replaced with simpler ones. For instance, ODEs are used instead of PDEs. The model fails when tanks connected in series are employed. The complexity of model is reduced through boundary location. Removing the upstream parts of the sewer mechanics reduces the size of the system.

Control theory:The programmable classical logic control theory employs a trial and error method of mathematical models. The advantage claimed then was minimal human expertise and thus was deemed as automated system. Further, the provision for manual intervention in case of catastrophic incidents was acclaimed as a remarkable way of disaster management. Now, continued stipulations are in the direction of alerting and automated control of disastrous moments.

Table 14 Comparison between plant performance indexes for Scenario 1 calculated for 20 years of mechanistic WWTP model (ASM3) and ANN predictions

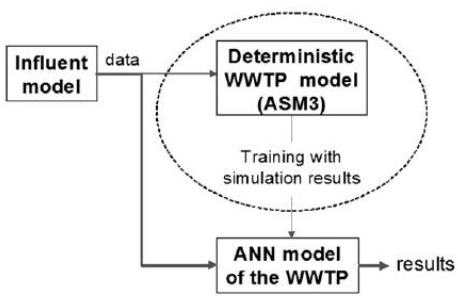
Variable	No. of violations	
	ASM3	ANN
BOD5 (g/m3)	0	0
SNH4 (g N/m3)	5894	5620
TN (g N/m3)	8081	8403
TSS (g/m3)	0	0
COD (g/m3)	0	0

ANN input variables:

- S_I – soluble inert material
- S_S – readily biodegradable substrate
- S_{NH4} – ammonium nitrogen
- X_I – particulate inert material
- X_S – slowly biodegradable substrate
- X_H – heterotrophs
- X_A – autotrophs
- TSS – total suspended solids
- Q – flow rate
- T – temperature

ANN output variables:

- BOD_5 – biochemical oxygen demand
- TKN – total Kjeldahl nitrogen
- S_{NH4} – soluble ammonium
- TN – total nitrogen
- TSS – total suspended solids
- COD_{TOT} – total chemical oxygen demand



Courtesy ref [164]

Table 14(b) Reduction of CPU time for simulation of WWTP [164]

Replacing mechanistic models with simple ones	ODE reduced to partial differential equations
Reduced activated sludge model	Integrated urban water system simulation
Activated sludge model 2d	Empirical model with WWTP data
Secondary classifier of WWTP	Mechanistic model replaced by empirical
Primary classifier	Empirical model
NN	Reduction in CPU

Table 14(c): Advantages of NNs over mechanistic models in WWTP[164]

- NNs function over wide range of operating conditions with adequate prediction accuracy
- Simulation is (36 times) faster than with mechanistic models
- Repeated training is not necessary when combined with integrated waste water system. The time reduces by a factor of 1300

NN models:In this decade, data driven evolutionary NNs with well proven supporting tools are not the alternative by choice or prejudice but based on their performance and growing theoretical proofs of their purpose under a variety of conditions. Raduly [164] replaced mechanistic model by NNs with lot many advantages. The data for a longer period (one year) is minimum as the seasonal temperature variation has profound influence. The current stipulation is to run the plant with comparable performance under all environmental conditions, unlike in yester years when the performance was assessed based on weather conditions of that day. Now, model should respond to changes in frequency, intensity and duration of rain events. Data for longer periods are essential to take care of rare occurrences of combined sewer overflows. For example, a three-year data cannot recognize overflow in case of a detention cycle of 5 years. Further, more accuracy is needed and complexity increases if it is integrated with urban waste water system.
However, models, (model driven or data driven), simple or complex do not explain all the experimental results in toto.

SLP_NN:Sridevi et al.[72] applied SLP_NN with LM training to predict biohydrogen production in distillery wastewater of a hybrid up flow anaerobic sludge blanket reactor (chart 75).

Chart 75: prediction of biohydrogen production in sludge blanket reactor	
SLP_NN 4-20-1 Trn: LM	NP : 231; Temp: (34 ± 1 °C) pH : 6.5

Fuzzy NN: Honggui et al.[93] introduced a fuzzy NN based online fault detection of sludge volume index (SVI) sensor. The results of earlier fault free operation of WWTP were the training data set and detection of fault was from residual of measured and predicted concentration values. The rigorous testing on a real WWTP system showed the efficiency of NN approach.

NN + Fuzzy logic+ rough sets:A hybrid fuzzy NN employing rough set theory for automating the control of processes in industrial wastewater treatmentis proposed. The analysis consists of three stage sequential procedure. It searches a set of multi-objective control strategies. Rough sets have greater indiscernable capability. GAs are parallel procedure in search space and they are the best to arrive at an optimum without the knowledge of derivative information. The choice of fitness function is the key factor. The combination of Gas, rough sets fuzzy logic with NNs is far superior compared to individual components or their binary- ternary- hybrid strategies (table 15). Fuzzy sets and rough sets are used to analyze inexact imprecise uncertain and vague knowledge.

NN + SVM:Betrie et al.[368] found NN to be better than SVM and integration of results of prediction of NN and SVM by aggregation is superior to component procedures (chart 76).

Table 15(a): The definitions of parameters for modeling analysis industrial waste water

Parameters	Definition
Control variables	
pH at B1	The pH value at B1
pH at H1	The pH value at H1
pH at I1	The pH value at I1
TP	Total phosphorous (mg/L)
TN	Total nitrogen (mg/L)
TFR	The flowrate of treatment effluent (m3/d)
EL	The amount of electricity consumption (kW h/d)
State variables	
HAC	Acetic acid at equalization basin

a	:	Acetic acid at equalization basin (mg/L).
b	:	Benzoic acid at equalization basin (mg/L).
c	:	Paratoluic acid at equalization basin (mg/L).
d	:	Terephthalic acid at equalization basin (mg/L).
e	:	Total organic carbon at equalization basin (mg/L).
f	:	The pH value at B1.
g	:	The pH value at H1.
h	:	The pH value at I1.
i	:	The flowrate of treatment effluent (m3/d).
j	:	The amount of electricity consumption (kW h/d).
k	:	Total phosphorus.

	(mg/L)
BA	Benzoic acid at equalization basin (mg/L)
Ptol	Paratoluic acid at equalization basin (mg/ L)
TA	Terephthalic acid at equalization basin
	(mg/L)
TOC	Total organic carbon at equalization basin (mg/L)
Control goals	
COD	COD in the effluent (mg/L)
SS	SS in the effluent (mg/L)
cost	Partial operatingcost (NT$/ton COD removal)

l	:	Total nitrogen

Table 15(b) : The derived fuzzy rule table based on GA and rough set theory

Rule no.	State variables						Control variables					
	a	b	c	d	e	f	g	h	i	j	k	l
1	4	3	—	—	6	2	1	2	3	3	—	—
2	5	3	—	—	6	4	2	3	7	6	—	—
3	4	3	—	—	4	3	2	4	6	2	—	—
4	3	3	—	—	4	2	1	2	3	3	—	—
5	5	3	—	—	7	3	2	4	6	2	—	—
6	4	3	—	—	5	3	3	3	6	5	—	—
7	5	3	—	—	4	2	2	3	5	5	—	—
8	3	3	—	—	6	2	3	3	7	5	—	—
9	2	2	—	—	4	2	2	3	3	5	—	—
10	4	3	—	—	3	3	2	4	6	2	—	—
11	2	3	—	—	3	2	1	2	3	3	—	—
12	5	3	—	—	5	4	2	3	7	6	—	—
13	2	3	—	—	5	4	2	4	7	5	—	—
14	2	2	—	—	2	4	3	1	2	3	—	—
15	4	2	—	—	5	3	3	4	5	4	—	—
16	2	3	—	—	4	2	2	3	3	5	—	—
17	3	3	—	—	5	2	3	3	7	5	—	—
18	2	2	—	—	5	4	2	3	7	6	—	—
19	3	3	—	—	3	3	2	4	6	2	—	—
20	2	3	—	—	2	4	2	3	7	6	—	—
21	5	2	—	—	5	2	2	1	4	6	—	—
22	2	2	—	—	3	2	1	3	4	2	—	—
23	4	2	—	—	6	2	1	3	4	2	—	—
24	2	2	—	—	6	2	2	3	5	6	—	—
25	1	3	—	—	3	3	2	4	6	2	—	—
26	4	2	—	—	7	2	3	3	6	6	—	—
27	1	3	—	—	2	4	2	3	7	6	—	—
28	4	2	—	—	3	2	2	3	5	5	—	—
29	5	2	—	—	3	4	3	1	2	3	—	—

W. C. Chen, N. Chang, J. Chen, Water research, 37(2003)95-107
Rough set-based hybrid fuzzy-neural controller design for industrial waste water

Chart 76: Prediction of acid rock drainage chemistry	
Aggregation method for - NN - SVM	Prediction of acid rock drainage chemistry
- Predictive uncertainties	Probability bounds analysis

Component	
1	2
Caffeine Cocaine Carbamazepine Diazepam Fluoxetine Hydrocodone Ketorolac	Tramadol Alcohols natural hormones Hormone-like chemicals

WWTP technologies

- Bioaugmentation
- Membrane reactors
- Advanced oxidation process
- Sorptiom
- Electrochemical methods

EDC

- Pharmaceuticals
- Personal care products
- Pesticides
- Industrial prodcuts
- Phytoestrogens

The limitations of individual component modules are diminished or eliminated while retaining the unique positive features. The information and knowledge bits generated out of the simulation experiments are pivotal in intelligent design of new WWTP plants. The objective is to enhance the functional aspects and decreasing the operational costs of the already running prototype plants. In yesteryears the performance indices were evaluated under dry weather. But, nowadays the efficiency of targets are focused in all hostile environmental conditions. Thus the data input requirements include historical incidents under varying intensity and duration of rainfall/temperature in addition to the rare sewer/detention pond over flow situations. Raduly [164] developed NN models separately for influent flow and the treatment process. He opines a one-year of influent data and decadal data for overflow of detention pond will result in reasonable conclusions. The CPU time for simulation of such a mega event is very large but a first step to quantify the control strategies in a real time operable WWTP.

NN + Fuzzy logic + GA (Multi objective optimization) :With a priori information of contaminants in the waste stream at the input of the plant, NN-predictive models guide personnel (operators) at WWTPs to maintain quality of effluents. In Houston city, an automated wastewater flow control at pilot level was studied. It controls the incoming flow by 14 pumps of different capacities. NN is employed to activate or deactivate the pumps based on weather conditions, time of the year and approved protocol. Prior to this, this task was done by human operators. A multi objective control strategy for WWTP was successfully applied for a plant in Taiwan [183]. A representative static function was generated in the model. The treatment plant is controlled through automatic tuning employing the fuzzy logic and GA is used along with NN. A sequential NN architecture consisting of two MLPs for WWTP with notable success is reported. The first NN is for a routine control, while second monitors the critical parameters. The output is to control measures like stopping the process or controlling the inputs. Here, SLP_NN (16-6-14) was used, where two of the variables are real numbers representing the average wastewater level over an hour and 2hours. The other 14 inputs are binary variables corresponding to the status (off or on) of the pumps. Based on 120 samples, the actual pump status and that predicted by NN are almost the same with a small error. Thus, NN mimics the human operator performance paving way to automation. It is based on past data and not on explicit decision rules. Phase wise automation and providing information for the operators will increase the efficiency of the wastewater treatment plant.

WWTP at El-Gabal El-Asfar:An NN model was applied to the WWTP located at El-Gabal El-Asfaron the east bank of Nile River, Egypt [183]. It is considered as the largest WWTP in Middle East. The operations include screening and grit removal, primary sedimentation, surface aeration, final clarification followed by chlorination. This plant is a non-nitrifying conventional type. BOD and SS at different locations in the treatment process for a period of 10 months are analysed with NNs. Fuzzy NNs to simulate up flow in anaerobic sludge blanket and fluidized bed reactor. Knowledge discovery from databases (KDD) is employed [391] for aqueous effluents from a manufacturing plant.

NN modeling found place in maintaining DO concentration in a WWTP [111], adaptive control dissolved oxygen [27], industrial wastewater treatment process in activated sludge treatment in a pulp mill [309], COD concentration of effluent [116] etc.

🗁 Combined sewer systems (CSS)

Although combined sewer systems are no longer constructed the existing ones require newer methods of control [165]. CSS collects and transports both urban wastewater and rain/storm water. It is a network of urban drainage system. Real time regulation involves control of gates pumps **and weirs**. CSSs contribute to the pollution of nearby water bodies especially when the load exceeds the discharge capacity of sewer or treatment plant. The modeling of CSS is complex in each of its sub goals. The typical modules are storm water runoff, sewer hydraulics etc. The simulation and appropriate use of the real time data are attempted. Rec.NN is applied for CSS in King County wastewater treatment division, Seattle, USA. Jordan-NN captures the dynamic and rapid response characteristics of the combined sewer systems [165]. The inputs are spatially distributed rainfall (current and past) previous controls optimal gate controls from OPTCON and UNSTDY. The network is retrained offline as and when new storm events occur.

Inadequacies of WWTP: Synergistic environmental toxic effects have been noticed even for binary mixtures and thus there is a concern regarding inadequate efficacies of WWTPs. Although each compound is less than toxic limit, their cumulative sum results in deleterious effects.Since many WWTPs are designed for removal of EDCs/ degradation products, they enter environment. The stringent protocols of REACH (Registration, Evaluation, Authorization, and Restriction of Chemicals) now impose restrictions on new chemicals should passes through environmental clearance of European Chemical Agency (ECHA) to minimize substances of very high concern (SVHCs).

III. Soil (12-13)

Soil pollution: Soil is not a homogeneous mixture of matter. The special heterogeneity is a good probe to follow dynamics of soil heavy metals (SHM), a consequence of man-made activities as well as nature's processes. Li et al. [344] studied special distribution and pollution of SHM in Huizhou City, Guangdong Province with NNs and combined results with GIS spatial correlation of SHM. And NNs, as universal function approximators, is one step forward in proposing a data driven models without explicit model driven equations.

12.1 Plant uptake Models for pollutants from contaminated soil: Takaki et al.[204] studied plant uptake models for neutral hydrophobic organic pollutants based on experiment data(chart 77). The plant uptake processes are good indicators to estimate effect on humans exposured to these toxic substances from polluted land. The crop yield is modelled using soil quality, nitrogen fertilizer and cropping year with radial basis function- (RBF-) NN.

Chart 77: Plant uptake models [204]

Model	**Uptake of Chemicals through**	**If**
EUSES	Root	logKOW > 8 logKOA > 11

ACC-HUMAN	Shoot	logKOW	> 10
		KAW	> 10^{-4}

Abbreviation	Partition coefficient
KAW	Air–water
KOW	Octanol–water

Other typical models

- RAIDAR
- CSOIL
- CLEA
- CalTOX

Surface vehicles: Peng et al.[323] proposed NN controller design for rendezvous autonomous surface vehicles. Lyapunov stability analysis of the distributed NN controllers using neighboring vehicles' information and graph theory showed that signals in the closed-loop and those with output feedback are uniformly bounded. These NN_ adaptive observers are found to estimate the unmeasured velocity of each vehicle driven in leaderless and leader–follower mode with real life dynamical uncertainties/ ocean disturbances etc.

Impervious surfaces: These are mainly artificial structures—such as pavements (roads, sidewalks, driveways and parking lots) that are covered by impenetrable materials such as asphalt, concrete, brick, and stone--and rooftops. Soils compacted by urban development are also highly impervious.

