



An Ensemble Meta-Modelling Approach Using the Dempster-Shafer Theory of Evidence for Developing Saltwater Intrusion Management Strategies in Coastal Aquifers

Dilip Kumar Roy¹  · Bithin Datta^{1,2}

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Abstract

The optimum abstraction policy of coastal groundwater resources is prescribed by solving a meta-model based saltwater intrusion management model. Groundwater parameter uncertainties are explicitly incorporated into the developed meta-models in order to address the uncertainties present in coastal aquifer processes. Nevertheless, the accuracy and consequent reliability of such a management model depends upon the right choice of meta-models or a combination of meta-models. The optimal combination of meta-models, also referred to as an ensemble meta-model, can be selected by applying the Dempster-Shafer (D-S) theory of evidence. D-S evidence theory provides a platform upon which to base the selection of the best meta-model or combination of meta-models to formulate the preferred ensemble. This study demonstrates the application of D-S theory to provide an ensemble of meta-models for developing saltwater intrusion management models in coastal aquifers. The prediction accuracy of the developed ensemble meta-model is compared with that of the best standalone meta-model in the ensemble. The results confirm that the ensemble meta-model performs equally well when compared with the best meta-model in the ensemble. The developed meta-models and their ensemble are then used to develop computationally feasible multiple objective saltwater intrusion management models by utilizing an integrated simulation-optimization approach. The solution results of the management models demonstrate the superiority of the ensemble meta-model approach over standalone meta-models in obtaining Pareto optimal groundwater abstraction patterns. The evaluation of the proposed methodology is demonstrated using an illustrative multilayer coastal aquifer system subjected to groundwater parameter uncertainties.

Keywords Coastal aquifer · Management model · Meta-models · Ensemble · Dempster-Shafer theory

✉ Dilip Kumar Roy
dilip.roy@my.jcu.edu.au

¹ Discipline of Civil Engineering, College of Science and Engineering, James Cook University, Townsville, QLD 4811, Australia

² Cooperative Research Centre for Contamination Assessment and Remediation of the Environment, University of New Castle, Callaghan, NSW 2308, Australia

1 Introduction

Saltwater intrusion has become one of the challenging issues in the sustainable management of coastal aquifers. An efficient saltwater intrusion management policy requires a planned and judicious exploitation of water resources. Unplanned over-abstraction accelerates the contamination of already vulnerable fresh groundwater resources in coastal aquifers. Therefore, a planned groundwater abstraction policy needs to be implemented for ensuring the stability of freshwater supplies to communities living near the coastal regions of the world. However, the modelling of coastal aquifer processes is associated with ubiquitous parameter and prediction uncertainties. Parameter uncertainty can be addressed by developing meta-models that explicitly incorporate groundwater parameter uncertainties. Prediction uncertainty can be addressed by using the best combination of meta-models: i.e., an ensemble of meta-models to predict the future scenarios of saltwater intrusion processes. In this study, we propose this ensemble approach with a new selection criterion for developing an optimal groundwater extraction strategy. Prediction uncertainty is addressed by employing the best combination of meta-models (referred to as an ensemble), from various possible combinations of meta-models, in order to predict the future scenarios of saltwater intrusion processes. The ensemble approach is utilized for developing a multiple objective groundwater extraction strategy for saltwater intrusion management in coastal aquifers.

In addition to planned abstraction from the production wells, hydraulic control measures such as barrier wells provide a reduction in the extent of saltwater intrusion in coastal aquifers (Sreekanth and Datta 2011a). These barrier wells create hydraulic barriers near the shoreline, and help to increase beneficial water abstraction from the production wells. However, groundwater abstracted from barrier wells is generally very saline and cannot be used for beneficial purposes; therefore, the objective should be to reduce water abstraction from these wells. Groundwater abstractions from both production and barrier wells are controlled in such a way that the resulting salinity concentrations at specified monitoring locations do not exceed the maximum permissible values. To create a negative hydraulic barrier along the coast in order to reduce the extent of saltwater intrusion, a set of negative hydraulic barrier wells are used in the present study. This methodology requires an integrated simulation-optimization (S/O) approach in which the simulation model calculates the corresponding salinity concentrations from the randomly generated groundwater abstraction patterns by means of the optimization algorithm. The calculated salinity concentrations are then evaluated by the optimization routine for the violation of pre-specified maximum permissible salinity concentrations. The process continues until the global Pareto optimal solutions are obtained. These repeated evaluations are generally associated with a huge computational burden (Dhar and Datta 2009).

One of the most promising ways of attaining computational effectiveness in an S/O method is the utilization of approximate meta-models (Blanning 1975). Previous studies in the literature of saltwater intrusion management models (Ataie-Ashtiani et al. 2014; Bhattacharjya and Datta 2005; Christelis et al. 2017; Hussain et al. 2015; Roy and Datta 2018; Sreekanth and Datta 2011b) have utilized S/O approaches in which the simulation model was replaced by either a standalone meta-model (Bhattacharjya and Datta 2009; Roy and Datta 2018) or an ensemble of meta-models (Roy and Datta 2017a; Sreekanth and Datta 2011b). Meta-models are developed by means of the input-output training datasets obtained from solution results of a numerical simulation model. Meta-models thus developed approximate and represent the complex physical processes of coastal aquifers. The nonlinear and complex processes of coastal aquifer systems are associated with uncertainties in groundwater parameters. Therefore,

the developed meta-models should capture the variations in uncertain groundwater parameters. This study proposes Multivariate Adaptive Regression Spline (MARS) (Friedman 1991) based meta-models, which are developed based on different realizations of a set of uncertain groundwater parameters.

Meta-models are also associated with a certain degree of prediction uncertainty. If not addressed properly, this prediction uncertainty may propagate to the integrated S/O approach and may influence the optimality of solutions. An ensemble of meta-models deals with this prediction uncertainty by minimizing the adverse effects of a standalone meta-model (Goel et al. 2007). An ensemble meta-model provides a more reliable, accurate and dependable prediction. Moreover, it provides better Pareto optimal solutions compared to a standalone meta-model in the integrated S/O based saltwater intrusion management models (Sreekanth and Datta 2011b). Therefore, to account for the prediction uncertainties of meta-models, a weighted average ensemble of MARS meta-models (called an ensemble meta-model hereafter) is proposed in this study. The ensemble approach utilizes the Dempster-Shafer (D-S) theory of evidence (Dempster 1968; Shafer 1976) to select the best combination of meta-models comprising the ensemble. The ensemble meta-model thus developed is externally linked to a Controlled Elitist Multi Objective Genetic Algorithm (CEMOGA) (Deb and Goel 2001) to develop optimal groundwater extraction strategies in coastal aquifers.

The D-S evidence theory is based on the combination of Dempster's original concepts of relaxing certain Bayesian restrictions and Shafer's contribution to expanding them (Caselton and Luo 1992). The D-S theory can be thought of as a conventional probability theory, which assumes a multiple valued mapping from one space to another (Dempster 1967). It is an evidence theory that offers methods of integrating conflicting, vague and uncertain information from diverse sources to provide a certain amount of belief. These imprecise segments of information are stored in a function called Basic Probability Assignments (BPA), which is associated with belief (Bel), plausibility (PI), and pignistic probability (BetP). In meta-modelling terms, the BPAs contain information about statistical indices of meta-model performances, e.g. the Coefficient of Correlation (R), Root Mean Squared Error (RMSE), Index of Agreement (IOA) etc. (Müller and Piché 2011). It must be noted that a particular meta-model may have conflicting characteristics in terms of statistical performance indices. These conflicting performance indices need to be addressed in determining the belief in the prediction capabilities of that meta-model. Dempster's rule of combination is used to incorporate these conflicts.

