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### **The inverse problem and ground water management**

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**Abstract:** The response of groundwater basins to natural and anthropogenic inputs depends on many interrelated factors such as the values of groundwater flow and mass transport parameters. This work presents a theoretical analysis of the impact of parameter uncertainty on groundwater management decisions. It is shown that under classical, Bayesian, and deterministic assumptions about the parameter structure, the resulting management decisions could be very different. This underscores the importance of adopting the proper parameter structure and the need for using consistent methods to solve the inverse problem.

**Key words:** Inverse problem, groundwater management, groundwater response function, stochastic control, consistent parameter estimation.

### **1 Introduction**

The implemetation of groundwater hydraulic/allocation and quality models requires specifying various parameters, e.g., hydraulic conductivities and hydrodynamic dispersion coefficients. Frequently, such parameters must be estimated from field data and subsequently used in the management model. The purpose of this research is to derive analytical expressions relating the decision variables (e.g. pumping rates) and the uncertainty of parameters (measured by the covariance of parameter estimators). Such analytical expressions show in closed-form the effect of parameter variability on groundwater management policies. In addition, this study also determines the impact of the assumptions concerning the structure of parameters upon management decisions. Three different parameter structures are considered: classical (the parameters are fixed and unknown); Bayesian (the parameters are random with some probability distribution); and deterministic (the parameters are fixed and known). The developments presented include the control of hydraulic (e.g., piezometric heads) and water quality (e.g., solute concentrations) variables by means of external inputs such as pumping or influx recharge rates.

### **2 The model equation**

Consider the equation of flow in a heterogeneous and isotropic (the approach is applicable to the anisotropic case as well) porous medium:

$$
\nabla \cdot (K^* \nabla \phi) - \sum_{i=1}^M Q_i \delta(\mathbf{x} - \mathbf{x}_i) = S \frac{\partial \phi}{\partial t}
$$
 (1)

in which  $\phi$  = piezometric head;  $K^* = K^*(x,y,z)$  represents hydraulic conductivity;  $Q_i$  = sink term;  $S = S(x,y,z)$  denotes specific storativity; and  $\delta(\cdot)$  = Dirac delta function. Initial and boundary value problems define the time and space distribution of the field variable,  $\phi$  over the entire domain. A time-space discretization of Eq. (1) by the finite element method (Loaiciga and Marifio 1986) gives

$$
\mathbf{\phi}_t = \Pi_0 \mathbf{\phi}_{t-1} + \Pi_1 \mathbf{x}_t + \Pi_2 \mathbf{z}_t + \mathbf{v}_t \tag{2}
$$

in which  $\phi = N \times 1$  vector of piezometric heads at time t;  $x_t = K \times 1$  vector of controllable or decision variables (e.g. pumping or recharge rates);  $z_t = M \times 1$  vector of uncontrollable variables involving boundary conditions;  $v_t = N \times 1$  vector accounting for modeling and measurement errors with zero expected value, which can be assumed autocorrelated over time; and the matrices  $\Pi_0$ ,  $\Pi_1$ , and  $\Pi_2$  have elements that are functions of the distributed parameters (i.e. hydraulic conductivities and storativities). Rewriting Eq. (2) in terms of initial conditions:

$$
\phi_t = \Pi'_0 \phi_0 + \sum_{m=0}^{t-1} \Pi''_0 \Pi_1 \mathbf{x}_{t-m} + \sum_{m=0}^{t-1} \Pi'''_0 \Pi_2 \mathbf{z}_{t-m} + \sum_{m=0}^{t-1} \Pi'''_0 \mathbf{v}_{t-m}
$$
(3)

which is valid for  $t = 1, 2, ..., T$ . Expressing Eq. (3) for all time periods at once

