Chapter 2

ON THE DETERMINATION OF HYDRAULIC MODEL PARAMETERS USING THE ADJOINT STATE FORMULATION

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I. ABSTRACT

The estimation of various parameters involved in numerical modeling of hydraulic systems is discussed. The method described here uses the adjoint equation approach, which has also been used in ground-water hydrology, with the strong constraint formulation in the relevant functional. The parameter-correction equation is used to modify parameter estimates, with the philosophy that there is no modification when the data misfit vanishes. The application to a set of equations (e.g., equations of motion) is illustrated. In particular, this data-assimilation method is used to determine the friction factor for tidal rivers. The method is thus an alternative to those suggested by Dronkers,\textsuperscript{17} Yeh and Becker,\textsuperscript{18} or Chiu and Isu.\textsuperscript{19}

II. INTRODUCTION

The mathematical modeling of almost all natural dynamical systems involves some physical aspects that defy convenient quantification, or render the equations too difficult to solve. Examples of these in the equations of motion are boundary stresses (bottom friction, wind shear), eddy viscosity, etc. Such physical processes are therefore included in the model in some parameterized form, but the associated unknown parameters usually cannot be estimated accurately from experiments. Values are assigned to them based on empirical relationships, experiments (where the circumstances are, in all likelihood, different from the situation under consideration), individual judgment, or precedent. If no data are available for the situation of interest, it is difficult to estimate the parameters.

We are concerned in this article with those cases where at least some data is available. This availability enables the model to then be "tuned", i.e., the model is run repeatedly for different values of the parameter until the model results match the data. This is often an expensive process, since the parameterized process may not bear a linear relationship to the data, or, for different values of the parameter, the departure of the model solutions from data may be small for different segments of the \((x,t)\) domain for which the data is available.

In the field of ground-water hydrology, a more systematic attempt has been made in recent years at estimating the model parameters (hydraulic transmissivities). Yeh\textsuperscript{1} gives a review of the various methods used in the inverse ground-water problem. Of particular interest is the adjoint-state method used by Neuman,\textsuperscript{2} Neuman and Carrera,\textsuperscript{3} and Carrera and Neuman\textsuperscript{4} to determine the transmissivities from data, and by Sykes et al.\textsuperscript{7} to study the sensitivity of ground-water model results to the input parameters. In these studies the ground-water flow is described by a single (diffusion-type) governing equation.

A method similar to the ground-water hydrologic case is described in this paper for estimating parameters of other flow models, such as those governed by the equations of momentum and continuity. The adjoint equation approach (described in Section IV) is combined with the strong constraint formulation of Sasaki,\textsuperscript{8} giving a general framework that is readily applicable to a set of steady or unsteady state equations. The philosophy adopted is that, if an initial estimate of the parameter yields a mismatch of the model results and data, this mismatch (hereafter referred to as "data misfit") should be minimized (reduced to noise level, if possible). One will then have obtained the desired value of the parameter that produced the data. As such, the data play a role in providing successively better values of the parameter. The method may briefly be described as follows:

Let \(D(x,t)\) be the variable for which data \(D'(x,T)\) exists at some locations \(x\) for duration \(T\). Let \(p(x,t)\) be some parameter (such as eddy viscosity, etc.) of the model which produces the data \(D'\). If the governing differential equations are written as:

\[
\sum_{j=1}^{N} a_j(D_t) = f, \quad (j = 1,2,\ldots,N)
\]  

then we will try to minimize the square of the data misfit,
subject to the constraints (Equation 1). Since minimizing Equation 2 will not necessarily yield the true value of \( p \) (unless, of course, this minimum is exactly zero), we will obtain only an estimate \( p' \) of \( p \), and we require that

\[
\int (p(x,t) - p'(x,t))^2 dxdt
\]

be a minimum. The above expression is the "plausibility criterion" of Neumann and Carrera.