In the present study, the selection of a single best meta-model or different combinations of meta-models are carefully chosen based on applying the evidence theory. Unlike the previous studies of saltwater intrusion management models, where either a single meta-model or a combination of a certain number of meta-models are linked to the optimization algorithm in order to develop the management model, the present study focuses on selecting the best combination of meta-models for approximating the saltwater intrusion processes in coastal aquifers. In addition, the individual meta-models are developed by using different realizations of uncertain model parameters. Therefore, the developed meta-models explicitly incorporate the groundwater parameter uncertainty.

This paper contributes to the development of meta-models that explicitly incorporate groundwater parameter uncertainties. It also aims at selecting the best meta-model as well as the best combination of meta-models (ensemble) to approximately emulate saltwater intrusion phenomena in coastal aquifers by utilizing the D-S theory of evidence. Finally, the study provides a comparison of the quality of the Pareto optimal groundwater abstraction patterns derived from the ensemble meta-model and the standalone meta-models.

2 Methodology

A number of MARS based meta-models are developed from the solutions of a numerical simulation model. The best meta-model and the best combinations of meta-models are selected through the application of the D-S theory of evidence. The meta-models thus obtained are integrated with the optimization algorithm in order to prescribe optimal groundwater abstraction strategies as solutions. Brief explanations for each of the constituents of the methodology are provided in the following subsections.

2.1 Numerical Modelling of Physical Processes in Coastal Aquifers

A three dimensional (3D) density reliant combined flow and salt transport numerical simulation model, FEMWATER (Lin et al. 1997) is utilized for simulating the coastal aquifer processes. The simulation results provide the required number of input-output training datasets for MARS based meta-models. The governing 3D flow and transport equations are provided in Lin et al. (1997), and are not repeated here.

2.1.1 Groundwater parameter uncertainty

Groundwater flow and transport processes are subjected to uncertain model parameters. Uncertainty in groundwater modelling systems arises primarily from variations in aquifer properties such as bulk density, compressibility, and hydraulic conductivity (Ababou and Al-Bitar 2004). Other causes of uncertainties may originate in changes in aquifer recharge and groundwater abstraction patterns. The present study incorporates uncertainties in aquifer recharge, bulk density, compressibility, and hydraulic conductivity in simulating the coupled flow and solute transport phenomena. The uncertain groundwater parameters are paired randomly with the transient groundwater abstraction patterns to acquire the resulting salinity concentrations at selected monitoring locations.

Realizations of hydraulic conductivity values are obtained from a lognormal distribution. Aquifer recharge, bulk density, and compressibility realizations are acquired through Latin Hypercube Sampling (LHS) (Pebesma and Heuvelink 1999). Different realizations of these uncertain model parameters are then integrated to generate a multivariate realization of these parameters.

2.1.2 Input-Output Training Patterns

Meta-models learn from the trends in input-output training datasets produced by using a simulation model. The simulation model is fed with input groundwater abstraction values to obtain the resulting salinity concentrations. One set of groundwater abstraction values and the corresponding salinity concentrations form one pattern of input-output dataset. A required quantity of these input-output datasets are used for training and validation of the meta-models.

Transient groundwater abstraction values are obtained from the LHS technique with specified lower and upper bounds of 0 m³/day and 1300 m³/day, respectively. For each set of uncertain groundwater parameters, 500 sets of groundwater abstraction values are used in order to generate 500 values of salinity concentrations. Five sets of uncertain model parameters are used to obtain 5 × 500 sets of salinity concentrations at specified locations within the aquifer. A meta-model is developed from each randomized parameter set. Therefore, 5 meta-

models are developed, each incorporating a particular set of uncertain groundwater model parameters.

2.2 Meta-Model

MARS based meta-models and their ensembles are used to obtain a reasonably accurate estimation of salinity intrusion processes. MARS is a rapid, flexible, adaptive, and nonparametric approach to developing regression models (Friedman 1991). MARS maps input-output relationships by dividing the solution domain into different intervals of inputs, and by fitting distinct Splines or Basis functions into these intervals (Bera et al. 2006). MARS adopts both a forward and a backward step during nonlinear mapping of the inputs and outputs. In the forward step, MARS builds a complex model by utilizing the specified maximum number of Basis functions. However, to prevent model overfitting and complexity, MARS adopts a backward stepwise procedure to parsimoniously select only the most influential input variables that provide accurate prediction of output variables (Salford-Systems 2016). In general, the input-output mapping of meta-models is expressed as

$$S_{output}(x) = M_{output}(x) + \varepsilon \quad (1)$$

where, $S_{output}(x)$ = output from the simulation model at point x , $M_{output}(x)$ = predicted output of the meta-model, and ε = error between simulation model outputs and meta-model predictions.

A commercial software package Salford Predictive Modeller (SPM v8.2) (SPM 2016) is used to develop the MARS based meta-models.

2.3 The Dempster-Shafer evidence theory

The D-S theory of evidence can be characterized as a conventional probability theory when a multiple valued mapping from one space to another is considered (Dempster 1967; Wasserman 1990). The basic concept of multiple valued mapping from T to Θ is presented in Fig. 1 (Wasserman 1990).

In Fig. 1, Θ denotes the parameter space, and θ represents each individual possible value within this parameter space of interest such that $\theta \in \Theta$. T defines a probability space with a probability density of μ_T on T . Then the multiple valued mapping from T to Θ is presented by $\Gamma(t) \subset \Theta$, i.e. an observation t in T is corresponding to the observation that the true value of θ is in $\Gamma(t) \subset \Theta$. The conventional probability distribution μ_T in T is referred to as an imprecise probability distribution on Θ (Walley 1991) or a basic probability assignment (BPA) (Shafer 1976). Shafer (1976) defined BPA as $m(A)$ for $A \subset \Theta$, that is $m(A : A = \Gamma(t)) = \mu_T(t)$. The collection of all subsets of Θ is known as the “frame” of Θ . Therefore, the “frame” of Θ is an “exhaustive set of mutually exclusive hypotheses or propositions”. This “frame” of Θ forms the essential concept of D-S.

