## R & D NOTES

# Optimization of Eigenvalues When Using the Galerkin Method

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### Introduction

Among the weighted residuals methods the Galerkin approach is one of the most popular among chemical engineers (Finlayson, 1972; Schechter, 1967).

It has been shown recently (Laura et al., 1985) that the inclusion of an undetermined parameter in the approximate coordinate function used to solve the governing differential system allows for the optimization of the fundamental eigenvalue in problems governed by the Helmholtz equation and in the case of domains of complicated boundary shape. This is due to the fact that the Galerkin method yields upper bounds for the eigenvalues. That approach is extended here in order to minimize higher eigenvalues. Two examples are given: (a) the classical Graetz problem, and (b) the determination of a concentration profile in a light-catalyzed reactor.

It is important to point out that use of the Rayleigh method and inclusion of a minimization parameter has been used extensively to determine fundamental eigenvalues in vibration and buckling problems (Schmidt, 1982; Bert, 1984).

#### **Proposed Approach**

Suppose the exact solution of an eigenvalue problem is of the form

$$y = y(x_1, x_2, \dots, x_N) \tag{1}$$

An approximate solution  $y_a$  can then be taken of the form

$$y_a = \sum a_i \psi_i(x_1, x_2, \dots, x_N, \gamma)$$
 (2)

where the  $a_i$ 's are arbitrary parameters which are determined according to the Galerkin method and  $\gamma$  is the minimization parameter. The functional relations  $\psi_i$ 's must satisfy all the boundary conditions (Finlayson, 1972).

Substituting Eq. 2 into the governing differential equation one obtains an "error" or "residual function"

$$\epsilon = \epsilon(x_1, x_2, \dots, x_N, a_1, a_2, \dots, a_p, \gamma, \lambda)$$
 (3)

where  $\lambda$  is the eigenvalue under investigation.

The Galerkin method requires that the error function  $\epsilon$  be orthogonal with respect to each coordinate function  $\psi_i$  on the domain under consideration

$$\int_{D} \epsilon \psi_{i} dD = 0 \quad (i = 1, 2, \dots, p)$$
 (4)

and a linear, homogeneous system of equations in the  $a_i$ 's results. From the nontriviality condition one obtains a secular determinant whose roots constitute the approximate eigenvalues of the problem  $\lambda_i$ . Obviously each eigenvalue  $\lambda_i$  is a function of the still undetermined minimization parameter  $\gamma$ :

$$\lambda_i = \lambda_i(\gamma) \tag{5}$$

It is required now that

$$\frac{\partial \lambda_i}{\partial \gamma} = 0 \tag{6}$$

and this minimization condition will certainly allow for the optimization of the eigenvalues. Admittedly, once the secular determinant has been generated it is convenient to perform Eq. 6 numerically.

It is important to point out that the method proposed in this note is limited to linear self-adjoint problems. Regarding the inclusion of  $\gamma$  in the general formulation, it appears at this point that in most cases it is convenient to use it as an exponential parameter in the approximate coordinate functions used to solve the differential system.

#### **Applications**

Consider first the Graetz problem governed by the differential system

$$\frac{d^2y}{dr^2} + \frac{1}{r}\frac{dy}{dr} + \lambda^2(1 - r^2)y = 0$$
 (7a)

$$y(1) = 0 \tag{7b}$$

Taking

$$y_a = \sum_{i=1}^2 a_i (1 - r^{\gamma - 1 + i}) = \sum_{i=1}^2 a_i \psi_i$$
 (8)

and following the previously explained procedure one obtains

$$(X_2X_4 - X_6^2)\lambda^4 + (X_1X_4 + X_2X_3 - X_5X_6 - X_6X_7)\lambda^2 + (X_1X_3 - X_5X_7) = 0$$
 (9)

where  $X_i = X_i(\gamma)$  and

$$X_{1} = \int_{0}^{1} (r\psi_{1}\psi_{1}'' + \psi_{1}\psi_{1}')dr; \quad X_{2} = \int_{0}^{1} (r - r^{3})\psi_{1}^{2}dr$$

$$X_{3} = \int_{0}^{1} (r\psi_{2}\psi_{2}'' + \psi_{2}\psi_{2}')dr; \quad X_{4} = \int_{0}^{1} (r - r^{3})\psi_{2}^{2}dr$$

$$X_{5} = \int_{0}^{1} (r\psi_{1}\psi_{2}'' + \psi_{1}\psi_{2}')dr; \quad X_{6} = \int_{0}^{1} (r - r^{3})\psi_{1}\psi_{2}dr$$

$$X_{7} = \int_{0}^{1} (r\psi_{2}\psi_{1}'' + \psi_{2}\psi_{1}')dr$$

$$(10)$$

As previously stated the minimization procedure is evaluated leading to the results:

$$(\gamma = 1.90)$$
  $\lambda_1 = 2.704$   $(\gamma = 1.10)$   $\lambda_2 = 7.07$ 

The first eigenvalue coincides with the exact result while the second differs from the exact value by 6% ( $\lambda_2 = 6.66$ ) (Schechter, 1967).

Consider now the determination of the concentration profile in a light-catalyzed reactor (Schechter and Wissler, 1960), which for the particular set of parameters considered by the authors in their interesting paper is expressed by the differential system

$$\frac{d^2y}{dr^2} + \frac{1}{r}\frac{dy}{dr} + \left[\lambda^2(1-r^2) - \frac{2}{r}\right] = 0$$
 (11a)

$$\frac{dy}{dr}(0) = 2y(0) \tag{11b}$$

$$\frac{dy}{dr}(1) = 0 ag{11c}$$

Taking now:

$$y_a = a_1 \left( -\frac{r^{\gamma}}{\gamma} + r + \frac{1}{2} \right) + a_2 \left( -\frac{2}{\gamma + 1} r^{\gamma + 1} + 2r + 1 \right)$$
 (12)

where each coordinate function satisfies the boundary conditions and applying a procedure similar to the one previously developed one obtains

$$(\gamma = 2.6)$$
  $\lambda_1 = 2.773$   
 $(\gamma = 1.4)$   $\lambda_2 = 6.33$ 

where the first eigenvalue again coincides with the exact results (Schechter and Wissler, 1960). (The second eigenvalue is not available.)

In conclusion it appears that the present approach possesses some inherent advantages in view of its simplicity and flexibility. It may also be of considerable value in the application of the finite element method based on the Galerkin formulation.

#### Notation

 $a_i = arbitrary constant$ 

 $\vec{D}$  = domain

r = dimensionless radial variable

 $x_i = independent variable$ 

 $X_i = \sec Eq. 10$ 

Y = dependent function

 $\gamma$  = minimization parameter

 $\lambda = eigenvalue$ 

 $\psi_i = \text{coordinate function}$ 

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