Hydrogeology Journal
https://doi.org/10.1007/s10040-019-01963-8

PAPER

Adaptive optimization of a vulnerable well field

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Received: 18 May 2018 / Accepted: 10 March 2019

Abstract

The contamination of groundwater resources is a challenge for drinking water supplies. To meet water quality standards, well-field operators need practical solutions to reduce the vulnerability of production wells. Strategies for several combinations of management variables such as well flow rate or water level in drains, are usually possible to satisfy the required production rate. However, these strategies may lead to contamination issues for the abstracted groundwater. A surrogate transport model was implemented in a well field vulnerable to a contaminated stream. An adaptive multi-objective optimization approach is proposed. The objective is to maximize the water production at the well field while minimizing the proportion of stream water abstracted. The optimization problem is adaptive to the stream level, which is a key parameter describing hydrological conditions. A systematic exploration of management settings is conducted and a three-dimensional Pareto front is extracted. From these optimum settings, a practical easy-to-use approach is developed. The well-field operator can adjust production settings to optimum conditions as a function of the observed stream water level and desired production rate.

Keywords Optimization · Well field · Groundwater/surface-water relations · Modeling

Introduction

Over the few last decades, population rise has led to increasing pressure on groundwater resources. As a consequence of human development and urbanization, numerous well fields are now located in urban or suburban areas where accidental and diffuse pollution risk is high (Derx et al. 2010; Doppler et al. 2007; Engeler et al. 2011; Kurtz et al. 2014). When a production well is affected by contamination from a pollution source, the well-field operator is generally constrained to stop the water production until the water quality returns to an acceptable level with respect to legal standards. When the source of the contamination cannot be removed or when residuals are likely to remain long term, a modification of the production scheme—i.e. the distribution of withdrawals among the different wells–may be sufficient to reduce the contamination of the extracted water. So as to find a better production scheme, operators frequently use trial and error methods based on the knowledge of the production site. This approach may contribute to the improvement of the production strategy of a well field but presents several limitations. Firstly, the “best” option may not be found by trial and error, and secondly, the production scheme may need to be adaptive to hydro-climatic conditions or to the occurrence of episodic pollution events. A more rational option is to implement a groundwater model for the study site and investigate the best pumping strategies by means of optimization algorithms (Peralta 2012).

An optimization of the management pattern, adaptable to hydrological conditions and production expectations, could help to produce groundwater of better quality, or to protect a vulnerable well field from a pollution vector like a stream or a contaminated area.

Over the past few years, several multiple-objective optimization techniques have been successfully applied to groundwater studies (Bauser et al. 2010, 2012; Marti et al. 2012; Peralta 2012; Yeh 2015) with Pareto front exploration (Erickson et al. 2002; Hansen et al. 2013), with for example evolutionary algorithms (Kollat and Reed 2007) and notably

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Published online: 26 March 2019

genetic algorithms (Kontos and Katsifarakis 2017; Bayer and Finkel 2004). These studies have provided an optimized well field management depending on dry or wet periods (Hansen et al. 2013) and have addressed optimization problems for both pollution and salinization issues (Kontos and Katsifarakis 2017); however, the optimization of management variables adaptive to both a decision variable (e.g. production rate) and an observed hydrological variable (e.g. stream level) is scarce.

The optimal solution can also be found by a systematic exploration of management solutions; however, one of the issues with systematic exploration is the computational burden of such an approach, which requires many model executions. The interest of algorithmic optimization is to reduce the number of executions to a few hundred or thousand, which is much lower than systematic exploration (Kontos and Katsifarakis 2017).

While flow models can have short computation times, advective-dispersive transport models are generally associated with prohibitive computation times, which makes optimization based on transport flow models hardly practical, even with finely tuned optimization algorithms (Hill 2006; Konikow 2011). Consequently, the optimization of groundwater production based on complex flow and transport models with relevant parameter estimation and uncertainty quantification is very scarce. Surrogate modeling constitutes an interesting approach to address this issue, whereby surrogate models have been employed to perform model analysis with numerous model runs in a reasonable amount of time (Burrows and Doherty 2016; Cousquer et al. 2018; Razavi et al. 2012).

This paper proposes, herein, a multiple-objective optimization with a Pareto front exploration based on a surrogate advective transport model. The main objective is to provide a solution for well field operators to optimize day-by-day production settings, depending on the required water volume, the acceptable water quality and current hydrological conditions, e.g. stream level.

