Application of Finite Element Method (FEM) Instruction to Graduate Courses in Biological and Agricultural Engineering

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Abstract

The application of *Finite Element Methods* (FEM) to a graduate level course in Biological Engineering, Advanced Transport Phenomena in Biological Engineering, is presented. First, the *Galerkin Weak Statement* (GWS) was introduced to the class to show the fundamental theory of FEM by solving a 1D steady state heat transfer problem. This technique provides a more accurate solution with the estimation of error. The concept of error reduction through mesh refinement was also introduced. Each student was required to conduct an independent semester project incorporating mathematical modeling and simulation of a biological engineering problem. One of these projects, fixed bed ion exchange modeling, is discussed in this paper. The outputs from these class projects illustrate that the students gained experience in using FEM to solve dynamic biological engineering problems.

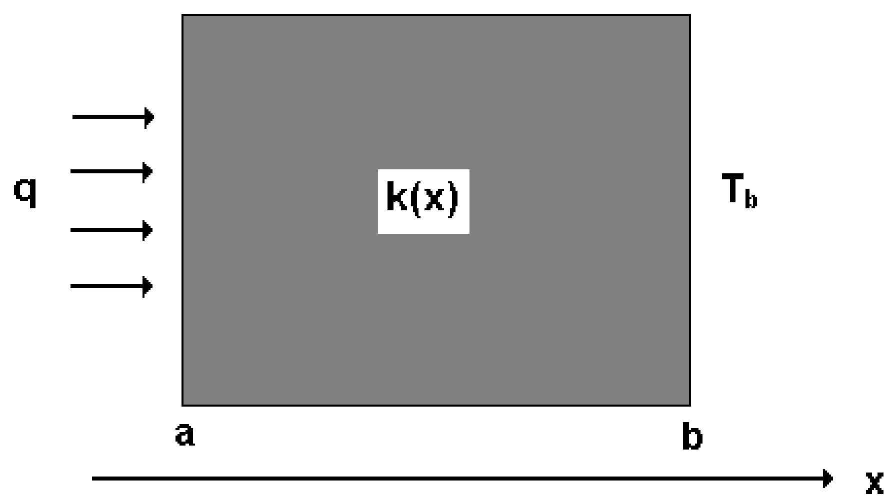
Introduction

Computer aided modeling of new products has allowed industry to quickly optimize design while spending less time and money on physical prototypes. Bioprocess and food process engineers often deal with complex heterogeneous system characterized by non-Newtonian behavior. Solutions to partial differential equations that describe these complex systems are difficult to obtain. Advantages of using Computer-Aided Engineering (CAE) prototyping in food and bioprocess development (Datta 1998; Baker et al. 1999) and application to mechanics of materials (Hillsman 1994) have been previously addressed They include: 1) quick and inexpensive testing of alternative scenarios that can result in reduced costs and increased profits, 2) clear understanding of the interactions between the physical processes and their sensitivity to various operational parameters, and 3) front-end engineering before prototyping, making the prototypes closer to optimum and reducing their number. Development of computer models to describe these complex bioprocessing systems is needed.

This paper addresses the experience in introducing Finite Element Methods (FEM) to a graduate level course in Biological Engineering in LSU, BE 7352, Advanced Transport Phenomena in Biological Engineering, during the fall semester of 2001. The course included two aspects of FEM development. First, the fundamentals of FEM using the *Galerkin Weak Statement* (GWS) were introduced to the class with discussion of error analysis. This technique provides a more accurate solution with the estimation of error. The concept of error reduction through mesh refinement was also introduced. An example one-dimensional steady state heat transfer problem was used to illustrate these concepts. Secondly, the students gained first-hand experience with FEM by application to independent semester projects in biological engineering. Each project was required to include computational modeling and simulation of a biological engineering problem, primarily from the student's research interest.

The fundamental theory of FEM

One dimensional heat transfer was used to present the fundamental theory of FEM. Simple 1-D heat transfer through a plane wall is shown in Figure 1. In this problem, the equation is given in terms of T (temperature) on the domain Σ, on the boundary a < x < b with corresponding Neumann (constant flux, q) and Dirichlet (constant temperature) boundary conditions.