$$
\begin{bmatrix}\n\phi_1 \\
\phi_2 \\
\vdots \\
\phi_T\n\end{bmatrix} = \begin{bmatrix}\n\Pi_0 \\
\Pi_0^2 \\
\vdots \\
\Pi_0^T\n\end{bmatrix}\n\phi_0 + \begin{bmatrix}\n\Pi_1 \\
\Pi_0\Pi_1 & \Pi_1 \\
\vdots \\
\Pi_0^T\n\end{bmatrix}\n\phi_0 + \begin{bmatrix}\n\Pi_1 \\
\Pi_0\Pi_1 & \Pi_1 \\
\vdots \\
\Pi_0^T\n\end{bmatrix}\n\phi_0 + \begin{bmatrix}\n\Pi_1 \\
\Pi_0\Pi_1 & \Pi_1^T\n\end{bmatrix}\n\phi_0 + \begin{bmatrix}\n\Pi_1 \\
\Pi_2 \\
\\
\Pi_2 \\
\Pi_2 \\
\Pi_1^T\n\end{bmatrix}\n\phi_0 + \begin{bmatrix}\n\Pi_1 \\
\Pi_2 \\
\Pi_2 \\
\Pi_
$$

or, with obvious redefinition,

 $\Omega \times \phi_0$  +  $\Psi \times x$  +  $\Lambda \times z$  + v (5)

$$
(TN \times 1) (TN \times N) \times (N \times 1) (TN \times TK) \times (TK \times 1) (TN \times TM) \times (TM \times 1) (TN \times 1)
$$

The importance of Eq. (5) cannot be overemphasized. It provides an explicit dependence of the field variables on the decision variables x. It is worth relating Eq. (5) to the discrete convolution or response equation (Maddock 1972)

$$
s(k, t) = \sum_{i=1}^{t} \sum_{j=1}^{K} \beta(k, j, t - i + 1) Q(j, i)
$$
 (6)

in which  $s(k, t)$  = the drawdown at point k at the end of the t<sup>th</sup> time period;  $Q(j, i)$  = pumping rate at the jth well (j may equal k) during the *i*th time period;  $\beta(k, j, t-i+1)$  = the change in drawdown at the kth point at the end of tth time period due to a unit quantity of water pumped from the jth well during the ith time period. Equation (6) is applicable to linear groundwater processes

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with homogeneous boundary and initial conditions. Let  $t = 1, 2, ..., T$ , and define

$$
s_t' = (s_1, s_2, \dots, s_N)
$$
  
\n
$$
x_t' = (Q_{1t}, Q_{2t}, \dots, Q_{Kt})
$$
  
\n
$$
B_t = [\beta_{kj}]_t, \quad k = 1, 2, \dots, N; \quad j = 1, 2, \dots, K.
$$
  
\nNote that the matrices  $B_t$  ( $t = 1, 2, \dots, T$ ) are of size  $N \times K$  each. By using Eqs. (7)-(9). Eq. (6) can be rewritten in matrix form as

$$
\begin{bmatrix}\n\mathbf{s}_1 \\
\mathbf{s}_2 \\
\mathbf{s}_3 \\
\mathbf{s}_4\n\end{bmatrix} = \begin{bmatrix}\nB_1 & & & \\
B_1 & B_2 & & \\
\vdots & & & \\
B_1 & B_2 & & \\
B_1 & B_2 & & B_T\n\end{bmatrix} \begin{bmatrix}\n\mathbf{x}_1 \\
\mathbf{x}_2 \\
\vdots \\
\mathbf{x}_T\n\end{bmatrix}
$$
\n(10)\n  
\n(TN×1) (TN×TK) (TK×1)

or, in shorthand notation,

$$
s = Yx \tag{11}
$$

Equation (11) is a subcase of Eq. (5). Boundary and initial conditions ( $z_t$  and  $\phi_0$ , respectively) vanish in Eq. (11) due to the homogeneity assumptions. The error term (v in Eq. (5)) does not appear in Eq. (11) because of the deterministic formulation of drawdowns, although it could be introduced if desired. Thus, it has been shown that the response model (see Eq. (5)) that describes the time evolution of piezometric heads is readily derived by forming the finite element matrices and is applicable to irregular finite domains with arbitrary initial and boundary conditions, provided that the underlying process is linear.