Solid waste: Bunsan et al.[79] predicted dioxin emission in incinerating treatment of municipal and industrial solid waste in Taiwan with SLP_NN (chart 78). The frequency of injection of activated carbon was found to be high impact factor in toxic emission.

Chart 78: Incineration municipal and industrial solid waste treatment [79]

+	-
Volume reduction of solid waste	Toxic pollutants emitted from incinerators →
Reduced landfill areas/ recycling	Health perturbation
Large energy generation	

Data	onitoring incinerator
# years	4
Location	Taiwan

Model	SLP_NN_BP
	5-8-1
R^2	0.99

Chart 79 : NN Prediction of suspended load in the Chelchay Watershed, northeast of Iran

# Data series	59
Location:	Four gravel bed-rivers Sand bed river

Model	**Architecture I#-[H#]-O#**	**RMSE$**
Chang formula best of nine formulas r = 0.69	----	0.013
SLP:	4-[4]-1	0.0009
M(2)LP:	4-[4-1]-1	0.001

Sludge: Han et al.[319] applied Hierarchical_NN trained withExt.ExtremeLrnMach for activated sludge of wastewater treatment processor (WWTP) with commendable success. Ongen et al.[248] used NNs for variations in synthetic (syn-) gas produced by dry air gasification of dewatered sludge from tannery wastewater treatment plant. The calorific value of synthetic gas was determined in a lab-scale updraft fixed-bed steel reactor. Haddadchi et al.[250] found that NNs predict suspended load in the Chelchay Watershed better than even the best nine models earlier proposed (chart 79). NN modeled ammonia emissions from sewage sludge [34].

13. Treatment/disposal of solid waste

Municipal solid waste (MSW): Sewage contains organic moieties, sulphurous and nitrogenous compounds producing directly or indirectly mal-odor[176]. Municipal solid waste (MSW) disposal is through land filling. The emission of gases and leachate production are the prime causes of environmental pollution. The limited barren land area also demands the treatment of municipal solid waste (MSW) (table 15) [388]. Combustion pyrolysis and gasification are the means of energy recovering but are criticized due to gaseous pollution.

Table 15: Hidden units and learning rate [388]

	ESS	1.7		
	Epochs	4000		
	Lrn_rate	0.05		
# hidden units	3	5	7	9
ESS	1.657	1.641	**1.636**	1.674
	ESS	1.8		
	# hidden units	7		
Lrn_rate	0.01	0.05	0.1	0.15
Epochs	2913	534	224	542

ESS : Error sum of squares ; Lrn_rate : Learning rate

Mal-odor: The concentration of odorant at the threshold is defined as one odor unit. It is a paradox that the odor of molecules with different molecular structure is similar although molecules with similar structures have distinctly different odors. In spite of considerable research, well-defined principles are not yet available relating the odor with principles of physics/chemistry/biology. In addition to it experimental measurement of odor is very complicated but humans are good at it without any effort. However some animals like dog and pig have 100 to 1000 fold neurons olfactory (responsible in the odor recognizing) organ. In the scientific front hitherto a panel of judges discriminate the flavour/odor and of course taste.

E-nose: Recent advances in sensors research electronics, computer science, information theory and artificial intelligence-2 revolutionized the odor measurement and electronic nose (E-nose) is a viable reliable and accurate device conforming to the routine needs. Yet they don't replace trained sniffer dogs and other animals in their natural habitat. E-Nose with embedded NNs is exposed to sewage samples collected from different locations viz. inlet works settlement tank activated sludge and final effluent of a WWTP producing 12 sensor array responses for each sample [176]. The total organic carbon (TOC) by flame ionization technique GC with MS and gas sensors with NNs are unbiased measures of odor. In fact there is no single sewage odor but several compounds with the distinct odor characteristics results in a typical sewage odor. Thus it is not necessary to use GC-MS for detection and quantification of each compound. Otherwise, left for longer periods of time especially in absence of O_2 results in unbearable odor due to anaerobic processes. Apart from human sensory panels H_2S analyzers and odor potential are employed in sewage odor measurement. BOD measurement takes five days yet the results are not reproducible. There are no perfect or reproducible quantification methods and thus measurement of odor is difficult.

Treatment:The treatment of solid waste comprises of collection treatment and disposal of potentially odorous materials in liquid form. The composition of MSW depends on climatic conditions and socio-economic factors in human activity. The major utility of MSW is for steam boilers in power station. The heating value depends upon elementary chemical composition which is composite. In a nut shell the relationship between the heating value of MSW and the interacting factors are not straightforward.

13.1 Activated sludge model 1 (ASM1):It is developed by international association on water pollution research and control (IAWPRC) task group on mathematical modeling for design and operation concerned with biological wastewater treatment. The simulation model distinguished between slow and rapid biodegradable substances as well as hetero-tropic and autotropic biomass.

- However ASM1 is not applicable for wastewater contaminated with coke.

MLP is put forward to estimate the concentration of nitrogen as ammonia in the effluent. The solid waste in Istanbul per day is around 9000 tons while the total MSW is 18000 m3(0.5 tons/m^3)[168]. These numbers have been growing with increase in population over time. The Odayeri sanitary landfill is in operation since 1995 and the dumpsite is contemplated for 25 years of usage.

Landfill leachate: It is formed when rain water melted from snow or the sewage liquid percolates through the landfill spaces and leaks out from the sides or flows through the bottom. The transportation of leachate carries widely different types of chemicals to the low-lying extremes of the landfill. There is a correlation between rain fall/precipitation and quantity of leachate. The sanitary landfill produces worst/dangerous pollution of environment. The design of landfill diminishes the ill effects of leachate flow. The critical situations are light rainfall for a long time and short burst of heavy rain cyclones etc. result in quick saturation of the cover material. The consequence is little net infiltration. Karaca[168]proposed NNs for prediction and management of leachate daily flow rates in municipal solid waste landfill site (Istanbul/Odayeri) using BP(table 16). The future scope of NN-LEAP study are given table 16(c) which will decrease the uncertainty in prediction of leachate flow rates and improve the odor estimation.

Table 16 Comparison of backpropagation algorithms[168]

Backpropagation algorithms		R-values	Mean squared error	Iteration number
Batch training	With weight and bias learning rules	0.202	0.8633	113
Conjugate gradient	FletcherePowell	0.773	0.2195	22
Conjugate gradient	PolakeRibiere	0.701	0.2808	19
Conjugate gradient	PowelleBeale	0.888	0.1216	28
Conjugate gradient	Scaled	0.779	0.2541	19
Gradient descent		0.250	0.8649	95
Gradient descent	With adaptive lr.	0.731	0.4286	210
Gradient descent	With momentum	0.217	0.8110	89
Gradient descent	With momentum and adaptive lr.	0.335	0.8791	20
LevenbergeMarquardt		0.847	0.0308	11
One step secant		0.713	0.1955	34
quasi-Newton	BFGS	0.774	0.1358	24
Resilient (Rprop)		0.676	0.2242	26

Table 16(b):Variables for NN-LEAP method [168] solid waste leachate municipal

Variable	Units
pH	
Temperature	^oC
Conductivity	mS cm^{-1}
Output parameter	
Leachate daily flow-rate	m^3 day^{-1}

Meteorological parameters (Daily means)	
Months	[1 to 12]
Temperature	^oC
Pressure (sea level)	mbar
Cloudiness	[0 to 1]
Relative humidity	%
Precipitation	mm

Maximum temperature	^oC
Minimum temperature	^oC

Table 16(c): Extended scope of NN-LEAP study

- Inclusion of forecasted meteorological parameters on the day of prediction
- Hourly flow rates
- Contribution of special areas for MSW

Table 16(d): Input variables biogas - landfill

Input parameters

- pH
- Alkalinity (mg/l CaCO3)
- COD (mg/l)
- Sulfate (mg/l)
- Conductivity
- Chloride (mg/l)
- Waste temperature (^oC)
- Refuse age (day)
- **Output parameter [T]**
- CH4 (%) of landfill gas

Table 16(e): comparision of BP algorithms and LM [167]

Alg.	Extention	SLP (8-12-1)		SLP (8-15-1)	
		R values	MSE (Mean Squared error)	R values	MSE
Levenberg Marquardt		0.951	0.0026	0.957	0.0025
Conjugate gradient	Scaled	0.927	0.0782	0.940	0.0565
BP	One-step secant	0.948	0.0459	0.946	0.0613
BP	QuasieNewton	0.946	0.0604	0.933	0.0379
Gradient descent	With adaptive learning rate BP	0.948	0.0799	0.931	0.1013
Gradient descent	BP	0.844	0.2464	0.867	0.2736
Gradient descent	With momentum And adaptive learning rate bp	0.950	0.0574	0.931	0.0829
Gradient descent BP	With momentum	0.787	0.5113	0.509	1.2622
BP	Resilient	0.941	0.0348	0.921	0.0503
Batch training with weight and bias learning rules		0.901	0.1672	0.878	0.1732

The prediction of activated sludge bulking [291], multi-elemental determination in soils under sewage sludge [379], removal of lead from industrial sludge leachate using red mud [75], sludge hygienization [94],anaerobic sludge blanket (UASB) to treat pharmaceutical wastewater containing 6-APA and amoxicillin [249] used NN paradigm.

13.2 Natural hazards/calamities/disasters

Landslides: The prediction of landslide susceptibility helps in reducing the consequent property loss as well as death toll of this natural hazard. Conforti et al. [74]applied MLP_NN with BP training algorithm to predict landslide zones in Turbolo River catchment of North Calabria in Southern Italy (chart 80).

13.3 Land use:The human activity alters the surface of terrine in a non-linear fashion and is referred as land use change. Its' modeling is still a challenge due to multifactor influences. Tayyebi et al. [147] investigated global and local models (chart 81) for changes in land use. NNs are superior to other models for short-time (5 years) intervals and coarse (one km) resolution in East Africa. The regression/classification trees and MARS exhibit similar accuracies in the case of long time (20 years) interval or fine (30 m) resolution with large numbers of cells for Muskegon River Watershed.
The prediction of (urban) heat island prediction in Athens (Greece)[376], effects of land use changes [129], landslide susceptibility assessment in the Hoa Binh province of Vietnam [225], Wenchuan

earthquake (China) triggered landslides (BS), [102], land-use patterns under drought scenarios [105] and heavy metal concentrations in rice [104] have positive impact in modeling with NNs.

Chart 80: Landslide prediction with MLP_NN

Tools	Categories
Air-photo interpretation Field surveys GIS	Landslide depletion zones Accumulation zones
Influential factors for landslide Lithology faults land use drainage network Topographic factors Elevation slope Aspect Plan curvature Topographic wetness index Stream power index % Classification : 85 ROC : 0.9	**Model** MLP_NN (BP) Software :Idrisi Taiga Performance for Test data Confusion matrix ROC Susceptibility classes Very low, Low Moderate High, Very high.

Chart 81: Land transformation models

Glogal parametric
- Land use change
- NN based land transformation

Local non-parametric models
- Classification
- Regression tree
- MARS

Region
- East Africa
  - Agricultural expansion
- Muskegon River Watershed in the United States
  - Forests are re-growing
- South-Eastern Wisconsin in the United States
  - Urbanization

Chart 82: Consequences of thermal effects of urbanization

Thermal contributionin urban areas	Increased emission of pollutants
Urban materials Urban geometry Air pollution Anthropogenic heat	*Power plants* *SO_2* *CO* *NOx* *Suspended* particulates

Chart 83: Prices of residential abodes in Taranto (Italy)

X	No rational behavior
Pollution level Landscaping Consequential health perturbations Asking price	Motivations, Tastes Budget availability Residential location choices Schools
Y Sale price of residential properties	**Model** y = NN(X; Weight)

Location

Taranto
- European biggest steel factory
- 2nd industrial harbour

Chart 84: NN model for electrocoagulation removal of Cr(VI)

Variable optimization
- Center composite design
- RSM

Models
- ANOVA
- Multiple response optimization Artificial neural network

Chart 85: Mobile robot applications

- Rescue operations
- Space missions
- Avoid exposition to risky environment
- Agriculture
  - Planting
  - Pesticides application
    - Minimal amounts to mitigate environmental pollution

13.4 Urban heat island:Compared to rural dwelling, urbanization (chart 82) has a new dimension as a result of thermal behavior of materials causing urban heat island (UHI) phenomenon.

13.5 Miscellaneous

Environmental quality vs. real estate price: Chiarazzo et al.[384] proposed NN model for real estate appraisal in Taranto (Italy) considering environmental quality and personal preferences (chart 83). Bhatti[115] used NN, experimental design and RSM for removal of Cr(VI) by electrocoagulation (chart 84)

HyperRectangular Composite_NN (HyperRectComp_NN): It is a two layer network. The hidden neurons are added as per requirement using supervised decision-directed learning (SupDecDirectLrn) algorithm. The weights imbibe classification knowledge, which can be extracted in Horn clauses (If-Then-Else-rules). Su et al. [218] reported that this NN is successful (> 99%) to distinguish and identify forest land, river, dam area, and built-up land from remote sensing images.

NNs find a niche in urban growth allocation model for valley [298], eco system mapping [238], quality planning policies at a regional scale in northern Italy [150], mobile robots in plantation [337], removal of organic micro pollutants by ozonation [80], biogas production [362] and exposure in embroidery workrooms [20].

Robots in agricultural plantation: Jodas et al. [337] reported a software implementation of SVM and NN to find out route in agricultural plantation by a real time robot which tracks the image features (chart 85).

14. State-of-knowledge-of- health of environment and its impact on health

The constituents of air themselves become toxicif their levels exceed threshold values.Apart from small molecules (NOx, SOx, COx, H2S, O3), PMx, PAHs, PCBs and POPs are noteworthy pollutants in air. Further, in the cycle of Ground → surface →soil→water→ air, pollutants reaching air traverse thousands of miles and even pollute water bodies and soil system. The fecal bacteria are other menace in this context. Environmental protection agency (EPA, US), European commission (EC) are environmental agencies looking forward for global clean environment with stipulations on emissions, industrial wastes etc. The prime objective is clean air to inhale and uncontaminated (treated) water to drink avoidinghealth hazards for human beings (children/old/susceptible subjects). At the same time, no hindrance for promotion of sustained growth of industries/agricultural or Mari cultural practices/land use, but with less contribution of pollutants to environment. Some governments started levying fines and stopping sanctions to discourage extent of contamination and even declared incentives for green processes/technologies with near zero harmful outputs.The state-of-art-technology is implemented in (automatic) sampling, analysis with high-end-hyphenated-software imbedded instruments, validating protocols for the results. Now, it has gone to the extent of personalized monitoring systems for high risk groups to keep them in safer zone, apart from alarming signals for all. The sharp ended research goes on to bring out more precise/accurate sensors even in harsh environments.

The precipitation, rainfall, streams, rivers levels and run-off, estuaries, absorption/penetration into soil, ground water flow, and evapotranspiration from ground are in the cycle natural water body. The contamination from ecosystems like fecal bacteria from cattle, fermented flora fauna and animals perturb the purity of water. The human activity, industrialization, land use, release of domestic/industrial/biological wastes into water streams is a major hazard. The natural calamities like floods, inundations, tsunamis, volcanic gases, earth quakes perturb local environmental scenarios. The EPA and other bodies have a target of supply of safe potable water and diminish the pollution scenarios at different stages.

