



# Optimizing conjunctive use of surface water and groundwater for irrigation to address human–nature water conflicts: A surrogate modeling approach



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## ABSTRACT

In arid and semi-arid areas where agriculture competes keenly with ecosystem for water, integrated management of both surface water (SW) and groundwater (GW) resources at a basin scale is crucial, but often lacks scientific support. This study implemented physically-based, fully integrated SW–GW modeling in optimizing water management, and performed surrogate modeling to replace the computationally expensive model with simple response surfaces. Water use conflicts between agriculture and ecosystem in Heihe River Basin (HRB), the second largest inland river basin in China, were investigated. Based on the integrated model GSFLOW (Coupled Ground–Water and Surface–Water Flow Model), the conjunctive use of SW and GW for irrigation in the study area was optimized using a surrogate-based approach named DYCORS (DYNAMIC COordinate search using Response Surface models). Overall, the study demonstrated that, with the surrogate modeling approach, an expensive integrated model could be efficiently incorporated into an optimization analysis, and the integrated modeling would make feasible a physically based interpretation of the optimization results. In the HRB case study, the surrogate-based optimization suggested a very different time schedule of water diversion in opposite to the existing one, indicating the critical role of SW–GW interactions in the water cycle. With the temporal optimization, a basin-scale water saving could be achieved by reducing non-beneficial evapotranspiration. In addition, the current flow regulation in HRB may not be sustainable, because the ecosystem recovery in the lower HRB would be at the cost of the ecosystem degradation in the middle HRB.

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## 1. Introduction

In many arid and semi-arid inland river basins, irrigated farmlands compete keenly with the regional ecosystem for scarce water resources (Krebs et al., 1999; Wichelns and Oster, 2006). Typically, the temporal mismatch between river flow and irrigation water demand is notable in such areas, and flow conservation for natural ecosystem is an important management concern. In areas where surface water (SW) and groundwater (GW) strongly interact, aquifers could behavior like “reservoirs”, with which the temporal mismatch and/or the human–nature competition may be alleviated (Forrester and Keane, 2009; Simons et al., 2015; Singh, 2014a). In water-limited environments, groundwater pumping in addition to surface water diversion for irrigation is a common practice

(Cosgrove and Johnson, 2005; Liu et al., 2010; Singh, 2014a; Smout and Gorantiwar, 2005), and optimizing the conjunctive use of SW and GW is an important research topic for agricultural water management (Bouwer, 2002; Khare et al., 2006; Kumar et al., 2013; Safavi and Esmikhani, 2013; Singh, 2014b).

Simulation–optimization (SO) approaches are widely used in water resources management and planning, which couple hydrologic or hydro–agronomic modeling with mathematical optimization (Singh, 2014a,b). They have been applied to address different irrigation water management issues, such as improving crop productivity by optimizing land and water allocation (Khare et al., 2006; Smout and Gorantiwar, 2005; Singh and Panda, 2012), altering Best Management Practices (BMPs) to adapt to climate change (Cai et al., 2015), assessing optimal locations and pumping rates in coastal aquifers to avoid saltwater intrusion (Bhattacharjya and Datta, 2005; Mantoglou and Papantoniou, 2008; Reichard and Johnson, 2005), and controlling non–point pollution of agriculture (Tan et al., 2011). SO has been implemented to the issue of con-

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conjunctive use of SW and GW as well (Safavi and Esmikhani, 2013; Singh, 2014b; Singh and Panda, 2013; Tabari and Soltani, 2012). However, to avoid the tremendous computational cost, most of the studies adopted hydrological simulation with no detailed description of SW–GW interactions. Some optimization studies involved the 3-D groundwater flow model MODFLOW (Chang et al., 2010; Harbaugh, 2005; Safavi and Esmikhani, 2013), but the groundwater recharge processes are highly simplified in MODFLOW. The widely used SWAT model (Arnold et al., 2011) has also been applied in SO studies on the conjunctive use issue (Cai et al., 2015), but SWAT conceptualizes the groundwater system as water tanks, and highly simplifies groundwater flow processes. In areas with strong and complicated SW–GW interactions (e.g., groundwater discharge into streams, riverbed leakage, groundwater exfiltration as springs, groundwater recharge by irrigation water, etc.), physically based, fully integrated SW–GW modeling is highly desired to appropriately account for the critical processes. Nevertheless, the complex modeling has been rarely attempted within the SO framework.

Many integrated SW–GW models have been developed, such as Hydrogeosphere (Brunner and Simmons, 2012), MIKE-SHE (Graham and Refsgaard, 2001), ParFlow (Kollet and Maxwell, 2006), CATHY (Weill et al., 2011) and GSFLOW (Markstrom et al., 2008; Tian et al., 2015). These models can provide a comprehensive and coherent understanding on the basin-scale water cycle. However, incorporating such complex models in optimization remains as a great challenge, because both gradient-based and heuristic optimization algorithms would encounter difficulties in this case. In gradient-based algorithms, like linear programming (e.g., Singh and Panda, 2012), dynamic programming (Prasad et al., 2006), and fuzzy dynamic programming (e.g., Zeng et al., 2010), calculation of derivatives is a key step. The integrated models represent “black-box” functions whose derivatives cannot be analytically determined, while finite-difference approximation of the derivatives is laborious and may encounter the discontinuity problem. On the other hand, heuristic algorithms, such as genetic algorithm (GA) (Goldberg, 1989; Holland, 1975), particle swarm optimization (PSO) (Clerc and Kennedy, 2002) and shuffled complex evolution (SCE-UA) (Duan et al., 1992), require no derivative-calculation and are more promising for finding global optima. But they usually involve a very large number of iterations, and the optimization would be extremely time-consuming with complex models. A potential solution to this would be to employ surrogate modeling.

