J. Indian Soc. Coastal Agric. Res. 38(2): 51-67 (2020)

Conceptual Framework for Groundwater Vulnerability Assessment Using Physical, Experimental and Machine Learning Based Approaches in Coastal Aquifers of India

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Received: 24.12.2019 Accepted: 08.08.2020

The exploitation of coastal aquifers results in intrusion of seawater and optimal management of coastal aquifers focuses mainly on adopting good operational strategies to contain aquifer salinity within a mandated limit, while simultaneously meeting the demand for water supply/recharge. Management of saltwater intrusion in coastal aquifers is thus a critical issue of modern times. In this study, we present a theoretical framework for assessing the groundwater vulnerability in coastal aquifers of India using physical, experimental, and machine learning-based approaches. The developed framework suggests the use of 2D experiment for understanding the saltwater intrusion processes and fate and transport of contaminants like fluoride and arsenic. Further, the obtained parameters from the 2D experiments will be used to develop a numerical model using a physical-based simulator (SEAWAT). Lastly, the physical-based simulator will be replaced by a machine learning-based model and later will be coupled with optimization approaches to solve the groundwater management problem in coastal aquifers. The suggested framework will be useful in developing the strategies for minimization of saltwater intrusion or maximization of freshwater pumping in coastal zones.

(***Key words:*** *Machine Learning, Physical based models, Salt water intrusion)*

Groundwater is the main source of water supply in many coastal regions and most of the aquifers in the coastal belt are overexploited due to an ever increasing demand for water. Thus, excessive pumping of water gives rise to saltwater intrusion. Under normal conditions, freshwater would flow into the sea, however, excessive abstraction of water results in a reversal of groundwater flow from the sea towards inland thereby causing saltwater intrusion. Saltwater intrusion can be defined as the inflow of seawater into an aquifer and is common in coastal aquifers where the aquifers are in hydraulic contact with the sea. Saltwater intrusion leads to an increase in the saline water volume and correspondingly a decrease in the freshwater volume. Salinization of groundwater is very important because mixing even a small quantity of saltwater (2 to 3%) with groundwater makes freshwater unsuitable for use and can result in abandonment of freshwater supply wells in case the salt concentration exceeds drinking water standards (Abd-Elhamid and Javadi, 2011). Thus, saltwater intrusion should be prevented or at least controlled to protect groundwater resources. Bear *et al*. (1999) suggest that uncontrolled abstraction of water from aquifers or seasonal variations in natural groundwater flow, barometric pressure, tidal effects, seismic waves, dispersion, and climate change could result into saltwater intrusion problems. Indian coastal aquifer systems continue to be affected by geogenic and anthropogenic contaminations. Major aquifers of India's coastal regions have already been highly affected by fluoride (Rao, 2009), heavy metals (Ranjan *et al*., 2008 a,b and c), arsenic (Chakraborti *et al*., 2004; Chatterjee *et al*., 2010).

Fluoride

The total population of fluoride endemic in 201 districts of India is 411 million (40% of Indian population) and more than 66 million people are

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estimated to be suffering from fluorosis including 6 million children below 14 years of age. In which total 103 coastal districts are highly affected by fluoride since the independence of India (Fig. 1). In Gujarat state, the number of affected districts is 24 out of a total of 26 districts. A higher level of fluoride in groundwater could be due to leaching of fluoride from various minerals like fluorite, fluorapatite, cryolite, etc. Sometimes mica group of minerals may be responsible for fluoride in water. Crops irrigated with fluoride contaminated water and rock salts rich in fluoride are also in use as food. Table 1 presents a summary of studies reported fluoride problems in different coastal districts of India.

Arsenic

Over 70.4 million people are potentially at risk from groundwater arsenic toxicity in India. Several districts (Murshidabad, Nadia, North 24 Parganas, and South 24 Parganas) of coastal and delta regions of West Bengal was reported high arsenic contaminations (Table 2). The mechanism of arsenic release from sediments to aquifers has been established by several theories such as oxidation, reduction, and recent inflow of carbon, microbial or geochemically mediated reductive dissolution (Anawar *et al*., 2011; Das *et al*., 1996).

Nitrate and heavy metals in coastal wetlands

A high concentration of Cd, Cr, Cu, Ni, Pb, Fe, Mn, Zn was reported in Pichavaram mangrove. High total nitrogen was observed in <10 μm than in <63 and>125 μm grain size and also in the densely forested area of Pichavaram mangrove. Likewise, high uptake and accumulation of Fe, Cu, and Zn by mangrove plants in Zuari estuary (Coastal area of Goa) were observed by Noronha-D'Mello and Nayak (2016). Panigrahi *et al*. (2007 and 2009) studied the pre-monsoon, monsoon, and post-monsoon water samples and analyzed dissolved oxygen; nutrient, salinity along with the phytoplankton chlorophyll density in the period December 2001-June 2013 in Chilka lagoon. The findings of the study