Governing Equation

$$-\frac{d}{dx}\left(k\frac{dT}{dx}\right)-s=0 \quad over \quad a<x<b$$

Boundary Conditions

$$-k\frac{dT}{dx}=q \quad at\ x=a$$

$$T=T_b \quad at\ x=b$$

Figure 1 Conduction through a plane wall with uniform thermal conductivity

The steps to obtain the finite element solution presented to the class are described as follows (Baker and Pepper, 1991):

1. State the governing equation, and initial and boundary conditions. Define the approximate solution in terms of known spatial functions multiplied by unknown expansion coefficients. Determine that the suitable spatial functions exist and determine the unknown expansion coefficients.

$$T^N(x) = a_1\phi_1(x) + a_2\phi_2(x) + a_3\phi_3(x) + \mathrm{K} + a_N\phi_N(x) = \sum_{i=1}^{N} a_N\phi_N(x) \qquad (1)$$

where T^N = approximate solution, a_i is the expansion coefficient, and N_N is the trial spatial function.

The relationship between the exact solution and approximate solution is

$$T(x) = T^N(x) + e^N(x) \qquad (2)$$

where $e^N(x)$ is the approximate solution error.

2. Define the *Galerkin Weak Statement* (GWS) to determine the expansion coefficients that ensure an absolute minimum approximate error. This procedure minimizes the "distance" between the T(x) and $T^N(x)$ for any specified number of terms in the approximation, N. To form the GWS, the weighted residual approach is used to meet the *Galerkin* criterion that the weight functions must be equal to the selected trial functions to minimize the error by making the set of functions orthogonal.

$$\mathrm{GWS} = \int_\Omega \phi_i(x) L(T^N) dx \equiv 0 \qquad (3)$$

where $\phi(x)$ is defined below and $L(T^N)$ is governing differential equation of the system in terms of the approximation variable T^N. The GWS for the given 1-D heat transfer problem with linear trial space functions is:

$$\phi_i(x) = \frac{x - x_{i-1}}{x_i - x_{i-1}} \quad \text{for} \quad x_{i-1} \le x \le x_i \qquad (4)$$

$$\phi_i(x) = \frac{x_{i+1} - x}{x_{i+1} - x_i} \quad \text{for} \quad x_i \le x \le x_{i+1} \qquad (5)$$

$$\phi_i(x) = 0 \quad \text{for} \quad x > x_{i+1} \text{ or } x < x_{i-1} \qquad (6)$$

3. Select piecewise continuous spatial functions (linear, quadratic, or cubic).
4. Define a discretization of the solution spatial domain in terms of finite elements to

evaluate the weak statement integrals and apply boundary condition to solve for the unknown expansion coefficients.

5. Determine the approximation accuracy by determining the error to validate solution quality.

The approximate solution of a 1-D heat transfer equation obtained through these steps can be obtained and compared to the analytical solution, if the analytical solution exists.

Asymptotic Error Estimation

The theoretical estimate of performance of the linear basis Finite Element implementation of the GWS is described by the error semi-norm $|e^h|_E$, which cannot be determined unless the exact solution is known. Thus, it is not possible to estimate error using a single solution on mesh domain, Ω^h. In practice, a mesh refinement process is followed using a sequence of nested meshes, Ω^h, $\Omega^{h/2}$, $\Omega^{h/4}$, etc.

The definition of approximation error for two such solutions yields

$$T^h + e^h = T = T^{h/2} + e^{h/2} \tag{7}$$

Similarly, the energy semi-norm relation is given as:

$$\left|T^h\right|_E + \left|e^h\right|_E = \left|T\right|_E = \left|T^{h/2}\right|_E + \left|e^{h/2}\right|_E . \tag{8}$$

The energy norm of the estimated solution for 1-D heat transfer equation can be obtained using following equation;

$$\begin{aligned} \left|T^h\right| = E\left|T^h, T^h\right| &\equiv \frac{1}{2}\int_\Omega k {T^h}^2 dx \\ &= \frac{1}{2}\sum_{e=1}^{M}\left(\{Q\}_e^T [DIFF]\{Q\}_e\right) \end{aligned} . \tag{9}$$

The relationship between these two energy semi-norms is derived as

$$\left|e^h\right| = 2^{2k} \cdot \left|e^{h/2}\right| . \tag{10}$$

Thus, the *asymptotic error estimate* is defined as

$$e^{h/2} = \frac{\Delta T^{h/2}}{2^{2k} - 1} \tag{11}$$

where $\Delta\left|T^{h/2}\right| = \left|T^{h/2}\right| - \left|T^h\right| = \left(2^{2k} - 1\right) \cdot \left|e^{h/2}\right|$.

The calculated error estimate for the example 1D heat transfer problem is tabulated in Table 1, which explains the relationship between mesh refinement and the improvement of approximate solution.