A well field that is vulnerable to a contaminated stream is used to illustrate this approach. The paper first describes the study site and the objectives. The optimization methodology with a surrogate model is then detailed. The results of optimization, and the benefits and limitations of the proposed approach are eventually discussed.

Study site

Site description and objectives

The case study used for developing the optimization approach is a well field that supplies ca. 20% of the urban area of Bordeaux (France). A stream prone to industrial contamination crosses the well field, which makes stream-aquifer interactions of strategic importance. The stream flows over Plio-Quaternary sandy materials, overlying an Oligocene limestone aquifer. These two geological formations are hydraulically connected, with similar hydraulic conductivity, and therefore considered herein as a single heterogeneous aquifer (Canik 1968).

Groundwater is abstracted with two pumping wells and two 500-m-long drainage galleries, each equipped with a pump that regulates the water level in the drain (Fig. 1). Field investigations shows that every production unit has a strong impact on stream–aquifer patterns of interaction (Cousquer et al. 2017). Depending on the well flow rates or the water level of the drainage galleries, the stream–aquifer hydraulic gradient can be altered and reversed. The usual global production rate is ca. 1,000 $m^3\ h^{-1}$ for the entire well field.

The aquifer mean hydraulic conductivity is of the order of $5 \cdot 10^{-4}$ m s^{-1}. The thickness of the aquifer varies between 40 and 60 m. The width of the stream varies between 10 and 15 m, with a depth of about 1 m.

Production from wells and drains has been stopped on several occasions during the last decade due to an industrial pollution issue, with several accidental peaks occurring in the stream that have contaminated production units. Stream level is of importance for the groundwater quality; the stream–aquifer head gradient can be reversed depending on stream level fluctuations (Valois et al. 2017). The operator was willing to find an adaptive management strategy that could maintain an acceptable production rate while staying within the drinking water quality standards. This motivated the investigations for an optimized management strategy adaptive to the stream level.

Mixing ratio as a proxy for stream contamination

As the stream is the principal contamination vector, an optimal management strategy consists in minimizing the intrusion of stream water toward the production points. Thereby, one needs to quantify the proportion of water originating from the stream at each production unit (wells and drains); this can be characterized with the so-called mixing ratio (Carrera et al. 2004; Cousquer et al. 2018). The mixing model is based on Ca^{2+} and HCO_3^- concentrations. These values are reported by orthogonal projection on a mixing line that links the two end-members considered (Carrera et al. 2004; Rueedi et al. 2005). Here, the first end-member is representative of stream water, while the second is representative of groundwater from a well sufficiently distant from the stream to avoid any mixing. Thus, a mixing ratio of 0% means pure groundwater, while a mixing ratio of 100% means pure stream water. Samples were collected nine times between October 2014 and February 2018. Concentrations were obtained with a DIONEX IC column for Ca^{2+} and titration for HCO_3^-. An uncertainty of about