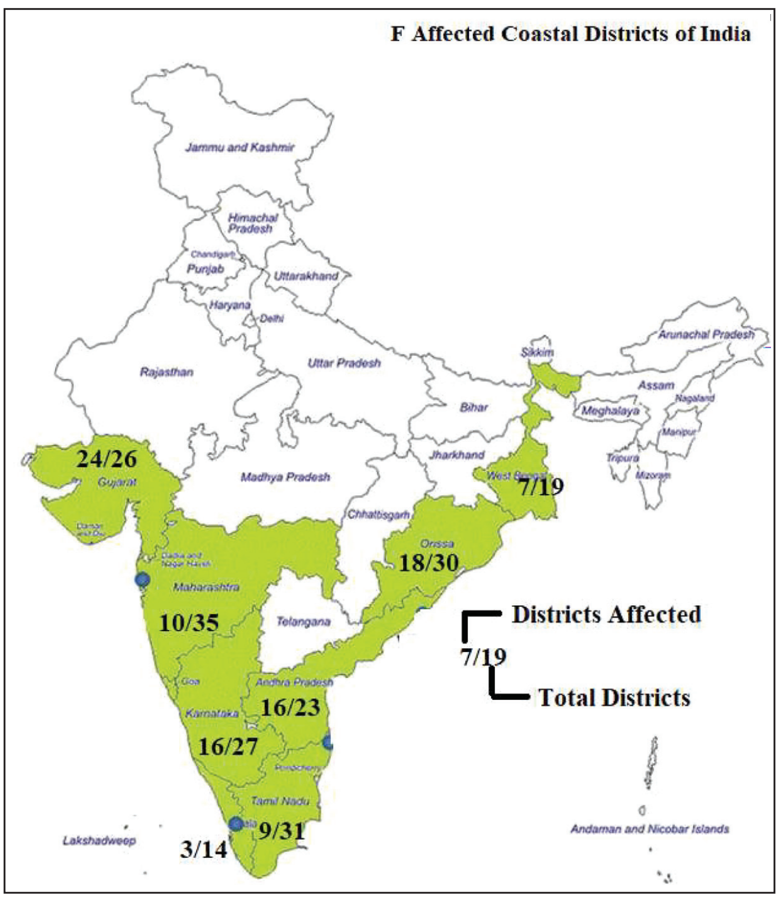

Fig. 1. *Fluoride affected Indian coastal districts (adopted from Chakraborti et al., 2016)*

Table 1. *Summary of studies reported high fluoride concentrations in Indian soil-water systems*

State	District	State/locality	Concentration range	Sources	References
Orissa	Nayagarh	Singhpur and Sagaragan	>1.5 mg L^{-1}	Mixing of hot spring water with groundwater	Kundu *et al.* (2001), Tripathy *et al.* (2005)
Andhra Pradesh	Guntur	Whole District	0.3-2.3 mg L^{-1}	F- rich salt due to high ET, low hydraulic conductivity and more contact time with weathered rock.	Subba Rao (2003)
Gujarat	District of North Gujarat	Cambay region	>5 ppm	Weathering of rocks of the Kumbhalgarh group, Ambaji Granites and Gneisses of Delhi super group, Lunawada group and Godhra granite	Gupta *et al.* (2005)
West Bengal	Birbhum	Nalhati-1	0.006-1.95 mg L^{-1}	Basaltic rock and water interaction	Gupta *et al.* (2006)
Andhra Pradesh	Prakasham	Whole district	0.5-9 mg L^{-1}	Fluorite and fluorapatite formation	Ramanaiah *et al.* (2006)
Gujarat	Mehsana	Whole district	0.14-5.6 mg L^{-1}	Quartz, calcite, albite and anorthite along with sodium bicarbonate waters	Dhiman and Keshari (2006)
Kerala	Palakkad	Whole District	0.2-5.75 mg L^{-1}	Hornblende biotite gneiss	Shaji *et al.* (2007)
Gujarat	Mehsana district	Kadi tehsil	0.9-2.08 mg L^{-1}	Alkaline water enhance F leaching	Salve *et al.* (2008)
Andhra Pradesh	Visakhapatnam	River Varaha Basin	1.15-1.28 mg L^{-1}	Leaching due to alkaline subsurface	Rao (2009)
West Bengal	Hooghly	Whole District	0.01-1.18 µg mL^{-1}	Geogenic along with application of super phosphate in cultivated land	Kundu and Mandal (2009 a and b)
Karnataka	Kolar and Tumkur	Bagepalli, Gudiabanda, Pavagada	0.36-3.34 mg L^{-1} (Kolar) and 0.78-5.35 mg L^{-1} (Tumkur)	Dissolution and calcite precipitation	Mamatha and Rao (2010)
Tamil Nadu	Kacheepuram	Palar River Basin	1-3.24 mg L^{-1}	Weathering of schistose and gneissose rocks.	Dar *et al.* (2011)
Tamil Nadu	Thoothukudi	Thoothukudi city	0-3.3 mg L^{-1}	High Na+ and pH causes F-leaching	Srinivasamoorthy *et al.* (2012)
Tamil Nadu	Dindigul	Whole District	0.02-3.3 mg L^{-1}	Weathering of hornblende biotite gneiss	Chidambaram *et al.* (2013), Magesh *et al.* (2013)
Kerala	Alappuzha	Whole District	0.6-2.88 mg L^{-1}	Not Specified	Raj and Shaji (2017)

Table 2. *Summary of studies reported As-contaminations in Indian soil-water systems*

State	District	Concentration range	Key findings	References
West Bengal	9 Districts-Maldah; Murshidabad; Bardhaman; Hugli; Howrah; Nadia; North 24-Parganas; Parganas; and Calcutta.	>50 µg L^{-1}	Out of 9 As affected districts, 7 districts reported high health issues (Skin lesions).	Chowdhury *et al.* (2000)
West Bengal	Murshidabad; 24 Parganas (north)	0.1-93.1 mg L^{-1}	As-concentration range 3.2-93.1 mg L^{-1} at depth 6-50 m in fine and medium sand layers	Acharyya *et al.* (2000)
West Bengal	24-Parganas (Ramnagar–Dhapdhapi block of Baruipur area)	>0.05 mg L^{-1}	Clay and peat layer contain more As than silt and sand layers.	Pal *et al.* (2002)
West Bengal	Area between Damodar fan-delta and west of Bhagirathi River	>300 µg L^{-1}	Maximum concentration i.e. 313 µg L^{-1} at Paigachi	Acharyya and Shah (2007)
West Bengal	Ganges-Brahmaputra-Meghna deltaic alluvium	0-0.29 mg L^{-1}	Fe(II)-Fe(III) cycling is the dominant process for the release of As from aquifer sediments to groundwater	Chakraborti *et al.* (2004); Chatterjee *et al.* (2010)

indicated a high nitrate in the monsoon then the pre and post-monsoon which also altered the phytoplankton growth and their decomposition. Likewise, Ram *et al*. (2018) reported pollution index for Cu, Mn, Ni, Pb, and V in the Sundarbans mangrove area (Eastern coast of India) and Elephanta island mangrove area (Western coast of India).

