*Water Resources Research*

Supporting Information for

**Analytical and numerical adjoint solutions for cumulative streamflow depletion**

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**Introduction**

This Supporting Information document contains two derivations. The first derivation (S1) describes a closed-form analytical solution for the calculation of cumulative streamflow depletion. The second derivation (S2) describes a numerical adjoint solution for cumulative streamflow depletion.

S1. Derivation of closed-form analytical solution for cumulative streamflow depletion

The volume of cumulative streamflow depletion () can be calculated as the temporal integral of an instantaneous streamflow depletion flux () resulting from a groundwater extraction flux () applied from = to =:

|  |  |
| --- | --- |
|  | (1) |

where is bore-stream separation distance (L), is the duration of time elapsed since the onset of groundwater extraction (T), is unconfined aquifer transmissivity (L2.T–1), is unconfined aquifer storage coefficient (unitless), is streambed leakance [L], is streambed hydraulic conductivity [L.T–1], is aquifer saturated thickness (L), = streambed thickness perpendicular to flow (L.T–1), and erfc is the complementary error function. To simplify the derivation of , the following substitutions are introduced:

|  |  |
| --- | --- |
|  | (2) |
|  | (3) |
|  | (4) |

The integral can be separated into two parts as:

|  |  |
| --- | --- |
|  | (5) |

The first integral can be evaluated as follows. The solution of the indefinite integral of a complementary error function multiplied by an integrand () raised to an exponent () is (Ng and Geller, 1969; Section 4, Equation 15):

|  |  |
| --- | --- |
|  | (6) |

Through substitution, we now manipulate the first integral presented in Equation 5 to achieve the form on the left-hand side of Equation 6. We define as:

|  |  |
| --- | --- |
|  | (7) |
|  | (8) |
|  | (9) |
|  | (10) |
|  |  |
|  |  |
|  | (11) |

The remaining indefinite integral can be evaluated as (Gradshteyn and Ryzhik, 2007; Section 2.33, Equation 23):

|  |  |
| --- | --- |
|  | (12) |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  | (13) |

When evaluated at between the limits = and =, the equivalent definite integral is:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  | (14) |

The second integral in Equation 5 can be simplified as:

|  |  |
| --- | --- |
|  | (15) |

This integral can be evaluated using integration by parts; i.e.:

The variables and are defined as:

|  |  |
| --- | --- |
|  | (16) |
|  | (17) |
|  | (18) |
|  | (19) |
|  | (20) |
|  | (21) |
|  | (22) |
|  |  |
|  | (23) |

The solution for (Eq. 4) can now be updated as:

|  |  |
| --- | --- |
|  |  |
|  | (24) |

The remaining integral term can be evaluated using -substitution. Let ; therefore:

|  |  |
| --- | --- |
|  | (25) |
|  | (26) |
|  | (27) |
|  | (28) |
|  | (29) |
|  | (30) |
|  | (31) |
|  | (32) |

New integration limits are calculated as:

The integral can now be integrated w.r.t , rather than w.r.t :

|  |  |
| --- | --- |
|  |  |
|  |  |
|  |  |
|  |  |
|  | (33) |

This expression can be expanded as:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  | (34) |

The first integral can be evaluated as the difference between two integrals as:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  | (35) |

The second integral can be evaluated as the difference between two integrals using integration by parts (with = and =) as:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  | (36) |

The two evaluated integrals can be re-combined as:

|  |  |
| --- | --- |
|  | (37) |

The solution for (Eq. 18) can now be expressed in closed form as:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  | (38) |

This expression can be expanded and rearranged as:

|  |  |
| --- | --- |
|  |  |
|  | (39) |

This can be simplified by collecting like terms as:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  | (40) |

When =0, this expression simplifies to:

|  |  |
| --- | --- |
|  | (41) |

S2. Derivation of numerical adjoint solution for cumulative streamflow depletion

In its simplest form, the exchange flux () between an unconfined aquifer and a fully connected river, stream, or stream network at a given time can be represented by a linear function of streambed hydraulic conductivity () and thickness (), and the hydraulic gradient between the groundwater and surface water domains. When this exchange occurs on a model domain boundary, a Cauchy boundary condition can be used. Alternatively, when this exchange occurs inside a model domain, a source/sink term can be used. For convenience, both representations are referred to here as the stream boundary. The total rate of exchange flow () over a river, stream, or stream network can be calculated by integrating the exchange flux over the cross-sectional area through which exchange occurs (which can be either the bank or base of the stream) along the total length of the stream (or stream network):

|  |  |
| --- | --- |
|  | (1) |

where is aquifer hydraulic head and is stream stage, and where both values are expressed relative to a consistent datum. Omega () represents the spatial domain of interest. is a dimensionless indicator function that has a value of unity at all stream locations and a value of zero elsewhere. Multiplication of the integrand by the indicator function and subsequent integration over the whole domain is equivalent to integration over the total cross-sectional area of the stream or stream network. Positive values of represent gaining stream conditions. It should be noted that the solution presented here is also valid for losing stream conditions (i.e. for negative values of ).