The variational formulation of the problem with the constraint (Equation 1) implies minimizing the functional \( F \), given by

\[
F = \int \int K_p (D - D')^2 dxdt + \int \int K_p (p - p')^2 dxdt + \sum_{j=1}^{N} \int \int \lambda_j L_j(D) dxdt
\]

where \( \lambda_j \) is the Lagrange multiplier associated with the \( j \)th equation, and the Gauss precision moduli \( K_0 \) and \( K_p \) are introduced for scaling purposes (these are discussed later). The above is a "strong constraint" formalism, following the classification of Sasaki. A "weak constraint" formalism could be used by replacing \( L(D) \) in Equation 4 by \( [L(D)]^2 \), and this formulation can be physically interpreted by saying that the governing equation is only approximately satisfied. This formalism has been used by Provost and Salmon. If necessary, filter terms can be added in Equation 4 to eliminate small-scale variability. They are desirable when the data are noisy or sparse, e.g., Provost and Salmon have included a filter term that describes spatial roughness, since the sparsely sampled data provide no information about length scales smaller than the data separation. The functional \( F \) can be minimized by differentiating, resulting in extra "adjoint" equations for the Lagrange multipliers and an algebraic equation for systematic correction of the initial estimate \( p' \).

The foregoing ideas are illustrated in this paper by application to the problem of estimating friction factors for a tidal river. The flow situation is described by one-dimensional time-dependent equations of motion and flow data from laboratory simulations that were taken from Harlemann and Lee. In Section III some details of the laboratory study and the governing equations are given. The formulation of the functional \( F \) and its minimization, together with a solution algorithm, are discussed in Section IV. The results of this study and concluding remarks are given in Section V.

III. ILLUSTRATIVE EXAMPLE

We consider a one-dimensional tidal-flow model, with the objective of determining the bottom friction coefficient. Harlemann and Lee have reported data pertaining to tidal-flow-simulation studies performed at the U.S. Waterways Experiment Station. The model consists of a rectangular flume, closed at one end, and connected at the other end to a large basin where sinusoidal tidal motion is produced. Harlemann and Lee have reported making a number of runs of their finite-difference model for various values of Manning’s \( n \) to obtain agreement of their computer model results with measurements along the flume. The data pertaining to Test 1 described in Harlemann and Lee are shown in Figure 1.

The phenomenon may be described by the following equations of continuity and momentum:
where $D(x,t)$ is the distance between the water surface and channel bottom, $q(x,t)$ is the flow per unit width, $g$ is the gravitational acceleration, and $f$ is the friction factor. The boundary conditions are

$$D (\text{in cm}) = 15.25 + 1.525 \sin \omega t \quad \text{at} \quad x = 0$$

($\omega = 2\pi/600$)

$$\frac{\partial q}{\partial x} = 0 \quad \text{at} \quad x = L$$

A finite-difference scheme staggered in space and time is used, and when the friction factor $f$ is assigned the value of 0.189 (determined by Harleman and Lee with hydraulic experiments and model tuning), the resulting surface elevations at one point in the flume (at $x = L/2$, approximately) are shown in Figure 1.

We will now assume that this data was available, and consider the inverse problem of determining $f$.

**IV. THE ADJOINT EQUATIONS**

Corresponding to Equation 4, the functional $F$ for the problem described in the preceding section is
where the third and fourth integrals contain the strong constraints (viz. the governing Equations 5 and 6), and \( \lambda_D(x,t) \) and \( \lambda_D(x,t) \) are the Lagrangian multipliers corresponding to these. 

\( L \) and \( T \) are characteristic length and time scales of the problem, introduced for proper scaling since the parameter \( f \) is not considered to be a function of \( x \) and \( t \), as in Equation 4. If, for instance, \( f = f(x) \), then the second term in Equation 7 would read:

\[
T \int K(f - f')^2 dx
\]

Here we choose \( L = 100 \text{ m} \) (length of the channel) and \( T = 600 \text{ s} \) (length of the data).

The functional \( F \) is minimized by differentiating:

\[
\frac{\partial F}{\partial \lambda_D} = 0, \quad \text{resulting in Equation 5}
\]

\[
\frac{\partial F}{\partial \lambda_A} = 0, \quad \text{resulting in Equation 6}
\]

\[
\frac{\partial F}{\partial f} = 0, \quad \text{resulting in} \quad f = f' - \frac{1}{LT} \iint \lambda_D q^2 dx dt
\]

\[
\frac{\partial F}{\partial D} = 0, \quad \text{resulting in} \quad \frac{\partial \lambda_D}{\partial t} + gD \frac{\partial \lambda_A}{\partial x} + \frac{\lambda_D q^2}{4D^3} - \Gamma K_D(D - D') = 0
\]

\[
\frac{\partial F}{\partial q} = 0, \quad \text{resulting in} \quad \frac{\partial \lambda_A}{\partial t} + \frac{\partial \lambda_D}{\partial x} - \frac{2 \lambda_D q^2}{8D^2} = 0
\]