Hydrocarbon and green house gaseous pollutants

Indian coastal aquifers are at high risk of hydrocarbon pollutants as most of the petrochemical refineries are located in these regions. Accumulation of hydrocarbon contaminants in aquifers and the use of contaminated groundwater for irrigation further deteriorate the situation and raises concern about their exposure to the public. Recently, many coastal soil-water systems were reported with high PAHs contaminations. Total petroleum hydrocarbons, which include acenaphthene, fluorene, phenanthrene, and fluoranthene in groundwater samples collected from Royapuram, Chennai city, Tamil Nadu to range between 1.6-12.9 µg L^{-1} were reported by Brindha and Elango (2014). Mitra *et al*. (2019) reported high (3.26-628.61 ng g^{-1}) PAHs, PCBs, PCBzs and OCPs in the surface sediments (0-5 cm) of the Hooghly River estuary in the Western Bengal basin. Likewise, Zanardi-Lamardo *et al*. (2019) found 15.4-1731 ng g^{-1} of PAHs in Sundarbans mangrove, the eastern coast of India. Recently, Duttagupta *et al*. (2019) reported PAHs (naphthalene, phenanthrene, and fluoranthene) of concentration ranges 1.15-23.13 ng g^{-1} in aquifer sediments of Western Bengal basin, India. While naphthalene was the dominant PAH with a maximum concentration of 8.25 mg L^{-1} in groundwater samples. Further study is needed to explore hydrocarbon contaminations in coastal aquifer systems.

Indian coastal wetlands are major sources of greenhouse gases (GHGs) which affects soil-water quality and ultimately agricultural productivity of the area. GHGs emission from different coastal wetlands of India has been listed in Table 3. A little attention has been paid to study the role of GHGs on groundwater quality in the coastal area of India.

Groundwater vulnerability assessment methods

Groundwater vulnerability is referred to as the relative susceptibility of aquifer systems to anthropogenic pollution. It has been extensively used

Table 3. *Summary of studies performed to investigate GHGs emissions from Indian coastal wetlands*

Reference	Study site	GHGs	Estimated emission
Sarma *et al*. (2001)	Mandovi-Zuari estuarine	CO_2	11-65 mmol m^{-2} day^{-1}
Bouillon *et al*. (2003)	Gautami Godavari estuary	CO_2	21.9±26.1 (Godavari); 70.2±127 (Mangroves); 8.3±13.6 (Kakinnada Bay) - mmol m^{-2} day^{-1}
Gupta *et al*. (2008)	Chilika logoon, Coastal Region on Orissa	CO_2	81-861 mmol m^{-2} day^{-1}
Muduli *et al*. (2012)	Chilika logoon, Coastal Region on Orissa	CO_2	10.28±4.79-195.86±39.79 mol C m^{-2} yr^{-1}
Gupta *et al*. (2009)	Cochin estuary	CO_2	65±80-267±131 mmol m^{-2} day^{-1}

worldwide to evaluate the risk of pollution and for protecting groundwater from pollution. In last three decades, several methods have been proposed for the assessment of groundwater vulnerability (Kumar *et al*., 2015; Machiwal *et al*., 2018; Wachniew *et al.*, 2016; Yadav *et al.*, 2018; Yadav *et al.*, 2019). Aquifer vulnerability may be distinguished as (a) intrinsic vulnerability, and (b) specific vulnerability (Fig. 2). The intrinsic vulnerability of groundwater generally focused on geological, hydrological, and hydrogeological characteristics, but independent of the nature of contaminants, to estimate contaminants generated by anthropogenic activities. While specific vulnerability accounts contaminant properties (fate and biogeochemical processes) in addition to transport characteristics and their relationship with various components of intrinsic vulnerability (Machiwal *et al*., 2018).

Index based models

Most of the groundwater vulnerability studies are based on either an index-based method (Kumar *et al*., 2015) or Geographic Information System (GIS)-based DRASTIC method (Shirazi *et al*., 2012). DRASTIC (Aller *et al*., 1987) and GOD (Foster and Chilton, 2003) are the most established methods. In GOD method, groundwater confinement, description of the strata, depth to groundwater table were considered to model the aquifer vulnerability index (AVI). While, DRASTIC model runs by considering depth to the water table, net recharge, aquifer media, soil media, topography, the impact of the vadose zone, and hydraulic conductivity. Thus, the DRASTIC model (integrated with GIS) is the most popular and widely used for groundwater vulnerability assessment (Kumar *et al*., 2015).

Attenuation potential of the vadose zone and soil

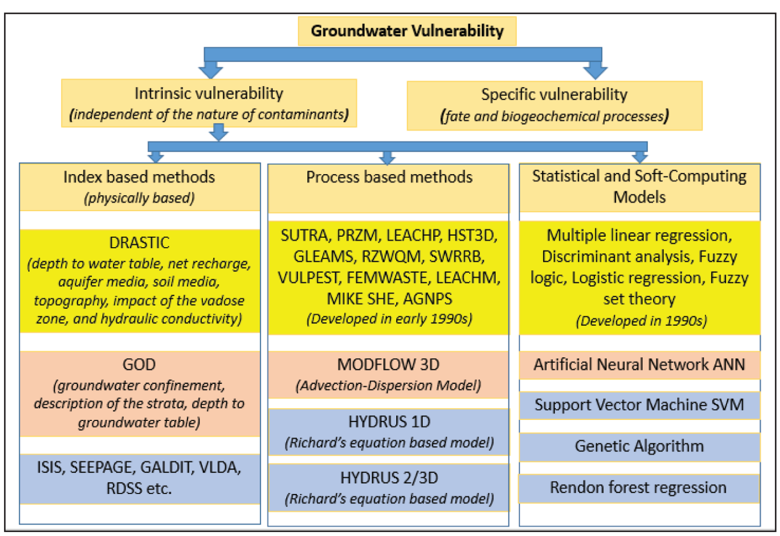

Fig. 2. *Classification of methods for the groundwater vulnerability assessment (adopted from Machiwal et al., 2018)*