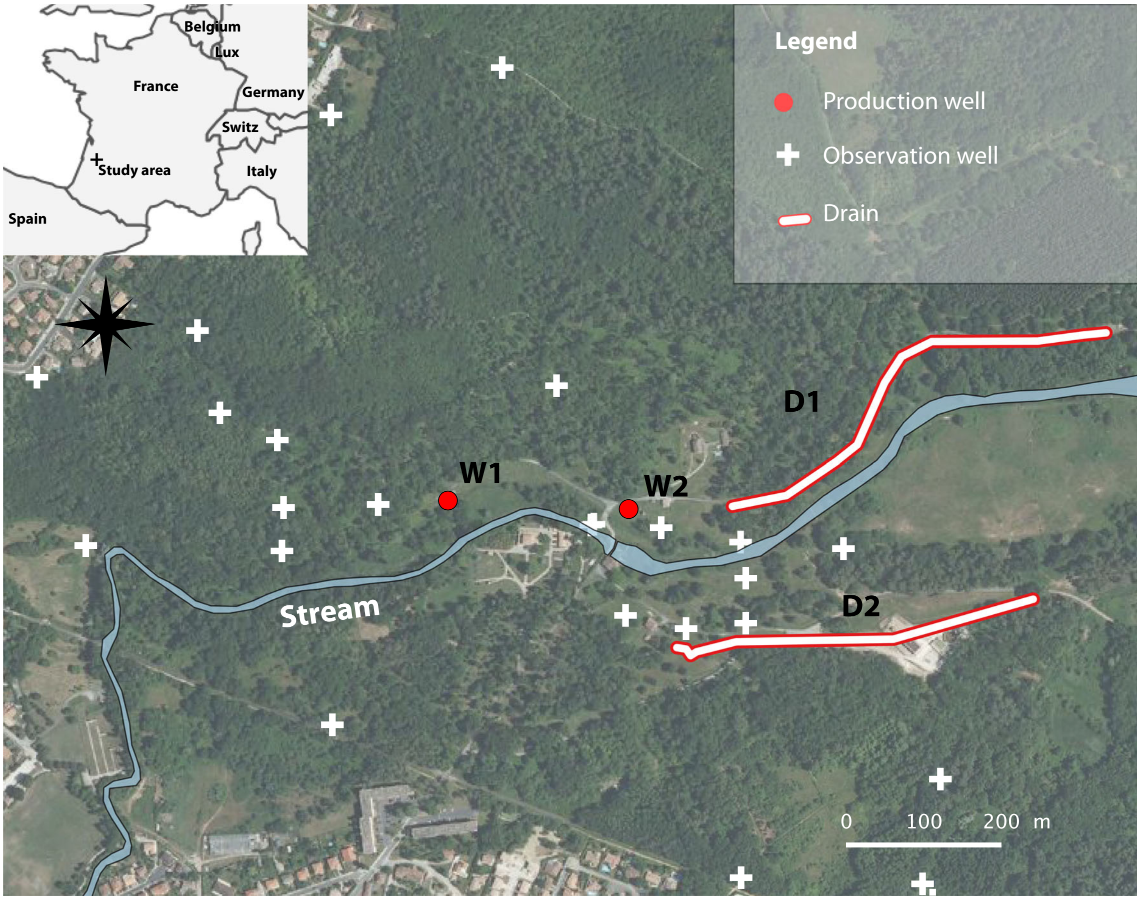

Fig. 1 The well field composed of two wells (W1, W2) and two drains (D1, D2), which is crossed by a stream. Groundwater is monitored in a series of observation wells (white crosses)

8% was found through error propagation on the orthogonal projection equation (Hughes and Hase 2010).

With the classic well field management strategy before any optimization, the average mixing ratios at wells W1 and W2 and drains D1 and D2 were about 10, 20, 40 and 0% of stream water, respectively, which yields a rate-weighted average of ca. 30%. The purpose of the approach presented hereafter is to optimize the production settings so as to reduce this mixing ratio.

Methods

Flow and transport modeling

Two models have been used for the optimization, a flow model and a transport model, with both models being based on the same spatial extents but differing in regards to temporal discretization. The first model simulates transient flow with MODFLOW-2005 (McDonald and Harbaugh 1988) and aims to reproduce observed water levels in the observation wells over a period of 700 days. Stream levels, drain levels, recharge and well flow rate are time-varying boundary conditions and were set according to field observations. The second model is an advective transport model under steady-state flow conditions. The second transport model simulates mixing ratios at production points based on the flow model. Advective-dispersive transport models, which are classically used, would be too time consuming to perform such optimization, which requires numerous model executions. A surrogate model developed by Cousquer et al. (2018) overcomes the issue by using a particle tracking method to simulate mixing ratio at production points. The flow model is based on MODFLOW-2005 (McDonald and Harbaugh 1988) and the surrogate transport model is based on backward particle tracking to determine the origins of a set of particles disseminated around a sink point of interest (well or drain; Cousquer et al. 2018). Particle tracking is conducted with MODPATH (Pollock 1994).

The model domain is centered on the well field and extends over ca. 12 km^2 (4.5 km by 2.6 km; Fig. 1). Model boundary conditions were set in accordance with regional groundwater head and flow directions (Cabaret 2011). North and south boundary conditions are head-dependent flux boundary conditions (GHB), while east and west boundary conditions are no flux. The domain is discretized with a 10 m · 10 m grid, with a total of ca. 120,000 cells. The stream and drains are simulated with head-dependent flux boundary conditions (Cauchy-type; Cousquer et al. 2017). Wells are represented by sink terms in corresponding aquifer cells. Groundwater recharge is calculated with a reservoir model (Ledoux et al. 1984) from climate data and applied uniformly to the entire model area. The computation time for this flow and advective transport model is 15 s.