Modeling plays a major role in monitoring, analyzing, planning and maintaining a sustained water system balance. Linear, transformed linear, polynomial models in all fields of research were coveted. Simultaneous multi-linear equations were solved with a paper and pencil or software. Least squares solution in statistical parlance has implicit assumptions viz. response is a random variable with normal errors and explanatory variables are error free and uncorrelated/ independent/ orthogonal. In early seventies of last century, COX models, ARMA settled a firm platform for to probe into empirical regression or time series data.

In late nineties, data driven NNs opened new era to account non-linear relations with only axiom that there is a functional relation between response and explanatory variables, but it need be known explicitly. NNs, non-linear model free data driven adaptive methods have been used in monitoring water contamination, potable water quality maintenance, water-levels, run-off, waste-water treatment plants etc. The color of ocean, wave height, precipitation on seas and oceans, sea surface (SS) temperauture/salinity has been predicted with NNs. The data here is mostly from satellites and high end modelling techniques for corroboration. The water global budget looks for causes and consequences of melting of ice caps on terrestrial and marine environment.

This was a boon to modelers not to hand write many models (brain waves). The subject specialists posed the lacuna, that the results are not in the frame of their discipline, although the experimental results are almost nearer to model output and forecast was also satisfactory for short values ahead. The point to remember at this juncture, is that with almost all empirical models and even mechanistic models with transformed equations, the domain is shifted another. Whatever it is, fuzzy-sets and rule-extraction algorithms brought out user readable if-then-else rules from trained NNs. This has wiped out the long standing blemish for NNs. Now, fully automated systems, deep-learning paradigms crossed all these boundaries and are a new world itself even for mega projects like LHC.

15. Future track (2015-) prospects-Afterword

NN models for prediction of PMx are accurate enough for forecasting. The governmental agencies can consider NNs as recommendable data analysis tools in addition to currently practicable ones. Complex systems require complex networks [397], sufficient training data covering all possible scenarios and advanced optimization algorithms. But it is worth noting that the recent reports in environment are pertained to NN technology used was of 1990s. A major finding is that even simple NNs function better than MLR, ARMA and parametric non-linear models. The recent improvements NN and other paradigms are to be brought to implementable stage in environmental data analysis. Further the frequency of data acquisition deserves attention.

The scientific domain is dynamic, the cobweb of data, information, knowledge and intelligence is very intricate to discern (chart A2-2). The definition, scope and applications also have been evolving with the needs and hurdles. What is amazing is that yesteryears' intelligence is today's common sense. Scientists refine the models with pumped in knowledge bits, leaving aside even time tested ones. The features not present in earlier models are smartly included and even the most coveted ones of yesterdays are graciously deleted. However, the choosy tendency of a modeler/ experimentalist /theoretician (save elite groups) is a hidden but highly influential factor that affects outcome of science. For instance, low end models do not precisely forecast weather conditions such as hurricanes, tornadoes, and blizzards and this partially mars the reputation of modelling approach.It is but a fact that simple models are ancesers of today's coveted ones and are useful for startup activity or for a sub goal of warning for low cost (equipment, expertise and hardware/software resources) pursuits. On the other hand, the lacuna of 'plug and chug' by amateur practitioners is a quick buck approach for data-in-result-out with no feel of either data or methods. But, the results are looked at by the credit of method only, as details of adherence of the current data to the method applied is not explicitly available.

Now, it is imperative that each of simplifying assumptions, necessary conditions, and failure warnings at every stage of model should be made transparent through the modeling software itself. Further, the validity of conclusions reachable from the output also should be displayed. This was emphasized in our earlier chemometric, environmetric, kinetometric, speciometric and piscimetric studies [295, 296 and references therein 303 to 392]. The scientists formulate mathematical formulae/ relationships with a paper and pencil. The data is operated on these mathematical forest to project what they prefer to look for or substantiate/defend/refute a proposal/hypothesis etc. The expert systems of 1960s broke the tradition. Genetic programming went a step forward to automatically derive sets of mathematical formulae with supplied set of operators, variables etc. This resulted in sets of functions different in form but functionally equivalent. The mathematical function approximation popular outside AI domain also has same core philosophy. Now, CERN is looking forward for an era of automatic learning with a new concept called 'deep learning'. It does not require manual creation of formulae by human scientists, not even traditional machine learning tools or human experts' insight. In this decade the buzz words are deep learning, peta-/exa-scale hardware/memory based computations, hyper intelligence and beyond. There is no final word for 'the theory' or 'highest level of experiment' in the rational scientific research. In fact, they are also evolving. 'Today's standard model of particle physics is not final, as it does not account for dark matter and dark energy. . The progress of science includes more and more precise measurements and observations with still higher and lower energy beating reteram scientist's capabilities. The outcome will focus on tracing cracks in the existing knowledge. This establishes a ground to take off into improvised theories /models /experiments/ computations including simulations. The findings of exploration for new particles with 14 TeV will culminate into science broadening its spectrum with a deep-sensed eye for reformed/ restructured/ reorganized bunch of fool proof scientific theories in the coming decades.

ACKNOWLEDGEMENTS

I profusely thank Prof Hopke, Clarkson University, Postsdam, USA for academic discussions during my visit to USA in 2002 for a lecture program in his laboratory.I thank Dr Ch Venkateswarlu, Scientist, BARC, for inviting to deliver an invited lecture on applications of Simplex in environmental chemical analysis in 1987 at 4th ISAS conference at Burdwan (west bangal). My respects to Prof. Khopkar for including state-of-art-of-environmetrics in invited talks at ICC conference in Mysore in 2004. Prof Y Anjaneyulu, center for environment, JNTU, Hyderabad arranged a series lectures on impact of chemometrics in pollution monitoring/ abatement, risk assessment for over a decade during mid-nineties and in early 2000. I am grateful to Prof D Satyanarayana, Marine chemistry and G S Murthy, Nuclear chemistry, Andhra University for their constant encouragement in our research pursuits. RSR thank Depart of Ocean development for an interdisciplinary project on 'predictive modeling on fisheries' (1998-2001) and Department of Environment (DOEn) for a bauxite ore exploration and benefaction with NN modeling in 2008.

REFERENCES

[1] Y. Cohen, R. Rallo, R. Liu, H. H. Liu,*Acc. Chem. Res.*, **2013,** 46, 3, 802–812.

[2] W. Bo. Chen, W.C. Liu, M. Hsi Hsu,*Advances in Eng. Software,* **2012,** 45,1, 69-79.

[3] J. Senthilnath, S. Bajpai, S.N. Omkar, P.G. Diwakar, V. Mani,*Advances in Space Res.*, **2012,** *50,* 9, 1274-1287.

[4] A. P. Piotrowski, J. J. Napiorkowski,*Advances in Water Resources,* **2012,** 49,97-113.
[5] E. Ward, W. Buytaert, L. Peaver, H. Wheater,*Advances in Water Resources,* **2011,** 34,10, 1222-1231.
[6] C. C. Yang, S. O. Prasher, J. AndreLandry, H. S. Ramaswamy,*Agricultural systems,* **2003,** 76, 561-574.
[7] W. Orzepowski, A. M. Paruch, K. Pulikowski, T. Kowalczyk, R. Pokładek,*Agricultural Water Manag.,* **2014,** 138,45-54.
[8] A. Singh, M. Imtiyaz, R.K. Isaac, D.M. Denis,*Agricultural Water Manag.,***2012,** 104,113-120.
[9] A.M. Melesse, S. Ahmad, M.E. McClain, X. Wang, Y.H. Lim,*Agricultural Water Manag.,* **2011,** 98,5, 855- 866.
[10] S. H. Elsafi,*Alexandria Engineering J.,* **2014,** 53,3, 655-662.
[11] S. H. Elsafi,*Alexandria Engineering Journal*,**2014,** 53, 655–662
[12] W. Zhao, P. K. Hopke, X. Qin K. A. Prather,*Anal. Chim. Acta,* **2005,** 549, 1-2, 179-187.
[13] V. O. Santos, Jr., F. C.C. Oliveira, D. G. Lima, A. C. Petry, E. Garcia, P. A.Z. Suarez J. C. Rubim,*Anal. Chim. Acta, **2005,** 547, 2, 188-196*
[14] Y. Ni, P. Qiu S. Kokot,*Anal. Chim. Acta,* **2005,** 537, 1-2, 321-330.
[15] J. F. F. Sánchez, A. S. Carretero, J. M. B. Sánchez, C. C. Blanco A. F. Gutiérrez,*Anal. Chim. Acta,* **2004,** 510, 2, 183-187.
[16] Y. Ni, P. Qiu S. Kokot,*Anal. Chim. Acta,* **2004,** 516, 1-2, 7-17.
[17] D. B. Von ina, D, Dob nik, M. Novi J. Zupan,*Anal. Chim. Acta,* **2002,** 462, 1, 87-100.
[18] K. Tuovinen, M. Kolehmainen H. Paakkanen,*Anal. Chim. Acta,* **2001,** 429, 2, 257-268
[19] C. Wan P. de B. Harrington,*Anal. Chim. Acta,* **2000,** 408, 1-2, 1-12.
[20] M. Aliabadi, R. Golmohammadi, M. Mansoorizadeh, H. Khotanlou, A. O. Hamadani,*Applied Acoustics,* **2013,** 74,364-374.
[21] Shivakumar, P. S. Pai, B.R. S. Rao,*Applied Energy,* **2011,** 88,7, 2344-2354.
[22] Y. Kim,*Applied Ocean Res.,* **2015,** 49,42-56.
[23] H. C. Lu, H. K. Liu,*Applied Ocean Res.,* **2013,** 42,43-54.
[24] H. Wahid, Q.P. Ha, H. Duc, M. Azzi,*Applied St Computing,* **2013,** 13,10, 4087-4096.
[25] M. Z. kermani, O. Kisi, T. Rajaee,*Applied St Computing,* **2013,** 13,12, 4633- 4644.
[26] E. Karadurmus, M. Cesmeci, M. Yuceer, R. Berber,*Applied St Computing,* **2012,** 12,1, 494-497.
[27] H. G. Han, J. F. Qiao,*Applied St Computing,* **2011,** 11,4, 3812-3820.
[28] Z. Zainuddin, O. Pauline,*Applied St Computing,* **2011,** *11,* 8, 4866- 4874.
[29] D. V. Kumar, P. R. Kumar, M. S. Kumari,*Artificial Neural Networks Procedia Eng.,* **2013,** 64,993-1002.
[30] Z. Wang, F. Lu, H. di He, Q. C. Lu, D. Wang, Z. R. Peng,*Atmos. Env.,* **2014,**In Press.
[31] R. Khatibi, L. Naghipour, M. A. Ghorbani, M. S. Smith, V. Karimi, R. Farhoudi, H. Delafrouz, H. Arvanaghi,*Atmos. Env.,* **2013,** 68,286-294.
[32] A. V. Carron, A. L. Dutot, T. Lombardo, A. Chabas,*Atmos. Env.,* **2012,** 54,141-148.
[33] P. Perez,*Atmos. Env.,* **2012,** 60,271-276.
[34] P. Boniecki, J. Dach, K. Pilarski, H. P. Boniecka,*Atmos. Env.,* **2012,** 57,49-54.
[35] G. Reikard,*Atmos. Env.,* **2012,** 60,593-600.
[36] A. Cazorla, F.J. Olmo, L. A. Arboledas,*Atmos. Env.,***2008** 42, 11, 2739-2745.
[37] U. Brunelli, V. Piazza, L. Pignato, F. Sorbello, S. Vitabile,*Atmos. Env.,* **2007,** 41, 2967-2995.

[38] S. P. Karakitsios, C. L. Papaloukas, P. A. Kassomenos, G. A. Pilidis,*Atmos. Env.,* **2007** 41, 40, 9555-9569.
[39] M. Dall'Osto R. M. Harrison,*Atmos. Env.,* **2006,** 40, 39, 7614-7631.
[40] J. Hooyberghs, C. Mensink, G. Dumont, F. Fierens, O. Brasseur,*Atmos. Env.,* **2005,** 39, 3279–3289.
[41] H. Junninena, H. Niska, K. Tuppurainen, J. Ruuskanen,M. Kolehmainen,*Atmos. Env.,* **2004,** 38, 2895–2907
[42] M. Tolock, D. A. Lakea, M. V. Johnstona, A. S. Wexler,*Atmos. Env.,* **2004,** 38, 3263-3273.
[43] S. Owega, G. J. Evans, R. E. Jervis, M. Fila, R. D'Souza, B. Uz-Zaman Khan,*Atmos. Env.,* **2004,** 38, 5545–5553.
[44] D. Jiang, Y. Zhang, X. Hu, Y. Zeng, J. Tan, D. Shao,*Atmos. Env.,* **2004,** 38, 7055–7064
[45] J. Kukkonen, L. Partanen, A. Karppinena, J. Ruuskanen, H. J. ninen, M. Kolehmainen, H. Niska, S. Dorling, T. Chatterton, R. Foxall, G. Cawley,*Atmos. Env.,* **2003,** 37, 4539–4550.
[46] H. Jin In, oon-UngPark,*Atmos. Env.,* **2003,** 37, 4625-4636.
[47] S. H. Pastor, J. O. Allen, L. S. Hughes, P. Bhave, G. R. Cass, K. A. Prather,*Atmos. Env.,* **2003,** 37, S239-S258.
[48] S.M.S. Nagendra, M. Khare,*Atmos. Env.,***2002,** 36, 2083–2098.
[49] P. Perez, J. Reyes,*Atmos. Env.,* **2002** 36 4555–4561.
[50] D. Podnar, D. Koracin, A. Panorska,*Atmos. Env.,***2002,** 36, 561–570.
[51] P. Perez,*Atmos. Env.,* **2001,** 35, 4929–4935.
[52] M. Plochl,*Atmos. Env.,* **2001,** 35, 5833-5841.
[53] M. Kolehmainen, H. Martikainen, J. Ruuskanen,*Atmos. Env.,* **2001,** 35, 815-825.
[54] P. PeH rez, A. Trier, J. Reyes,*Atmos. Env.,***2000,** 34, 1189-1196.
[55] M.W.Gardener, S. R. Dorling,*Atmos. Env.,* **2000,**34,171-176
[56] M. W. Gardener, S. R. Dorling,*Atmos. Env.,***2000,**34,21-34.
[57] S.L. Reich, D.R. Gomez, L.E. Dawidowski,*Atmos. Env.,* **1999,** 33, 3045-3052.
[58] M.W. Gardner, S.R. Dorling,*Atmos. Env.,* **1999** 33 709-719.
[59] E. L. Kalman, F.winquist, I. lundstrom,*Atmos. Env.,* **1997,** 31, 1715-1719.
[60] R. C. Deo, M. Şahin,*Atmos. Res.,***2015,** 153,512-525.
[61] J. Abbot, J. Marohasy,*Atmos. Res.,* **2014** 138,166-178.
[62] C. Roy, R. Kovordányi,*Atmos. Res.,* **2012,** 104–105,40-69.
[63] S. Khedairia, M. T. Khadir,*Atmos. Res.,* **2012,**113,89-101.
[64] Ü. A. Şahin, C. Bayat, O. N. Uçan,*Atmos. Res.,* **2011,** 101,1–2, 314-326.
[65] P. C. Chu, Y. Chen, S. Lu,*Atmos. Res.,* **2008,** 89, 4, 365-373.
[66] A. Ezcurra, J. Saenz, G. Ibarra-Berastegi, J. Areitio,*Atmos. Res.,* **2008,** 89, 3, 233-242.
[67] A. Manzato,*Atmos. Res.,* **2007,** 83, 2-4, 349-365.
[68] M. Lacinová, J. Munzar, M. Franc, *Atmos. Res.,* **2007,** 83, 2-4, 488-497.
[69] M. A. Martinez, M. Velazquez, M. Manso, I. Mas,*Atmos. Res.,* **2007,** 83, 2-4, 366-379.
[70] M. A. Martinez, M. Velazquez, M. Manso, I. Mas,*Atmos. Res.,* **2007,** 83, 2-4, 366-379.
[71] C. Zhou, L.Y. Ding, R. He,*Automation in Construction,* **2013,** 36,208-217.
[72] K. Sridevi, E. Sivaraman, P. Mullai,*Bioresource Technology,* **2014,** 165,233-240.
[73] Hong-di He, Wei-Zhen Lu, Yu Xue,*Building and Env.,***2014,** 78,111-117.
[74] M. Conforti, S. Pascale, G. Robustelli, F. Sdao,*CATENA,* **2014,** 113,236-250.
[75] F. Geyikçi, E. Kılıç, S. Çoruh, S. Elevli,*Chemical Eng. J.,* **2012,** 183,53-59.