was considered in the SINTACS method which makes it more applicable pollution source indexing (Civita and De Maio, 2004). Likewise, the ISIS method was designed by integrating the rating systems and weights of DRASTIC and SINTACS methods and the GOD scheme (Gogu and Dassargues, 2000). For coastal aquifers, the GALDIT method was developed in the framework of the EU-India COASTIN project with the aim of aquifer vulnerability assessment to seawater intrusion (Ferreira, and Chachadi, 2005). In which, groundwater occurrence, hydraulic conductivity, depth to groundwater level above the sea, distance inland perpendicular from the shoreline, the impact of existing seawater intrusion status, and aquifer thickness were considered to model the vulnerability. The majority of index-based modeling approaches are limited to evaluate a complex soil-water system for varying range of pollutants. Thus, process-based models were introduced concurrently to evaluate or consider fate and transport mechanisms in the performance of vulnerability assessment methods.

Process-based models

Process-based models utilize natural processes occurring within the hydrogeologic settings of underlying vadose-zone and aquifer systems. Such simulation models usually determine specific (or pollutant-specific) vulnerability for diffuse pollution sources by incorporating various physical, chemical, and biological (microbial) processes dictating the fate and transport of contaminants in unsaturated and saturated zones. These models predict contaminant transport at both spatial and temporal scales. The most popular and widely used process-based models are SEAWAT, MIKE SHE, MODFLOW 1D, HYDRUS 1D, HYDRUS 2/3D (Machiwal *et al.*, 2018). SEAWAT is used to simulate saltwater intrusion in a coastal aquifer. The software simulates three-dimensional, variable-density, transient ground-water flow in a porous media by solving the coupled flow and solute transport equations. The fluid density is assumed to be solely a function of the concentration of dissolved constituents and the effects of temperature on fluid density are not considered.

The governing flow equation solved by SEAWAT (Guo and Langevin, 2002) is as follows:

$$\nabla\left[\rho K_f\left(\nabla h_f+\frac{\rho-\rho_f}{\rho_f}\nabla z\right)\right]=\rho S_{Sf}\frac{\partial h_f}{\partial t}+n\frac{\partial\rho}{\partial C_m}\frac{\partial C_m}{\partial t}-\rho_S q_S' \qquad \dots (1)$$

where is the fresh water specific storage [L^{-1}] defined as the volume of water released from storage per unit volume per unit decline of freshwater head and is the concentration of solute mass per unit volume of fluid [M L^{-3}]. Likewise, the solute transport equation solved by the SEAWAT (Zheng and Wang, 1999) is:

$$\frac{\partial(nC_m)}{\partial t}=\nabla\cdot(nD\cdot\nabla C_m)-\nabla\cdot(qC_m)-q_S' C_S \qquad \dots (2)$$

where D is the hydrodynamic dispersion coefficient tensor [$L^2\ T^{-1}$] and C_s is the source or sink concentration [M L^{-3}].

HYDRUS (finite element method) generally used to model water flow and solute transport with transient boundary conditions, where the van Genuchten-Mualem hydraulic model (van Genuchten, 1980) is adopted for modeling water flow, and a general form of the advection-dispersion equation is used for modeling solute transport (Šimůnek and van Genuchten, 2008).

$$\frac{\partial\theta_m}{\partial t}=\frac{\partial}{\partial x}\left[K_x(h)\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial y}\left[K_y(h)\frac{\partial h}{\partial y}\right]+\frac{\partial}{\partial z}\left[K_y(h)\frac{\partial h}{\partial z}+K(h)\right]-S_m-\Gamma_w$$
$$\frac{\partial\theta_{im}}{\partial t}=-S_{im}+\Gamma_w \qquad \dots (3)$$

where θ is the volumetric water content defined as the volume of water per unit volume of soil (dimensionless), h is the pressure head of mobile region [L], S is a sink function that represents the water extraction by surface vegetation [T^{-1}], z is the depth of vadose zone measured positive upwards [L], is the water transfer rate between mobile and immobile region [T^{-1}], K is the hydraulic conductivity of the soil [L T^{-1}] and t is the time [T]. To solve this equation, explicit expressions for the soil constitutive relationship between the dependent variable h and the nonlinear terms K and θ are required. Out of the many soil moisture constitutive relationships reported in the literature, the most popular ones are by van Genuchten (1980). The closed form θ-h relationship developed by fitting mathematical equations to field experiments data yields

$$\theta(h)=\begin{cases}\theta_s & h\geq 0\\ \theta_r+[\theta_s-\theta_r]\Big/\left[1+|\alpha h|^n\right]^m & h<0\end{cases} \qquad \dots (4)$$

where θ_s is the saturated water content, θ_r is the residual water content (irreducible) and is the moisture content at soil matrix potential, h, n, m, α are curve fitting parameters Likewise, van Genuchten (1980) used the statistical pore size distribution model along with equation 2a to yield the K-h relationship.

$$K(h)=K_s S_e^l \left[1-\left(1-S_e^{1/m}\right)^m\right]^2 \quad \ldots (5)$$

where K_s is the saturated hydraulic conductivity of the soil, m =1-1/n and S_e is the effective saturation.

