

*Water Resources Research*

Supporting Information for

The Multi-scale Dynamics of Groundwater Depletion

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**Introduction**

This supporting information gives a detailed description of the nonlinear optimization procedure and the multi-scale groundwater model summarized in the Approach section of the main paper.

Text S1

*Multi-scale groundwater model*

The governing equation for the entire aquifer is the following unconfined vertically-averaged two-dimensional groundwater flow equation, based on the Dupuit-Forcheimer assumption discussed in the main portion of this paper (Bear, 1979):

 (S-1a) (S-1b)

 (S-1c)

 (S-1d)

where:

= two-dimensional region covered by the aquifer

, = Dirichlet (specified head) and Neumann (specified flux) portions of the boundary  of .

aquifer head at two-dimensional location (L) in  and at time  (T)

 aquifer specific yield (--), see Table 1

aquifer hydraulic conductivity (LT-1) , see Table 1

volumetric pumping flux per unit area (LT-1)

initial head (L)



specified head on Dirichlet boundaries (L)

specified aquifer bottom elevation (L)

 vector of specified volumetric flux per unit width on Neumann boundaries

(L2 T-1)

In our application the pumping rate  can change from year to year but remains constant within each year’s irrigation season, which lasts  days. Pumping is assumed to be continuous during each year’s irrigation season but zero outside this season. It is defined at each of the well locations included in the analysis and is determined by the optimization procedure.

We obtain a regional aquifer-scale description of the groundwater head distribution by solving (S1) in Cartesian coordinates  over the entire aquifer region :

 (S-2a)

 (S-2b)

 (S-2c)

 (S-2d)

 (S-2e)

where:

aquifer-scale head at two-dimensional location  (L) and time  (*T*)

= unit area pumping rate for *t* in year *n* and  for  (LT-1)



 otherwise (LT-1)

total volumetric rate of water pumped from well *w* in year *n* (L3T-1)

radius of the well circle  (L)

area of the well circle  (L)

, *x* and *y* components of the specified boundary flux vector 

The aquifer-scale solution is obtained by discretizing this equation over space on a triangular finite element grid and performing a variable time-step integration over time. The solution is reported at a daily time step for use in subsequent pumping cost computations (see below). The grid includes extra detail in  well circles  located within the overall aquifer region . In our example =9. Well circle  is centered on the location of well *w* and is assigned a radius , which is selected to ensure that mass is conserved across the circular boundary (see below). It’s area is In the aquifer-scale solution the volumetric pumping rate from well *w* is distributed uniformly throughout . This solution is implemented with functions from the MATLAB Partial Differential Equation Toolbox, documented at <https://www.mathworks.com/help/pde/>.

This aquifer-scale solution procedure can resolve variability over distances compatible with the smallest finite element grid scale, which is on the order of 100 meters for our application. This scale is significantly larger than both the well radius and the radial extent of the region near the well center where drawdown is greatest.

We obtain the higher-resolution local well-scale solutions needed to compute realistic well costs at individual wells by solving a separate small-scale groundwater flow problem within each well circle . In circle  the two-dimensional unconfined flow equation is expressed in local polar coordinates with the origin located at the center of well *w*. An assumption of approximate radial symmetry  within the well circle allows the unknown head  inside  to be expressed as a function of the radial coordinate *r* only and solved in one dimension, along *r*. This gives the following nonlinear local-scale flow equation for well circle *w*:

 (S-3a)

 (S-3b)

 (S-3c)

where:

well-scale head at radius *r* (L) and time  (*T*)

 = unit area well pumping rate for day *t* in year *n* and  for (LT-1)

 otherwise

radius of the well *w* borehole (L) = 0.5 m for our example

area of the well *w* borehole (L2)

Equation (S-3b) is a Neumann boundary condition (imposed at the well center) that follows from the assumption of axial symmetry. Equation (S-3c) is a Dirichlet condition that specifies that the well-scale head  along the circular boundary  must be equal to the average of the aquifer-scale head values  computed on this boundary (where ). In our implementation the one-dimensional well-scale nonlinear differential equation is solved with the MATLAB library function *pdepe,* documented at <https://www.mathworks.com/help/matlab/ref/pdepe.html>. The head boundary condition of (S-3c) provides the link between the local and regional scales of our multi-scale groundwater model.