[76] F. Gharagheizi, Ali Eslamimanesh, A. H. Mohammadi, D. Richon,*Chemical Eng. Science,* **2012,** 68,1, 290-304.
[77] Y. Li, Li Su, X. Zhang, X. Huang, H. Zhai,*Chemomet. Intel. Lab. Syst.,* **2011,** 105,1, 106-113.
[78] P. Zheng, P. de B. Harrington, d. M. Davis,*Chemomet. Intel. Lab. Syst.*, **1996,** 33, 121-132.
[79] S. Bunsan, Wei-Yea Chen, Ho-Wen Chen, Y. H. Chuang, N. Grisdanurak,*Chemosphere,***2013,** 92,3, 258-264.
[80] S. Sudhakaran, J. Calvin, G. L. Amy,*Chemosphere,* **2012,** 87,2, 144-150.
[81] S. Fdez-Ortiz de Vallejuelo, G. Arana, A. de Diego, J. M. Madariaga,*Chemosphere,* **2011,** *85,* 8, 1347-1352.
[82] M.L. Martın, I.J. Turias, F.J. Gonzalez, P.L. Galindo, F.J. Trujillo, *Chemosphere,***2008,** 70, 1190–1195.
[83] E. Ma. Pena-Mendez, K. Novotna, D. Gajdosova,V. Gonzalez, J. Havel,*Chemosphere,***2007,** 68, 2047–2053.
[84] A. Samecka-Cymerman, A. Stankiewicz, K. Kolon, A.J. Kempers,*Chemosphere,***2007,** 67, 954-960.
[85] Y. Yildirim, M. Bayramoglu,*Chemosphere,* **2006,** 63, 1575-1582.
[86] J. G.Watson, T. Zhu, J. C. Chow, J. Engelbrecht, E. M. Fujita, W. E. Wilson,*Chemosphere,***2002,** 49, 1093-1136.
[87] R. Żbikowski,*Coastal and Shelf Science,* **2011,** 94,2, 138-143.
[88] X. Yi, G. Li, Y. Yin,*Cold Regions Science and Technology,* **2013,** 88,10-16.
[89] L. Zhao, F.E. Hicks, A. R. Fayek,*Cold Regions Science and Technology,* **2012,** 70,32-42.
[90] C. Cojocaru, M. Macoveanu, I. Cretescu,*Colloids and Surfaces A: Physicochemical and Eng. Aspects,* **2011,** 384,1–3, 675-684.
[91] T. Tirelli, M. Gamba, D. Pessani,*Comptes Rendus Biologies,* **2012,** 335,10–11, 680-686.
[92] T. Tirelli, L. Favaro, M. Gamba, D. Pessani,*Comptes Rendus Biologies,* **2011,** *334,* 10, 695- 704.
[93] H. Honggui, Li Ying, Q. Junfei,*Computers & Electrical Engineering,* **2014,** 40,7, 2216-2226.
[94] A.K. Mahendra, A. Sanyal, G. Gouthaman,*Computers & Fluids,* **2011,** 46,1, 333-340.
[95] M. Liu, X. Liu, Da Liu, C. Ding, J. Jiang,*Computers & Geosciences,* **2015,** 75,44-56.
[96] A. P. Piotrowski, M. Osuch, M. J. Napiorkowski, P. M. Rowinski, J. J. Napiorkowski,*Computers & Geosciences,* **2014** 64,136-151.
[97] M. B. Gueye, A. Niang, S. Arnault, S. Thiria, M. Crépon,*Computers & Geosciences,* **2014,** 72,201-209.
[98] A. D. Mehr, E. Kahya, C. Yerdelen,*Computers & Geosciences,* **2014,** 70,63-72.
[99] A. M. Kalteh,*Computers & Geosciences,* **2013,** 54,1-8.
[100] S. Karimi, O. Kisi, J. Shiri, O. Makarynskyy,*Computers & Geosciences,* **2013,** 52,50-59.
[101] A. J. Cannon,*Computers & Geosciences,* **2012,** 41,126-135.
[102] C. Xu, X. Xu, F. Dai, A. K. Saraf,*Computers & Geosciences,* **2012,** 46,317-329.
[103] O. Kisi, J. Shiri,*Computers & Geosciences,* **2012,** 43,73-82.
[104] M. Liu, X. Liu, M. Wu, L. Li, L. Xiu,*Computers & Geosciences,* **2011,** 37, 10, 1642- 1652.
[105] H. Wang, X. Li, H. Long, Y. Qiao, Y. Li,*Computers & Geosciences,* **2011,** 37,7, 831-843.
[106] S. Liu, L. Xu, D. Li, Q. Li, Yu Jiang, H. Tai, L. Zeng,*Computers and Electronics in Agriculture,* **2013,** 95,82- 91.
[107] C. L. Chan, B. K. Low,*Computers and Geotechnics,* **2012,** 43,101-110.

[108] S. Kiranyaz, T. Ince, J. Pulkkinen, M. Gabbouj, J. Ärje, S. Kärkkäinen, V. Tirronen, M. Juhola, T. Turpeinen, K. Meissner,*Computers in Biology and Medicine,* **2011,** 41,7, 463-472.

[109] J. Karami, A. Alimohammadi, T. Seifouri,*Computers, Env. and Urban Systems,* **2014,** 43,25-33.

[110] [110] E. F. Geiger, M. D. Grossi, A. C. Trembanis, J. T. Kohut, M. J. Oliver,*Continental Shelf Res.,* **2013,** 63,S235-S242.

[111] Hong-Gui Han, Jun-Fei Qiao, Qi-Li Chen,*Control Eng. Practice,* **2012,** 20,4, 465- 476.

[112] C. Ribeiro, A. R. Ribeiro, A. S. Maia, V. M. F. Gonc¸ alves, M. E. Tiritan,*Critical Rev. Anal. Chem.,* **2014,** 44, 142–185.

[113] Y. Elipot, H. Hinaux, J. Callebert, S. Rétaux,*Current Biology,* **2013,** 23,1, 1-10.

[114] M. Ojha, S. Maiti,*Deep Sea Res. Part II: Topical Studies in Oceanography,* **2013, In Press.**

[115] M. S. Bhatti, A. S. Reddy, R. K. Kalia, A. K. Thukral,*Desalination,* **2011,** 269,1–3, 157-162.

[116] X. Xi, Y. Cui, Z. Wang, J. Qian, J. Wang, L. Yang, S. Zhao,*Desalination,* **2011,** 272,1–3, 27-35.

[117] Tsai-Fu Chuang, Yuan-Hsiou Chang,*Ecological Eng.,* **2013,** 58,255-261.

[118] J. He, A. Chu, M. C. Ryan, C. Valeo, B. Zaitlin,*Ecological Eng.,* **2011,** 37,11, 1804- 1814.

[119] Tsai-Fu Chuang, Yuan-Hsiou Chang,*Ecological Engineering,* **2014,** 68,223-232.

[120] M. Dukowska, A. Kruk, M. Grzybkowska,*Ecological Informatics,* **2014,** 24,112-123.

[121] M. Awad,*Ecological Informatics,* **2014,** 24,60-68.

[122] S. Fukuda, T. Tanakura, K. Hiramatsu, M. Harada,*Ecological Informatics,* **2014,(**In Press).

[123] K. Lock, P. L.M. Goethals,*Ecological Informatics,* **2013,** 17,30-35.

[124] B. Özbay, G. A. Keskin, Ş. C. Doğruparmak, S. Ayberk,*Ecological Informatics,* **2011,** 6,3–4, 242-247.

[125] Q. Chen, Q. Yang, Y. Lin,*Ecological Informatics,* **2011,** *6,* 6, 407-413.

[126] M. Kim, N. Park, R.I. (Bob) McKay, H. Shin, Yun-Geun Lee, Kwang-Seuk Jeong, Dong-Kyun Kim,*Ecological Modelling,* **2014,** 291,205-217.

[127] N. Tremblay, T. Werner, K. Huenerlage, F. Buchholz, D. Abele, B. Meyer, T. Brey,*Ecological Modelling,* **2014,** 291,233-241.

[128] M. Dukowska, M. Grzybkowska, A. Kruk, E. Szczerkowska- Majchrzak,*Ecological Modelling,* **2013,** 265,221-229.

[129] F. Li, Mi-Jung Bae, Yong-Su Kwon, N. Chung, Soon-Jin Hwang, Sang-Jung Park, Hae-Kyung Park, D. Soo Kong, Young-Seuk Park,*Ecological Modelling,* **2013,** 252,53-62.

[130] T. Penczak, Ł. Głowacki, A. Kruk, W. Galicka,*Ecological Modelling,* **2012,** 227,64-71.

[131] D.R. Pontin, S. Schliebs, S.P. Worner, M.J. Watts,*Ecological Modelling,* **2011,** 222,10, 1657-1665.

[132] T. Czech, F. Gambuś, J. Wieczorek,*Ecotoxicology and Env. Safety,* **2014,** *110,* 232-238.

[133] B. ZareNezhad, A. Aminian,*Energy Conversion and Manag.,***2011,** *52,* 2, 911-916.

[134] P. Lauret, M. Diagne, M. David,*Energy Procedia,* **2014,** 57,1044-1052.

[135] C.J. T. Renald, P. Somasundaram,*Energy Procedia,* **2012,** 14,1427-1438.

[136] A. Albostan, B. Barutcu, B. Onoz,*Energy Procedia,* **2011,** 6,331-336.

[137] Hsueh-Hsien Chang,*Energy,* **2011,** 36,1, 181-190.

[138] P. S.G. de M. Neto, F. Madeiro, T. A.E. Ferreira, G. D.C. Cavalcanti,*Eng. Appl. Artificial Intelligence,* **2014,** 32,185-191.

[139] K. Siwek, S. Osowski,*Eng. Appl. Artificial Intelligence,* **2012,** 25,6, 1246-1258.

[140] D. Gacquer, V. Delcroix, F. Delmotte, S. Piechowiak,*Eng. Appl. Artificial Intelligence,* **2011,** 24,6, 1070-1083.

[141] S. Nativi, P. Mazzetti, M. Santoro, F. Papeschi, M. Craglia, O. Ochiai,*Env. Model. Software,* **2015,** 68 June 1-26
[142] Chih-Chiang Wei,*Env. Model. Software,* **2015,** 63,137- 155.
[143] L. Carrera, G. Standardi, F. Bosello, J. Mysiak,*Env. Model. Software,***2015,** 63,109-122.
[144] X. Li, H. R. Maier, A. C. Zecchin,*Env. Model. Software,***2015,** 65,15-29.
[145] S. A. Hale, B. Gardiner, A. Peace, B. Nicoll, P. Taylor, S. Pizzirani,*Env. Model. Software,* **2015,** 68 June 27-41
[146] Jean-Luc de Kok, G. Engelen, J. Maes,*Env. Model. Software,* **2015,** 68 June 42-54
[147] A. Tayyebi, B. C. Pijanowski, M. Linderman, C. Gratton,*Env. Model. Software,* **2014,** 59,202-221.
[148] R. Muñoz-Mas, F. Martínez-Capel, V. Garófano-Gómez, A.M. Mouton,*Env. Model. Software,* **2014,** 59,30- 43.
[149] P. Coad, B. Cathers, J. E. Ball, R. Kadluczka,*Env. Model. Software,* **2014,** 61,393- 409.
[150] C. Carnevale, G. Finzi, G. Guariso, E. Pisoni, M. Volta,*Env. Model. Software,* **2012,** 34,44-50.
[151] D. B. May, M. Sivakumar,*Env. Model. Software,* **2009,** 24, 2, 296-302.
[152] S. A. Dellana, D. West,*Env. Model. Software,* **2009,** 24, 1, 96-106.
[153] E. Salazar-Ruiz, J.B. Ordieres, E.P. Vergara, S.F. Capuz-Rizo,*Env. Model. Software,* **2008,** 23, 8, 1056-1069.
[154] R. J. May, G. C. Dandy, H. R. Maier, J. B. Nixon,*Env. Model. Software,* **2008,** 23, 10-11, 1289-1299.
[155] R. J. May, H. R. Maier, G. C. Dandy, T.M.K. G. Fernando,*Env. Model. Software,* **2008,** 23, 10-11, 1312-1326.
[156] A. Coman, A. Ionescu, Y. Candau,*Env. Model. Software,* **2008,** 23, 12, 1407-1421.
[157] R. Wieland, W. Mirschel,*Env. Model. Software,* **2008,** 23, 2, 215-224.
[158] N.G. Tait, R.M. Davison, S.A. Leharne, D.N. Lerner, *Env. Model. Software,* **2008,** 23, 5, 611-621.
[159] G. Ibarra-Berastegi, A. Elias, A. Barona, J. Saenz, A. Ezcurra, J. Diaz de Argandoña,*Env. Model. Software,* **2008,** 23, 5, 622-637.
[160] B. Lin, M. Syed, R.A. Falconer,*Env. Model. Software,* **2008,** 23, 6, 729-740.
[161] A.M. Kalteh, P. Hjorth, R. Berndtsson,*Env. Model. Software,* **2008,** 23, 7, 835-845.
[162] A. Vellido, E. Martı, J. Comas, I. Rodrı´guez-Roda, F. Sabater,*Env. Model. Software,* **2007,** 22, 1053-1065.
[163] L. S. Iliadis, F. Maris,*Env. Model. Software,* **2007,** 22, 1066-1072.
[164] B. Raduly, K.V. Gernaey, A.G. Capodaglio, P.S. Mikkelsen, M. Henze,*Env. Model. Software,* **2007,** 22, 1208-1216.
[165] S. Darsono, J. W. Labadie,*Env. Model. Software,* **2007,** 22, 1349-1361.
[166] I. Machon, H. Lopez, J. Rodrıguez-Iglesias, E. Maranon, I. Vazquez,*Env. Model. Software,* **2007,** 22, 1382-1387.
[167] B. Ozkaya, A. Demir, M. S. Bilgili,*Env. Model. Software,***2007,** 22, 815-822.
[168] F. Karaca, B. Ozkaya,*Env. Model. Software,* **2006,** 21,1190-1197.
[169] S. Shanmuganathan, P. Sallis, J. Buckeridge,*Env. Model. Software,***2006,** 21, 1247-1256.
[170] E. Agirre-Basurko, G. Ibarra-Berastegi, I. Madariag,*Env. Model. Software,* **2006,** 21, 430-446.
[171] T. Slini, A. Kaprara, K. Karatzas, N. Moussiopoulos,*Env. Model. Software,* **2006,** 21, 4, 59-565.
[172] D. W. McCann, *Env. Model. Software,* **2005,** 20, 1335–1342.
[173] B. Sivakumar,*Env. Model. Software,* **2005,** 20, 515-519.