Hydrodynamic parameters are interpolated on computation grid cells by kriging from pilot points (de Marsily et al. 1984). Parameter estimation has been conducted with the Gauss-Levemberg-Marqart algorithm (GLMA), a nonlinear Newton method for parameter estimation, implemented in PEST++ (Welter et al. 2015). A hybrid regularization Tikhonov-TSVD has also been conducted to stabilize the solution (Fienen et al. 2009). The simulated values showed a reasonably good adjustment with observed values, with root mean square errors (RMSE) of 0.19 m for heads in the observation wells, 11.7 $m^3 h^{-1}$ for flow in for both drainage galleries; and 11% for mixing ratios at the four production points (Cousquer et al. 2018).

Optimization

The calibrated flow and transport model described in the previous section is used for the optimization, considering as inputs the stream level (H_S) and the well field operating variables: well discharge rates (Q_{W1} and Q_{W2}) and drain levels (H_{D1} and H_{D2}). From this data, the model computes drain discharge rates (Q_{D1} and Q_{D2}) and the associated wells and drains mixing ratios, (α_{W1}, α_{W2}) and (α_{D1}, αo_{D2}), respectively (Fig. 2). The well field total production rate is the sum of production rates at each production unit: $Q_{tot} = Q_{W1} + Q_{W2} + Q_{D1} + Q_{D2}$ and the global mixing ratio is obtained from the weighted mean of mixing ratios at each production unit:

$$\alpha_{tot} = (Q_{W1} \cdot \alpha_{W1} + Q_{W2} \cdot \alpha_{W2} + Q_{D1} \cdot \alpha_{D1} + Q_{D2} \cdot \alpha_{D2}) / Q_{tot} \tag{1}$$

The objective of the optimization is to adjust the decision variables (discharge rates for wells, water level for drains) so as to reach the minimum vulnerability to stream water expressed as a mixing ratio (α_{tot}), while supplying a sufficient production rate (Q_{tot}). For a given value of H_{riv}, this multi-objective optimization problem can be expressed as follows:

$$\min \alpha_{tot} = \frac{(Q_{W1} \cdot \alpha_{W1} + Q_{W2} \cdot \alpha_{W2} + Q_{D1} \cdot \alpha_{D1} + Q_{D2} \cdot \alpha_{D2})}{Q_{W1} \cdot + Q_{W2} + Q_{D1} + Q_{D2}} \tag{2}$$

$$\max \mathrm{Q}_{tot} = Q_{W1} + Q_{W2} + Q_{D1} + Q_{D2} \tag{3}$$

where the constraints on model input variables Q_{W1}, Q_{W2}, H_{D1} and H_{D1} are given in Table 1. This optimization (minimize α_{tot}) is constrained by H_{riv}.

As mentioned previously, the stream has been identified as the main controlling factor for hydrological variations. The optimal setting therefore not only depends on the required production rate, but also on the stream water level. The objective is to adjust management variables for a given stream level and water production rate. The use of a model with a particularly short computation time makes the random exploration of numerous production scenarios possible. The exploration has been conducted by random sampling of stream level and decision variables. Field observations showed that stream levels, wells discharge and drainage gallery levels, are the main controlling factors on mixing ratios. In order to investigate the entire range of realistic values, uniform distributions were considered for all of these variables. For each production unit, the lower and upper bounds have been defined depending on the pumping capacities for the wells and the levels for the drains, with a global pumping rate ranging from 700 to 1,200 $m^3 h^{-1}$. The range of stream water levels has been defined based on historic records (Table 1).

The flow and transport model has been run for $1.5 \cdot 10^5$ samples, each representative of distinct management scenarios. The obtained mixing ratios can be plotted against the total production rate and stream level (Fig. 3). The samples of interest minimize the mixing ratio and are bounded by the so-called Pareto front. The Pareto front is first selected with the help of a Python library that provides a nondominated sorting for multi-objective problems (Woodruff and Herman 2013).