The BPA is the fundamental method of expressing uncertainty in the D-S theory of evidence. The BPA is a type of probability assignment in which probability values are assigned to both subsets and singleton elements (the “frame” of Θ). “A BPA value on a subset represents the belief that is exactly committed to that subset and to nothing smaller” (Caselton and Luo 1992). Information on a certain hypothesis or proposition is stored in BPA to obtain the reliability of a given hypothesis. The sum of BPA values over the frame Θ must be equal to 1, i.e. $\sum_{A \subset \Theta} m(A) = 1$. BPAs are associated with three functions: belief (Bel),

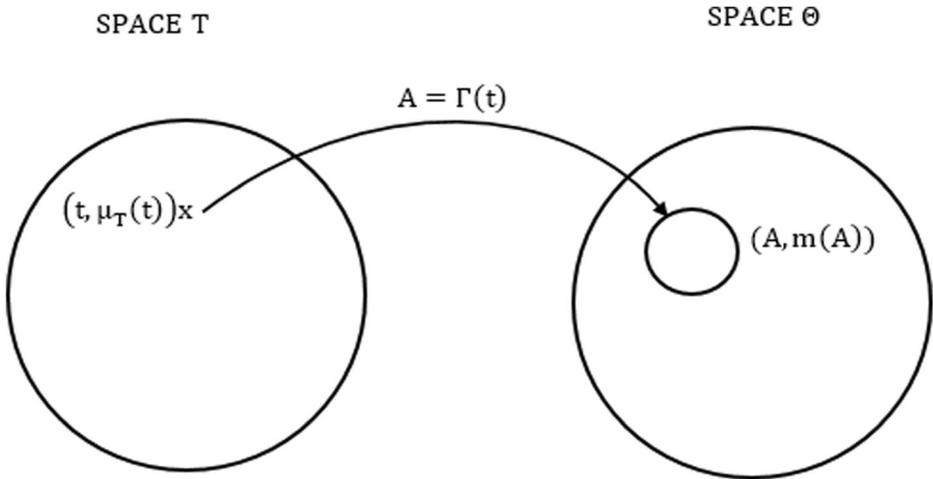


Fig. 1 The multiple valued mapping from T to Θ that generates a BPA on Θ (after Wasserman (1990))

plausibility (PI), and commonality (H) (Caselton and Luo 1992). For a subset $A \subset \Theta$, belief and plausibility of A can be calculated from the BPA on Θ as

$$Bel(A) = \sum_{B \subset A} m(B) \tag{2}$$

$$PI(A) = \sum_{B \cap A \neq \phi} m(B) \tag{3}$$

where, $\phi =$ null set.

The commonality of subset A accumulates all of the probability values in the BPA that could potentially be dedicated to A from all of the supersets that include A . The commonality for the subset $A \subset \Theta$ is defined as

$$H(A) = \sum_{B \subset \Theta, A \subset B} m(B) \tag{4}$$

The rule to integrate two belief functions is introduced by Shafer (Shafer 1976). This rule of combining two belief functions is referred to as Dempster’s rule of combination. This is an “associative and commutative operation” designed to map two belief functions, both defined on the same parameter space Θ into a new belief function on Θ . Let m_1 and m_2 be two BPAs on Θ . Then, Dempster’s combination rule provides the new combined BPA m ($m = m_1 \oplus m_2$) that can be expressed as

$$m(A) = m_1 \oplus m_2(A) = \begin{cases} 0, & A = \phi \\ \frac{\sum_{B \cap C = A} m_1(B)m_2(C)}{1-K}, & A \neq \phi \end{cases} \tag{5}$$

$$K = \sum_{B \cap C = \phi} m_1(B)m_2(C), \quad K \in (0, 1) \tag{6}$$

where \oplus denotes orthogonal sum of m_1 and m_2 . B and C are the subsets of hypotheses in Θ .

2.4 Ensemble of meta-models using Dempster-Shafer theory of evidence

It is often difficult to decide in advance on the suitability of a particular meta-model for the problem at hand. Therefore, the effectiveness of different meta-models or different combination of meta-models needs to be investigated in order to obtain the most effective approximation of the physical processes of interest. The combination of meta-models is commonly referred to as an ensemble of meta-models. In ensemble approach, the output from each individual meta-model are integrated to provide a combined output. Mathematically this can be expressed as

$$Y_{ensemble} = \sum_{i=1}^n \frac{Y_{meta-model_i}}{n} \tag{7}$$

where, $Y_{ensemble}$ = output of the ensemble, $Y_{meta-model_i}$ = output from the i^{th} meta-model, and n is the number of meta-models in the ensemble.

Furthermore, not all meta-models perform equally well for particular problems. Therefore, the influence of each meta-model in the ensemble needs to be adjusted based on its performance on the test dataset. This approach is known as weighted average ensemble, and the prediction $Y(x)$ of such an ensemble is represented by

$$Y(x) = \sum_{i=1}^n \omega_i \times y_i(x) \tag{8}$$

$$\sum_{i=1}^n \omega_i = 1 \tag{9}$$

where, $y_i(x)$ = prediction of the i^{th} meta-model constituting the ensemble, ω_i = corresponding weights to i^{th} meta-model, and n is the number of meta-models.

The D-S theory of evidence is applied to calculate the weight of each of the contributing meta-models. The performance indices of meta-models are considered as BPA (Müller and Piché 2011) of the D-S theory. Five performance indices have been selected as meta-model characteristics. They are Coefficient of Correlation (R), Index of Agreement (IOA), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Median Absolute Deviation (MAD). These meta-model characteristics are calculated from the meta-model’s predicted and simulation model outputs. Ideally, the best meta-model should have higher values of R and IOA as well as lower values of RMSE, MAE, and MAD.

The meta-model characteristics are normalized to satisfy the condition that the sum of BPA values over the frame Θ must be equal to 1, i.e. $\sum_{A \subset \Theta} m(A) = 1$. The normalization is performed by using the following sets of equations (Müller and Piché 2011):

$$m_i^R = \frac{R_i}{\sum_{j \in \mathcal{R}} R_j}; m_i^{IOA} = \frac{IOA_i}{\sum_{j \in \mathcal{R}} IOA_j} \tag{10}$$

$$m_i^{RMSE} = \frac{1}{\sum_{j \in \mathcal{R}} \frac{1}{RMSE_j}}; m_i^{MAE} = \frac{1}{\sum_{j \in \mathcal{R}} \frac{1}{MAE_j}}; m_i^{MAD} = \frac{1}{\sum_{j \in \mathcal{R}} \frac{1}{MAD_j}}$$

where, \mathcal{R} represents the set of meta-models in the ensemble.

These normalized BPAs are used to calculate the pignistic probabilities of each meta-model. Pignistic probabilities are important elements of the decision making process. At the onset of decision making, belief is at the credal level (Smets 1999), and is characterized by the basic belief assignment, m defined on the “frame of discernment”, Θ . This belief induces a probability function at the ‘pignistic’ level, $BetP$ defined on the same “frame of discernment”, Θ . Smets (1990) labels this transformation as “pignistic transformation”, mathematically expressed as

$$BetP(x) = \sum_{A \subseteq \Theta, x \in A} \frac{m(A)}{1-m(\phi)} \frac{1}{|A|} \text{ for every } x \in \Theta \quad (11)$$

The $BetP$ can be used to make decisions based on the theory of expected utilities, the justification of which relies on rationality requirements explained in details in Smets and Kennes (1994).

Based on the pignistic probability values, the weights assigned to each meta-model in different combinations of ensembles are determined. This can be mathematically expressed as

$$\omega_i = \frac{BetP_i}{\sum_{i=1}^n BetP_i} \quad (12)$$

where, ω_i = weights assigned to i^{th} meta-model for a particular combination, $BetP_i$ = pignistic probability of the i^{th} meta-model for the corresponding combination, and n = number of meta-models contributing to form the corresponding combination.