While the first three derivatives are easily derived, the derivation of the last two is described in Appendix A. It is therefore seen that by minimizing the functional, the original governing equations are recovered, along with Equation 8 for estimating a corrected value \( f \) from the original estimate \( f' \), and two adjoint Equations 9 and 10 which allow the calculation of the Lagrangian multiplier needed in Equation 8. A more formal minimization of the functional, resulting in Equations 8 to 10, is presented in Appendix B.

Some simplification of Equations 8, 9, and 10 is wrought by letting \( \lambda_D/K_D = \Lambda_D \) and \( \lambda_D/K_D = \Lambda_D \) and \( K_D/K_D = K' \), so that we have only one Gauss precision modulus \( K \) instead of \( K_D \) and \( K' \). Equations 8, 9, and 10 then take the form:

\[
f = f' - \frac{1}{LT} \iint \frac{q^2}{8D^2} \Lambda_D dx dt
\]

or,

\[
f = f' - \Delta f
\]

\[
\frac{\partial \Lambda_D}{\partial t} + gD \frac{\partial \Lambda_A}{\partial x} + \frac{\Lambda_D q^2}{4D^3} - \Gamma K(D - D') = 0
\]
The adjoint equations have two important features. We note that the friction terms in
the governing Equation 6 and the corresponding adjoint Equation 10a have opposite signs.
This implies that the adjoint equations have to be integrated backwards in time. Secondly,
if the initial and boundary conditions for this backward integration are chosen to be
\[ \Lambda_\alpha(x,T) = 0 \quad \text{and} \quad \Lambda_\beta(x,T) = 0 \]
\[ = 0 \quad \text{since } q \text{ is specified at } L,t \]
\[ = 0 \quad \text{since } D \text{ is specified at } 0,t \]
then the adjoint equations are forced only by the data misfit term in Equation 9a. The data
misfit thus plays the dominant role in determining the corrected friction factor (Equation
8a), since the \( \Lambda \)'s depend on this forcing function. The procedure for determining the
parameter \( \nu \) can be outlined as follows:

1. Choose an initial estimate \( \nu = \nu_i \).
2. Run the model for the governing Equations 5 and 6 with this value of \( \nu \). Obtain \( q(x,t) \)
   and \( D(x,t) \) for \( 0 < x < L \) and \( 0 < t < T \).
3. Calculate the resulting data misfits \( D(x_t,t) - D'(x_t,t) \).
4. Run the adjoint model equations 9 and 10 backwards in time, using the \( q \)'s and \( D \)'s
calculated in 2. The numerical scheme for this will be very similar to that of the
original model, as the \( \Lambda \)-equations are very similar.
5. Use the \( \Lambda \)'s calculated in 4 and the \( q \)'s and \( D \)'s calculated in 2 to determine \( \nu_{i+1} = \nu_i - \Delta \nu \) (Equation 8a). If \( |\Delta \nu| < \) some prescribed tolerance, the solution is reached,
STOP.
6. Set \( \nu = \nu_{i+1} \), and go to 2.

The use of the parameter-correction equation in step 5 above is a direct realization of the
philosophy set out in Section II, since \( \Delta \nu \) is dependent on \( \lambda_\alpha(x,t) \), which is forced only by
the data misfit in the adjoint equations, as mentioned earlier.

The parameter correction Equation 8 can also be discussed in the context of an optim-
ization procedure. Consider the minimization of the data misfit:

\[ F' = \frac{1}{LT} \int \int \frac{K}{2} [D(x,t) - D'(x,t)]^2 dx dt \]

We can deduce (from Equation B7) that

\[ \frac{1}{LT} \int \int \frac{\lambda_\alpha |q|^2}{K_\alpha D^2} dx dt = \Delta \nu = \frac{\partial F'}{\partial \nu} \]

and Equation 8 may be rewritten as

\[ \nu_{i+1} = \nu_i - \left( \frac{\partial F'}{\partial \nu} \right) \]