It is common in groundwater quality models to use linear advective-dispersive equations to model miscible displacement of ideal tracers (see, e.g. Willis 1979)

$$
\eta \frac{\partial uC}{\partial t} = \nabla \cdot (\eta D_h \cdot \nabla C) - \mathbf{q} \cdot \nabla C - f \tag{12}
$$

in which  $C =$  the solute concentration;  $q =$  the specific discharge;  $D_h =$  the hydrodynamic dispersion tensor;  $\eta$  = the medium porosity; and  $f$  = the flux of solute across the boundaries of the liquid phase. Assuming a steady-state velocity field to ensure time independence of  $\bar{D}_h$ , and after discretizing Eq. (12) by the finite element method (finite differences could be used too), gives the model system equation for all time steps

$$
C = \Omega C_0 + \Psi w + \Lambda y + u \tag{13}
$$

in which  $C = TN \times 1$  vector of concentrations;  $C_0 = N \times 1$  vector of initial conditions; w, y, and  $\mathbf{u} = T\mathbf{K} \times 1$ ,  $T\mathbf{M} \times 1$ , and  $T\mathbf{N} \times 1$  vectors of decision (i.e. fluxes  $f$ ), uncontrollable (boundary conditions), and error variables, respectively. The suitably dimensioned matrices  $\Omega$ ,  $\Psi$ , and  $\Lambda$  have elements that are functions of the dispersion tensor. The developments that follow are illustrated with piezometric head as the field variable (see Eq. (5)) but one can proceed in a similar manner when the concentration of solute in the aquifer is the field variable (Eq. (13)).

### **3 Choice of management criterion**

The objective is to minimize a quadratic loss function that represents the decision maker's preferences

$$
L = E(\phi'Q\phi) \tag{14}
$$

in which  $Q = TN \times TN$  matrix that typically includes a discount factor in addition to relative target weights on the dependent variables  $\phi$ . Costs on decision variables can be imposed by augmenting the model Eq. (5) with  $x = Ix$  and including their penalties in a suitably enlarged matrix  $Q$ , and desired paths of variables can be incorporated by subtracting them from both sides of Eq. (5). It is assumed that estimation of parameters is based on  $\tau$  observations prior to the control horizon. Furthermore, inequality constraints (e.g. nonnegative decision vectors) are assumed nonbinding so that the convex minimization problem at hand is fully characterized by Eq. (14) subject to Eq. (5). Quadratic loss functions arise quite often in groundwater management models (see, e.g. Casola et al. 1986).

#### **4 Classical and Bayesian decision policies**

In order to derive an open-loop solution to the management problem, the following matrix-vector identities are useful (Neudecker 1969)-(primed notation denotes the transpose):

$$
A \otimes B = \begin{bmatrix} a_{11}B & \dots & a_{1N}B \\ \vdots & \dots & \vdots \\ a_{M1}B & \dots & a_{MN}B \end{bmatrix}
$$
 (15)

$$
\text{vec}(ABC) = (C'\otimes A)\text{vec}(B) \tag{16}
$$

 $tr(ABCDF) = vec(B')'[A'F'\otimes C]vec(D)$  (17)

$$
tr(\mathbf{a}' A \mathbf{b}) = tr(\mathbf{b} \mathbf{a}' A) \tag{18}
$$

$$
\text{vec}(\mathbf{a}' \otimes I) = T_a \mathbf{a} \tag{19}
$$

in which A, B, C, D, and  $F =$  suitably dimensioned matrices; a and  $\mathbf{b} =$  suitably dimensioned vectors;  $vec()$  = operator that stacks consecutive columns of a matrix below one another;  $tr()$  = trace of a square matrix;  $I$  = identity matrix;  $T_a$  = aggregator matrix with elements equal to either zero or one, and they are arranged through rows and columns to make Eq. (19) valid. Notice that if a and I in Eq. (19) are of dimensions  $N \times 1$  and  $M \times M$ , respectively, the aggregator  $T_a$ will be of dimension  $MNM \times N$ .