Every possible combination of ensembles is evaluated, i.e. different combinations of two-, three-, and four-model blends, standalone individual meta-models, and all meta-models together are considered. Five MARS based meta-models (denoted by M1-M5) constitute 31 focal elements. For single models, the focal elements are [M1], [M2], [M3], [M4], and [M5], respectively. For two model combinations the corresponding focal elements are [M1, M2], [M1, M3], [M1, M4], [M1, M5], [M2, M3], [M2, M4], [M2, M5], [M3, M4], [M3, M5], and [M4, M5], respectively. The focal elements for the three model combinations are [M1, M2, M3], [M1, M2, M4], [M1, M2, M5], [M1, M3, M4], [M1, M3, M5], [M1, M4, M5], [M2, M3, M4], [M2, M3, M5], [M2, M4, M5], and [M3, M4, M5], respectively. Four model combinations have the following focal elements: [M1, M2, M3, M4], [M1, M2, M3, M4], [M1, M2, M4, M5], [M1, M3, M4, M5], and [M2, M3, M4, M5], respectively. The focal element corresponding to the five model combination is [M1, M2, M3, M4, M5]. Statistical performance indices are calculated for each combination of meta-models, and normalized to obtain the BPAs of the corresponding combinations. Then D-S is applied to the BPAs of the combinations of meta-models in order to calculate the corresponding pignistic probabilities. The calculated pignistic probability values provide an indication of which of all of the considered combinations of meta-models is the best. The higher the value of pignistic probability, the better the performance of the combination meta-model is.

A MATLAB toolbox, Surrogate Model Optimization Toolbox (Müller 2012) is used to calculate the weights of combination meta-models by applying the D-S theory of evidence. The code is slightly modified for using five meta-models in developing different combinations of meta-models.

2.5 Saltwater intrusion management model

The selected best combination of meta-models and the standalone meta-models are linked externally to the optimization algorithm CEMOGA, in order to develop S/O based saltwater

intrusion management models. The multi-objective management models provide optimal abstraction values in terms of a Pareto optimal front. The Pareto front specifies two contradictory objectives of coastal groundwater management strategies. The first objective ensures maximum abstraction of groundwater from a group of production wells. The second objective minimizes the abstraction of water from a group of barrier wells placed near the coastline to hydraulically control saltwater intrusion. Both of these objectives need to be satisfied while meeting the requirement of maximum permissible salinity concentrations at specified monitoring locations. The multi-objective optimization formulation is expressed as (after Dhar and Datta (2009))

$$\text{Maximize : } f_1 = \sum_{r=1}^R \sum_{t=1}^T Q(PW)_r^t \quad (13)$$

$$\text{Minimize : } f_2 = \sum_{s=1}^S \sum_{t=1}^T Q(BW)_s^t \quad (14)$$

Subject to

$$C_i = f(Q(PW), Q(BW)) \quad (15)$$

$$C_i \leq C_{max} \quad (16)$$

$$Q(PW)_{min} \leq Q(PW)_r \leq Q(PW)_{max} \quad (17)$$

$$Q(BW)_{min} \leq Q(BW)_s \leq Q(BW)_{max} \quad (18)$$

where, PW = production wells, BW = barrier extraction wells, R = total number of production wells, S = total number of barrier extraction wells, T = total number of time steps, $Q(PW)_r^t$ = groundwater abstraction from the r^{th} production well at t^{th} time period, $Q(BW)_s^t$ = groundwater abstraction from the s^{th} barrier well at t^{th} time period, C_i = salinity concentrations at i^{th} monitoring location at the end of the management period, eq. (15) indicates linking of the combination of meta-models within the optimization model, eq. (16) restricts the salinity concentrations at i^{th} monitoring location below the maximum permissible salinity concentrations for that location, Eqs. (17) and (18) sets the lower and upper bounds of the groundwater extraction rates from the production and barrier wells, respectively.

The solutions obtained from the multiple objective coastal groundwater management model are verified and compared by using the constraint method (Datta and Peralta 1986) of solving the multiple objective model, i.e. by converting it to a series of single objective optimization formulations. For this purpose, one of the objectives is specified explicitly and the other objective is introduced as a constraint ensuring specified different minimum levels. This process is repeated multiple times for specified values of the second objectives. This ensures solution of a single objective optimization model each time, with the solution representing a single point on the Pareto Optimal front. The single objective formulation is expressed as

$$\text{Maximize : } f = \sum_{R=1}^R \sum_{t=1}^T Q(PW)_r^t \quad (19)$$

Subject to

$$C_i = f(Q(PW), Q(BW)) \quad (20)$$

$$C_i \leq C_{max} \quad (21)$$

$$\sum_{s=1}^S \sum_{t=1}^T Q(BW)_s^t \leq Q(BW)_{specified} \quad (22)$$

$$Q(PW)_{min} \leq Q(PW)_r \leq Q(PW)_{max} \quad (23)$$

$$Q(BW)_{min} \leq Q(BW)_s \leq Q(BW)_{max} \quad (24)$$

where, $Q(BW)_{specified}$ = total specified amount of water abstraction from the barrier extraction wells. Both management models are executed in the MATLAB environment utilizing parallel computing platforms. The multiple objective optimization problem is solved using the Controlled Elitist Multiple Objective Genetic Algorithm (CEMOGA) solver in MATLAB (MATLAB 2017). The single objective formulation is solved using GlobalSearch (MATLAB 2017) optimization approach, which utilizes repeated runs of a local solver ('fmincon' (MATLAB 2017)) to obtain the global optimal solution. The flow diagram of the proposed ensemble based methodology is showed in Fig. 2.

2.6 Performance evaluation indices

Performances of the standalone meta-models and the ensemble meta-model are evaluated by using the following statistical performance indices.

$$R = \frac{\sum_{i=1}^n (C_{i,S} - \overline{C}_S) (C_{i,S} - \overline{C}_P)}{\sqrt{\sum_{i=1}^n (C_{i,S} - \overline{C}_S)^2} \sqrt{\sum_{i=1}^n (C_{i,P} - \overline{C}_P)^2}} \quad (25)$$

$$IOA = 1 - \frac{\sum_{i=1}^n (C_{i,S} - C_{i,P})^2}{\sum_{i=1}^n (|C_{i,P} - \overline{C}_S| + |C_{i,S} - \overline{C}_S|)^2} \quad (26)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (C_{i,S} - C_{i,P})^2} \quad (27)$$

$$RRMSE = \frac{RMSE}{\frac{1}{n} \sum_i C_{i,S}} \quad (28)$$

$$MAE = \sum_{i=1}^n \frac{|C_{i,S} - C_{i,P}|}{n} \tag{29}$$

$$MAD(C_S, C_P) = median(|C_{1,S} - C_{1,P}|, |C_{2,S} - C_{2,P}|, \dots, |C_{n,S} - C_{n,P}|) \tag{30}$$

for $i = 1, 2, \dots, n$

$$MAPRE = \frac{1}{n} \sum_{i=1}^n \left| \frac{C_{i,S} - C_{i,P}}{C_{i,S}} \right| \times 100 \tag{31}$$