In general, surrogate modeling refers to replacing a complex model with much simpler and computationally cheaper mathematical relationships in an iterative model evaluation process (e.g., Monte Carlo Simulation, heuristic optimization, etc.). There are two major types of surrogate modeling approaches. One is response surface approaches aimed at finding a data-driven relationship between multiple explanatory variables and a model output variable. This type of approaches have been increasing used in optimization studies recently (Razavi et al., 2012). Representative ones include Probabilistic Collocation Method (PCM) (e.g., Zheng et al., 2011; Wu et al., 2014), Kriging (e.g., Baú and Mayer, 2006), Support Vector Machine (SVM) (e.g., Cai et al., 2015) and radial basis function (RBF) (e.g., Regis and Shoemaker, 2007). There are two typical strategies to perform a surrogate-based optimization using response surface. One is batch approaches (e.g., Johnson and Rogers, 2000; Liong et al., 2001; Cai et al., 2015) which establish globally satisfactory response surfaces once for all, using a very large training set. The other is adaptive approaches which use a small training set to establish initial response surfaces (usually unsatisfactory) and iteratively update them with additional training points (e.g., Forrester and Keane, 2009; Ostfeld and Salomons, 2005; Regis and Shoemaker, 2007). DYCORS (DYNAMIC COordinate search using Response Surface models) by Regis and Shoemaker (2013) is a typical adaptive response surface approach.

The other type of surrogate modeling approaches is often referred to as model reduction or reduced-order modelling (Castelletti et al., 2012; McPhee and Yeh, 2008; Pasetto et al., 2011; Razavi et al., 2012), which yields a low-order, physically based, dynamic surrogate model of the original complex model. This type of approaches has also been adopted in optimization studies (e.g., Galelli et al., 2010). Although different surrogate modeling approaches have been employed for both surface water modeling (e.g., Ostfeld and Salomons, 2005; Cai et al., 2015) and groundwater modeling (e.g., Johnson and Rogers, 2000; Mugunthan and Shoemaker, 2006), they have been rarely used for fully integrated SW–GW modeling (Wu et al., 2015).

This study investigated the human-nature water conflicts in Heihe River Basin (HRB) in inland China. Farmlands in the middle HRB divert a great amount of the river flow, significantly reducing the water available to the lower HRB, a Gobi desert area with poor vegetation. Before 2000, the ecosystem in the lower HRB had experienced a fast degradation, and the end lake of the Heihe River were even dried out in certain years. A river flow regulation, starting from 2000, has refrained the surface water diversion, but stimulated groundwater pumping and caused a decline of the regional groundwater storage. The water issues in HRB are typical of inland river basins in the world. This study performed temporal optimization for the conjunctive use of river flow and groundwater in the Zhangye Basin (ZB), the core part of the middle HRB. GSFLOW and DYCORS were used as the integrated SW–GW model and surrogate-based optimization approach, respectively. The study objective was to explore how integrated hydrological modeling and surrogate-based optimization could benefit each other, and collaboratively solve complex real-world problems. The study results can also provide insights into the water resources management in HRB.

## 2. Data and method

### 2.1. The DYCORS algorithm

This study chose DYCORS (Regis and Shoemaker, 2009, 2013) as the surrogate-based optimization approach. The surrogate modeling in DYCORS adopts radial basis functions (RBFs) as the response surfaces. It has been demonstrated that, for optimization problems involving a complex hydrological model, DYCORS can effectively find optimal (or near-optimal) solution(s) with a reasonable computational cost (Espinete et al., 2013; Li et al., 2015). The main reason for using DYCORS in this study was two-fold. First, DYCORS adaptively updates its response surfaces during the optimization process. This is an innovative design which would substantially enhance the algorithm's searching efficiency. Second, the response surface approach in DYCORS aims to emulate a specific aspect(s) of the original model through a data training procedure, rather than to replace the original model as a whole based on a model-reduction analysis. This would offer great flexibility to the adaptive searching in DYCORS.

Let  $y = f(\mathbf{x})$  denote a computationally expensive function, which incorporates a complex “black-box” model, to be minimized, where  $\mathbf{x}$  represents a vector of decision variables. Also, let  $g(\mathbf{x})$  denote a surrogate model for  $f(\mathbf{x})$ . In general, DYCORS takes the following steps:

- i) Randomly sample  $n_0$  initial points of  $\mathbf{x}_i$  ( $i = 1, 2, \dots, n_0$ ) and compute the corresponding objective value  $y_i$ . Let  $\mathcal{A}$  denote the set of the sampled points, and  $\mathcal{B}$  denotes the corresponding set of objective function values. In this initial step, we have the iteration number (denoted as  $l$ ) equal to 1,  $\mathcal{A} = \{\mathbf{x}_1, \dots, \mathbf{x}_{n_0}\}$ , and  $\mathcal{B} = \{y_1, \dots, y_{n_0}\}$ , and the cumulative number of objective function evaluations (denoted as  $N$ ) equals to  $n_0$ . In the following steps,  $\mathcal{A}$

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