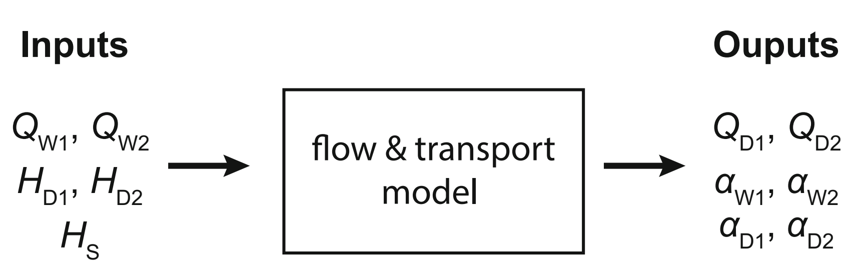

Fig. 2 The flow and transport model used for the optimization. This model considers the well field decision variables and stream level as inputs and yields drain discharge rates, together with mixing ratios at each production unit. Where Q_{D1} and Q_{D2} are drain discharge rates, Q_{W1} and Q_{W2} are well discharge rates, H_{D1} and H_{D2} are drain levels and α_{W1}, α_{W2}, α_{D1}, α_{D2} are wells and drains mixing ratios respectively

Table 1 Distribution ranges of stream level and decision variables used for the random sampling in the uniform distributions

Variable	Unit	Lower bound	Upper bound
Q_{W1}	[m^3 h^{-1}]	0.0	500.0
Q_{W2}	[m^3 h^{-1}]	0.0	500.0
H_{D1}	[m]	7.0	9.0
H_{D2}	[m]	9.2	9.7
H_{riv}	[m]	10.2	11.2

Second, the Pareto fringe (red points on Fig. 3) is extracted based on a distance shorter than 5% of the mixing ratio from the Pareto front. It should be noted that points lying close to one another in Fig. 3 may correspond to contrasting decision variables. The interest of extracting the Pareto *fringe* rather than the *front* alone is to avoid erratic change in optimal settings. In doing so, the adaptation of operating variables to stream level changes remains relatively smooth.

The points located in the Pareto fringe are associated with the optimal value of decision variables as a function of the stream level. For the adaptive optimum management to become practical, these optimal decision variables should be described as continuous functions of the required discharge rate (Q_{tot}) and stream level (H_S). To this effect, polynomial functions are adjusted from the Pareto fringe dataset for each decision variable (Q_{W1}, Q_{W2}, H_{D1}, H_{D2}) and for informative purposes, the total mixing ratio (α_{tot}). Such a polynomial function can be noted as follows:

$$P(Q_{tot}, H_S) = \sum_{i,j} c_{i,j} \cdot {Q_{tot}}^i \cdot {H_S}^j (2) \quad (4)$$

where P is the polynomial function and $c_{i,j}$ are the polynomial coefficients. A 4th order polynomial function has been found to be sufficiently smooth, while remaining sufficiently close to the Pareto fringe values; however, a higher order has been tested without changing this result.

So as to identify whether the number of samples (10^5) is sufficient to describe the optimum settings, the sampling method is then validated by cross-validation. To this effect, another sample of 10^5 is used as a validation set to be compared to the first calibration set. The polynomial functions of optimum management settings (Eq. 2) are now obtained from the calibration set alone. For each production unit, one considers the residuals between the values obtained from the polynomial function and the associated values obtained from the samples lying in the Pareto fringe, either from the calibration or from the validation set. The mean residual values for the calibration and validation sets are presented in Table 2. The mean residuals for the calibration set are low, while the mean values or residuals obtained from the validation set are slightly higher, but close to the associated values obtained from the calibration set, which validates the sample size.

Results

The polynomial functions describing the optimal values of mixing ratio and management settings can be represented as two-dimensional plots. The optimal mixing ratio presented in Fig. 4 is obtained with the optimum production settings described in Fig. 5. As expected, the optimal mixing ratio rises with increasing stream water levels and increasing global production rates, which result in increasing stream-to-aquifer