Thus, using Equation 8 is equivalent to minimizing \( F' \) by the method of steepest descent
which may be written more generally as
ITERATION:

FIGURE 2. Convergence of $f$ when initial estimate $f_1 = 101.2$. Changes made in $K$ during the convergence process are indicated.

$$f_{i+1} = f_i - \alpha \left( \frac{\partial F'}{\partial f} \right)$$

where $\alpha$ is a variable weighting factor (implicitly represented here by $1/K$) used to ensure that $F'$ is reduced. It is also possible to use other minimization schemes, such as the conjugate gradient method, which may be written generally as:

$$f_{i+1} = f_i + \gamma_i d_i$$

where $d_i = - \left( \Delta f \right)_i + \beta_{i-1} d_{i-1}$.

The $\gamma$ and $\beta$ are determined by appropriate formulae (e.g., Walsh). Steepest descent and conjugate gradient algorithms, or some variations thereof, have been commonly used in adjoint ground-water modeling studies (e.g., Chen et al., Chavent et al., Neumann, Carrera and Neumann, Yziquel and Bernard) and although several comparisons have been made, there appears to be no consensus as to which algorithm is superior.

V. RESULTS AND DISCUSSION

It is seen from the algorithm given in the preceding section that $\Delta f \to 0$ when the data misfits $(D - D_0) \to 0$. The number of iterations required to obtain the solution will therefore depend on the magnitude of the departure of the first solution from the data. If a good initial estimate $f_1$ can be made, the data misfit will be small to start with, and the process will converge quickly. Otherwise more iterations are required. Figures 2 and 3 show the convergence of $f$ when the initial estimates $f_1 = 101.2$ (an inordinately high value which damps out almost all motion, deliberately chosen) and $f_1 = 0.067$, respectively. In both cases, $f$
converges to a value of 0.189, which corresponds to a Manning's $n = 0.02$ (determined by Harleman and Lee by hydraulic experiments and model tuning). Figures 4 and 5 show how the data misfit is reduced during successive iterations. (In this study, no effort was made to accelerate convergence.)

Some remarks are appropriate regarding the choice of $K$. It is best to choose a large value for $K$ first, and if, during the succeeding iteration, some measure of the data misfit (like $\int (D - \tilde{D})^2 \, dt$) is found to have increased, then $K$ can be reduced. It is easy to see from Equations 8a to 10a that $\Delta f(x,t)$, and hence $\Delta f$ are directly proportional to $K$. In the case where $f_1$ was chosen to be 101.2, a value of $K$ larger than $10^8$ in the initial stages would give more rapid convergence. However, Figure 3 shows one case where the second iterate is actually farther from the solution than the first iterate, due to $K$ being too large ($10,000$). This, however, only increases the number of iterations required to obtain the true solution. If $K = 1000$ this does not happen and convergence is rapid. Also, if during the convergence process, $\Delta f$ is seen to reverse sign after a few iterations, then this is an indication that the solution region has been reached, but a large $K$ causes $f$ to overshoot. Oscillations may be then observed if $K$ is not reduced, since the overshoot reverses the sign of the data misfit. In this study, $K$ is reduced by a factor of 10 (see Figure 2) whenever $\Delta f$ changed sign. (This reduction factor could also be allowed to vary for greater efficiency.) Similar treatment of $K$ is necessary if a large $K$ yields a negative $f$, or, alternatively, the constraint that $f \geq 0$ can be included in the functional. In any case, $K$ can be easily treated as a self-adjusting parameter based on $\Delta f$ and the above criteria or similar ones can be built into the
program, so that the iterations can proceed unmonitored. The most important observation is that, regardless of the magnitude of $K$, the method always modifies a given iterate in the direction of the true friction factor, and never away from it.

Unlike the laboratory data used in the above calculations, most field data are usually contaminated by noise. In order to assess the effect of noisy data on the performance of the adjoint model, Gaussian noise was superimposed (Figure 6) on the data used previously. Figure 7 shows the data misfit shrinking to noise level when the true value of the friction
FIGURE 6. Variation of surface elevation with time, at \( x = 0.5L \) (as in Figure 1), with noise superimposed on model output.

FIGURE 7. Reduction of data misfit \((f, = 101.2)\) for data shown in Figure 6.

factor is obtained from the algorithm. At least in the case of this well-posed problem, the model appears to be unaffected by the noise in the data.