[174] J.B. Ordieres, E.P. Vergara, R.S. Capuz, R.E. Salazar,*Env. Model. Software,* **2005,** 20, 547-559.
[175] D. P.B.T.B. Strik, A. M. Domnanovich, L. Zani, Rudolf Braun, P. Holubar,*Env. Model. Software,* **2005,** 20, 803–810.
[176] G. Onkal-Engin, I. Demir, S. N. Engin,*Env. Model. Software,* **2005,** 20, 843-850.
[177] M. N. Almasri, J. J. Kaluarachchi,*Env. Model. Software,* **2005,** 20, 851-871.
[178] C. E.N. Gattsa, Alvaro R.C. Ovalle, Cleide F. Silva,*Env. Model. Software,* **2005,** 20, 883-889.
[179] Jean-Baptiste Filippi, P. Bisgambiglia,*Env. Model. Software,* **2004,** 19, 261–274.
[180] J.F. Mas, H. Puig, J.L. Palacio, A. Sosa-Lopez,*Env. Model. Software,* **2004,** 19,461–471.
[181] H. R. Maier, N. Morgan, C. W.K. Chow,*Env. Model. Software,* **2004,** 19, 485–494.
[182] G. Nunnari, S. Dorling, U. Schlink, G. Cawley, R. Foxall,T. Chatterton,*Env. Model. Software,* **2004,** 19, 887–905.
[183] M. M. Hamed, M. G. Khalafallah, E. A. Hassanien,*Env. Model. Software,* **2004,** 19, 919-928.
[184] D. De la Rosa, F. Mayol, E. Diaz-Pereira, M. Fernandez, D. de la Rosa Jr.,*Env. Model. Software,* **2004,** 19, 929–942.
[185] S. Kralisch, M. Fink, W.A. Flugel, C.Beckstein,*Env. Model. Software,* **2003,** 18, 815-823.
[186] A. B. Chelani, C.V. Chalapati Rao, K.M. Phadke, M.Z. Hasan,*Env. Model. Software,* **2002** 17, 161–168.
[187] E. Kalapanidas, N. Avouris,*Env. Model. Software,* **2001,** 16, 263–272.
[188] M.K. Purvis, Q. Zhou, S.J.S. Cranefield, R. Ward, R. Raykov, D. Jessberger,*Env. Model. Software,* **2001,** 16, 439–445.
[189] W.G. Booty, D.C.L. Lam, I.W.S. Wong, P. Siconolfi,*Env. Model. Software,* **2001,** 16, 453–458.
[190] Jean-B. Serodes, M. J. Rodriguez, A. Ponton,*Env. Model. Software,* **2001,** 16, 53-62.
[191] Holger R. Maier, Graeme C. Dandy,*Env. Model. Software,* **2000,** 15, 101-124.
[192] L. A. Belanche, J. J. Valdes, J. Comas, I. R. Roda, M. Poch,*Env. Model. Software,* **1999,** 14, 409-419.
[193] A. Bockreis, J. Jager,*Env. Model. Software,* **1999,** 14, 421-426.
[194] M. J. Rodriguez, J. B. Serodes,*Env. Model. Software,* **1999,** 14, 93-102.
[195] M. J. Rodriguez, J. B. Sérodes,*Env. Model. Software,* **1998,** 14, 1, 93-102.
[196] I. Machon, H. Lopez, J. Rodrıguez-Iglesias, E. Maranon, I. Vazquez,*Env. Model. Software.,***2007,** 22, 1382-1387.
[197] Franc¸ ois Anctil, C. Perrin, V. Andre´assian, *Env. Model. Software.,***2004,** 19, 357–368.
[198] H.J.S. Fernando, M.C. Mammarella, G. Grandoni, P. Fedele, R. Di Marco, R. Dimitrova, P. Hyde,*Env. Pollution,* **2012,** 163,62-67.
[199] Y.F. Huang, G.Q. Wang, G.H. Huang, H.N. Xiao, A. Chakma,*Env. Pollution,* **2008,** 151, 3, 460-469.
[200] M. Kampa, E. Castanas, **2008**, 151, 2, 362-367.
[201] Inn-Sil Kwaka, Tae-Soo Chona, Hyun-Min Kangb, Nam-Il Chunga, Jong-Sang Kimc, Sung Cheol Kohd, Sung-Kyu Leee, Yoo-Shin Kim,*Env. Pollution,* **2002,** 120, 671–681.
[202] S. K. Mohanty, A. A. Torkelson, H. Dodd, K. L. Nelson, A. B. Boehm,*Environ. Sci. Technol.* **2013,** 47, 10791−10798.
[203] S. Xu, G. Kozerski, D. Mackay,*Environ. Sci. Technol.,* **2014,** 48, 11748−11759.
[204] K. Takaki, A. J. Wade, C. D. Collins,*Environ. Sci. Technol.,* **2014,** 48, 12073−12082.
[205] J. Nasir, X. Wang, B. Xu, C. Wang, D. R. Joswiak, S. Rehman, A. Lodhi, S. Shafiq, R. Jilani,*Environ. Sci. Technol.,* **2014,** 48, 2610−2618.

[206] Jia Guo, Staci L. Capozzi, Thomas M. Kraeutler, Lisa A. Rodenburg,*Environ. Sci. Technol.,* **2014,** 48, 8573−8580

[207] E. G. Snyder, T. H. Watkins, P. A. Solomon, E. D. Thoma, R. W. Williams, G. S. W. Hagler, D. Shelow, D. A. Hindin, V. J. Kilaru, P. W. Preuss,*Environ. Sci. Technol.,* **2013,** 47, 11369−11377.

[208] S. Jeannottat D. Hunkeler,*Environ. Sci. Technol.,* **2013,** 47, 12115−12122.

[209] L. M. Persson, M. Breitholtz, I. T. Cousins, C. A. de Wit, M. MacLeod, M. S. McLachlan,*Environ. Sci. Technol.,***2013,** 47,12619−12622.

[210] M. E. Dueker, G. D. O'Mullan, A. R. Juhl, K. C. Weathers, M. Uriarte,*Environ. Sci. Technol.,* **2012,** 46, 10926−10933.

[211] H. Wöhrnschimmel, P. Tay, H. von Waldow, H. Hung, Yi-Fan Li,M. MacLeod, K. Hungerbuhler,*Environ. Sci. Technol.,* **2012,** 46, 2047−2054.

[212] G. H. Reischer, D. Kollanur, J. Vierheilig, C. Wehrspaun, R. L. Mach, R. Sommer, H. Stadler, A. H. Farnleitner,*Environ. Sci. Technol.,* **2011,** 45, 4038–4045.

[213] Sung-Deuk Choi F. Wania,*Environ. Sci. Technol.,* **2011,** 45, 8834–8841.

[214] G. Ćirović, D. Pamučar, D. Božanić,*Expert Systems with Appl.,***2014,**41,9,4245-4258.

[215] R. Olawoyin, A. Nieto, R. L. Grayson, F. Hardisty, S. Oyewole,*Expert Systems with Appl.,* **2013,** 40,9, 3634-3648.

[216] J.M. Barrón-Adame, M.G. Cortina-Januchs, A. Vega-Corona, D. Andina,*Expert Systems with Appl.,* **2012,** 39,1, 107-116.

[217] A. P. Piotrowski, P. M. Rowinski, J. J. Napiorkowski,*Expert Systems with Appl.,* **2012,** *39,* 1, 1354-1361.

[218] Mu-Chun Su, De-Yuan Huang, Jieh-Haur Chen, Wei-Zhe Lu, L.C. Tsai, Jia- Zheng Lin,*Expert Systems with Appl.,* **2011,** 38,10, 12917-12922.

[219] H. Riahi-Madvar, S. Ali Ayyoubzadeh, M. G. Atani,*Expert Systems with Appl.,* **2011,** 38,1, 215-222.

[220] I. A. Juma, H. H. Hussein, M. F. Al-Sarraj,*Flow Measurement and Instrumentation,* **2014,** 38,49-53.

[221] M. Sahu, K.K. Khatua, S.S. Mahapatra,*Flow Measurement and Instrumentation,* **2011,** 22,5, 438-446.

[222] A. H. Zaji, H. Bonakdari,*Flow Measurement Instrumentation,* **2015,** 41,81-89.

[223] S. Jimenez, J. Ballester,*FUEL,* **2007,** 86, 486-493.

[224] Qian-Jin Liu, Zhi-Hua Shi, Nu-Fang Fang, Hua-De Zhu, Lei Ai,*Geomorphology,* **2013,** 186,181-190.

[225] D. T. Bui, B. Pradhan, O. Lman, I. Revhaug, O. B. Dick,*Geomorphology,* **2012,** 171–172,12-29.

[226] D. Wallach, F. Lamare, G. Kontaxakis, D. Visvikis,*IEEE Transactions On Medical Imaging,* **2012,** 31 2

[227] T. Basile, A. Petrella, M. Petrella, G. Boghetich, V. Petruzzelli,S. Colasuonno, D. Petruzzelli,*Ind. Eng. Chem. Res,* **2011,** 50, 8389–8401.

[228] A. Rahman, Md S. Shahriar, C. D'Este, G. Smith, J. McCulloch, G. Timms,*Information Processing in Agriculture,* **2014,** 1,1, 42-50.

[229] J.T. Schoof, S.C.Pryor, S. M. Robeson,*Int. J. Climatol* **2007** 27 4 439–454

[230] F. S. Mpelosoka, A. B.Mullan, R. G. Heerdegen,*Int. J. Climatol.,* **2001,** 21, 1415-1433.

[231] A. Tayyebi, B. C. Pijanowski,*Internat. J. Applied Earth Observation and Geoinformation,* **2014,** 28,102-116.

[232] B. Jena, P.J. Kurian, D. Swain, A. Tyagi, R. Ravindra,*Internat. J. Applied Earth Observation and Geoinformation*, **2012,** 16,1-4.
[233] Z. Z. Sirdari, A. Ab ghani, Z. Abu hassan,*Internat. J. Sediment Res.*, **2014,** 29,4, 481-490.
[234] K. Song, Lin Li, L. P Tedesco, S. Li, Bob E Hall, Jia Du,*ISPRS J. Photogrammetry and Remote Sensing*, **2014,** 95,68-80.
[235] D. Mackay, Jon A. Arnot,*J. Chem. Eng. Data* **2011,** 56, 1348–1355
[236] A. B. Levine, S. Liu, F. Vince, M. Li, A. Ostfeld,*J. Env. Manag.*,**2014,** 143,8- 16.
[237] Y. Jiang, Z. Nan, S. Yang,*J. Env. Manag.*,**2013,** 122,130- 136.
[238] H. Zhang, J. Song, C. Su, M. He,*J. Env. Manag.*,**2013,** 115,227-234.
[239] S. Cheng, Li Li, D. Chen, J. Li,*J. Env. Manag.*,**2012,** 112,404-414.
[240] B. He, T. Oki, F. Sun, D. Komori, S. Kanae, Yi Wang, H. Kim, D. Yamazaki,*J. Env. Manag.*,**2011,** *92*, 1, 172-177.
[241] F. S. Mjalli, S. Al-Asheh, H.E. Alfadala,*J. Env. Manag.*,**2007,** 83, 329–338.
[242] K. Chau,*J. Env. Manag.*,**2006,** 80, 47–57.
[243] I. Stanimirovaa, M. Daszykowskia, D.L. Massarta, F. Questiera, V. Simeonovb, H. Puxbaum,*J. Env. Manag.*,**2005,** 74, 349–363.
[244] M. N. Almasri1, J. J. Kaluarachchi,*J. Env. Manag.*,**2005,** 74, 365–381.
[245] Fi-John Chang, Yu-Hsuan Tsai, Pin-An Chen, A. Coynel, G. Vachaud,*J. Env. Management*, **2015,** 151,15, 87- 96.
[246] Lu Zhang, Wei-hua Xu, Zhi-yun Ouyang, Chun-quan Zhu,*J. for Nature Conservation*, **2014,** 22,4, 326-336.
[247] A. Beucher, P. Österholm, A. Martinkauppi, P. Edén, S. Fröjdö,*J. Geochemical Exploration*, **2013,** 125,46- 55.
[248] A. Ongen, H. K. Ozcan, S. Arayıc,*J. Hazardous Materials*, **2013,** Volume 263, Part 2, 15361-366.
[249] Z. Chen, H. Wang, Z. Chen, N. Ren, A. Wang, Yue Shi, X. Li,*J. Hazardous Materials, Volume Issues 30 January Pages***2011,** 185,2–3, 905-913.
[250] A. Haddadchi, N. Movahedi, E. Vahidi, M. H. Omid, A. A. Dehghani,*J. Hydrodynamics, Ser. B,* **2013,** 25,3, 459-470.
[251] W. Thoe, S.H.C. Wong, K.W. Choi, J.H.W. Lee,*J. Hydro-Env. Res.*, **2012,** 6,3, 164-180.
[252] M. López-Lineros, J. Estévez, J.V. Giráldez, A. Madueño,*J. Hydrology*, **2014,** 510,103-109.
[253] J. T. DeWeber, T. Wagner,*J. Hydrology*, **2014,** 517,187-200.
[254] D. Antanasijević, V. Pocajt, A. Perić-Grujić, M. Ristić,*J. Hydrology*, **2014,** 519, Part B,1895-1907.
[255] A. K. Lohani, N.K. Goel, K.K.S. Bhatia,*J. Hydrology*, **2014,** 509,25-41.
[256] G. Tayfur, G. Zucco, L. Brocca, T. Moramarco,*J. Hydrology*, **2014** 510,363-371.
[257] Z. He, X. Wen, Hu Liu, J. Du,*J. Hydrology*, **2014,** 509,379-386.
[258] A. Belayneh, J. Adamowski, B. Khalil, B. Ozga-Zielinski,*J. Hydrology*, **2014,** 508,418-429.
[259] J. C. Cole, K. O. Maloney, M. Schmid, J. E. McKenna Jr.,*J. Hydrology*, **2014,** 519, Part A,588-598.
[260] F. Mekanik, M.A. Imteaz, S. Gato-Trinidad, A. Elmahdi,*J. Hydrology*, **2013,** 503,11-21.
[261] Jian-Ping Suen, Hung-Nien Lai,*J. Hydrology*, **2013,** 493,124-131.
[262] Z. Li, D. Yang, Y. Hong,*J. Hydrology*, **2013,** 500,157-169.
[263] Shi-Peng Yu, Jing-Song Yang, Guang-Ming Liu,*J. Hydrology*, **2013,** 497,189-197.
[264] Chang-Han Chung, Fi-J. Chang,*J. Hydrology*, **2013,** 486,224-233.

[265] A. D. Mehr, E. Kahya, E. Olyaie,*J. Hydrology,* **2013,** 505,240-249.

[266] Fi-John Chang, Wen-Ping Tsai, Hung-kwai Chen, R. Sau-Wai Yam, E. E. Herricks,*J. Hydrology,* **2013** 476,280-289.

[267] S. Mohanty, M. K. Jha, Ashwani Kumar, D.K. Panda,*J. Hydrology,* **2013,** 495,38-51.

[268] E. K. Lafdani, A. M. Nia, A. Ahmadi,*J. Hydrology,* **2013,** 478,50-62.