Applying Eq. (16) to Eq. (5) gives

$$
\phi = (\phi_0' \otimes I_{TN}) \text{vec}(\Omega) + (z' \otimes I_{TN}) \text{vec}(\Lambda) + (x' \otimes I_{TN}) \text{vec}(\Psi) + v \tag{20}
$$

Substituting Eq. (20) into Eq. (14) and expanding yields  $(I_{TN}$  denotes a  $TN \times TN$ identity matrix)

$$
L = E \{ \text{vec}(\Omega)'(\phi_0' \otimes I_{TN})' Q(\phi_0' \otimes I_{TN}) \text{vec}(\Omega) + \text{vec}(\Lambda)'(\mathbf{z}' \otimes I_{TN})' Q(\mathbf{z}' \otimes I_{TN}) \text{vec}(\Lambda) + \text{vec}(\Psi)'(\mathbf{x}' \otimes I_{TN})' Q(\mathbf{x}' \otimes I_{TN}) \text{vec}(\Psi) + 2 \text{vec}(\Omega)'(\phi_0' \otimes I_{TN})' Q(\mathbf{z}' \otimes I_{TN}) \text{vec}(\Lambda)
$$

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+ 
$$
2\text{vec}(\Omega)'(\phi_0' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN})\text{vec}(\Psi)
$$
  
+  $2\text{vec}(\Omega)'(\phi_0' \otimes I_{TN})'Q\mathbf{v} + 2\text{vec}(\Lambda)'(\mathbf{z}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN})\text{vec}(\Psi)$   
+  $2\text{vec}(\Lambda)'(\mathbf{z}' \otimes I_{TN})'Q\mathbf{v} + \text{vec}(\Psi)'(\mathbf{x}' \otimes I_{TN})'Q\mathbf{v} + \mathbf{v}'Q\mathbf{v}.$  (21)

In Eq.  $(21)$ , all the terms with a single error term v vanish since v has a zero expected value. In addition, those terms not involving  $x$  are irrelevant to the optimization and are collected in a single term  $L^*$ , simplifying Eq. (21) to

$$
L = L^* + E[vec(\Psi)'(\mathbf{x}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN})vec(\Psi)]
$$
  
+ 2E[vec(\Omega)'(\phi\_0' \otimes I\_{TN})'Q(\mathbf{x}' \otimes I\_{TN})vec(\Psi)]  
+ 2E[vec(\Lambda)'(\mathbf{z}' \otimes I\_{TN})'Q(\mathbf{x}' \otimes I\_{TN})vec(\Psi)]. (22)

Next, Eqs. (18), (17), and (19) (in this sequence) are applied to Eq. (22) to yield  $L = L^* + x'T$   $\left\{E$  [vec( $\Psi$ )vec( $\Psi$ )<sup>'</sup>]  $\otimes Q$  }  $T_x$ **x** 

+ 
$$
2\phi_0 T_\phi{'}
$$
{ $E$ [vec( $\Omega$ )vec( $\Psi$ )'] $\otimes$   $Q$ } $T_x$ **x**  
+  $2z'T_z{'}$ { $E$ [vec( $\Lambda$ )vec( $\Psi$ )'] $\otimes$   $Q$ } $T_x$ **x**. (23)

Define

$$
L_{xx} = T_x \langle E[\text{vec}(\Psi)\text{vec}(\Psi)'] \otimes Q \rangle T_x \mathbf{x} \tag{24}
$$

$$
\mathbf{L}_{\mathbf{x}} = T_{\mathbf{x}}^{\prime} \{ E \left[ \text{vec}(\Psi) \text{vec}(\Omega) \right] \otimes Q \} T_{\phi} \phi_0 + T_{\mathbf{x}}^{\prime} \{ E \left[ \text{vec}(\Psi) \text{vec}(\Lambda) \right] \otimes Q \} T_{\mathbf{z}} \mathbf{z} \,. \tag{25}
$$

Differentiating Eq.  $(23)$  with respect to x, equating the resulting expression to zero, and solving for x gives

$$
\mathbf{x}^* = -L_{xx}^{-1} \mathbf{L}_x \,. \tag{26}
$$

#### **5 The classical solution**

Equation (26) represents the optimal solution. However, the matrices  $\Omega$ ,  $\Psi$  and  $\Lambda$ are unknown, and to make the optimal solution computationally feasible, Eq. (26) must be expressed in terms of observable quantities. At this point, we introduce the classical and Bayesian assumptions on the parameters. Under the classical assumption, matrices  $\Lambda$ ,  $\Omega$ , and  $\Psi$  are assumed fixed (i.e. nonrandom) and unk-<br>nown. Their estimators, i.e.  $\Lambda$ ,  $\Omega$ , and  $\Psi$ , are statistical entities, and their second moments are expressed by