The discretization of the well-scale solution procedure is fine enough in our application to allow an estimate of the daily average well head, well lift and saturated depth to be computed at a borehole radius that is less than 1m. This provides a realistic small-scale estimate of the local well lift that agents actually use when making pumping decisions. The well-scale estimate of pumping lift can be much greater than the one that provided by the lower resolution aquifer-scale solution at the well location (especially when the aquifer transmissivity is low). At well *w* the pumping decision of agent *w* for year *n* is based on an estimate of the total annual pumping cost made at the beginning of the irrigation season:

 (S-4)

where:

well-scale pumping lift over day *t* at  borehole radius of

well *w* (L)

ground surface elevation at well *w* = 30m. in our example

= average well-scale pumping lift over year *n* at  borehole radius of well *w* (L)

volume (L3) pumped in one day during irrigation season, at well *w* in year *n*, assuming the annual pumping rate (L3 yr-1) is constant over the days of the irrigation season (the pumping rate is assumed to be zero outside the irrigation season)

number of days that well *w* is pumped during the irrigation season = 182 days in our example

= pumping cost per unit energy expended when pumping water ($ M-1L-2T2) =

$ 0.15 (kWhr)-1 in our example

= pump efficiency (--) = 0.5 in our example

= density of water (ML-3) = 1000 kg m-3

= gravitational acceleration (LT-2) = 9.8 m sec-2

The multi-scale solution procedure described above yields two solutions within the individual well circles, since the aquifer and well solution domains overlap there. The lower-resolution aquifer-scale head solution is discarded within the well circles. However, the aquifer-scale head gradient projection  along the boundary of well circle defines the total flux crossing the boundary . A second boundary flux value is provided by the well-scale head gradient along the same boundary. The line integrals of the aquifer-scale and well-scale point flux values along need to be the same if the total mass of water crossing the well circle for well *w* is to be conserved. Due to numerical approximations, the mass flux estimates from the well-scale and aquifer-scale solutions are not identical. The exact value of the mass flux error for each well depends on the case simulated and the time, but can generally be brought to within a few percent of the aquifer-scale by proper choice of the well radius. In our application this radius is 500 m. for all wells.

Text S2

*Optimization procedure: Objective functions*

The cooperative and uncooperative well pumping strategies considered in this paper are derived from optimization problems that maximize similar measures of net benefit. In both cases the net annual benefit is the difference between the annual demand for irrigation water ($ T-1) for any well *w* and year *n* and the annual pumping cost ($ T-1) , where (L3T-1) is the annual volumetric pumping rate (constant over the pumping period) and  (L) is the average annual pumping lift (see (S-3))

The demand function is assumed to be quadratic and concave:

 (S-5)

where are specified time-invariant positive coefficients and  is defined over the range of values where the quadratic function increases with . The concave shape of the revenue function reflects the diminishing marginal demand for additional irrigation water [Negri, 1990]. In our example the linear demand coefficient is varied while the quadratic coefficient is fixed.

The total annual pumping (energy) cost  ($ yr-1) over the irrigation season for year *n* and well *w* is given in (S-4):



Although the annual cost and revenue expressions given above are the same for the cooperative and uncooperative strategies the total benefit functions differ, reflecting 1) differences in the information available for making a decision in any given year and 2) different approaches to discounting.