The classical convection dispersion equation is used for contaminant fate and transport in multi-dimensions considering a contaminant attenuation/sink term. Fick's law coupled with the mass balance equation yields the following modified form of the advective-dispersive equation.

$$\frac{\partial(\rho_s S_D)}{\partial t}+\frac{\partial(\theta C)}{\partial t}=\frac{\partial}{\partial x_i}\left[D_{ij}\theta\frac{\partial C}{\partial x_i}-q_i C\right]+S_c-\Gamma_s$$

$$\frac{\partial(\rho_s S_D)}{\partial t}+\frac{\partial(\theta C)}{\partial t}=\Gamma_s+S_c \quad \ldots (6)$$

where C is the contaminant concentrations in the soil water solution (mg per unit volume of soil solution), S_D is the amount of solute adsorbed by the soil solids (mg of contaminant per kg of soil), q_i is the i-th component of soil water flow velocity [L T^{-1}] (i = 1, 2, 3), D_{ij} is the tensor of hydrodynamic dispersion coefficient [L^2 T^{-1}] (i, j = 1, 2, 3), p_s is the bulk density of soil, q is the soil water flux, and S_c is the sink term (mg per unit volume of soil per unit time). The tensor of hydrodynamic dispersion coefficient (or diffusion-dispersion coefficient) D_{ij} is a pore water velocity-dependent function and is evaluated by adding the mechanical dispersion and molecular diffusion coefficients as:

$$D_{ij}=(\alpha_L-\alpha_T)\frac{v_i v_j}{v}+\alpha_T v\delta_{ij}+D_o \quad \ldots (7)$$

where α_L and α_T are longitudinal and transverse dispersivities [L], v is the pore water velocity (q/θ), δij is the Kronecker delta (δ_{ij} = 1 if $i = j$, and δ_{ij} = 0 otherwise), and D_o is the molecular diffusion [L^2 T^{-1}]. Yadav and Junaid, (2014) estimated the vulnerability index using HYDRUS 1D for Doon valley. They considered the reciprocal of time required for the surface solute to reach the underground water resources, considering constant and atmospheric boundary conditions, is used for quantifying the vulnerability index. A similar study was also performed by Joshi and Gupta, (2018) and compared with the GIS-based DRASTIC model.

The main limitation of the process-based methods is the difficulty in acquiring extensive field data. This limitation is overcome to a limited extent by developing index-based simplified models under the assumption of steady-state flow and uniform homogeneous ideal medium. Most of the process-based models are still unable to consider complex soil microbial dynamics and biogeochemical mechanisms like biodegradation, nitrifications, denitrifications, etc. Only a few process-based models have been linked with GIS. For example, the NLEAP (Nitrate Leaching and Economic Analysis Package) model was used with the GIS framework to predict the spatial distribution of nitrate leaching (Shaffer *et al*., 1995). Thus, index-based qualitative models have been preferred over process-based models in the past, because the latter requires a large amount of field data, and it is difficult to obtain reliable data for a complex subsurface process especially in the resource-poor developing countries. In contrast to the index-based models that have been exhaustively utilized in vulnerability assessment over large areas, the studies dealing with process-based models were only undertaken for very small areas, for example, part of an aquifer system, watershed/catchment, agricultural fields, etc.

Machine learning-based models

Machine learning techniques will be helpful to evaluate and reduce the complexity of large data sets. Sensitivity analysis based on a machine learning approach will provide a more accurate understanding of governing processes and associate parameters. A management strategy for saltwater intrusion is based on simulation of flow and transport processes. Simulation of these processes becomes more difficult particularly in coastal aquifers as they are density-dependent. Moreover, the coupling of the simulation model with optimization techniques makes all this more complex and time consuming (Bhattacharjya and Datta, 2009). Bhattacharjya *et al*. (2007) proposed an ANN model to simulate a density-dependent saltwater intrusion process in coastal aquifers and suggested that data-based model like ANN can reduce the computational burden significantly without impairing the simulation accuracy. Later, Bhattacharjya and Datta (2009) used ANN-GA based approach to solve multiple objective management problems of a coastal aquifer. The results of their study show that the proposed methodology could be adapted successfully to solve multiple objective management models for coastal aquifers. Likewise, Sreekanth and Datta (2010) developed a simulation-optimization model using genetic programming (GP) as a replacement for FEMWATER and found that GP was better suited for optimization using an adaptive search method. Similarly, Banerjee *et al*. (2011) successfully used ANN to predict groundwater salinity of an island aquifer. In the same way, Ashtiani *et al*. (2013) proposed a combination of ANN-GA to manage freshwater in small islands and suggested that ANN could provide a more effective framework for minimizing seawater intrusion. Hussain *et al*. (2015) presented a surrogate modeling technique Evolutionary Polynomial Regression (EPR) for simulation of saltwater intrusion and successfully used it in a coupled simulation-optimization model to minimize the economic and environmental costs. Roy and Datta (2017) used a Sugeno type Fuzzy Inference System (FIS) replacing FEMWATER to predict saltwater concentration at different monitoring locations and suggested that FIS can simulate the complex physical processes of heterogeneous coastal aquifers. The literature review thus indicates that data-based models could be used to simulate the saltwater intrusion process accurately. It is also evident from the literature that only a few data-based models (ANN, GP, FIS) have been tested so far, however, the recent research in the field of machine learning has shown that new and efficient models like SVM (Vapnik, 1995) and ELM (Huang *et al*., 2004) have been developed very recently successfully used in various water resources problems (Himanshu *et al.*, 2017a; Himanshu *et al*., 2017b; Yadav and Eliza, 2017; Yadav *et al.*, 2016a; Yadav *et al.*, 2016b; Yadav *et al.*, 2017). These models have been used in various water quantity and quality problems and can overcome all shortcomings associated with the traditional models like ANN and GP. Further, Yadav *et al*. (2018) used physical (SEAWAT) and data-based models (ANN, SVM, GP, ELM) to develop a management strategy for coastal aquifers.