$$
\sum_{\Psi\Omega} = E[\text{vec}(\hat{\Psi})\text{vec}(\hat{\Omega})'] - E[\text{vec}(\Psi)\text{vec}(\hat{\Omega})'] \tag{27}
$$

in which  $\Sigma_{\Psi O}$  = covariance of vec( $\Psi$ ) with vec( $\Omega$ ). Analogous definitions hold for  $\sum_{\psi\psi}$ ,  $\sum_{\psi\chi}$ , etc. Notice that the second term on the right-hand side of Eq.  $(27)$  is equal to vec( $\Psi$ )vec( $\Omega$ )' under the classical assumption, since  $\Psi$  and  $\Omega$  are considered fixed and known. In addition, it is implicit in Eq.  $(27)$  that  $E$  [vec( $\Psi$ )] = vec( $\Psi$ ), i.e.,  $\Psi$  is an unbiased estimator of  $\Psi$ . Matrices  $\Lambda$  and  $\Omega$  are unbiased as well. From Eq. (27), it follows that

$$
E[\text{vec}(\Psi)\text{vec}(\Omega)'] = E[\text{vec}(\hat{\Psi})\text{vec}(\hat{\Omega})'] - \sum_{\Psi\Omega}.
$$
 (28)

The population second moments in the right-hand side of Eq. (28) are replaced by their sample estimates, leading to a redefinition of the Hessian (Eq. (24)) and gradient (Eq. (25)) under the classical assumption

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$$
\hat{L}_{xx} = T_x' \{ [vec(\hat{\Psi})vec(\hat{\Psi})' - \hat{\Sigma}_{\Psi\Psi}] \otimes Q] \} T_x
$$
\n
$$
\hat{\mathbf{I}} = T_x' \{ [vec(\hat{\Psi})vec(\hat{\mathbf{I}})' - \hat{\Sigma}_{\Psi\Psi}] \otimes Q] \} T_x
$$
\n(29)

$$
\mathbf{L}_{x} = T_{x} \{ \left[ \text{vec}(\mathbf{\Psi}) \text{vec}(\mathbf{\Omega})' - \sum_{\mathbf{\Psi} \mathbf{\Omega}} \left[ \mathbf{\Psi} \mathbf{\Omega} \right] \right\} T_{\phi} \mathbf{\Phi}_{0} + T_{x} \left\{ \left[ \text{vec}(\mathbf{\hat{\Psi}}) \text{vec}(\hat{\mathbf{\Lambda}})' - \sum_{\mathbf{\Psi} \mathbf{\Lambda}} \left[ \mathbf{\Psi} \mathbf{\Omega} \right] \right\} T_{z} z \right\}.
$$
 (30)

The optimal management policy in terms of estimated quantities is given by  $x = - \hat{L}_{xx}^{-1} \hat{L}_{x}$  (31)

Equation (31) represents the solution to the groundwater management problem unaer the classical assumption lor me parameters. Lne parameters and their covariances in Eqs. (28) and (29) are computed from the solution of the inverse problem, prior to the control horizon (Loaiciga and Marifio, 1986).

#### **6 The Bayesian solution**

The Bayesian assumption, in which the parameters are random variables, leads to a modification in Eq. (27)

$$
\sum_{\Psi\Omega} = E[\text{vec}(\Psi)\text{vec}(\Omega)'] - \text{vec}(\overline{\Psi})\text{vec}(\overline{\Omega})'
$$
(32)

in which  $E(\Psi) = \Psi$  and  $E(\Omega) = \Omega$ . The outer product in the second term of the right-hand side of Eq. (32) as well as  $\sum_{\mu} \varphi_{\Omega}$  are replaced with their sample estimates, so that Eq. (32) can be rewritten as:

$$
E[\text{vec}(\Psi)\text{vec}(\Omega)'] = \text{vec}(\hat{\Psi})\text{vec}(\Omega)' + \sum_{\Psi\Omega}.
$$
 (33)