The total volume of water () exchanged over a given duration (e.g. from to ) can be calculated by integrating through time; i.e.:

|  |  |
| --- | --- |
|  | (2) |

Here, represents the volume of water discharged from an aquifer into a stream or stream network (i.e. losing stream conditions), in which case the sign of is positive. Conversely, the sign is negative if an aquifer is recharged by water infiltrated from a stream or stream network (i.e. gaining stream conditions).

The rate of change in exchange volume at time = resulting from groundwater extraction at a rate of at the location and over the period = to = can be calculated as the change in flux through the stream boundary; i.e.:

|  |  |
| --- | --- |
|  | (3) |

where it is assumed that stream stage heights are independent of (or not substantially affected by) groundwater extraction. It is noted here that the derivative of aquifer hydraulic head with respect to changes in extraction rate will be negative. Since streambed hydraulic conductivity and thickness values will be positive, the derivative of aquifer–stream exchange volume with respect to changes in extraction rate will also be negative.

To increase the clarity of the derivation (here and subsequently), the variable is now substituted for the derivative of aquifer hydraulic head with respect to changes in groundwater extraction; i.e.:

|  |  |
| --- | --- |
|  | (4) |

where the dependence of this derivative on the location of groundwater extraction is shown explicitly. For the remainder of this derivation, this extended notation will be omitted for clarity. The variable is also known as the direct sensitivity term, or as the tangent linear model state variable. Equation 3 therefore simplifies to:

|  |  |
| --- | --- |
|  | (5) |

Equation 5 is the focus of the present study and represents the performance function of interest. The primary aim of the remainder of the following derivation is to achieve an alternative formulation of (5) which is not dependent on the direct sensitivity, . The reduction in groundwater–surface water exchange volume over a given duration, , can be expressed as a function of (5) as:

|  |  |
| --- | --- |
|  | (6) |

To clarify, represents the reduction in volume of water discharged from an aquifer to a gaining stream; therefore, the sign of this term is positive. The derivative represents the rate of change in the volume of water discharged to a stream and, by definition, will be negative. For this reason, the negative sign on the right-hand side of (6) is required to ensure that the sign of remains positive.

Three-dimensional groundwater flow in an unconfined aquifer that is hydraulically connected to a river, stream, or stream network is described by the following governing equation:

|  |  |
| --- | --- |
|  | (7) |

Where represents source/sink terms, and is the aquifer bottom elevation; therefore is equal to the saturated thickness of the unconfined aquifer. Initial conditions can be specified as:

|  |  |
| --- | --- |
|  | (8) |

The following boundary condition types can be applied as necessary (1=Dirichlet, 2=Neumann, 3=Cauchy):

|  |  |
| --- | --- |
|  | (9) |
|  | (10) |
|  | (11) |

where (L.T–1) represents the parameterization of a Cauchy boundary condition.

If the saturated thickness of the unconfined aquifer is not substantially affected by groundwater extraction (specifically, the area of aquifer located between the bore and stream) then the hydraulic conductivity tensor can be replaced by a transmissivity tensor; i.e.:

|  |  |
| --- | --- |
|  | (12) |

The governing equation for the forward model (7) can then be simplified as:

|  |  |
| --- | --- |
|  | (13) |

For 3-D groundwater flow in an unconfined aquifer, the change in hydraulic head due to groundwater extraction is described by taking the derivative of each term with respect to the bore extraction rate, :

|  |  |
| --- | --- |
|  |  |
|  | (14) |

where was again used to represent the sensitivity of aquifer hydraulic head to changes in groundwater extraction; i.e. . Equation 14 is known as the tangent linear model of the associated forward model (13). Importantly, it was assumed that the stream stage () is not considerably affected by groundwater extraction. The following boundary condition types can be applied as necessary (1=Dirichlet, 2=Neumann, 3=Cauchy):

|  |  |
| --- | --- |
|  | (15) |
|  | (16) |
|  | (17) |

And the following initial condition:

|  |  |
| --- | --- |
|  | (18) |

A new arbitrary state variable () can be combined with the tangent linear model by taking the inner product of  with each term in (14):

|  |  |
| --- | --- |
|  |  |
|  | (19) |

The left-hand side of (19) is equal to zero and can therefore be added to the performance measure of interest (5) as:

|  |  |
| --- | --- |
|  |  |
|  | (20) |

The aim here is to exchange the tangent linear model state variable () for the adjoint state variable () in each temporal and spatial derivative term in the previous equation. For temporal derivatives, this is achieved through use of integration by parts, where storage terms are moved outside of the derivative terms. Integration by parts states that:

|  |  |
| --- | --- |
|  | (21) |

Let and ;

|  |  |
| --- | --- |
|  | (22) |

For spatial derivatives, the product rule of differentiation is used. The product rule states that:

|  |  |
| --- | --- |
|  | (23) |

Which, for spatial derivatives (i.e. gradient and divergence operators) is equivalent to:

|  |  |
| --- | --- |
|  | (24) |

Which can be rearranged as:

|  |  |
| --- | --- |
|  | (25) |

For the spatial derivative of unconfined groundwater flow; i.e.:

|  |  |
| --- | --- |
|  | (26) |

Let and ;

|  |  |
| --- | --- |
|  | (27) |

Since is symmetric (i.e. = ) then the last term can be redefined by rearranging (27) as:

|  |  |
| --- | --- |
|  | (28) |

Equation 26 can now be substituted for the following expression:

|  |  |
| --- | --- |
|  | (29) |

A new expression for the performance measure of interest (5) can now be written as:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  | (30) |