Conceptual framework for coastal aquifers of India

Data and information sources

To understand the behaviour of a coastal aquifer, it is important to gather a large number of data from several agencies. For example, meteorological data can be collected from the Indian Meteorological Department (IMD). Likewise, land use and land cover data can be collected from different remote sensing and satellite based observatory like USGS Earth Explorer (www.earthexplorer.com). District and block-wise groundwater data can be obtained from India-WRIS (http://indiawris.gov.in) and Central Ground Water Board (CGWB). Furthermore, information regarding coastal rivers, basin, pollution, and so on can be obtained from ENVIS Centre for Coastal Zone Management and Coastal Shelterbelt (http://www.iomenvis.in/) as well as from state-level coastal management information systems, for example, Karnataka state's coastal management information systems site (http://cmiskarnataka.in/). Furthermore, soil-water quality, coastal processes & hazards, agriculture, habitats & ecosystems, and more data can be collected from some specialized coastal research institutes like National Centre for Coastal Research, Chennai, Suganthi Devadason Marine Research Institute (SDMRI), National Geophysical Research Institute, ICAR-Central Coastal Agricultural Institute, National Institute of Ocean Technology, CSIR coastal and hydraulics laboratory, etc. Information on coastal research can be obtained from the Ministry of Environment, Forest, and Climate Change, Ministry of Water Resource (JalSakti), and Ministry of Earth Science, Government of India. National Project on Aquifer Mapping and Management (NAQUIM) will facilitate data gaps especially physical and hydraulic characteristics, groundwater chemical characteristics, and resource availability (Saha *et al*., 2019). District or watershed level information can be explored with local public health engineering departments (PHEDs), municipalities, hospitals, and gram panchayat in and around pollution affected or target study area. Collected data can be categorized and then machine learning techniques can be applied to evaluate and determine sensitive parameters (Fig. 3).

Integrated physical, experimental and machine learning-based modeling

Indian coastal aquifers are continuing be to affected by multiple pollutants as discussed in the introductory section. None of the data providing agencies have information about realistic biogeochemical parameters, fate and transport parameters, or any contaminant hydrological information of any site. Most of the aquifer vulnerability studies performed in the past were not considered realistic contaminant behaviour. Thus, extensive laboratory and field experiments are needed to investigate the governing fate and transport processes under dynamic coastal aquifers conditions. In the laboratory, basic physical parameters like porosity, hydraulic conductivity, dispersivity can be determined

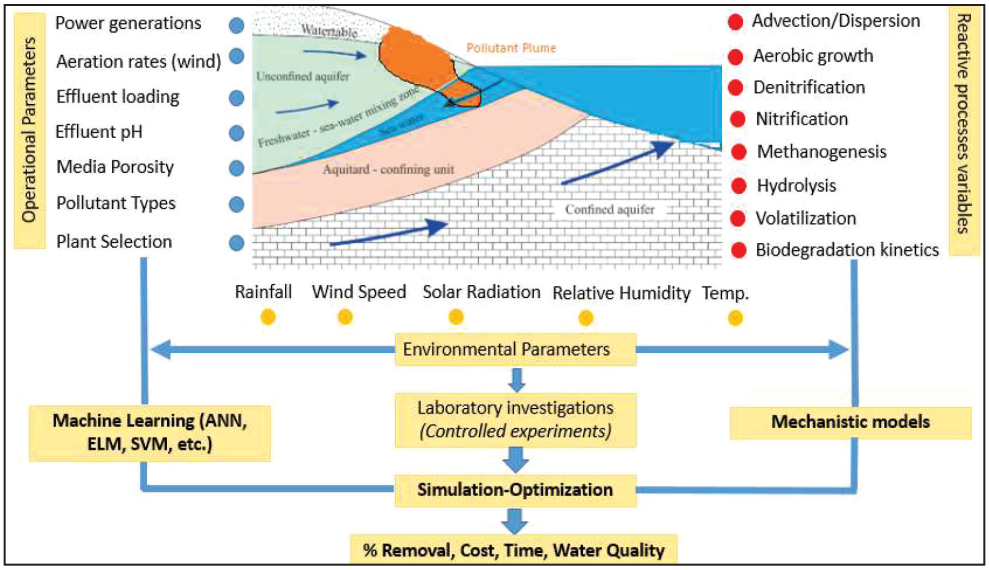

Fig. 3. *Conceptual framework to evaluate the aquifer vulnerability to multiple contaminations in coastal regions under climate change conditions*

using the oven-dry method, constant head permeameter, and tracer test experiments. Similarly, pressure plate experiments can be performed for soil-moisture curve analysis. Small scale batch scale experiments can be performed for biodegradation, adsorption of multi-pollutants under varying environmental conditions (Gupta *et al.*, 2019). Furthermore, 1D column experiments can be performed to estimate pollutant movements, multi-phase movements, and gaseous diffusion analysis. These experiments will also be conducted to evaluate the role of operational and environmental parameters on fate and transport processes of single or multiple pollutants, like fluoride and arsenic interactions with the salt-water intrusion. Likewise, the role of freshwater on salt-water intrusion and *vice-versa* can be obtained by conducting large scale experiments by incorporating recharge rates, density-driven flow, and underlying aquifer conditions as shown in Fig. 4. Consideration of realistic characteristics of pollutants is rare in vulnerability assessment studies performed in the past. Thus, laboratory experiments will add significant values inaccurate estimation of aquifer vulnerability, especially in coastal aquifers where groundwater systems are more dynamics than other inland aquifers.