Kling–Gupta efficiency (KGE) is calculated as

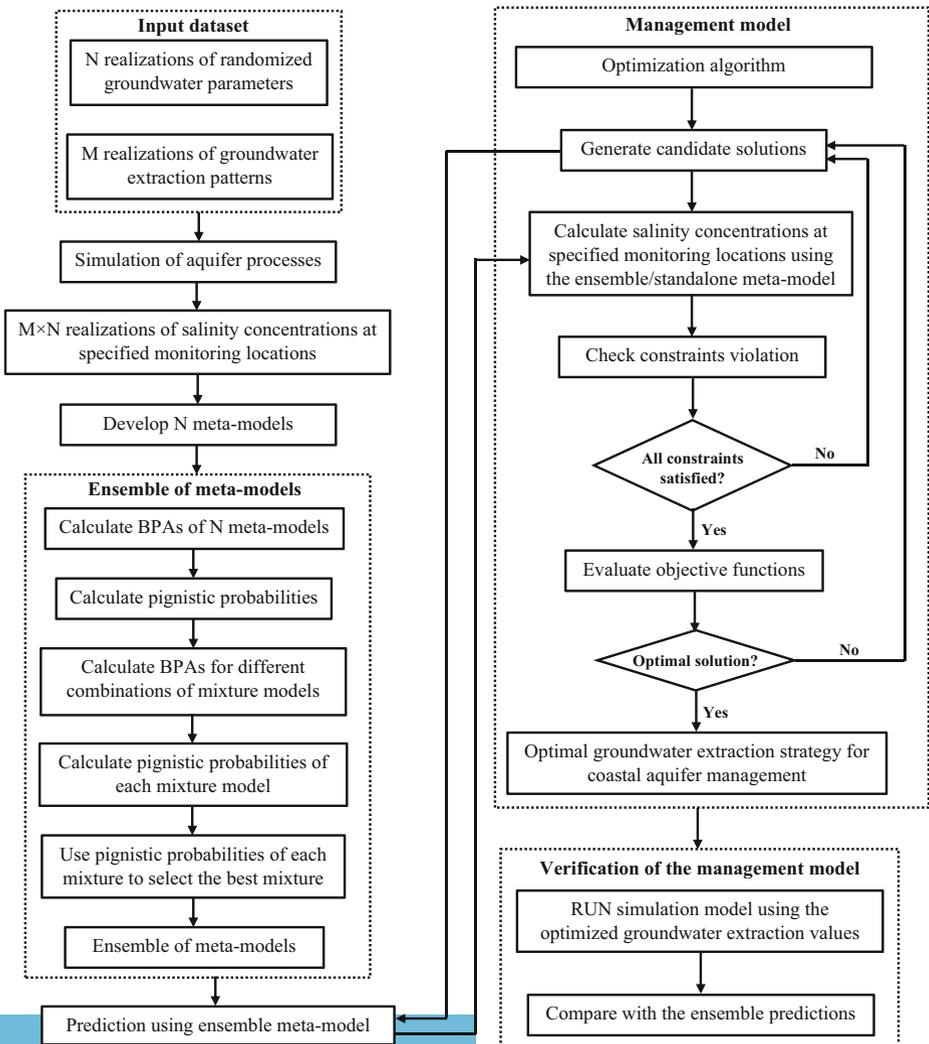


Fig. 2 Flow diagram of the proposed methodology for ensemble based management strategy development

$$KGE = 1-ED = 1-\sqrt{(R-1)^2 + (\alpha-1)^2 + (\beta-1)^2} \quad (32)$$

$$\alpha = \frac{\sqrt{\frac{1}{n} \sum_{i=1}^n (C_{i,P} - \overline{C}_P)^2}}{\sqrt{\frac{1}{n} \sum_{i=1}^n (C_{i,S} - \overline{C}_S)^2}} \quad (33)$$

$$\beta = \frac{\frac{1}{n} \sum_{i=1}^n C_{i,P}}{\frac{1}{n} \sum_{i=1}^n C_{i,S}} \quad (34)$$

where, $C_{i,S}$ = simulated salinity concentration values, and $C_{i,P}$ = predicted salinity concentration values, \overline{C}_S = mean values of the simulated salinity concentration values, \overline{C}_P = mean values of the predicted salinity concentration values, n = number of data points, ED = Euclidian distance from the ideal data points, α = relative variability in the predicted and simulated salinity concentration values, β = ratio between the mean predicted and mean simulated salinity concentration values representing the bias.

3 Application of the proposed methodology

The performance of the ensemble meta-model based saltwater intrusion management model is assessed for an illustrative multilayered coastal aquifer study area. The aquifer system is subjected to transient groundwater abstractions from a collection of production and barrier abstraction wells. Uncertainty in some of the groundwater parameters are considered. A three-dimensional view of the illustrative study area (Roy and Datta 2017b) is presented in Fig. 3 below.

The illustrative multilayered coastal aquifer system covers a study area of 4.35 km². The unconfined aquifer system is 80 m thick, divided into four individual layers with different materials. A stream flowing through the right side of the aquifer provides a specified stream water head of 1 m at the upstream end. This head varies linearly along the stream and reaches to 0 m at the coastal boundary. Both ends of the coastal boundary are assigned an initial head of 0 m. The salinity concentration at the coastal boundary is assumed to have a constant value of 35,000 mg/l. Eleven (11) production and five barrier extraction wells with a well density of 3.68 wells/km² are considered. The production and barrier wells are denoted by PW1-PW11 and BW1-BW5, respectively, in Fig. 3. The entire simulation time of five years is divided into identical time steps of five days. The management period of five years is divided into five identical time steps of one year each. Water abstraction from the wells is assumed to be constant during each one-year period. Salinity concentrations are measured at the end of each management horizon, at specified monitoring locations. Five monitoring locations are sited at different salinity regions of the aquifer.

The proposed management model considers 80 decision variables (X1-X80). These variables represent groundwater abstractions from 16 wells (11 production wells +5 barrier wells) in the five-year management period. Variables X1-X55 denotes groundwater abstraction from

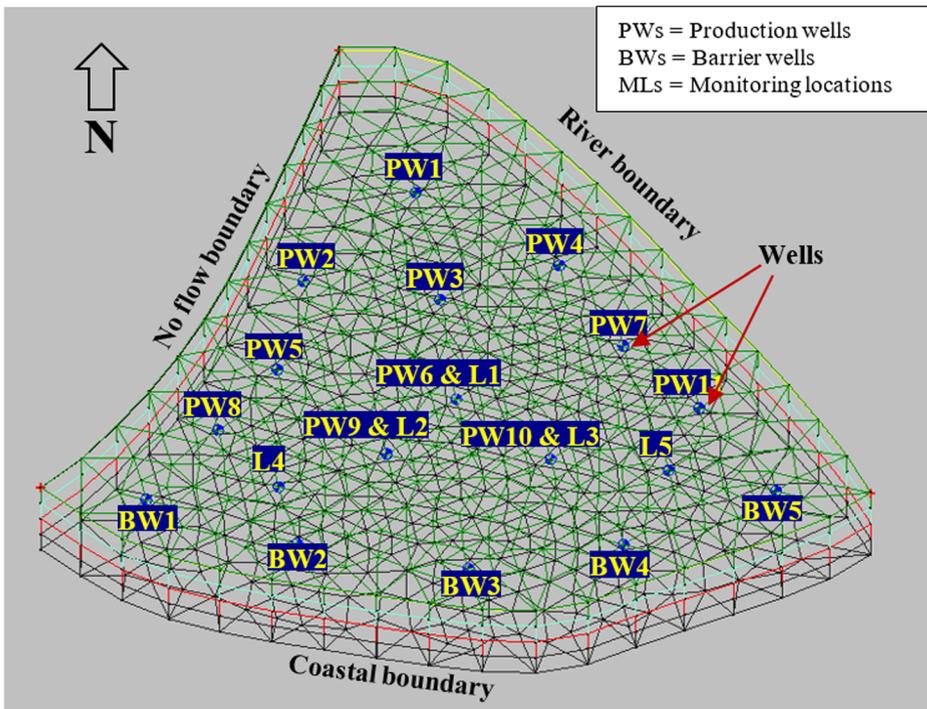


Fig. 3 3D view of the coastal aquifer system (after Roy and Datta (2017b))

the production wells in space and time. Variables representing water abstraction from barrier extraction wells are represented by X56-X80 in space and time.