The above example demonstrates that the strong constraint variational formulation can be used successfully to determine friction factors for tidal rivers. Dronkers\(^{17}\) has suggested a rather elementary method for estimating the Chezy coefficient for short river sections, by algebraically manipulating governing equations similar to equation 5 and 6, and assuming a linear variation of \( D_s \) and other quantities along the section. The data required for this
method consists of the tidal elevations at the ends of the channel section and discharge measurements at some point within. The method proposed in this paper also requires boundary conditions (for the original forward model) but can utilize either surface elevations or discharge measurements as data, and makes no simplifying assumptions. It may be considered an alternative to other more sophisticated methods of estimating the friction factor in open channel flow, e.g., Yeh and Becker,19 who have devised a linear programming formulation to minimize the data misfit; or Chiu and Isu,19 who have used Kalman filtering in conjunction with the standard-step method to compute the friction factor from steady-state flow data in the Rio Grande.

This paper has discussed another adaptation of a data assimilation technique (e.g., Harlan and O'Brien,20 Talagrand and Courtier,21 Courtier and Talagrand22) to water-resources engineering. The technique determines the friction factor for river flows, by utilizing the parameter-correction equation in conjunction with the adjoint model. The approach can be used for other hydraulic models as well, in the context of model tuning, as a viable alternative to the laborious process of varying the parameters (probably arbitrarily) and comparing results for many runs. The iterative scheme suggested here automatically stops when the data misfit is reduced, essentially, to noise level. As such, the data is used as a guide to obtain better estimates of the parameter.

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APPENDIX A

We first rewrite Equation 7 after integrating once the last two of the four terms in the right hand side

\[
F(D,q,\lambda_b,\lambda_q,f) = \int \int \frac{K_b}{2} \Gamma_i (D - D')^2 dx dt + LT \frac{K_f}{2} (f - f')^2 + \int \lambda_b D' |_{x=0}^{x=L} dx - \int \int \frac{\partial \lambda_b}{\partial t} dx dt + \int \lambda_q q^2 |_{x=0}^{x=L} dt
\]

\[
- \int \int \frac{\partial \lambda_b}{\partial x} \cdot q dx dt + \int \lambda_q q^2 |_{x=0}^{x=L} dx - \int q \frac{\partial \lambda_q}{\partial t} dx + \int \int \frac{gD^2}{2} \lambda_q |_{x=0}^{x=L} dx dt - \int \int \frac{gD^2}{2} \frac{\partial \lambda_q}{\partial x} dx dt + \int \lambda_q \cdot \frac{f_0 q}{8D^2} dx dt
\]

The boundary integrals (viz. the third, fifth, seventh, and ninth terms on the right-hand side) are all equal to zero, as explained in Appendix B. Differentiation of the remaining terms in F with respect to D and q yields equations 9 and 10.

APPENDIX B

In the following, we assume that \( f = f(x) \), since this case has been briefly alluded to in the text. The functional F is formulated slightly differently, including only the least squares error and the plausibility criteria (as in Neuman), and the governing equations are subsequently accounted for.
Let \( F = \int \int_{x} \frac{K_{p}}{2} [D(x,t) - D'(x,t)]^2 dx dt + T \int_{x=0}^{L} \frac{K_{f}}{2} [f(x) - f'(x)]^2 dx \)

To minimize \( F \), \( \delta F = 0 \)

\[ \delta F = \int \int K_{p} [D(x,t) - D'(x,t)] \delta D dx dt + T \int_{x=0}^{L} K_{f} [f(x) - f'(x)] \delta f dx = 0 \]

Taking the first variation of Equation 5 gives:

\[ \delta (D_{x} + q_{x}) = 0 \]
\[ \frac{\partial}{\partial t} (\delta D) + \frac{\partial}{\partial x} (\delta q) = 0 \]

(Multiplying Equation B3 by an arbitrary function \( \lambda_{o}(x,t) \), and integrating over all \( x \) and \( t \),

\[ \int \int \lambda_{o} \frac{\partial}{\partial t} (\delta D) dx dt + \int \int \lambda_{o} \frac{\partial}{\partial x} (\delta q) dx dt = 0 \]