Based on laboratory experiments, large scale numerical simulation can be performed for accurate estimation of pollutant transports through heterogeneous aquifer media under local and landscape scale boundary conditions. Such large scale simulation can also be performed for future projection of pollutants loading and ultimately vulnerability at different time scales. This has been completely ignored in previous studies. Furthermore, a better estimate of the mean travel (residence) time taken by a contaminant through the vadose zone requires consideration of preferential flow paths that are difficult to be correctly delineated in the field or laboratory. Thus, numerical simulation should focus on the development of improved vulnerability assessment methods considering dual-porosity (preferential or fracture flow) or triple porosity (karst systems) and other shortcomings of the existing methods. For example, the HYDRUS 2/3D model can successfully model dual-porosity for heterogeneous media (Šimůnek and van Genuchten, 2008). Solute transport modeling can be evaluated by considering indirect and direct hydraulic connections between surface water bodies and groundwater. This provides accurate spatio-temporal dynamics of stream-aquifer exchange due to subsurface heterogeneity and scale problems. In conclusion, there is a need for more and more in-depth field investigations in different hydrogeological and hydro-climatic settings to improve the understanding of physical, chemical, and biological processes, and develop adequate and good-quality databases.

The steps to develop such integrated models (Fig. 5) are explained below.

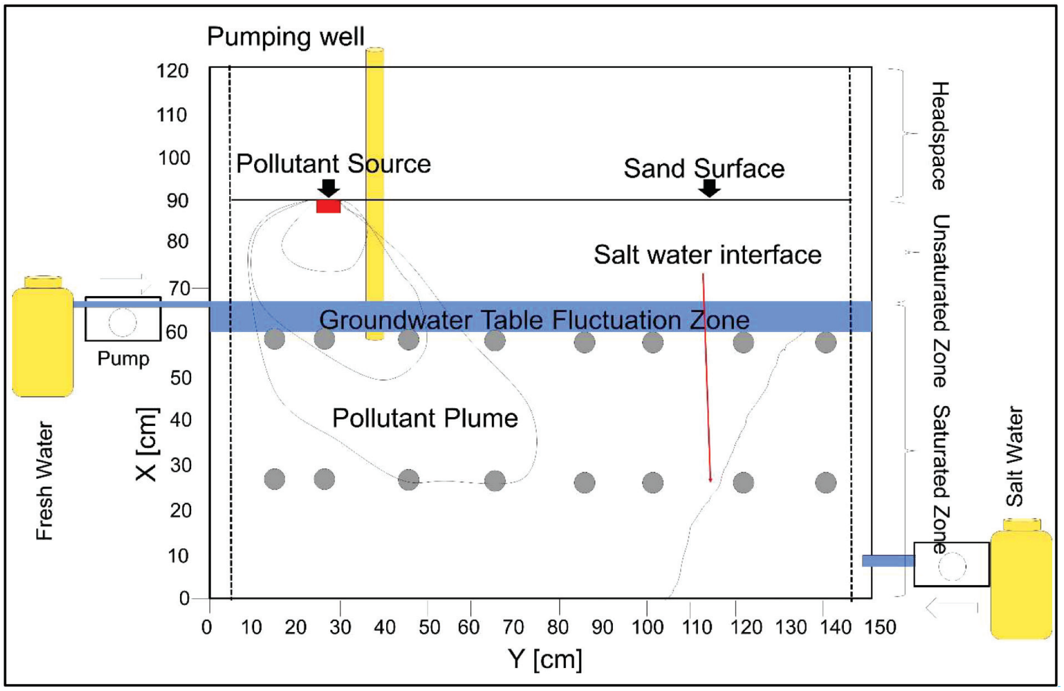

***Fig. 4.** Laboratory experiments for salt-water intrusion and pollutant fate and transport parameters analysis*

Step 1. Experimental analysis: A 2D experiment (Fig. 4) can be conducted to understand the saltwater intrusion process and also to understand the fate and transport of associated contaminant.

Step 2. Selection of the input and output data: Further, the obtained parameters from the 2D experiment can be used in a physical-based model (SEAWAT) to generate the set of pumping rates and associated contaminant concentration at different locations in the modeling area.

Step 3. Training and testing of the ML model: The randomly generated pumping rates are used as input data and output obtained from physical-based models (maximum allowable concentration or maximum head or minimum head) is considered as the target output. In this method, a large number of pumping patterns are required which can be divided as training, testing, and validation sets as 70%, 15% and 15%, After training or learning the network with ML, a final weight matrix is obtained. This is further applied to the independent input in a "test" phase. The outcome is then compared with the simulated output of the physical-based model.

Step 4. Coupling of optimization technique: The trained ML model is then suitably coupled with optimization approaches like PSO in a single MATLAB program.

Step 5. Optimization of the objective function: The developed model is then used to solve the problem of optimizing the groundwater management strategy either minimizing the saltwater intrusion or maximizing the freshwater pumping rates.

Use of ML/AI in contaminant transport study

Machines learning, such as artificial neural networks (ANN), extensively used as surrogates for the mathematical model. Historically, as some successful applications, ML/AI have been utilized to "learn" to accurately mimic the behaviour of a solute transport so that it can be later employed in an optimization framework for remediation purposes. Previously, a large number of studies have used machines learning approach, the neural network, particle swarm optimization (PSO) algorithm (Mategaonkar and Eldho 2012; Yadav *et al*., 2016); the Pareto tabu search (NPTS) (Yang *et al*., 2012); the firefly algorithm (FA), Fuzzy Transformation Method (FTM) (Taravatrooy *et al*., 2019), to design an in-situ bioremediation system for the polluted saturated zone instant of contaminant transport models like BIOPLUME II (Shieh and Peralta, 2005), BIOFDM (Kumar *et al*., 2013); BIOPLUME III (Kumar *et al*., 2013; Taravatrooy *et al*., 2019; Yadav *et al*., 2016). Shieh and Peralta (2005) evaluated the performance of in-