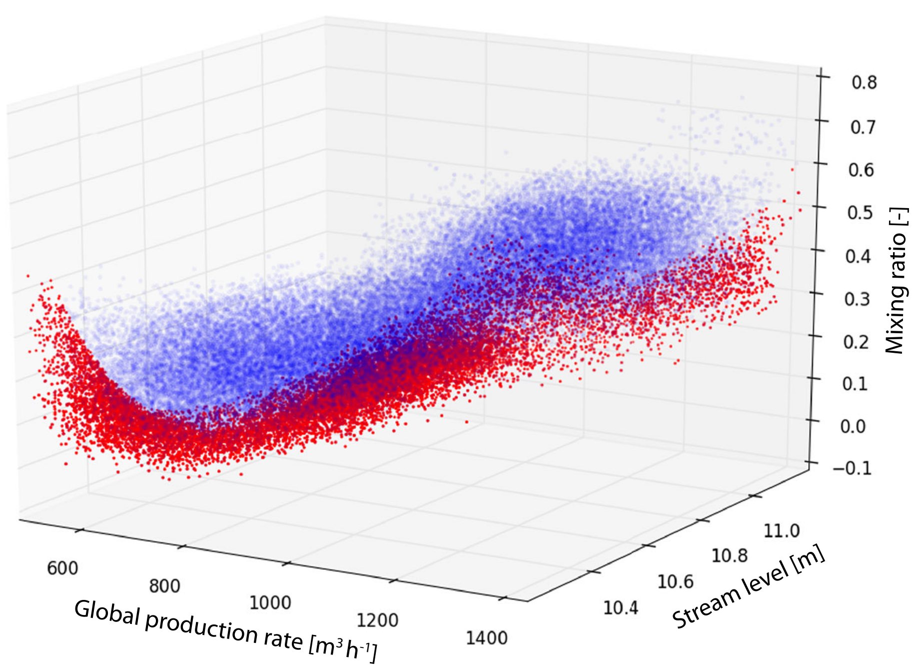

Fig. 3 Total mixing ratio, production rate and stream level for the 10^5 sampled settings. In red, the points lying in the Pareto fringe, which present mixing ratios between +0 and +5% from the Pareto front

Table 2 Comparison of mean residuals between Pareto fringe values for both subsets (calibration and validation) and their projection on the polynomial surface of the calibration subset. Mean residuals of each subset are low and sufficiently close to validate the described methodology and the sampling

Variable	Unit	Mean residuals	
		Calibration	Validation
Q_{W1}	[$m^3\ h^{-1}$]	0.22	0.24
Q_{W2}	[$m^3\ h^{-1}$]	0.057	0.062
H_{D1}	[m]	$1.7 \cdot 10^{-2}$	$2.4 \cdot 10^{-2}$
H_{D2}	[m]	$3.2 \cdot 10^{-2}$	$4.4 \cdot 10^{-2}$

flow (Fig. 4). For a global production rate at 1,000 $m^3\ h^{-1}$, the mixing ratio can be maintained below 15%, regardless of the stream level.

For each production point, the optimum setting depends on the observed stream level and the desired global flow rate of the well field (Fig. 5). When the stream level increases, the optimum level for drains also increases so as to reduce stream to aquifer flow. It can also be noted in Fig. 5 that when a higher production rate is needed, the optimum production rate increases for wells, while optimum drain levels decrease. However, the flow decreases for wells and increases for the level of drains.

In order to illustrate the interest of such optimization, the optimum management settings can be compared to the historical settings of January 3, 2015, which represent the classical management scenario before optimization (Table 3). It appears that with optimum settings, the total mixing ratio could have been reduced by 18%. The entire optimization (see Fig. 5) has not been tested in the field due to operational constrains; however, the practitioner has now used optimization results and general optimal ways, which is discussed in the next section.

Discussion

The implementation of the optimization approach greatly reduced the contribution of stream water in the abstracted water at the well field of interest, thus making the extraction of drinking water that meets quality standards possible even for relatively high global water needs and a high-flow regime in the stream. The results will now be implemented to a practical decision tool for the management of a well field which is used for daily management. Currently, the main results of the optimization are applied in practice with good results. D2 level has been turned up and D1 has been put down; the flow rate of D1 is then better with a very low mixing ratio and compensates for the loss of the D2 flow rate. Thanks to this management, in February 2018, a mixing ratio of 0% in D1 for a flow rate of 550 $m^3\ h^{-1}$ and a mixing ratio of 25% for D2 with a flow rate of 200 $m^3\ h^{-1}$ was observed. The global flow rate was 950 $m^3\ h^{-1}$ for a global mixing ratio of 5%; however, the 'instructions' regarding Fig. 5 were not perfectly followed because of technical constraints (pipe size, pump, etc.) at the time of the study.