[269] P.C. Nayak, B. Venkatesh, B. Krishna, Sharad K. Jain,*J. Hydrology,* **2013,** 493,57-67.

[270] H. Badrzadeh, R. Sarukkalige, A.W. Jayawardena,*J. Hydrology,* **2013,** 507,75-85.

[271] A. P. Piotrowski, J. J. Napiorkowski,*J. Hydrology,* **2013,** 476,97-111.

[272] Fi-John Chang, Chang-Han Chung,*J. Hydrology,* **2012,** 440–441,102-112.

[273] O. Kisi,*J. Hydrology,* **2012,** 456–457,110-120.

[274] Y. S. T. Hong,*J. Hydrology,* **2012,** 468–469,11-21.

[275] M. E. Akiner, A. Akkoyunlu,*J. Hydrology,* **2012,** 456–457,121-129.

[276] Z. Huo, S. Feng, S. Kang, G. Huang, F. Wang, Ping Guo,*J. Hydrology,* **2012,** 420–421,159-170.

[277] X. Zeng, K. L. Kiviat, K. Sakaguchi, Ala M.A. Mahmoud,*J. Hydrology,* **2012,** 452–453,226-231.

[278] A. K. Lohani, R. Kumar, R. D. Singh,*J. Hydrology,* **2012,** 442–443,23-35.

[279] V. Jothiprakash, R.B. Magar,*J. Hydrology,* **2012,** 450–451,293-307.

[280] R. Maheswaran, R. Khosa,*J. Hydrology,* **2012,** 450–451,320-335.

[281] O. Kisi, A. H. Dailr, M. Cimen, J. Shiri,*J. Hydrology,* **2012,** 450–451,48-58.

[282] O. Kisi, C. Ozkan, B. Akay,*J. Hydrology,* **2012,** 428–429,94-103.

[283] A. P. Piotrowski, J. J. Napiorkowski,*J. Hydrology,* **2011,** 407,1–4, 12-27.

[284] R. Khatibi, M. Ali Ghorbani, M. H. Kashani, O. Kisi,*J. Hydrology,* **2011,** 403,3–4, 201-212.

[285] I. F. Cruz, O. Pedrollo, N. M.R. Castro, P. Girard, P. Zeilher, S. K. Hamilton,*J. Hydrology,* **2011,** 399,3–4, 376- 384.

[286] S. Araghinejad, M. Azmi, M. Kholghi,*J. Hydrology,* **2011,** 407,1–4, 94-104.

[287] Wen-ping XIE, Jing-song YANG,*J. Integrative Agriculture,* **2013,** 12,4, 711-722.

[288] A. A. Masrur Ahmed,*J. King Saud University - Eng. Sciences,***2014, In Press.**

[289] A. Velo, F.F. Pérez, T. Tanhua, M. Gilcoto, A.F. Ríos, R. M. Key,*J. Marine Systems,* **2013,** 111–112,11-18.

[290] R. Vendramea, R. S. Braga, Y. Takahata, D.S. GalvaÄo,*J. Mol. Struct., (Theochem,)* **2001,** 539, 253-265.

[291] H. G. Han, J. F. Qiao,*J. Process Control,* **2012,** 22,6, 1103- 1112.

[292] D. Rengaraj, W. S. Kwon, M. G. Pang,*J. Proteome Res.,* **2015,** 14, 22−37

[293] N. Jaafarzadeh, M. Ahmadi, H. Amiri, M. H. Yassin, S. S. Martinez,*J. the Taiwan Institute Chemical Engineers,* **2012,** *43,* 6, 873-878.

[294] M. Nyhan, A. McNabol, B. Misstear,*J. Transport & Health,* **2014,** *1,* 4, 305-315.

[295] K. Ramakrishna, R. Sambasiva Rao,*Journal of Applicable Chemistry,* **2015,**4,1,1-98.

[296] K. RamaKrishna, V. A. Ramam, R. Sambasiva Rao,*Journal of Applicable Chemistry,* ***2014,****3,* 6, 2209-2311.

[297] K. RamaKrishna, Ch. V. K. Rao, V. A. Ramam R. Sambasiva Rao,*Journal of Applicable Chemistry,****2014,****3,*1, *6-29.*

[298] R. B. Thapa, Y. Murayama,*Landscape and Urban Planning,* **2012,** 105,1–2, 140-148.

[299] L. Wei, Z. Hu, L. Dong, W. Zhao,*Mar. Pollut. Bull.* ***2014****,* http://dx.doi.org/ *10.1016/j.marpolbul.2014.11.036*

[300] K. W. Allen, M. Rayner,*Marine Chem.,* **2014,** 167,135-149.

[301] M. Schulz, M. Matthies,*Marine Env. Res.,* **2014,** 98,14-20.

[302] B. S. Marx, F. Giraud, E. Mattioli, Y. Gally, N. Barbarin, L. Beaufort,*Marine Micropaleontology,* **2014,** 111,15-25.

[303] S. Singh, D. Velotto, S. Lehner,*Marine Pollution Bulletin,* **2014,** 86,1–2, 379-390.

[304] L. Wei, Z. Hu, L. Dong, W. Zhao,*Marine Pollution Bulletin,* **2014, (**In Press).

[305] N. M. Gazzaz, M. K. Yusf, A. Z. Aris, H. Juahir, M. F. Ramli,*Marine Pollution Bulletin,* **2012,** 64,11, 2409-2420.

[306] Y. Cheng, X. Li, Q. Xu, O. G. Pineda, O. B. Andersen, W. G. Pichel,*Marine Pollution Bulletin,* **2011,** 62,2, 350- 363.

[307] S. Liu, H. Tai, Q. Ding, D. Li, L. Xu, Y. Wei,*Mathematical and Computer Modelling,* **2013,** 58,3–4, 458-465.

[308] J. Huang, J. Xu, X. Liu, J. Liu, L. Wang,*Mathematical and Computer Modelling,* **2011,** 54,3–4, 995-1004.

[309] M. Heikkinen, H. Poutiainen, M. Liukkonen, T. Heikkinen, Y. Hiltunen,*Mathematics and Computers in Simulation,* **2011,** 82,3, 450-459.

[310] S. Cho, B. Lim, J. Jung, S. Kim, H. Chae, J. Park, S. Park, J. K. Park,*Measurement,* **2014,** 53,224-233.

[311] D. I.A. Pereira, S. F.A. Bruggraber, N. Faria, L. K. Poots, M. A. Tagmount, M. F. Aslam, D. M. Frazer, C. D. Vulpe, G. J. Anderson, J. J. Powell, *Nanomedicine: Nanotechnology, Biology, and Medicine*,**2014,** 10 1877–1886.

[312] P. Perez J. Reyes,*Neural Comput.* **2001,** 10, 165–171.

[313] A. J. Cannon,*Neural Networks.*,**2007,** 20, 444–453.

[314] R. van der Merwe, T. K. Leen, Z. Lu, S. Frolov, A. M. Baptista,*Neural Networks.,* **2007,** 20, 462-478.

[315] G. Corzo, D. Solomatine,*Neural Networks.*,**2007,** 20, 528-536.

[316] G. C. Cawley, G. J. Janacek, M. R. Haylock, S. R. Dorling,*Neural Networks.,* **2007,** 20, 537–549.

[317] G. Acciani, E. Chairantoni, G. Fornarelli, S. Vergura,*Neural Networks.,* **2003,** 16, 427-436.

[318] F. C. Morabito, M. Versaci,*Neural Networks.*,**2003,** 16, 493-506.

[319] H. G. Han, Li-Dan Wang, Jun-Fei Qiao,*Neurocomputing,* **2014,** 128,128-135.

[320] H. Wang, D. Wang, Z. Peng,*Neurocomputing,* **2014,** 133,170-178.

[321] C. C. Wei,*Neurocomputing,* **2014,** 136,71-81.

[322] P. Szymczyk, M. Szymczyk,*Neurocomputing,* **2014,**In Press.

[323] Z. Peng, D. Wang, H. H.T. Liu, G. Sun, H. Wang,*Neurocomputing,* **2013,** 115,130-141.

[324] K. Yan Chan, Le Jian,*Neurocomputing,* **2013,** 99,564-569.

[325] Z. Yao, M. Feia, K. Li, H. Kong, Bo Zhao,*Neurocomputing.*,**2007,** 70, 641-647.

[326] B. Bhattacharya, D.P. Solomatine,*Neurocomputing*.,**2005,** 63, 381–396.

[327] A. Montanari, A. Londei, B. Staniscia,*Ocean & Coastal Manag.*,**2014,** 101, Part B,114- 122.

[328] P. C. Deka, R. Prahlada,*Ocean Eng.,* **2012,** 43,32-42.

[329] G. Reikard, P. Pinson, J. R. Bidlot,*Ocean Eng.,* **2011,** 38,10, 1089-1099.

[330] S. G. Patil, S. Mandal, A.V. Hegde, S. Alavanda,*Ocean Eng.,* **2011,** 38,1, 186-196.

[331] P. Jain, M.C. Deo, G. Latha, V. Rajendran,*Ocean Modelling,* **2011,** 36,26-39.

[332] A. Girone, P. Maiorano, M. Marino, M. Kucera,*Palaeogeography, Palaeoclimatology, Palaeoecology,* **2013,** 392,105-116.

[333] T.R. Nkuna, J.O. Odiyo,*Physics and Chem. the Earth,* **2011,** 36, Parts A/B/C,14–15, 830-835.

[334] S. Alvisi, M. Franchini,*Physics and Chem. the Earth, A/B/C,* **2012,** 42–44,108-118.
[335] F.D. Mawale, A.J. Adeloye, R. Rustum,*Physics and Chem. the Earth, Parts A/B/C,* **2012,** 50–52,34-43.
[336] R. M. Puscasu,*Procedia Computer Science,* **2014,** 29,1156-1170.
[337] D. S. Jodas, N. Marranghello, A. S. Pereira, R. C. Guido,*Procedia Computer Science,* **2013,** 18,240-249.
[338] T. Kajiyama, D. D'Alimonte, J. C. Cunha,*Procedia Computer Science,* **2011,** 4,2186-2195.
[339] G. Tan, J. Yan, C. Gao, S. Yang,*Procedia Eng.,* **2012,** 31,1194-1199.
[340] A. Rai, N. S. Kumar, Srinivasa Pai P., B.R. S. Rao,*Procedia Eng.,* **2012,** 38,280-292.
[341] S. De Vito, G. Fattoruso, R. Liguoro, A. Oliviero, E. Massera, C. Sansone, V. Casola, G. Di Francia,*Procedia Eng.,* **2011,** 25,84-87.
[342] P. K. Gupta, K. Das M. Sharma,*Procedia Engineering,* **2014** 92 9 – 18
[343] J. Sun, Z. Wang, R. Li, D. Ma, B. Liu,*Procedia Env. Sciences,* **2011,** 8,161-165.
[344] Y. Li, C. kui Li, J. jun Tao, Li-dong Wang,*Procedia Env. Sciences,* **2011,** 10, Part C,1953-1960.
[345] J. C. G. Estrada, I. P. Calvo,*Progress in Oceanography,* **2015,** 130,112-124.
[346] B. Su, X. Zeng, J. Zhai, Y. Wang, X. Li,*Quaternary Internat.,* **2014, In Press,**
[347] X. Zeng, Z. W. Kundzewicz, J. Zhou, B. Su,*Quaternary Internat.,* **2012,** 282,113-121.
[348] S. C.J. Palmer, P. D. Hunter, T. Lankester, S. Hubbard, E. Spyrakos, A. N. Tyler, M. Présing, H. Horváth, A. Lamb, H. Balzter, V. R. Tóth,*Remote Sensing Env.,* **2015,** 157,158-169.
[349] Di Long, Y. Shen, A. Sun, Y. Hong, L. Longuevergne, Y. Yang, Bin Li, Lu Chen,*Remote Sensing Env.,* **2014,** 155,145-160.
[350] A. Ghosh, A. K. Varma, S. Shah, B.S. Gohil, P. K. Pal,*Remote Sensing Env.,***2014,** 142,20-32.
[351] J. Chen, W. Quan, T. Cui, Q. Song, C. Lin,*Remote Sensing Env.,* **2014,** 149,213-226.
[352] E. Zabolotskikh, L. Mitnik, B. Chapron,*Remote Sensing Env.,***2014,** 147,89-98.
[353] Z. B. Mustapha, S. Alvain, C. Jamet, H. Loisel, D. Dessailly,*Remote Sensing Env.,* **2014,** 146,97-112.
[354] C. Goyens, C. Jamet, T. Schroeder,*Remote Sensing Env.,***2013,** 131,63-75.
[355] I. Ioannou, A. Gilerson, B. Gross, F. Moshary, S. Ahmed,*Remote Sensing Env.,***2013,** 134,78-91.
[356] T. Lammoglia, C. R. de S. Filho,*Remote Sensing Env.,* **2012,** 123,381-389.
[357] D. D'Alimonte, G. Zibordi, J. F. Berthon, E. Canuti, T. Kajiyama,*Remote Sensing Env.,* **2012,** 124,402-412.
[358] J. Brajard, R. Santer, M. Crépon, S. Thiria,*Remote Sensing Env.,***2012,** 126,51-61.
[359] E. A. Urquhart, B. F. Zaitchik, M. J. Hfman, S. D. Guikema, E. F. Geiger,*Remote Sensing Env.,* **2012,** 123,522-531.
[360] E. Spyrakos, L. G. Vilas, J. M. T. Palenzuela, E. D. Barton,*Remote Sensing Env.,* **2011,** 115,10, 2471-2485.
[361] L. G. Vilas, E. Spyrakos, J. M. T. Palenzuela,*Remote Sensing Env.,***2011,** 115,2, 524-535.
[362] E.B. G. Kana, J.K. Oloke, A. Lateef, M.O. Adesiyan,*Renewable Energy,* **2012,** 46,276-281.
[363] H. Yang, Z. Jiang, S. Shi,*Sci. Total Env.,***2006,** 358, 265– 276.
[364] Y. S. Park, T. S. Chon, Inn-Sil Kwak, S. Lek,*Sci. Total Env.,***2004,** 327, 105–122.
[365] Y. Hongwei, J. Zhanpeng, S. Shaoqi,*Sci. Total Env.,***2004,** 322, 209-219.
[366] M. Nadal, M. Schuhmacher, J.L. Domingo,*Sci. Total Env.,***2004,** 321, 59–69.
[367] P. Wang, Y. Liu, Z. Qin, G. Zhang,*Science The Total Env.,***2015,** 505,1202-1212.
[368] G. D. Betrie, R. Sadiq, K. A. Morin, S. Tesfamariam,*Science The Total Env.,***2014** 490,182- 190.