Table 1 The calculated error estimate

Number of mesh	$\|\|T^h\|\|$	$\Delta\|\|T^{h/2}\|\|$	$\|\|e^{h/2}\|\|$
2	4.2250e+003		
4	4.3813e+003	156.2500	52.0833
8	4.4203e+003	39.0625	13.0208
16	4.4301e+003	9.7656	3.2552
32	4.4325e+003	2.4414	0.8138
64	4.4331e+003	0.6104	0.2035

FEM software

The FEM program that was selected was FEMLAB (Comsol, Inc), which is an interactive MATLAB-based environment for modeling and solving scientific and engineering problems based on partial differential equations (PDEs). FEMLAB integrates computation, visualization, and programming in an easy-to-use environment. FEMLAB frequently uses MATLAB's syntax and data structures. One benefit of this integration is that you can save and export FEMLAB models as MATLAB programs that run directly in that environment, which allows the freedom to combine FEM-based modeling, simulation, analysis with other engineering algorithms.

Application of FEM to Biological Engineering Problems – Student Project

An ion exchange model with linear driving force was developed to describe color removal from a biological mixture using ion exchange resins. Color removal in ion exchange resins can be modeled as an adsorption process of a dilute species. Little interaction between different molecules in the fluid is assumed, which allows the application of single component adsorption models. Material is introduced as a bulk fluid at the top of a fixed-bed of spherical ion exchange resin beads. Local equilibrium is assumed around the adsorbent bead, i.e. the adsorption reaction is fast, allowing the amount of material adsorbed onto the bead surface to be determined by an equilibrium isotherm relationship. The temperature of the columns is controlled so isothermal conditions are assumed. A concentration boundary layer (film) forms around the bead and will be accounted for by the classical linear driving force (LDF) approximation (Rice 1982). The flux of material to the bead is determined by a mass transfer coefficient multiplied by the difference in concentration between the bulk and film. The beads have a bidisperse pore distribution, being an agglomeration of many micro-beads. It is assumed that the bead structure may be reduced into a lumped parameter, effective mass transfer coefficient (Rice 1982). The LDF mass transfer coefficient now becomes an effective parameter that is assumed to take into account the pore diffusion effects.

Assuming that the bed porosity is constant and that there is no concentration gradient in the radial direction, a one-dimensional, time dependent axial dispersion model may be used for the fixed bed:

$$v_0 \frac{\partial C}{\partial z} - D_{ax} \frac{\partial^2 C}{\partial z^2} + \varepsilon \frac{\partial C}{\partial t} + (1-\varepsilon)\frac{\partial q}{\partial t} = 0 \qquad (13)$$

where v_0 is velocity, C is the bulk fluid concentration, z is the axial direction, D_{ax} the dispersion coefficient in the axial direction, ε is the porosity, and q is the concentration of the adsorbed species. This partial differential equation (PDE) is coupled to the LDF approximation of the film.

$$(1-\varepsilon)\frac{\partial q}{\partial t} = k_c a\left(C - C^*\right) \qquad (14)$$

where k_c is the effective mass transfer coefficient, a the interfacial area, C^* is the concentration in the film. The parameters k_c and a will be lumped together as $k_c a$, for this discussion. The concentration of the adsorbed species, q, is related to the concentration in the film, C^*, by an isotherm, described in general as $q = f\left(C^*\right)$. This may be inverted to yield q and substituted into (Equation 14):

$$(1-\varepsilon)\frac{\partial q}{\partial t} = k_c a\left(C - f^{-1}(q)\right). \qquad (15)$$

Two hyperbolic PDE's describing the adsorption under the LDF approximation have been developed. These two equations were converted to dimensionless form to reduce the number of parameters involved:

$$\frac{\partial \phi}{\partial \eta} - \frac{1}{Pe}\frac{\partial^2 \phi}{\partial \eta^2} + \frac{\partial \phi}{\partial \theta} + \frac{(1-\varepsilon)x}{C_0 \varepsilon}\frac{\partial \psi}{\partial \theta} = 0 \qquad (16)$$

$$\frac{\partial \psi}{\partial \theta} = St\left(\phi - \xi^{-1}(\psi)\right) \qquad (17)$$

where $\phi = \frac{C}{C_0}$, C_0 = concentration at time 0; $\eta = \frac{z}{L}$, $Pe = \frac{v_0 L}{D_{ax}} = \frac{\text{bulk convection}}{\text{axial dispersion}}$, $\theta = \frac{t}{\tau}$, $\tau = \frac{\varepsilon L}{v_0}$, L = total bed length, $\psi = \frac{q}{x}$, $x = \frac{\varepsilon}{1-\varepsilon}C_0$ (i.e. $\psi = \frac{1-\varepsilon}{\varepsilon}\frac{q}{C_0}$), and $St = \frac{k_c a L}{v_0} = \frac{\text{film mass transfer}}{\text{bulk convection}}$.