4 Results and Discussion

The results of the prediction capabilities of standalone meta-models and their ensembles are presented in this section. In addition, the results of the saltwater intrusion management models prescribing optimal groundwater abstraction strategies for the coastal aquifer are also presented.

The performances of MARS meta-models at monitoring location L1 are presented in Table 1.

It is observed from Table 1 that the developed MARS meta-models produce higher values of R and IOA as well as lower values of MAD, MAE, and RMSE. However, meta-model predictions show a contradictory nature in terms of different statistical indices. For example, meta-model M5 can be considered the best among five meta-models when IOA, MAE, and RMSE criteria are considered. On the other hand, MAD criterion indicates the better performance of M1 among the meta-models. In addition, meta-models M1 and M5 produce the same value of R. Therefore, based on this evidence at hand, it is difficult to select the best meta-model. Similar results are obtained for all developed meta-models at all five monitoring locations (L1-L5). This conflicting nature of meta-model performance necessitates the incorporation of all the contradictory performance indicators in the selection process of meta-models. The D-S theory of evidence is applied in this study to resolve this conflict in prediction

Table 1 Performance of MARS meta-models at monitoring location L1

Statistical indices	M1	M2	M3	M4	M5
IOA	0.86	0.83	0.81	0.91	0.93
R	0.87	0.80	0.85	0.86	0.87
MAD	0.71	0.83	1.40	0.86	0.80
MAE	0.98	1.06	1.56	0.90	0.80
RMSE	1.32	1.42	1.92	1.11	0.97

*M1-M5 represents MARS based meta-models. *M1* Meta-model 1, *M2* Meta-model 2, *M3* Meta-model 3, *M4* Meta-model 4, *M5* Meta-model 5

capabilities. The D-S theory incorporates all model characteristics as bases upon which to select the best meta-model.

4.1 The D-S Evidence Theory in the Selection of Meta-Models and their Ensembles

The D-S theory of evidence is applied to calculate the pignistic probabilities of standalone meta-models at five monitoring locations. It is noted that the pignistic probability values of meta-model M5 are the highest among all meta-models considered (Table 2). Therefore, M5 is the best performing meta-model in predicting salinity concentrations at specified monitoring locations.

However, a standalone meta-model often fails to capture the true trends in the nonlinear relationships of the input-output patterns. An ensemble of such meta-models addresses this prediction uncertainty by incorporating the distinct features of standalone meta-models. However, including an ill-performing meta-model in the ensemble often causes the overall performance of the ensemble to deteriorate. Therefore, each contributing meta-model in the ensemble needs to be judiciously chosen to reduce the ill effects of poorly performing meta-models. This is done by assigning weights to each contributing meta-model in the ensemble. The pignistic probabilities of each meta-model are used to calculate the corresponding weights in the different combinations of meta-models. The weights are assigned to two-, three-, and four-model combinations at all monitoring location (L1-L5).

These weights are used to compute the prediction of each of the meta-model combinations. The corresponding performance indices are calculated for all combinations at all monitoring locations (L1-L5).

These statistical indices are then scaled (normalized) so that the sum over all meta-models for each BPA equals one. Then, the D-S theory of evidence is applied to find the pignistic probabilities of each combination of meta-models. Based on the pignistic probability values, a decision is made on the best meta-model combination among all considered meta-model

Table 2 Pignistic probabilities of each MARS meta-model

Monitoring locations	M1	M2	M3	M4	M5	SUM
L1	0.217	0.144	0.044	0.245	0.350	1
L2	0.213	0.204	0.046	0.206	0.331	1
L3	0.210	0.220	0.050	0.202	0.316	1
L4	0.177	0.191	0.046	0.234	0.353	1
L5	0.186	0.178	0.054	0.244	0.338	1

*L1-L5 represents five monitoring locations

combinations. The combined meta-model with the highest pignistic probability is designated as the best combination of meta-models (ensemble). A combination of M1-M2-M4-M5 produced the highest pignistic probabilities of 0.816, 0.818, 0.817, 0.818, and 0.817 for monitoring locations L1, L2, L3, L4, and L5, respectively. The weights of the contributing meta-models in the best combination of meta-models are then calculated.

These weights are used to calculate the predictions of the ensemble meta-models at different monitoring locations. The performance of the ensemble meta-models on the test dataset is calculated, and compared with the best performing meta-models (Table 3).

The performance is evaluated based on several performance indices. It can be observed from Table 3 that the ensemble meta-model provides similar results when compared with the best meta-model in the ensemble. R criterion indicates the superior performance of the ensemble meta-model compared to the best meta-model at monitoring locations L1, L2, L3, and L4. At location L5, the best meta-model produces slightly higher values of R than the ensemble meta-model. The performances of the meta-models are also assessed using IOA index (Willmott 1984). The IOA index is a measure of the extent of model prediction errors. The values of the IOA index varies between 0 and 1. An IOA index of 1 indicates a perfect match between predicted and observed salinity concentrations, and a value of 0 specifies no match at all (Willmott 1984). Based on the IOA index, the best meta-model's predictions at all monitoring locations are slightly better than the ensemble meta-model's predictions. The differences in predictions are negligible, and therefore the ensemble meta-model can be used to predict salinity concentrations at all locations. Moreover, the best meta-model's performance may not be equally well when it is presented with a new unseen test dataset. As the ensemble meta-model contains distinct features of different standalone meta-models, the ensemble approach is likely to provide better predictions in a diverse range of datasets. Notably, the IOA index is excessively sensitive to extreme values arising from the use of the squared differences (Legates and McCabe 1999).