The equation for the performance measure can be rearranged, in order to isolate the tangent linear model state variable (), as:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  | (31) |

The temporal derivative term outside of the curly braces can be evaluated using the quantities at the initial and final times as:

|  |  |
| --- | --- |
|  | (32) |

Using the divergence theorem, the spatial derivative terms outside of the curly braces can be evaluated as sums of the temporal integrals of fluxes through each of the three possible boundary condition types; i.e.:

|  |  |
| --- | --- |
|  | (33) |

The equation for the performance measure can now be written as:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  | (34) |

The governing equation for the adjoint model is obtained by setting the terms inside the curly braces to a value of zero, in order to eliminate the unknown variable from (34); i.e.:

|  |  |
| --- | --- |
|  | (35) |

This expression can be simplified by combining the third and fourth terms on the left-hand side as:

|  |  |
| --- | --- |
|  | (36) |

The third term on the left-hand side is equivalent to a Cauchy boundary condition but will typically be located within the model domain, so is retained in the governing equation as a source/sink term. This includes a loading term that is a constant source with a magnitude equal to unity.

To simplify the specification of the initial condition for the adjoint state model, the time variable, , can be replaced by an alternative variable, . Consequently, the adjoint state model is run backwards in time, from to . The governing equation for the adjoint state model (36) therefore becomes:

|  |  |
| --- | --- |
|  | (37) |

By setting the terminal condition:

|  |  |
| --- | --- |
|  | (38) |

and since (as defined by the initial condition of the tangent linear model):

|  |  |
| --- | --- |
|  | (39) |

By specifying the following boundary conditions for the adjoint model as necessary (1=Dirichlet, 2=Neumann, 3=Cauchy):

|  |  |
| --- | --- |
|  | (40) |
|  | (41) |
|  | (42) |

Therefore, the spatial derivatives evaluated as sums of the temporal integrals of fluxes through each of the three possible boundary condition types are also equal to zero; i.e.:

|  |  |
| --- | --- |
|  | (43) |

The performance measure (5) can now be written using the only non-zero term remaining from (34); i.e.:

|  |  |
| --- | --- |
|  | (44) |

Which is equivalent to:

|  |  |
| --- | --- |
|  | (45) |

Consequently, the reduction in groundwater–surface water exchange volume can be expressed as a function of the adjoint state variable as:

|  |  |
| --- | --- |
|  | (46) |

Additionally, through a change of variables, *VS* can be defined for extraction at any arbitrary location ; i.e.:

|  |  |
| --- | --- |
|  | (47) |

This states that the sensitivity of cumulative groundwater discharge from an unconfined aquifer to a fully connected stream over the duration == to == resulting from continuous groundwater extraction from an underlying confined aquifer over the same time period can be calculated at any potential extraction location as the (backwards in time) definite temporal integral of the adjoint state variable. The diffusion of the adjoint state variable through the groundwater flow system is described by the governing equation (37), with boundary conditions defined by (40-42) and terminal conditions at all locations described by (38).

The value of the adjoint state variable at any given simulated time will range from zero (at domain boundaries) to the value of the loading term (at the source of adjoint state; here, cells representing streams). Unlike the state variable in the forward model (i.e. hydraulic head), which has units of length, the adjoint state variable is dimensionless. Nonetheless, because the adjoint model governing equation is of the same form as the forward model governing equation, the same numerical code can be used for its solution. However, the magnitude of the adjoint state relative to the magnitude of the aquifer bottom elevation can affect the stability of the numerical solution. Specifically, when the latter exceeds the former, the affected cell is excluded from the numerical solution. To avoid this unwanted outcome, an offset can be applied to the adjoint state variable. Adjoint state variable values may be much smaller than the offset value required, causing spatio-temporal variations in adjoint state variable values to be obscured by numerical precision limits. For this reason, a multiplier can also be applied to the adjoint state variable. Both adjustments were applied by projecting the adjoint state variable linearly as:

|  |  |
| --- | --- |
|  | (48) |

where is a scaling parameter and is an offset parameter. The value of should be sufficiently large that adjoint state model outputs do not vary with increasing values. As discussed, the value of should exceed the aquifer bottom elevation in order to ensure the stability of the numerical solution. Following the rescaling of adjoint state variable values, the governing equation (37) becomes:

|  |  |
| --- | --- |
|  | (49) |

With boundary and terminal conditions:

|  |  |
| --- | --- |
|  | (50) |
|  | (51) |
|  | (52) |
|  | (53) |

During the post-processing of numerical model outputs, the reverse transformation is used to convert numerical adjoint state variable values () to “true” adjoint state variable values (); i.e.:

|  |  |
| --- | --- |
|  | (54) |