Integrating by parts once

\[ \int \lambda_{o} \delta D \int_{x=0}^{L} dx - \int \int \frac{\partial \lambda_{o}}{\partial t} \delta D dx dt + \int \lambda_{o} \delta q \int_{x=0}^{L} dx dt - \int \int \frac{\partial \lambda_{o}}{\partial x} \delta q dx dt = 0 \]

We then take the first variation of Equation 6,

\[ \delta \left( q_{x} + \frac{g}{2} (D^2)_{x} + \frac{f a q l}{8D^2} \right) = 0 \]
\[ \frac{\partial}{\partial t} (\delta q) + \frac{g}{2} \frac{\partial}{\partial x} (\delta D^2) + \frac{f a q l}{8D^2} \delta f - \frac{f a q l}{4D} \delta D + \frac{f}{8D^2} 2q |\delta q| = 0 \]

(Multiplying Equation B5 by an arbitrary function \( \lambda_{e}(x,t) \) and integrating,

\[ \int \int \lambda_{e} \frac{\partial}{\partial t} (\delta q) dx dt + \frac{g}{2} \int \int \lambda_{e} \frac{\partial}{\partial x} (\delta D^2) dx dt + \int \int \lambda_{e} \frac{\partial |\delta q|}{8D^2} \delta f dx dt - \int \int \lambda_{e} \frac{f a q l}{4D} \delta D dx dt + \frac{f}{4D^2} \int \int |q| \delta q dx dt = 0 \]

Integrating by parts once gives
\[
\int \lambda q \delta q|_{t=0}^{T} dx - \int \int \frac{\partial \lambda}{\partial t} \delta q dx \, dt \\
+ \frac{\delta}{2} \int \int \lambda \delta D \delta q|_{t=0}^{T} dx \, dt - \frac{\delta}{2} \int \int \frac{\partial \lambda}{\partial x} \delta D dx \, dt \\
+ \int \int \frac{\lambda \delta q}{8D^2} \delta q dx \, dt - \int \int \frac{\lambda \delta q}{4D^2} \delta q dx \, dt \\
+ \int \int \frac{\delta q}{4D^2} \delta q dx \, dt = 0
\]

Adding Equations B2, B4, and B6 (collecting terms in $\delta f$, $\delta q$, $\delta D$), yields

\[
\delta F = \int_{-\infty}^{\infty} \left[ \int \frac{\lambda \delta q}{8D^2} \, dt + TK_q(f(x) - f'(x)) \right] \delta f dx \\
- \int \int \left( \frac{\partial \lambda}{\partial t} + \frac{\partial \lambda}{\partial x} gD + \frac{\delta q}{4D^2} \lambda \delta q - K_0[D(x,t) - D'(x,t)] \right) \delta D \cdot dx \, dt \\
+ \int_{-\infty}^{L} \left( \lambda \delta D + \lambda \delta q \right)|_{t=0}^{T} dx + \int_{-\infty}^{T} \left( \lambda \delta q + gD\lambda \delta D \right)|_{t=0}^{T} dt = 0
\]

For the forward model, initial conditions must be specified. This implies $\delta D(x,0) = \delta q(x,0) = 0$, so that the lower limit (i.e., $t = 0$) of the integrand in the first boundary integral in Equation B7 vanishes. The upper limit (i.e., $t = T$) vanishes if $\lambda_0(x,T) = \lambda_0(x,T) = 0$, and these are the conditions imposed on the adjoint model, as described in the text. Thus, the first boundary integral vanishes. Similarly the second boundary integral in Equation B7 vanishes, since $\delta q(L,t) = \delta D(0,t) = 0$, $q$ and $D$ being given at $x = L$ and $x = 0$, respectively, and due to the boundary conditions used for the adjoint model, viz. $\lambda_0(L,t) = \lambda_0(0,t) = 0$.

Having dispensed with the boundary terms, the arbitrary quantities $\lambda_0$ and $\lambda_0$ can be so chosen that the coefficients of $\delta q$ and $\delta D$ in Equation B7 (i.e., the second and third terms) vanish. This yields the adjoint Equations 9 and 10, respectively. Consequently $\delta F = 0$ implies that the coefficient of $\delta f$ must also vanish, resulting in the parameter-correction equation (similar to Equation 8).

REFERENCES