The model posed was solved using FEMLAB, a plug-in to the mathematics application of MATLAB. The problem defined here is a 1-dimensional, time-dependent system with two dependent variables (ϕ,ψ) and one independent variable (η). The sensitivity of the breakthrough curve to a parameter can be analyzed by conducting repeated simulations. For example, the breakthrough curve is very sensitive to changes to Peclet (Pe) number and insensitive to the Stanton (St) number (Figures 3 and 4).

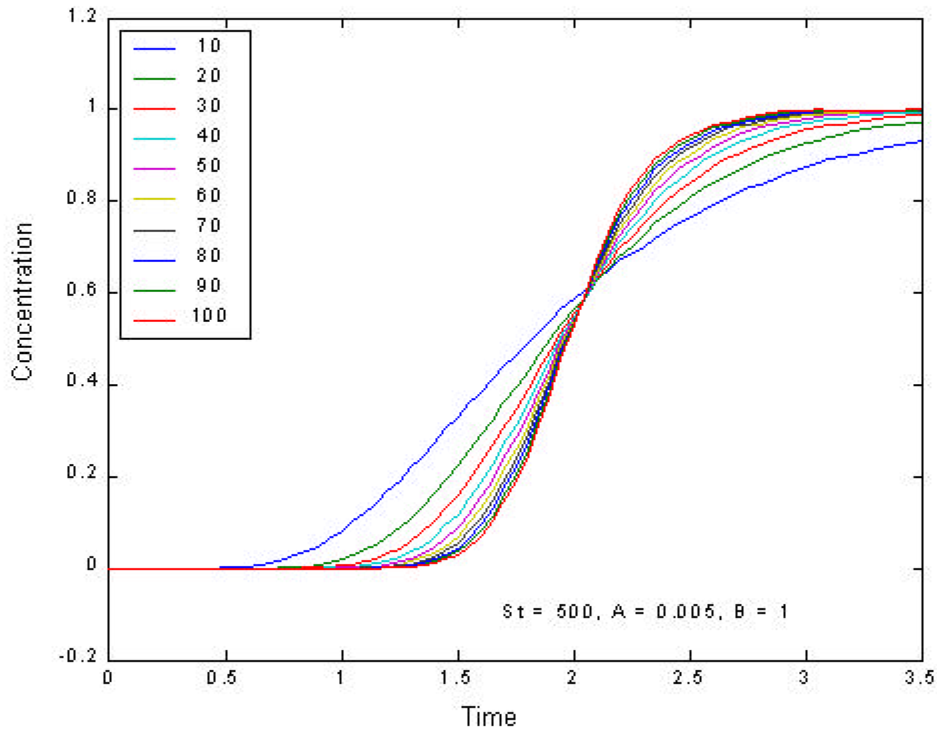


Figure 3. Sensitivity of adsorption breakthrough curves to the Peclet number

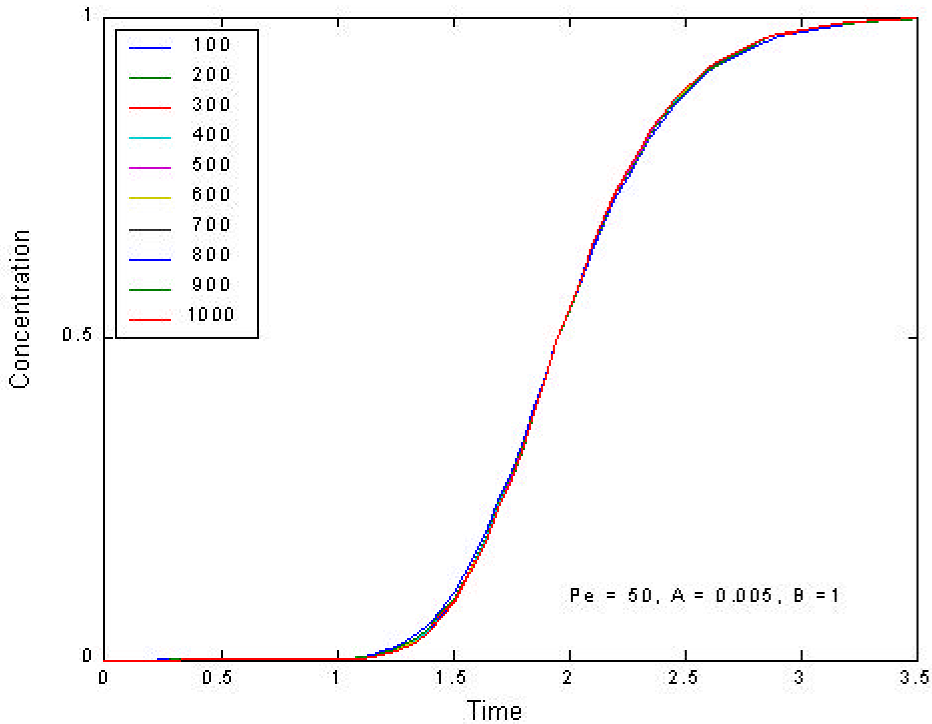


Figure 4. Sensitivity of adsorption breakthrough curves to the Stanton number

Student feedback

The evaluation from the students at the end of fall semester of 2001 was conducted concerning instruction in the application of computational finite element methods using FEMLAB. The evaluation questions given to the student are summarized at Table 2. The evaluation results are shown in Figure 5. The majority of the students responded that applying computational methods to biological engineering problems was beneficial and expect to use computational FEM in the future for their other project, labs, employment, and etc.