The optimization approach required 10^5 model runs so as to test a large set of management scenarios, a sampling strategy which has been validated by cross-validation. Such a large number of model executions becomes realistic only with short computation times, which is rarely possible with

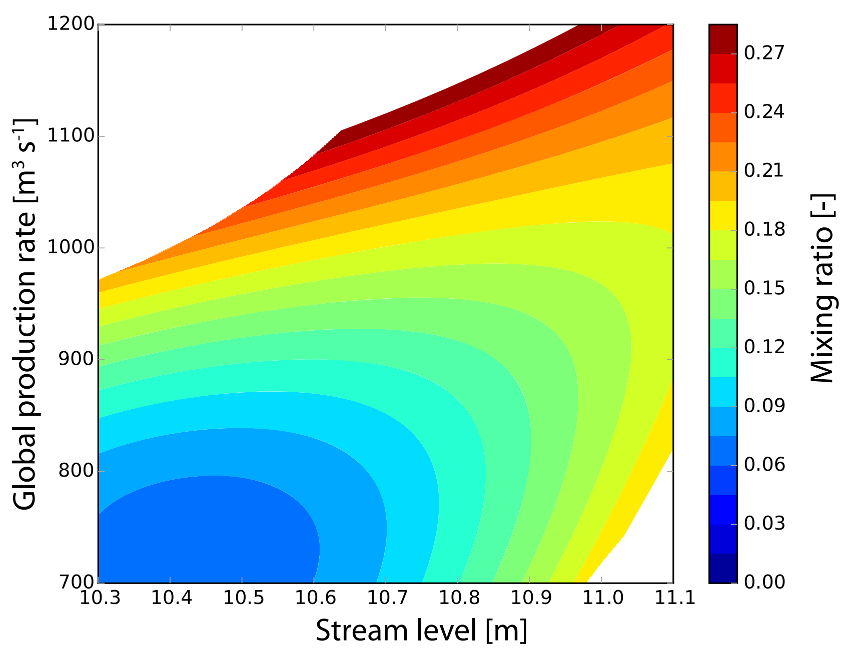

Fig. 4 Global mixing ratios obtained with optimized production settings. Given the observed stream level and the desired global production flow, the operator obtains the expected global optimal mixing ratio