The cooperative-with-foresight strategy takes advantage of its knowledge of the future consequences of pumping by simultaneously adjusting all  well pumping rates to maximize the present value of the stream of benefits obtained from all  wells over the entire planning horizon of years. The associated objective function is:



 (S-6)

where *r* is the annual discount rate. The cooperative-with-foresight information structure assumes that the cooperating agents have access, at the beginning of the planning horizon, to model predictions of the set of all annual average well lifts , the set of all annual pumping costs obtained for any set of proposed annual pumping rates , and the set of annual minimum daily aquifer outflows  (see S5).

The uncooperative-without-foresight strategy operates in real time by selecting the scalar pumping rate for each agent’s well at the beginning of each year. At the beginning of year *n* agent *w* maximizes the current net benefit function  with respect to the pumping rate  for only well *w* and year *n*:

 (S-7)

Note that the lift estimate used in this myopic benefit function is the previous year’s average pumping lift . This is the best lift information available to the myopic player for deciding on the next year’s pumping rate. The uncooperative agent does not consider the future consequences of current pumping from any of the wells. Also, the benefit function is not discounted because the uncooperative agents do not take into account any future benefits. In effect, these agents adopt very high annual discount rates. Nevertheless, it is possible to evaluate the total present value  of the stream of benefits that uncooperative agents collectively receive:

 (S-8)

This discounted uncooperative benefit can be directly compared to its cooperative counterpart of (S-5). Both describe the total benefit extracted from the aquifer by  agents over the planning horizon.

Text S3

*Optimization procedure: Groundwater model constraints*

In order to complete the formulation of either the cooperative or uncooperative optimization problems we need to relate the lifts appearing in the objective function to the pumping rates, which are the optimization decision variables. This can be done by incorporating all of the discretized groundwater model equations from Section S1 above as equality constraints in the optimization procedure. The nonlinear model equations are defined at all days in the multi-year planning horizon and at all model grid points within the well circles and in the rest of the aquifer.

The model constraints can be greatly simplified if we take advantage of the fact that the optimization procedure only requires average annual well pumping lifts and annual minimum aquifer outflows and only optimizes annual pumping rates. The daily and grid point values computed in the groundwater model are needed only to obtain accurate estimates of these annual quantities.

To exploit this property, we can use a nonlinear version of the response matrix method (*Gorelick*, 1983) to derive a smaller set of well-oriented annual groundwater constraints from the much larger set of daily grid-oriented model equations. Since the unconfined groundwater flow equations are nonlinear (see S1) and the classical response matrix method is based on linearized approximations to these equations, we need to update the response matrix constraints within the iterative loop of our nonlinear programming optimization algorithm. The quadratic structure of the objective functions discussed in S2 makes it attractive to adopt an iterative sequential quadratic programming (SQP) algorithm for our problem. This algorithm uses the MATLAB *quadprog* function, documented at [https://www.mathworks.com/help/matlab/ref/quadprog.html](https://www.mathworks.com/help/matlab/ref/pdepe.html) to solve the quadratic programming problem that results when linear response matrix constraints are used within the iteration loop of the SQP search algorithm. These constraints need to be updated on each iteration.

In our application, the response matrix approach can be viewed as a way to approximate the complex nonlinear vector function  that relates the annual average lift to the complete vector *u* of all annual pumping rates for all agents:

  (S-9)

Note that  is the unpumped steady-state lift. For our unconfined aquifer application  is nonlinear due to the dependence of transmissivity on head, through saturated depth.

A linear approximation of  at any given iteration *i* can be obtained from a first-order Taylor expansion, linearized around the pumping rate vector obtained from the previous iteration of the optimization algorithm:

 (S-10)

where:

= optimal pumping rate generated on iteration *i* of the SQP search algorithm

= specified nominal pumping rate used to initialize the search algorithm

= average annual lift computed by the complete nonlinear groundwater model on iteration *i*, from 

number of optimization iterations

The four-dimensional array that appears in the linear term is a time-dependent extension of the traditional steady state system response matrix, computed on iteration *i* (*Gorelick*, 1983). The array element  specifies the effect of pumping at well *v* during year *m* on the average lift at well *w* during year *n*. Causality implies that elements with *m>n* are zero. Each element of *G* is approximated by a finite difference ratio of individual lift and pumping rate perturbations from the previous solution:

 (S-11)

where:

= a perturbation in the element of the -dimensional pumping rate vector corresponding to (*v,m*)

= the resulting perturbation in the element of the - dimensional vector  corresponding to (*w,n*)

The perturbed lifts are obtained from simulations of the groundwater model that are run inside the overall optimization iteration loop. Thus requires +1 simulations in each iteration, one giving the unperturbed lift vector corresponding to the previous iteration’s vector of optimal

pumping rates and one giving the perturbed lift for each of the perturbed annual pumping rates.

Our experience indicates that this procedure is less computationally demanding than standard quasi-Newton search procedures that require numerical gradient evaluations and line searches. The computational effort can be further reduced by re-simulating only the period after the time that each pumping rate is perturbed and exploiting sparsity properties that reflect the diminishing influence of a pumping perturbation in any given year on lifts in future years. The resulting SQP algorithm generally converges in just a few iterations, except when the saturated depth drops low enough to greatly increase the nonlinearity of the system.

The set of linear equality constraints summarized in (S-9) conveys to the quadratic programming algorithm all the lift information needed from the multi-scale groundwater model, including the effects of aquifer boundary conditions and well interactions. This information is updated and the quadratic programming algorithm is rerun in each iteration until the optimal pumping solution converges.

Text S4

*Optimization procedure:**Well yield constraints*

In many situations well pumping rates may be more limited by well yield than by the cost of pumping (*Foster et al,* 2015). In such cases inequality constraints can be added to the optimization problem to ensure that the optimized pumping rate does not exceed the well yield. A convenient way to do this in our application is to use the well-scale portion of our groundwater model to identify the maximum pumping rate (or well yield) that always gives a positive saturated depth at the well borehole, for a given regional head distribution and hydraulic conductivity (*Foster et al.,* 2017; *Hecox et al.,* 2002; and *Upton et al.,* 2019). This maximum value constrains the pumping rate selected by the optimization procedure, as follows:

 (S-12)

where:

well yield at well *w* in year *n,* written as a function of the minimum saturated depth at the boundary of well circle *w* during year *n,* for a given horizontal hydraulic conductivity *K*.

 saturated depth on the last day of the pumping period in year *n* on the boundary (of radius ) of well circle *w.*

 = head on the boundary of well circle *w* at 

The well yield constraint is written in terms of the well circle boundary head  at the end of the pumping period. This head determines the local effects of aquifer-scale depletion (see S-3c). The well yield function  is derived from off-line simulations of the well-scale groundwater model, stored as a table, and interpolated in real-time within the optimization iteration loop. These simulations identify the maximum well pumping rate that can be sustained without dewatering the well, expressed as a function of .

The yield at a given well can be expected to gradually drop when the aquifer is being depleted and the well circle boundary head decreases. In some situations, the well yield may always be above the economically desirable pumping rate. Then the well yield constraints will be inactive and have no effect on pumping. However, when the hydraulic conductivity and saturated depth are small, well yield constraints may be the dominant factors controlling pumping rates.

Text S5

*Optimization procedure: Outflow constraints* (*Cooperative optimization only*)

For reasons discussed in the main paper, a cooperative pumping strategy may be able to reduce pumping to maintain aquifer outflows at or above levels needed to satisfy downstream water demands. This requires sufficient foresight to ensure that high pumping rates are decreased soon enough for the delayed impact of these decreases to have the desired effect at distant boundaries. Outflow boundary constraints on pumping may be formulated much like the lift constraints discussed in S2, by constructing an outflow response matrix that approximates the impact of pumping on the minimum daily outflow experienced during each year in the planning horizon.

We define a boundary outflow function:

 (S-13)

where:

the smallest daily volumetric flux (L3T-1) crossing a designated specified head aquifer boundary in year *n*

function relating the boundary flux to the annual well pumping rates assembled in the vector Q defined in S-8.