Equation (33) corresponds to the Bayesian assumption and differs from Eq. (28) (applicable under the classical viewpoint) by an important sign inversion on its right-hand side. Notice that in Eq. (28) a minus sign appears on its right-hand side, whereas the sign is positive on the right-hand side of Eq.  $(33)$ . The Hessian matrix (see Eq. (24)) and gradient vector (see Eq. (25)) are redefined appropriately in view of Eq. (33) to yield their Bayesian version,

$$
\tilde{L}_{xx} = T_x' \{ [vec(\hat{\Psi})vec(\hat{\Psi})' + \hat{\Sigma}_{\Psi\Psi}] \otimes Q \} T_x
$$
\n(34)

$$
\mathbf{L}_{x} = T_{x} \{ [vec(\Psi)]vec(\Omega) + \sum \Psi \Omega} \otimes Q \} T_{\phi} \Phi_{0}
$$
  
+ 
$$
T_{x} \{ [vec(\Psi)]vec(\hat{\Lambda}) + \sum \Psi \Omega} \otimes Q \} T_{z} z
$$
 (35)

The optimal Bayesian management decision is

$$
\tilde{\mathbf{x}} = -\tilde{L}_{xx}^{-1} \tilde{\mathbf{L}}_{x} \,. \tag{36}
$$

The deterministic approach consists of using the parameter estimates in the management model but disregarding their statistical variability. The deterministic solution can be obtained by setting to zero the covariances  $\sum \psi q_1$ ,  $\sum \psi q_2$ , and  $\sum \psi \wedge q_1$ in Eqs. (29) and (30), or in Eqs. (34) and (35), and then using either Eq. (31) or Eq. (36) to compute the deterministic management policies.

#### **7 Discussion and conclusions**

The analytical solutions provided for the classical and Bayesian cases make clear that the statistical variability of parameter estimators affects both the Hessian and the gradient of the optimal solution. In the classical case, groundwater parameters<br>are fixed and unknown. Based on field data, those parameters are estimated and used in the management model. The covariances of those estimators are also available from the solution to the inverse problem. It has been shown that those covariances appear as negative terms in the factors involving sample second moments in the Hessian and gradient expressions. If the estimation method used in the inverse

approach is consistent (so that parameter covariances tend to zero as the sample size increases), then for large samples, the effect of the statistical variability of parameter estimators on management policies should be negligible. It is usually the case in hydrogeologic modeling that data are scarce and the large sample properties of consistent parameter estimators are of little practical significance for small sample estimation. For most applications, the small sample properties will govern the behavior of parameter estimators, and, in particular, their variability as measured by the covariance matrix.

The covariances of parameter estimators also affect groundwater management solutions under the Bayesian assumption. The Bayesian approach stipulates groundwater parameters as random entities. A typical example is the logarithm of transmissivity that is known to follow approximately a normal distribution. The Bayesian solution to groundwater management problems differs from the classical solution by an important sign inversion in the factors involving sample second moments in the Hessian and gradient equations. Somewhere in between the classical and Bayesian solutions, the deterministic approach disregards the statistical variability of parameter estimators. In the deterministic case, parameter covariances are set equal to zero.

Groundwater management studies typically report deterministic results, even though the solution to the inverse problem is approached from either a classical or Bayesian standpoint. Once the estimates of parameters are obtained, they are used in the management models as if they were deterministic quantities. The analytical results provided above clearly indicate that mixing the two worlds, i.e., taking a classical or Bayesian viewpoint when solving the inverse problem but adopting a deterministic stance in the management model, may lead to gross numerical bias. The magnitudes of the resulting errors are determined by the covariance matrices of parameter estimators. From a practical standpoint, our findings-indicate the need to maintain the same assumptions on the parameters' structure throughout the solution of the inverse and management problems. It is usually the case that mathematical complexities compel the analyst to adopt a deterministic stance in the management model even though a classical viewpoint is taken in the inverse problem. In this case, we have shown that it is necessary to select adequate sample sizes in the solution of the inverse problem. Large sample sizes will minimize the impact of parameter variability in the management policies, provided that a consistent method is used to solve the inverse problem.

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#### **Appendix A Notation**

 $B_t = N \times K$  response matrices,

 $C = TN \times 1$  vector of concentrations,





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