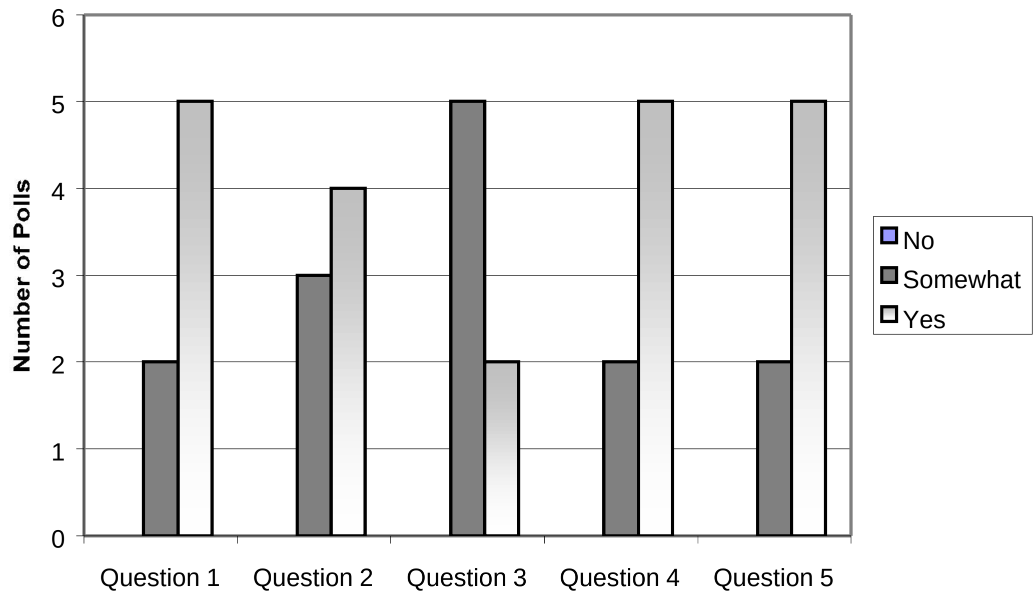


Table 2 Evaluation questions, which were asked to answer based on the scale: 1-no, 2-somewhat, and 3-yes

Practical Training Evaluation USDA Higher Education Challenge Grant
1. Did you like applying computational finite element methods (FEM) using FEMLAB (and MATLAB)?
2. Did the application of computational FEM benefit you in the learning of transport phenomena?
3. Do you understand the basic concept of numerical methods or the finite element method?
4. Did the instructor (instructors) explain the use of FEM and FEMLAB adequately?
5. Do you expect to use computational FEM in the future (other projects, labs, employment, etc)?

Figure 5. Student evaluations.

Summary

The introduction of fundamental theory of FEM and the use of FEM software, FEMLAB, has been a positive step in the introduction of numerical techniques to the Biological Engineering graduate curriculum.

Thus far, only linear basis functions in finite element analysis have been utilized. The concept of basis function will be expanded to include higher polynomial-degree, quadratic, and cubic finite element basis functions. The accuracy issue of these basis functions will be compared using error estimate with energy semi-norm.

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