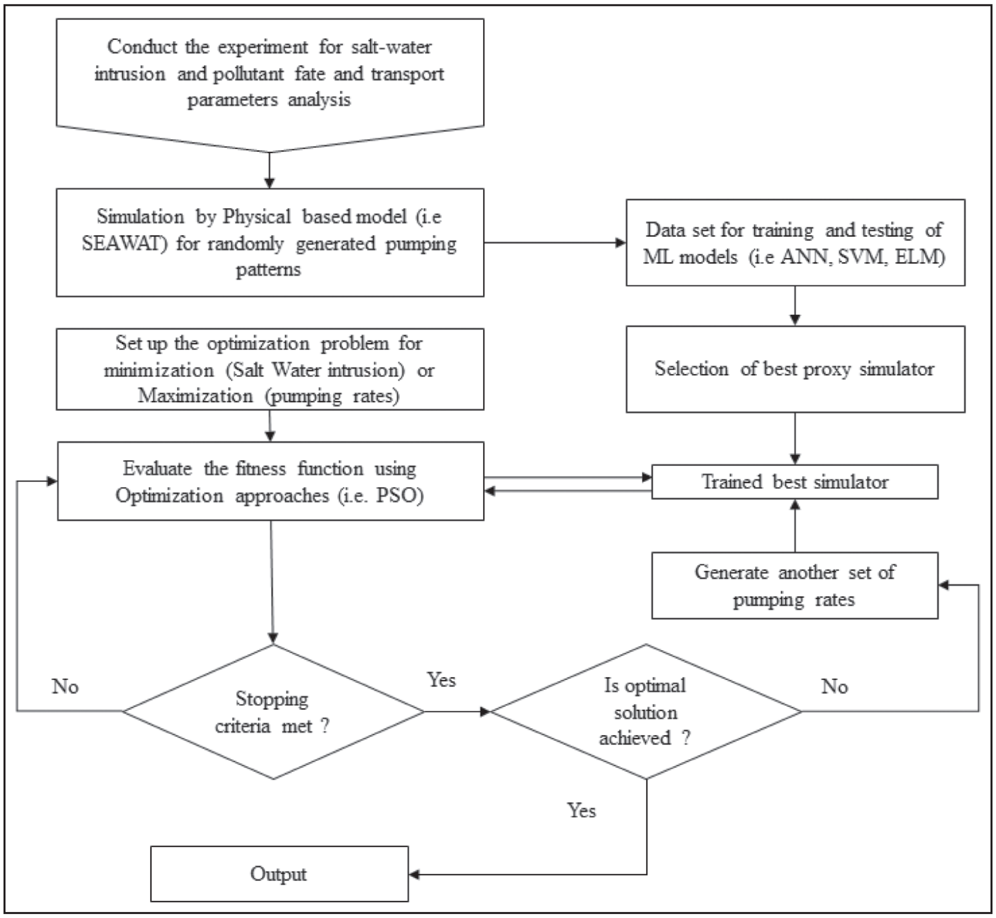

Fig. 5. *Intergraded physical, experimental, and machine learning (ML) based conceptual model for the management of coastal aquifers*

situ bioremediation systems by incorporating a genetic algorithm (Akbarnejad-Nesheli *et al*., 2016); Artificial Neural Networks (ANN), Support Vector Machines (SVM) and Extreme Learning Machines (ELM) (Yadav *et al*., 2016). Thus, ML/AI can be successfully applied to predict contaminant movement in the vadose zone and the saturated zone.

Role of climate change

Climate-driven changes in subsurface water resources play a more prominent role in 1) semi-arid and arid regions, where climate variability and changes accelerate high evapotranspiration rates and cause the significant subsurface water losses which ultimately leads to the high salinity problems; 2) coastal regions, the sea level rises to cause the reversal of hydraulic gradient between the sea and groundwater. This reversal of the hydraulic gradient causes the seawater intrusion towards the aquifer system, which may cause high salinity and deplete the quality of fresh groundwater (Loaiciga, 2009).

Increasing water table fluctuation, associated with climate change, may alter fate and transport of pollutants in the subsurface, especially in coastal aquifers (Gupta *et al*., 2019). Climate variability affects moisture variability both directly by altering surface water flux and indirectly via changes in groundwater extraction patterns. Dynamic climatic conditions are responsible for both the quantitative and qualitative aspects associated with contaminant movements (Ward *et al*., 1992). It has been observed that a dry vadose zone may accelerate aerobic growth of microbes, thus biodegradation kinetics, but significantly retard the advective flow. Lowering the water table may increase the thickness of the vadose zone which further increases the longevity of solute and retardation. Furthermore, denitrification may also be impacted by varying water table conditions (Sugita and Nakane, 2007). Thus, the qualitative assessments incorporating the fate and transport of subsurface pollutants are needed under climatic variation and boundary conditions using various ML/AI approaches.

Indian coastal aquifer systems continue to be affected by geogenic and anthropogenic contaminations. Over 480 million peoples are living in arsenic and fluoride endemic Indian districts. In this situation, a groundwater vulnerability assessment is a key tool to evaluate the relative susceptibility of aquifer systems to anthropogenic pollution for polluted site management. The index-based methods developed, like DRASTIC or its modified version is the most widely used method across the globe for aquifer vulnerability. Similarly, process-based methods have also been employed to assess aquifer vulnerability at different scales. However, there is a lack of a proper framework for coastal aquifer vulnerability assessment methods. Thus, an effort has been made to discuss a conceptual framework for coastal aquifer vulnerability by integrating physical, experimental, and machine learning techniques. It is recommended to develop an integrated approach for the accurate forecasting of water quality in coastal aquifers. Historically, the lack of hydrogeological data has been the major issue for modeling and aquifer vulnerability assessment, therefore it is suggested that the data-based models must be developed for the coastal aquifer system in India. This study will help environmental scientists, geochemists, field practitioners to plan remediation and management for Indian coastal polluted or highly vulnerable sites.

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