[369] D. Z. Antanasijević, V. V. Pocajt, D. S. Povrenović, M. D. Ristić, A. A. Perić-Grujić,*Science The Total Env.,* **2013,** 443,511- 519.
[370] Y. Wu, J. Guo, X. Zhang, X. Tian, J. Zhang, Y. Wang, J. Duan, X. Li,*Science The Total Env.,* **2012,** 433,20- 30.
[371] E. J. O. Marín, F. M. Capel, R. M. S. Costa, J. D. A. Hernández,*Science The Total Env.,* **2012,** 440,95- 105.
[372] D. Voukantsis, K. Karatzas, J. Kukkonen, T. Räsänen, A. Karppinen, M. Kolehmainen,*Science The Total Env.,* **2011,** 409,7, 1266-1276.
[373] T. Rajaee,*Science The Total Env.***2011,** 409,15, 2917-2928.
[374] R. Carafa, L. Faggiano, M. Real, A. Munné, A. Ginebreda, H. Guasch, M. Flo, L. Tirapu, P. C. von der Ohe,*Science The Total Env.,* **2011,** 409,20, 4269-4279.
[375] R. Derk, D. C. Davidson, A. Manke, T. A. Stueckle, Yon Rojanasakul, L. Wang,*Sensing and Bio-Sensing Research,* **2015,** 3 38–45
[376] K. Gobakis, D. Kolokotsa, A. Synnefa, M. Saliari, K. Giannopoulou, M. Santamouris,*Sustainable Cities and Society,* **2011,** 1,2, 104- 115.
[377] D. Wilson, M. del Valle, S. Alegret, C. Valderrama, A. Florido,*Talanta,* **2013,** 114,17-24.
[378] C. H. Kowalski, G. A. da Silva, H. T. Godoy, R. J. Poppi, F. Augusto,*Talanta,* **2013,** 116,315-321.
[379] E. C. Ferreira, D. M. B. P. Milori, E. J. Ferreira, L. M. dos Santos, L. M. Neto, A. Rita de A. Nogueira,*Talanta,* **2011,** 85,1, 435-440.
[380] G. C. Lalor, C. Zhang,*The Sci. Total Env.,***2001,** 281, 99-109.
[381] H. Cana, A. Dimoglo, V. Kovalishync,*Theochem,* **2005,** 723, 183-188.
[382] Y. Maa, S. Elankumaran, L. C. Marra, E. P. Vejerano, A. Pruden,*Toxicology Reports* **2014,** 1, 871–876
[383] P. Kumar, S.P. Nigam, N. Kumar,*Transportation Res. Part C: Emerging Technologies,* **2014,** 40,111-122.
[384] V. Chiarazzo, L. Caggiani, M. Marinelli, M. Ottomanelli,*Transportation Res. Procedia,* **2014,** 3,810-817.
[385] A. H. Lobbrecht, D. P. Solomatine,*Urban Water,* **2002,** 4, 283-289.
[386] Y. S. Hong, M. R. Rosen,*Urban water,* **2001,** 3, 193-204.
[387] A. Mukhopadhyay, A. Akber, A. Al-Awadi, *Urban water,* **2001,** 3, 53-62.
[388] C. Dong, B. Jin, D. Li,*Waste Management,***2004,** 23, 103-106.
[389] P. Filipponi, A. Polettini, R. Pomi, P. Sirini,*Waste Management,* **2003,** 23, 145–156.
[390] J.A. Stegemann, N.R. Buenfeld,*Waste Management,* **2003,** 2, 321–33.
[391] B. Yuan, X.Z. Wang, T. Morris,*Waste Management,* **2000,** 20, 677-686.
[392] W. Thoe, M. Gold, A. Griesbach, M. Grimmer, M.L. Taggart, A.B. Boehm,*Water research,* **2014,** 67,105-117.
[393] F. Xiao, J. S. Gulliver, M. F. Simcik,*Water research,* **2013,** 47,20, 7264-7272.
[394] S. Motamarri, D. L. Boccelli,*Water research,* **2012,** 46,14, 4508-4520.
[395] W. S. Chana, F. Recknagel, H. Cao, Ho-D. Park,*Water research,***2007,** 41, 2247-2255.
[396] J. T. Kuo, Y. Yi Wang, Wu-S. Lung,*Water research,* **2006,** 40 1367- 1376.
[397] S. Lek, M. Guiresse, J. L. Giraudel,*Water research,* **1999** 33, 16, 3469-3478.
[398] J. Farajzadeh, A. F. Fard, S. Lotfi,*Water Resources and Industry,* **2014,** 7–8,38-48.

Appendix-1: Environment and Science

Chart A1-1. Environment protection bodies

Agency	Abb
Department for Environment, Food and Rural Affairs	DEFRA, UK
European Environment Agency	EEA
Environmental protection agency, US	EPA_USA
Ministry of the Environment (Japan)	MoEn
Ministry of Environment and Forests(India)	MoEnF
National Ambient Air Quality Standards	NAAQS
Registration, Evaluation, Authorization, and Restriction of Chemicals	REACH

AQI	Canada	Great Vancouver regional district
IMECA	Air quality metropolitan	Mexico
PSI		Singapore
API	Air pollution	Hong Kong
API		China (1997)

Chart A1-2. Environmental Science (ES, Env.Sci.) Tasks

Environment (Env.)	
Phases	**Interfaces**
Air	Air_Water
Water	Water_ Soil
Soil	Soil_ Air

Extended environment
Vegetation
Food(veg),
Edible animals

Water-environment

Water budget
Ground
Surface
Hot water springs
Glaciers
Water inside living species

Atmosphere water
Lower/Upper
Cloud
Atmosphere Water vapor

Surface water		
	Still	Ponds
Surface	Flowing	Streams
		rivers
	Salty	Seas
		Oceans
	Estuarine	

Water types
Ultra-pure
Potable
Agriculture/aquaculture/Mari culture
Industry/domestic use
Bath/wash
Effluent
Polluted /contaminated

Influencing variables on pollution
Microbiological
Hydrological
Meteriological
Chemo_physical
Geological
……..

Water
Single molecule
Dimers, trimers, tetramers
Nano clusters
Large clusters
Bound water

Phases of Water	
Vapor	
Water	
Ice	$<0^{o}C$
	High pressure & High temperature

Bound water
Proteins
Minerals/ores
Materials

Water Quality indices
SWAN
PIG
….

Science of water
Chemistry
Physics
Biophysics
Geology

Water Theories
Thermodynamics
Statistical thermodynamics
CQC/ MD
…….

Environmental factors
Pressure
Temperature
Volume
Radiation/ Energy
Gravity

Natural calamities/ disasters

Catastrophes -- Natural
Earth quakes
Tsunami, Typhoon, cyclone …
Meteorites
Whirl wind
Glacier in equilibrium

Catastrophes
Oil spills
Ship wreck

Eco imbalance
Bacteria, virus
Pesticides residues
Industrial wastes/ byproducts/ organic solvents …

Civilisation/industry/Defense
Vehicles on ground
Ships/submarines
Aeroplanes/Satellites
………

Whirlwinds		
Major	Minor	Lesser
Tornadoes	Gustnado	Dust devils
Waterspouts	Fire whirl	Steam devils
Landspouts		Snow devils

Chart A1-3 Inter-/intra-/cross- disciplinary chemical sciences

Air, Water, Soil

Alchemy → Chemistry → [Organic, Inorganic, Physical]

Binary hybrid disciplines

Chemical biology	Bio[logical]chemistry
Chemical physics	Bio[logical]physics
Chemical geology	Geo chemistry
Chemical genetics	Genetic[s] chemistry

Chemical statistics
Chemo informatics
Chemometrics

Chemical computations	Computational chemistry

Chemical physics
Physical chemistry
Chemometrics

Ternary hybrid disciplines

Bio inorganic chemistry
Bio physical chemistry
Bio organic chemistry
…..
Biochemical genetics

Inorganic bio chemistry
Physical Bio chemistry
Organic Bio chemistry
……
Analytical Biochemistry

Quaternary hybrid disciplines

Physical chemistry chemical physics (PCCP)	BioChemistry ChemicalBiology (BCCB)
ComputatonalChemistry ChemicalComputations (C^4)	ChemicalStatistics StatisticalChemistry (CSSC)
…..	

Appendix-2: State-of-art-of-Modeling evolution in research mode

Chart A2-1: Process → Models

Processes	
Nature (Lab) NL	-13.7 billion years
	-4.6 billion years
	Now
	4.6 billion years Future
	….
Man-made Lab ventures	Satellites
	WWW
	Synthetic materials
	Virtual reality/ Artificial life
	……..

Understanding of processes	
Human senses	Observation
Lab(oratory)	Experiment
	Instruments
	Simulation
	Computations
Theory(computations, simulations) [TCS]	Conceptual First principles Empirical Hybrid …..

Discipline specific models		
Chemistry	ॐ Schrodinger wave equation	♎ Computational quantum chemistry
	ॐ Bose_Einstein	♎ Statistical thermodynamics
Particle physics	ॐ Standard model Theory of almost everything (TOAE)	
Environment	Single site	

	Regional Compartmental Global

Chart A2-2: Intelligent Computational Laboratory (Int.Comput.Lab, ICL)

Basis
Model driven
Data driven

Type
Persistence
Deterministic
Stochastic
Mechanistic
Empirical

Transparency
Black box
grey-box
white-box
Expert system based

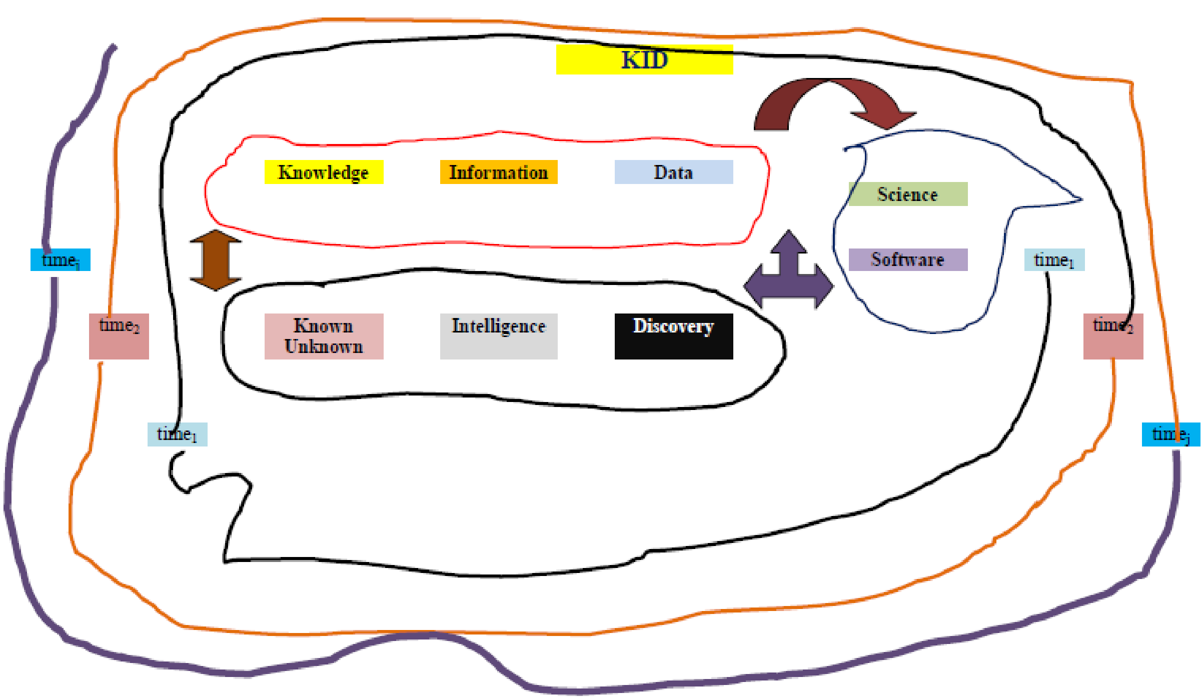
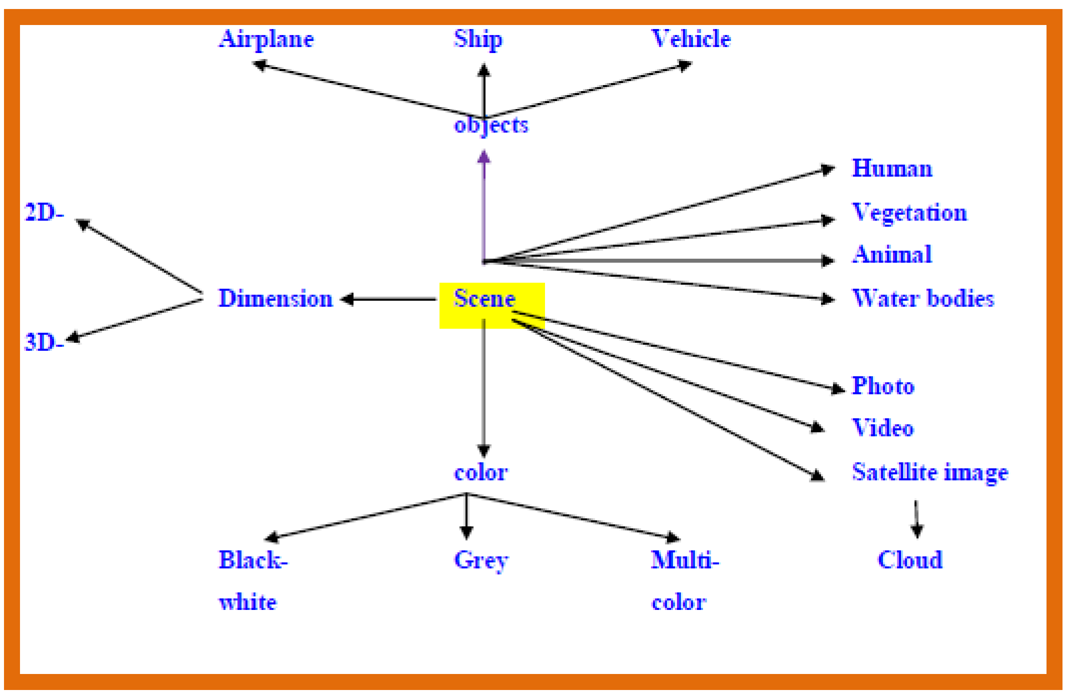


Chart A2-3: Tasks in Mathematical parlance

Object		**Components**
Tasks	:	[Function approximation, Parameterization, optimization, knowledge extraction]
Pattern recognition	:	[Classification, Discrimination, clustering],] [Profile recognition, image, scene] [Static, Dynamic, movie]

[knowledge extraction]	:	[Rule generation, rule selection]
Time series	:	[Single, multiple], [Discrete, continuous]; [deterministic, [stochastic, chaotic]]
Equations	:	[Algebraic, differential, integral]
[DE]	:	[ODE, PDE, EDE] [parabolic, elliptical, hyperbolic]
PDE	:	[Linear, non-linear [stiff]]

Function approximation	min(func(residual))
Classification	min(misclassification) max(generalizability)
Parameterization	min(var(par), corr(par))



Regression

In linear regression, the constraint is the linearity of the mapping function. Even though the system to be modeled may not be linear, the explanatory variables showing different trends are transformed rendering them amenable for application of linear regression.