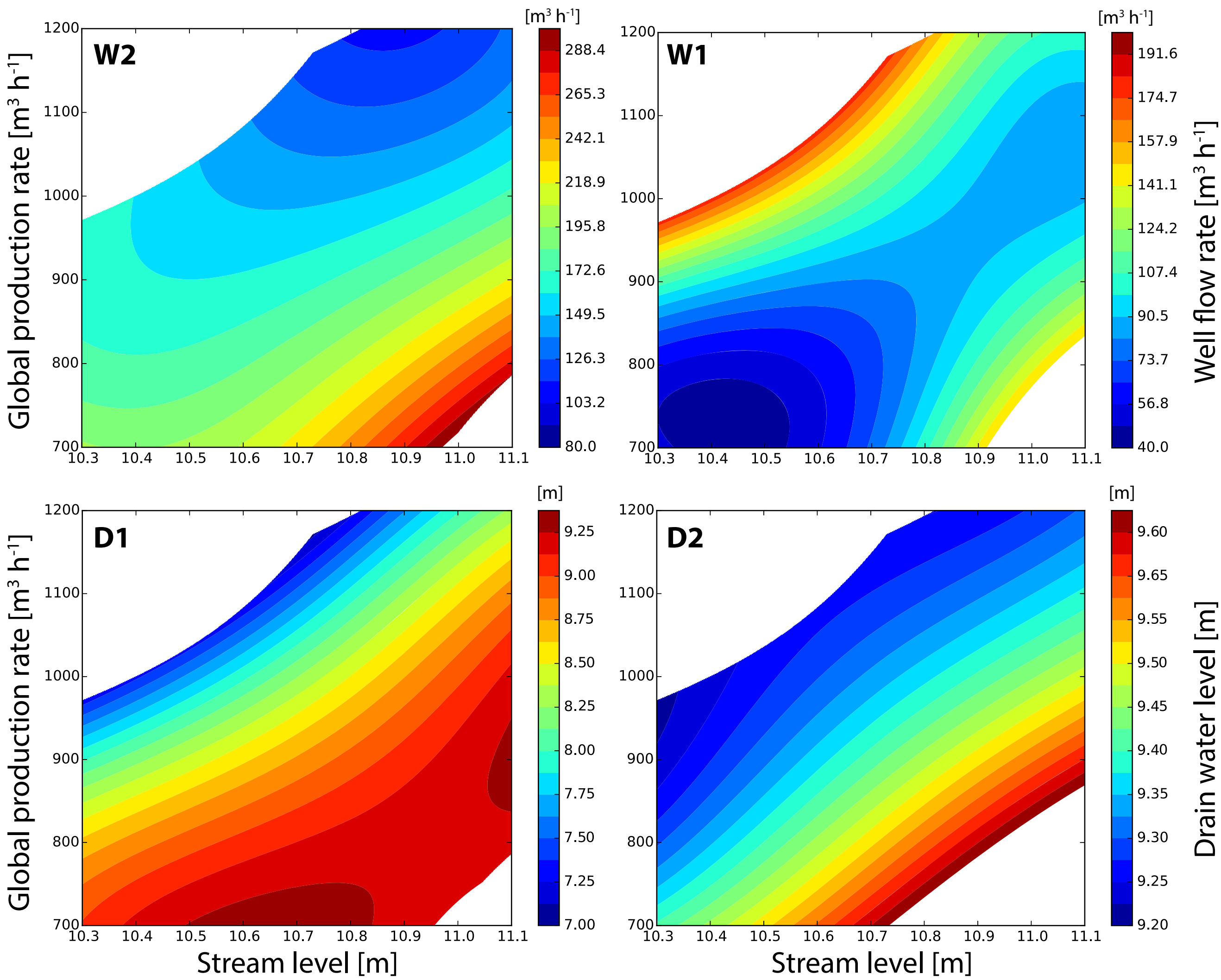

Fig. 5 Instructions for the management of each production unit of the well field. For a given stream level and a global production flow needed, the optimal mixing ratio presented (Fig. 4) can be obtained following the instruction for each point

classical transport models. In this study, the issue of computational burden is addressed with a surrogate model that has been subject to validation and uncertainty analysis (Cousquer 2017; Cousquer et al. 2018). This approach is the result of a meticulous modeling task that leads to a particularly fast flow and transport model obtained with relevant simplification hypothesis. However, it can appear that in other contexts, such an efficient surrogate model may not be obtained with reasonable hypothesis and the random exploration of input variables becomes impractical. As an alternative, optimization methods such as genetic algorithms can reduce the computational burden, while concentrating model runs with parameters leading close to the Pareto front (e.g. Bauser et al. 2012; Bayer and Finkel 2004; Erickson et al. 2002; Hansen et al. 2013, Peralta 2012). It should be recalled that in the present case, the optimization problem should be considered with three parameters: total production rate, total mixing ratio and stream level. This makes the implementation of algorithms and the visualization of results challenging (Blasco et al. 2008; Kollat and Reed 2007).

The employed approach, with a random exploration, leads to numerous waste executions far away from the Pareto front

Table 3 Application of the optimal management scheme on a historical event, the global mixing ratio is greatly improved with a reduction of 19% of surface water in product water

	Historical settings		Optimal settings	
Production point	Parameter	Mixing ratio	Parameter	Mixing ratio
D1	8.4 m	25%	8 m	8%
D2	9.7 m	0%	9.3 m	0%
W1	200 $m^3\ h^{-1}$	22%	250 $m^3\ h^{-1}$	17%
W2	320 $m^3\ h^{-1}$	33%	180 $m^3\ h^{-1}$	0%
Total	–	25%	–	6%

(Fig. 3); however, it has the advantage to yield a Pareto fringe instead of a single front. Extracting the fringe along the Pareto front and fitting continuous polynomial functions leads to relatively smooth adaptation of the decision variables to a changing stream level. The translation of optimum management settings to polynomial functions also greatly facilitates the implementation of the method by the well field operator.

The objective of the approach presented herein was to provide a tool which is easy to implement and useable by the operator for an efficient daily management of a water resource subjected to a contamination issue. The practical implementation of a model-based optimization approach adaptive to hydrologic conditions (here, the stream level) is not common in groundwater literature.

Conclusion

The proposed optimization approach has proven its efficiency to improve the management of a vulnerable well field. The method is based on a robust flow and surrogate transport model with a short computation time. An approach based on random sampling, Pareto fringe extraction and polynomial function fitting has been developed that has now been implemented as an optimum adaptive management tool of a well field and will improve the production of drinking water for a large city. The approach may be useful to operators of a large number of water production sites.

Acknowledgments The authors are grateful to the editor and the two anonymous reviewers for their constructive comments. We also thank Clotilde Thompson for her help in improving the English.

Funding information This work was conducted in the framework of the Mhyqadeau project supported by Suez Environnement (LyRE) and the French Aquitaine regional council.

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