Another performance evaluation criterion used for performance evaluation is the KGE. The KGE criterion is based on three components: correlation, bias, and variability. The KGE criterion is obtained by calculating the Euclidian distance of these three constituents from the ideal point (Gupta et al. 2009). The KGE criterion also provides a prediction of performance of the ensemble meta-models compared to the best meta-model at all monitoring locations (Table 3). Model performances are also assessed using RRMSE criterion, which integrates the variance and the bias of the forecast errors, and provides a good measure of prediction capability. Both the ensemble meta-models and the best meta-models at all monitoring locations provide similar results when the RRMSE criterion is used. The MAPRE criterion, providing information on the distribution of errors, is also used in the performance evaluation. At monitoring location L1, the ensemble meta-model provides better

Table 3 Performance of the ensemble meta-model and the best standalone meta-model on test dataset

Monitoring locations	R		IOA		KGE		RRMSE		MAPRE, %	
	B	E	B	E	B	E	B	E	B	E
L1	0.868	0.875	0.927	0.924	0.831	0.802	0.032	0.032	2.583	2.516
L2	0.794	0.796	0.884	0.874	0.765	0.745	0.067	0.070	5.395	5.460
L3	0.893	0.893	0.942	0.935	0.868	0.848	0.074	0.078	6.014	6.160
L4	0.683	0.688	0.805	0.796	0.609	0.602	0.053	0.054	4.299	4.415
L5	0.741	0.739	0.846	0.836	0.677	0.666	0.038	0.039	3.091	3.257

*B and E represents the best meta-model and the ensemble meta-model, respectively

results in terms of the MAPRE criterion. At all other monitoring locations, the ensemble meta-model performs equally well when compared to the best meta-model. Therefore, it can be concluded from the preceding discussion that an ensemble of meta-models based on the D-S theory of evidence can be applied to provide a reasonable prediction of the extent of saltwater intrusion phenomena in coastal aquifers. As the ensemble meta-model contains distinct features of the contributing meta-models, the ensemble approach is likely to provide more reliable Pareto optimal solutions in the saltwater intrusion management models. The quality of the Pareto optimal solutions obtained from both the ensemble and the standalone meta-models is presented in the next section.

4.2 Meta-Model Based Saltwater Intrusion Management Models

Ensemble meta-model and standalone meta-models are integrated separately with a multiple objective optimization algorithm (CEMOGA) in order to develop the management models. The CEMOGA parameters are selected by performing a sensitivity analysis, which evaluates various combinations of different parameters. The optimal combination of different parameters thus selected are: population size = 3000, crossover rate = 0.95, Pareto front population fraction = 0.7, function tolerance = $1e-05$, constraint tolerance = $1e-05$. The ensemble meta-model and five standalone meta-models are utilized to develop six management models. The resulting Pareto fronts are presented in Fig. 4. The Pareto fronts in Fig. 4 provide non-dominated optimal solutions of groundwater abstraction values, which are obtained by satisfying the constraints of maximum permissible salinity concentrations at specified monitoring locations. From the alternative feasible optimal solutions, the appropriate combinations of water abstraction from the production and barrier wells can be selected.

Figure 4 demonstrates that the ensemble meta-model provides better solutions than the best meta-model (M5), as well as M3 and M4. For total barrier well abstractions of 9000 m³/day the corresponding total production well abstractions are approximately 35,800 m³/day, 35,200 m³/day, 31,200 m³/day, and 34,500 m³/day for the ensemble meta-model, M5, M3, and M4, respectively. This implies that the better generalization capability of the ensemble meta-model captures the randomly generated groundwater abstractions by the optimization algorithm more accurately than the standalone meta-models. However, meta-models M1 and M2 produce relatively better solutions than both the other standalone meta-models and the ensemble meta-model. For the same 9000 m³/day of barrier well abstractions, meta-models M1 and M2 provide approximately 38,800 m³/day and 39,500 m³/day of total water abstractions from the production wells. The probable reason is that a standalone meta-model fails to capture the true trends in the randomly generated groundwater abstractions with the optimization algorithm. As the generalization capability of a meta-model decreases, the probability of the corresponding Pareto optimal front being infeasible increases. Since optimal solutions are obtained from a constrained optimization, i.e. optimal solutions are constrained by the maximum permissible upper limit on salinity concentrations, the uncertainties associated with the standalone meta-model often forces the optimal solution to move into the infeasible region (Sreekanth and Datta 2011a).

The stochastic nature of CEMOGA may produce different results for different runs of the same optimization problem. Therefore, the Pareto optimal solutions obtained from the multi-objective optimization formulation are compared with those obtained from a single objective formulation. The multi-objective formulation is converted to single objective one by assigning one of the objectives as a binding constraint. For this purpose, total barrier well abstractions are used as the constraint of the optimization problem. Abstraction values of 0–20,000 m³/day

with an interval of 1000 m³/day are used to obtain the corresponding total production well abstractions. Results are illustrated in Fig. 5. Figure 5 presents the resulting Pareto optimal fronts produced by the ensemble meta-model and the standalone meta-models. It is noted that the single objective optimization formulation provides relatively higher values of total production well abstractions. However, the results follow a similar trend when compared to the multiple objective formulation. The ensemble meta-model provides better solutions than the M3, M4, and M5 meta-models in terms of total production well abstractions. On the other hand, meta-models M1 and M2 produce better solutions than the ensemble meta-model. While the quantity is different, the two optimization procedures provide similar trends of results.

It is important to note that a better solution in terms of the objective function value may result from inaccurate prediction of the aquifer responses as obtained by using different standalone meta-models. It is expected that the ensemble meta-model predictions are more accurate, and hence the optimum solution based on the ensemble meta-model is more accurate and reliable. It is also noted from Figs. 4 and 5 that the ensemble based optimum solutions are placed somewhere in between the solutions based on other models. This can be intuitively justified, as it is plausible to assume that the better optimal solutions are due to less accurate prediction of the aquifer responses, and therefore may represent actual constraint violations. Therefore, the obtained optimum management strategies based on different meta-models are tested by solving the more accurate numerical simulation model.

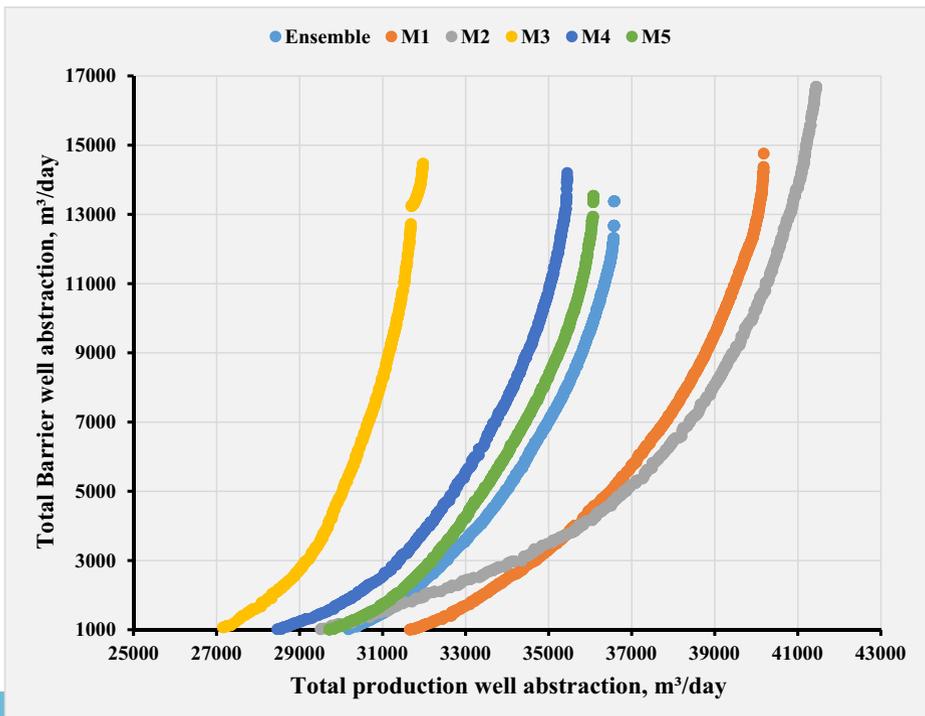


Fig. 4 Pareto optimal fronts obtained from the ensemble and standalone meta-models