Chart A2-4: Evolution of Cause-effect, classification models

Cause-Effect	[Theoretical, Empirical] [Linear, non-linear] [distribution-free] [Mathematical, Stochastic, Fuzzy] [parameter, non-parameter] [Hard, soft] [Model driven, data-driven] [Nature inspired] **Hybrid** Hybrid [fusionLevel, number of modules, paradigms] Number of modules [binary, ternary, quaternary ..]] Hybrid.fusionLevel : [loose coupled, tight, fusion] Hybrid. Paradigms : [homogeneous, heterogeneous] Hybrid.Paradigms.homogeneous : [ACO PSO Firefly]

Classification	DA: Discriminant analysis [Linear DA, Quadratic DA, Flexible DA, Mixture DA, Penalised DA] [Bayesian]
Clustering	k-means, c-means, Fuzzy-c-means, hierarchical clustering

Cause-Effect models

Model	Parameters	Variables
Linear	Linear	Linear
Multiple Linear	Linear	Linear
	Linear	Non-linear
	Non-Linear	Linear
	Non-Linear	Non-Linear
Non-linear	Non-linear Product of two linear terms Polynomial Gaussian Log/ exp /transcendental	

Models based on noise in measurement

Data		Noise		Model	Name
X	y	X	y		
FP	FP	No	No	y(t+1) = y(t)	Persistence
				y=fn(X;par)	Deterministic
		No	Norm(mean, sd)	y + N(.) =fn(X;par)	Stochastic
		No	Fuzzy(mf)	y + Fuz(.) =fn(X;par)	Fuzzy

		No	Chaotic	y + Chaos(.) =fn(X;par)	Chaotic
		FP:Floating point			

Chart A2-5: Heuristics and meta-heuristics for models

KB. A2.1: Meta rules for modeling

If There is no independent variable &
Response measured as a function of time
Then Analyse data with time-series models

If Independent & dependent variables
Then x-y model

If x-y data &
model is from first principles of discipline
Then Discipline specific model

If x-y data &
Model from first principles of discipline not available
Then Empirical model

KB. A2.2: Heuristics for type of models based on errors in y

If Noise isprobabilistic
Then Statistical models

If Noise is fuzzy
Then Fuzzy_regression

KB. A2.3: Heuristics for type of models based on data type

If Binary values
Then Binary regression
If Non-numerical data
Then Symbolic regression

If Empirical models
Then Choice is based on data structure, noise etc.

If Several theoretical models &
Empirical models
Then Develop a global one

Chart A2-6: Method_base of cause-effect models with eXpert System approach

Regression
Likelihood function
Based on residual

Likelihood
Maximum likelihood estimators
Absolute deviations
Least absolute deviations
Maximum absolute deviations
Constraint: Parameters > 0
Non-negative LS
Positive definite matrix
……
Residuals
Least Squares

Method	Goal
Least squares	Min ($Resid^T$ * Resid)
Least absolute deviations	Min (sum (Resid))
Max absolute deviations	Max (sum (Resid))
Least Median squares	Min (median($Resid^T$ * Resid))

Outliers
If Outliers are present in y

Least median squares
Iterative Recursive LS
Alternate LS

Then	Least median squares

	Variance-based
If	Errors in y is normal distribution & Homoscedastic
Then	Unit weighted LS
If	Error in y is normal distribution & heteroscedastic
Then	Weighted LS

Soft regression
Principal component regression (PCR)
Partial least squares regression (PLSR)
….

If	**Then**
PCs vs y linear	PCR
PCs vs y quadratic	QPCR
PLSCs vs y linear	PLSR
PLSCs vs y quadratic	QPLSR

Statistical linear correlation,
Mathematical independence,
Orthogonality of variables

If	**Then**
X uncorrelated	Linear LS
X correlated	PCA
X correlated & number of ys	PLSC

Nature inspired algorithms
Genetic algorithm
Immune algorithm
Predator-prey algorithm
Honey bee mating algorithm
Mosquito algorithm
……..

Appendix 3: Object functions in different tasks

There are tasks with either single or multiple object functions in estimating the free parameters of the model. Further, these functions vary depending upon the tasks like regression, classification, pattern detection etc. Minimization of a function of residuals for supervised data is generally employed. Sometimes, even maximization of performance measures also is a sought after in industry. In addition to residuals in Y with current model, a function of weight is also included which looks like Bayesian approach of parameter refinement obj_fun = ESS + f(W). In weight decay and true weight decay methods, scaled Euclidian distance of W from origin is added. The distance of W from true values ($P0^{-1}$) is considered in standard RLS procedure.

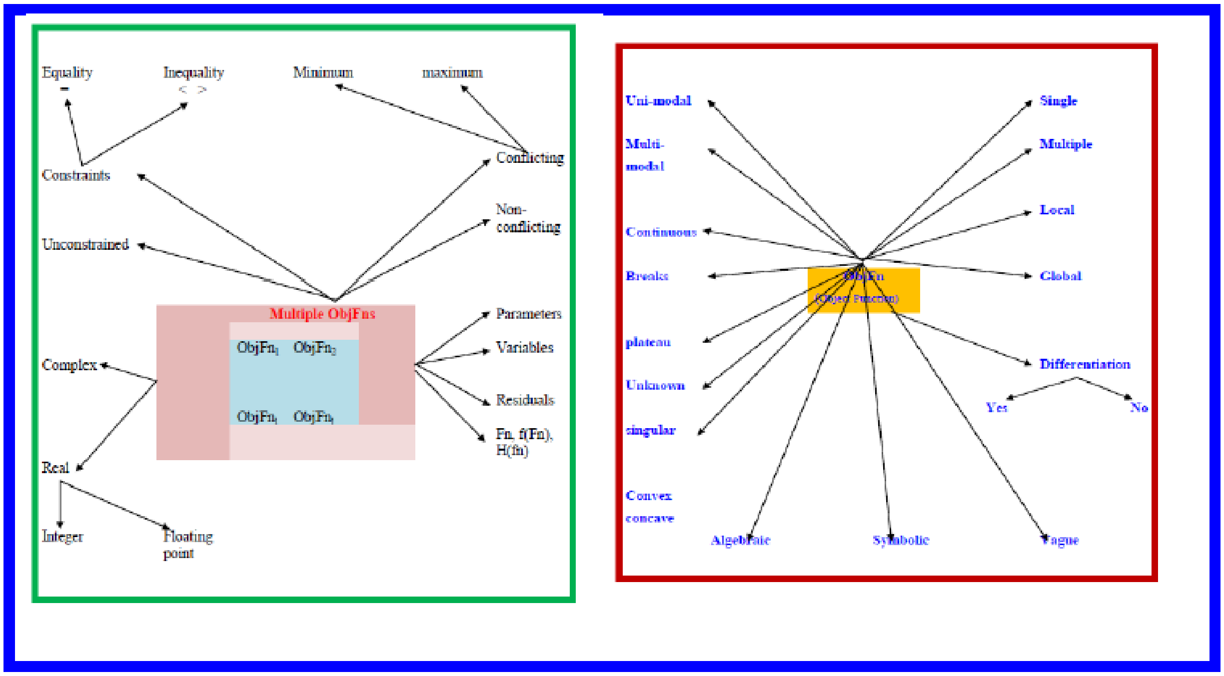


Chart A3-1: Categories of object functions

Popular object-functions and first derivatives

Object function: Abbreviation	Object function: function	$\frac{d\,f(e)}{de}$		
ESS	$e^T * e$	$2*\sum_{i=1}^{n} e_i$	*	$\frac{\partial e_i}{\partial par}$
Error	e_i			$\frac{\partial e_i}{\partial par}$
Sum of errors	$\sum_{i=1}^{n} e_i$			$\frac{\partial e_i}{\partial par}$
Regularized ESS	$ESS + \lambda * \lVert w \rVert^2$	$2*\sum_{i=1}^{n} e_i$	*	$\frac{\partial e_i}{\partial par}$
	$\frac{\beta}{2} * \ln\left[1+\frac{e_i^2}{\beta}\right]$	$\frac{e_i}{1+\frac{e_i^2}{\beta}}$	*	$\frac{\partial e_i}{\partial par}$

Novel object-functions and gradient

Object function	$\frac{dESS}{dx}$	Order of polynomial
$0.5 * \sum (y_i - ynn_i)^2$	$\sum (y_i - ynn_i) * g[TF(x)]$	Quadratic
$\frac{1}{3} * \sum \lvert (y_i - ynn_i) \rvert^3$	$\sum (y_i - ynn_i)^2 * g[TF(x)]$	Cubic
$\frac{1}{4} * \sum \lvert (y_i - ynn_i) \rvert^4$	$\sum (y_i - ynn_i)^3 * g[TF(x)]$	Quartic

Chart A3-2: object functions and derivatives

Error in input variable (EIV) based cost function: Gorp (2000) introduced EIV-object function to train data by FF-NNs with and without errors only in input or both in input and output variables. This function works in the stochastic framework.

Castillo method: The error in the input scale is used instead of age-old errors in output scale. The object functions are ESS and maximum of absolute of errors.

Typical object-functions

	MAE	$\frac{\sum \lvert e_i \rvert}{N}$
Weight decay	WD-ESS	ESS + α * 2W2²
True Weight decay	T WD-ESS	ESS + α * 2W2² + (1/n) * (w-w0)ᵀ * P0⁻¹ * (w-w0)
Standard RLS fn(ESS)	RLS LogResid	ESS + (1/n) * (w-w0)ᵀ * P0⁻¹ * (w-w0) log(1-resid²)
$cross\_entropy$	Cross_ent	$\sum \left[-ynn_i * \ln(y_i) - (1-ynn_i) * \ln(1-y_i) \right]$

$$ycal_i = fn(X; par)\ ;\ e_i = (ycal_i - yobs_i)\ ;$$
$$ynn_i : ycal_i\ from\ NNs$$

min(WD-ESS) ≈ max(posterior output probability)
if α = 0, TWD-ESS --> RLS

The linear programming methods were used for max (abs (error)), while linear equation in the case of ESS. This approach results in robust W and global optimum on the error surface. The errors in input scale need learning neural function, a new concept and superior to the known sigmoid and the like. It is implemented with polynomial (linear) combination of invertible basis functions (tanh and arc tanh). Even FT can also perform the job. This method is ten times faster compared to earlier ones.

Regularization methods:A penalty criterion is added to the objective function. But, the penalty term creates additional local minima increasing the possibility of settling in a bad local minimum. The object function is generally a function of residual (error) viz. error sum of squares, sum of absolute errors, regularized ESS, Bayesian error and so on.

Errors/ noise/ outliers in Data

Any measurement (chart A3-3) is contaminated with known/unknown distortion (chart A3-4). If the true value is known, the difference (ytrue-yobserved) is called an error. In mathematical analysis, constant and proportional errors are prevalent with pessimistic and optimistic limits. Respecting the law of classical statistics that small errors occur more frequently than larger ones (normal distribution), the distortion in replicate measurements was attributed to statistical probability. However, many probabilistic distributions (log normal, beta, exponential etc) were derived from seven distributions of Pearson. Stochastic processes also contribute to the perturbation of signal. The contribution of probabilistic component in the measured signal is called noise. The error/noise may also arise as a result of another sub-process. The errors in y, function (f(x;par)), variables (x), parameters of model are mathematical, statistical or fuzzy. The various pre-processing procedures are cited in chart A3-4.

Chart A3-3: Types of Data

Data	:	[simulated, observed] [Direct observation, indirect observation, derived from data] [Numerical, non-numerical]
[Non-numerical]	:	[Nominal, attribute], [symbol, character], image [: pixel/voxel], sound Literal : [word, sentence, abstract], [tactile-senses] Character: [alphabets, special character, graphic character, shapes]

Characteristic_ of data	:	[contradictory, redundant, non-informative]

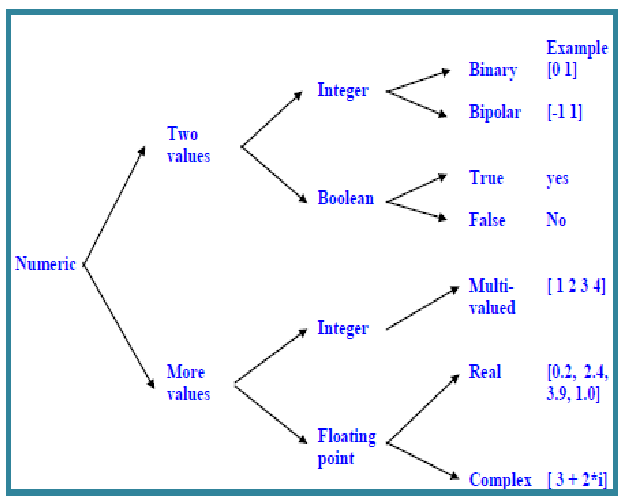


Chart A3-3b: Noise in data

Type of error in data	:	[No_error, fuzzy, probabilistic, possibility]

Chart A3-4:Preprocessing of data

Preprocessing	:	[scaling, Dimension reduction, increase of dimension,noise reduction]

Numerical	:	[constant, proportional, distribution based, Fuzzy, interval, grey, rough sets] [outliers], [trend]
Distribution	:	[probabilistic, Fuzzy]
Character	:	[rotation, translation, reflection, zoom-in, zoom-out, intensity-of-light, distortion]

Dimension reduction	:	[[SVD, PCA, PLS]; [Independent Component Aanalysis]; [Forward selection, backward elimination, GA]]
Noise reduction	:	[transform, filter]
Transform	:	[Kalman, Savitzky-Golay, Hadamart, FT, wavelet]
Kalman filter	:	[Extended KF, Ordinary KF]
Scaling	:	[Mathematical, statistical, fuzzy, interval, Grey]
Linear	:	[mean centered, variance-zero2one, minimum2one,zero2one]
Mathematical	:	[linear, non-linear]
Non-linear	:	[log, exp, power, tanh, boolean]

The numerical magnitudes of data sets of many tasks are on different orders and thus scaling is mandatory. ScaleX.m is a MATLAB function converting the matrix in the chosen range (lower to upper). Since the realistic comparison of residuals for model validation and prediction errors is to be performed in measurement scale, the unscaling function is also developed.

Optimization methods

Optimization (minimization or maximization) of response and error are crucial in every activity viz. high yield of product with minimum impurities, high quality of a finished product with a lower cost etc. The categories of optimization are without and with (linear/non-linear/equal/unequal) constraints. Depending upon the viability of calculating the function, first and second order gradients, a galaxy of optimization methods have proposed (Chart A3-5 and A3-6).

Chart A3-5: Optimization (training) methods

Optimization:
[Static, adaptive, dynamic]

[self-starting, non-self-starting]

Heuristics for choice of training methods

If	Object function has derivatives
Then	Gradient methods are used
Else	Direct search methods
If	Derivatives are not calculable & Function value is not available
Then	Simplex

Gradient based

First order	:	[Steepest descent (BP), One-step-secant, Resilent]		
		BP	:	[non adaptive {Without momentum, With momentum}, adaptive {Without momentum, With momentum}]
		[delta rule]	:	[Delta rule, Cum-delta, Norm-cum-delta, Delta-Bar Delta, Ext-DBD, Rumelhart and McClelland's delta] [Quick Propogation, Max Prop, Directed random search]
Second	:	Newton Raphson		

order		
Quasi-Newton	:	[Broyden-Fletcher-Goldberg-Shano (BFGS), Limited memory BFGS, Davidon-Fletcher-Powell (DFP)] [Marquardt] [Conjugate gradient] [Powell-Beale, Fletcher Powell, Polak-Ribiere, Fletcher Reeves]
Direct search (Non-gradient)	:	[Bisection, Golden search, False position, Brent, Simplex]
Direct search + gradient	:	[DBrent]

Chart A3-6a: Global optimization methods

Global optimization Methods	:	[SAA, GA]
[SAA]	:	[SAA-SS error, SAA-WTA error, SAA-WWTA error]

Chart A3-6b: Hybrid and adaptive methods

Hybrid	:	[{GN + SAA}, {Simplex + Kalman}, {GA+GN+BFGS+GA}]		
Adaptive	:	[Marquardt,CR, non-linear-CR]		
		Non-linear CR	:	[CR, NN]
		CR	:	[MLR, PCR, PLSR]
		Marquardt	:	[Steepest descent, GN, NR]

SAA : simulated annealing algorithm GA :genetic algorithm
CR : Continuous regression GN : Gauss-Newton