As in S3, we derive a linear approximation to this expression from the perturbed outflows generated in the response matrix perturbation runs of the multi-scale groundwater model:

 (S-14)

where:

 (S-15)

= perturbation in caused by a perturbation in 

Note that  is the unpumped aquifer outflow. For our unconfined aquifer application  is nonlinear due to the dependence of transmissivity on head, through saturated depth.

The outflow constraint on iteration *i* is implemented with the linearized outflow expression, as follows:

 (S-16)

where specified minimum daily outflow (L3T-1) across the designated boundary in year *n*

The set of linear equality constraints summarized in (S-14 to S-16) conveys to the quadratic programming algorithm all the aquifer outflow information needed from the multi-scale groundwater model. As with the lift response matrix, this information is updated on each iteration of the SQP search algorithm. Issues that might arise in implementing the outflow constraints are discussed in the main paper.

Text S6

*Optimization procedure: Summary*

*Cooperative pumping: one *- *dimensional* *optimization problem*:

In each iteration of the SQP search algorithm optimize the objective with a quadratic programming search algorithm:

; ; 



 *Single* *objective*

*lift constraints for all w,n*

 *yield constraints for all w,n*

 *outflow constraints for all w,n*

where is the **- dimensional vector of optimal cooperative pumping rates generated from the quadratic programming solver on iteration *i*.

*Uncooperative pumping:  separate optimization problems*

In each iteration of the SQP search algorithm for each *w* and *n*:



 *Objective for each w,n*

 *lift constraint for each w,n*

 *yield constraint for each w,n*

where is the scalar optimal uncooperative pumping rate for well *w* and year *n* generated from the quadratic programming solver on iteration *i*.

**Table S1***:* **Model and optimization inputs**

|  |  |  |
| --- | --- | --- |
| **Input** | **Units** | **Value** |
| Aquifer length | m | 15000 |
| Aquifer width | m | 10000 |
| Hydraulic conductivity, *K* | m day-1 | Case 1: 30  Case 2: 20  Case 3: 90 |
| Specific yield, *SY* |  | Case 1,3: 0.3;  Case 2: 0.1 |
| Length of outflow region on the western boundary | m | 3000 |
| Days in a year |  | 365 |
| Number of pumping days, *Np* |  | 182 |
| Number of non-pumping days |  | 183 |
| Ground surface elevation, *hg* | m | 40 |
| Aquifer bottom elevation, *hb* , eastern boundary | m | Case 1: shallow: -50; deep: -110  Case 2: shallow: -50  Case 3: shallow: -50 |
| Aquifer bottom elevation, *hb* , western boundary | m | -10 |
| Well centers (x,y) | m | [3500, 3000]; [3500,6000]; [4500,8000]; [5000,1500]; [5500,4000]; [6000,7000]; [6500, 5500]; [8000,3000]; [8500,7500] |
| Well circle radius | m | 500 |
| Well borehole radius | m | 0.5 |
| Western outflow boundary head | m | 0 |
| Northern boundary recharge flux, *R* | m2 day-1 | 2 |
| Minimum daily aquifer outflow *qoutmin* (Case 3) | m3 day-1 | 15,000 |
| Linear coefficient of quadratic benefit function, *b1* | $m-3yr | Case 1: high: 0.08; low: 0.02  Case 2 and 3: high: 0.08 |
| Quadratic coefficient of quadratic benefit function, *b2* | $m-6yr2 | 0.01\*10-6 |
| Pumping cost per unit energy, *c* | $kWhr-1 | 0.3 |
| Discount rate, *r* | % | Case 1 and 2: low: 3%  Case 3: high: 6%; low: 3% |
| Number of years of operation, *Ny* | yr | Case 1 and 2: 50  Case 3: 25 |
| Number of wells, *Nw* |  | 9 |