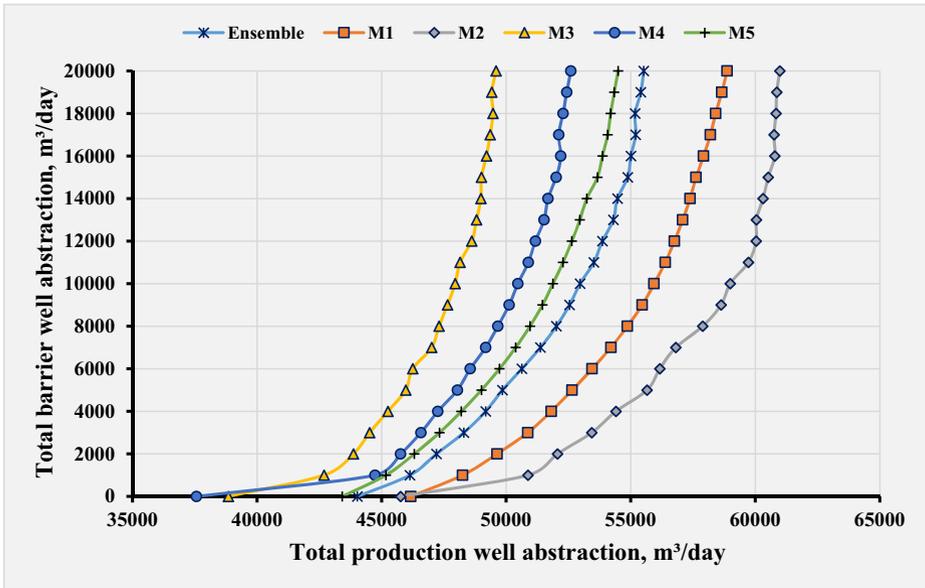


Fig. 5 Pareto optimal fronts produced by the ensemble and standalone meta-models for selected total amount of barrier well abstractions for the single objective formulation

4.3 Validation of the Pareto optimal solutions of the management models

The reliability of the optimal solutions is validated by comparing the corresponding salinity concentration values obtained from meta-models and the simulation model. For this, a number of solutions are arbitrarily chosen from the Pareto optimal fronts. The optimal solutions are then used as inputs to the ensemble meta-model, standalone meta-models, and the numerical simulation model. Corresponding salinity concentrations are obtained as solutions at specified monitoring locations. Percentage Relative Error (PRE) values are then computed from the meta-model predictions and the simulation model outputs (Table 4). It is observed from Table 4 that accuracy in terms of PRE values vary at different solutions for a particular monitoring location. For example, at location L1, the best meta-model outperforms the ensemble in solution S1 whereas the ensemble predictions are better than the best meta-model in solution S2. Likewise, at location L3, ensemble predictions are better for solution S1 whereas best meta-model predictions are better for solution S2.

The PRE values (Table 4) for all but one standalone meta-models (M5) utilized for prediction show that the ensemble model predictions of salinity for the chosen optimal management strategy are smaller than the PRE values from the stand alone meta-models. However, the errors are comparable and similar for the best meta-model in the ensemble (M5 is the best performing meta-model). It needs to be noted that for an illustrative aquifer, it may be relatively easy to identify the best performing meta-model as the parameters, inputs, and measurement are assumed to be available for different scenarios of management. In real life aquifers, where there are uncertainties and errors in estimation of parameters and measurements, it is very difficult to clearly identify the best performing meta-model amongst a set of candidate meta-models. This issue is actually addressed by using the ensemble meta-model, when it is no longer required to identify a best performing standalone meta-model. The

Table 4 Percentage relative error between meta-model predicted and simulation model outputs for selected optimal solutions

	Ensemble		M1		M2		M3		M4		M5	
	S1	S2	S1	S2	S1	S2	S1	S2	S1	S2	S1	S2
L1	2.15	1.21	6.62	4.95	13.23	16.54	4.25	4.99	6.38	3.94	1.78	1.93
L2	5.90	4.00	5.82	9.66	19.35	25.30	5.17	6.26	5.25	6.26	5.03	5.00
L3	5.37	1.74	8.34	12.41	24.31	25.48	14.36	14.83	9.18	9.08	3.67	3.61
L4	0.22	1.21	6.50	9.94	11.61	9.09	5.26	10.39	2.78	4.70	0.27	1.19
L5	0.70	0.88	3.22	7.13	11.95	11.36	4.51	7.98	1.89	3.08	1.00	0.60

*S1 and S2 represents solution 1 and solution 2, respectively

ensemble meta-model ensures improved accuracy of the predicted salinity values resulting from the chosen optimal management strategy.

In general, it can be argued that the ensemble meta-model provides relatively stable solutions at all monitoring locations. Therefore, the proposed ensemble meta-model based management model can be successfully applied to achieve optimal groundwater abstractions to control saltwater intrusion in a coastal aquifer subject to prediction and parameter uncertainties.

5 Summary and Conclusions

This study presents the application of the D-S theory of evidence to select an ensemble meta-model based on the optimal combination of meta-models, in order to improve the accuracy of approximating density reliant combined flow and solute transport processes in coastal aquifer systems. The study also applies the ensemble meta-model in the development of management models for prescribing optimal values of groundwater abstractions. This abstraction policy satisfies the constraints on maximum permissible salinity concentrations at specified monitoring locations. The management policy explicitly incorporates uncertainties associated with groundwater parameters and meta-model predictions. Use of the chosen ensemble model instead of standalone meta-models ensures improved accuracy of salinity prediction in the aquifer. Five MARS based standalone meta-models are developed from randomly paired realizations of uncertain model parameters and transient groundwater abstractions. Different combinations of these meta-models are assigned different weights determined by the D-S theory of evidence. The best meta-model combination is selected by comparing the pignistic probabilities of each combination as per the D-S theory of evidence. The higher the value of pignistic probability the better is the prediction capability of the meta-models or the combination of meta-models. The best combination of meta-models, M1-M2-M4-M5 has the highest pignistic probability values of 0.816, 0.818, 0.817, 0.818, and 0.817 at monitoring locations L1, L2, L3, L4, and L5 respectively. This ensemble meta-model and all the five standalone meta-models are separately linked to the optimization algorithm (CEMOGA) in order to develop the coastal aquifer saltwater intrusion management models.

The performance of the proposed approach is assessed by using an illustrative multilayered coastal aquifer study area. Comparison results indicate the superiority of the management strategies prescribed by the proposed ensemble meta-model over those produced by most of the standalone meta-models contributing to the ensemble. The Ensemble meta-model also provides a

more accurate and therefore more reliable solution in terms of the quality of the Pareto optimal front. Therefore, the proposed D-S based ensemble meta-model can potentially be applied to develop optimal groundwater abstraction policies for multilayered coastal aquifers.

The study assumes only vertical heterogeneity in terms of multiple layers of materials. The application of the developed methodology in a more complex heterogeneous coastal aquifer system would be an interesting topic for future research. Moreover, the findings of the study may be extended to using multiple algorithms of meta-models in order to develop a heterogeneous ensemble of meta-models.

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Compliance with Ethical Standards

Conflict of Interest The authors declare that they have no conflict of interest.

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