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A 2D Finite Element Simulation of Liquid Coupled Ultrasonic NDT System

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Abstract. The aim of this work is to improve modelling capabilities and reliability of wave propagation models using a commercial finite element package (COMSOL). The current model focuses on investigating the error and accuracy with the change in spatial and temporal discretization. To increase the reliability and inclusiveness of the finite element method, wave propagation has been modelled in solid medium with a cylindrical defect (side drilled hole), in a fluid medium and in a fluid-solid immersion model. The numerical predictions are validated through comparisons with available analytical solutions and experimental data. The model is being developed to incorporate additional complexity and ranges of properties, including operation at elevated temperature.

INTRODUCTION

A pulse-echo ultrasonic non-destructive testing (NDT) system using longitudinal waves in high temperature liquid medium (water, liquid metal or a molten salt) has been proposed in the past for inspection of advanced small modular reactors [1, 2]. Performing experiments in a molten salt or liquid metal at temperature (~250°C) is both experimentally challenging and expensive. In the past, many authors have studied piezo-electric materials and their performance parameters at high temperature [2, 3, and 4]. To provide greater insight into transducer performance and to reduce the cost of experimental verification, a modeling approach can be adopted. This paper focuses on validation and verification of base models for the wave propagation in solids and fluids. The purpose of such basic validation is to help build complex computational models with temperature dependency, including performance phenomenon which are closer to the NDT inspection needed for small modular reactors.

The current work discusses the finite element modelling of piezoelectric transducers for application in liquid coupled NDT system. The model will initially be validated with experiments at room temperature using coolant surrogates which is in this case is simply, water. For simulating the wave propagation phenomenon, it is necessary to resolve the shortest wavelength and hence the highest frequency in the spectrum. This requires greater emphasis on the maximum element size to be used in the meshing and time step for convergence of the solution. The present work contributes towards determining the optimal element size and time step through an iterative approach with consideration towards the accuracy and solution time for the computational model. The required data generated by these iterations can be used to make the design cycle more efficient by applying different combinations of element size and time step. The model uses a two dimensional finite element method and employs commercially available code (COMSOL) which solves the equations of dynamic equilibrium in the time domain. Three simple cases are investigated: wave propagation in an aluminum block with a side drilled hole (SDH), wave propagation in water and in water with an immersed aluminum plate. In the past, many authors have studied modelling of absorbing boundary to reduce the computational grid size. A task to investigate the potential for use of absorbing boundaries in COMSOL is discussed. Finally, the model results from three distinct cases are validated with the experimental data.
THEORETICAL BACKGROUND

The accuracy of the finite element model depends upon the constitutive equations of the models, material properties and discretization of the model.

Constitutive Equations of Piezoelectric Finite Elements

Several authors have implanted a finite element method to model the piezoelectric transducer and measure the performance parameters [5, 6]. In the piezoelectric device, the governing matrix equation relating to mechanical and electrical quantitates are given by:

\[ T = \varepsilon^E S + eE \]
\[ D = eS + \varepsilon^E E \]

where \( T \) is mechanical stress, \( \varepsilon^E \) is the elastic stiffness matrix under constant electric field, \( S \) is the mechanical strain, \( e \) is piezoelectric stress constant, \( E \) is the electric field, \( D \) is the electric displacement and \( \varepsilon^E \) is the electrical permittivity under constant strain \( S \). This form of equation is called the stress-charge equation which has been implemented in this model. The piezoelectric device can also be modelled using the strain-charge equations given by:

\[ S = S^E T + dE \]
\[ D = dT + \varepsilon^T E \]

Where \( S^E \) the mechanical strain under constant electric field \( E \), \( d \) is the piezoelectric charge constant, and \( \varepsilon^T \) is the electrical permittivity under constant mechanical stress. During analysis, the mechanical displacement and electric potential are found at each nodal point in the piezoelectric device. Moreover, a polynomial interpolation basis needs to be used to describe the continuity for displacement and electric field [6]. Hence, by applying the variation principle to equation (1), (2), a discrete finite element equation system can be obtained as follows [7]:

\[ \begin{bmatrix} M^{ee} & C^{ee} \\ C^{ee} & K^{ee} \end{bmatrix} \begin{bmatrix} \frac{\partial^2 u^e}{\partial t^2} \\ \frac{\partial u^e}{\partial t} \end{bmatrix} + \begin{bmatrix} 0 \\ K^{ee} \end{bmatrix} \begin{bmatrix} d^e \\ \phi^e \end{bmatrix} = \begin{bmatrix} F^e \\ Q^e \end{bmatrix} \]

where \( u^e \) is the mechanical displacement vector, \( \phi^e \) is the electric potential vector, \( F^e \) is the mechanical force vector and \( Q^e \) is the electric charge vector for each element defined in the piezoelectric device, \( M^{ee} \) is the mass matrix, \( C^{ee} \) is the mechanical damping matrix, \( K^{ee} \) is the mechanical stiffness matrix, \( K^{ee} \) is the di-electric matrix, \( K^{ee} \) is the piezo-electric coupling matrix. These terms are completely defined by Lerch [6]. The solution for the piezoelectric elements can be obtained by solving a set of linear algebraic equations with a symmetric band structure. The values of \( u, \phi, F, \) and \( Q \) are the globally assembled field quantities.

Mechanical damping plays an important role in the dynamic response, attenuation of vibration and hence radiated acoustic waveform [7]. Rayleigh damping can be applied to the time domain and it assumes that the damping matrix \( C^{ee} \) is the linear combination of mass matrix and mechanical stiffness matrix as defined in equations 5 and 6. This can be represented as:

\[ C^{ee} = \alpha M^{ee} + \beta K^{ee} \]

where \( \alpha \) and \( \beta \) are the Rayleigh constants for the mass and stiffness matrices respectively.

In the current model, viscous damping is considered in which \( \alpha = 0 \) and \( \beta > 0 \). Moreover, the backing material, matching layer and insulating case and steel outer body casing have been assigned nodes with linear elastic material properties and Rayleigh damping coefficients. For these linear elastic materials, the piezoelectric coupling matrix \( K^{ee} \) becomes a null matrix [5] and hence there is no coupling between the mechanical force vector and electric charge vector as defined in equations (5) and (6). As a result, computational model distinguishes the piezo-element from the other set of materials and the piezoelectric effect is only modeled as a real time phenomenon.
Pressure Acoustics Modelling

The pressure acoustics module consists of the wave propagating medium and a reflector. The attenuation in the acoustic medium can be modelled by using complex valued speed of sound and density [8]. Pressure acoustics problems modelled using COMSOL involve solving for the small acoustic pressure variations $p$ on top of the stationary background pressure $P_0$. Mathematically, this represents a linearization (small parameter expansion) of the dependent variables around the stationary quiescent values [8]. The governing equations for these problems are the momentum conservation equation (Euler’s equation) and the mass conservation equation (continuity equation). In pressure acoustics all processes are assumed to be reversible adiabatic (isentropic). Thus the wave propagating media for the current model is a lossless fluid medium. The governing equation for the pressure acoustics transient analysis problem is given by:

$$\frac{1}{\rho c^2} \frac{\partial^2 p}{\partial t^2} + \nabla \left( -\frac{1}{\rho} \left( \nabla P_t - q_d \right) \right) = Q_m$$

(8)

$$\nabla P_t = P + P_b$$

(9)

$$\frac{\rho}{\partial t} \frac{\partial^2 u}{\partial t^2} - \nabla T = F_v$$

(10)

where $\rho$ is the density of the wave propagating medium, $c$ is the speed of sound in the medium, $P_b$ is the gauge pressure, $q_d$ is dipole source, $Q_m$ is the monopole acoustic source [8] and $f_v$ is the body force per unit volume. The term $\rho c^2$ represents bulk modulus of the fluid.

MATERIALS AND GEOMETRY

Lead Zirconate Titanate (PZT)-5A is used as the active element in the piezoelectric transducer. The material properties for PZT-5A can be found in the COMSOL user guide and the material library [8]. The backing material for the piezoelectric transducer is assumed to be epoxy loaded tungsten powder. The matching layer consists of epoxy. Performance of the matching layer and backing material is affected by the operating temperature of the ultrasonic measurement system. The insulating case is made of nylon while the transducer outer body casing is made of stainless steel. Properties for these materials are given in several references including Medina et al. [7].

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (Kg/m³)</th>
<th>Poison Ratio</th>
<th>Elasticity module(N/m²)</th>
<th>β damping</th>
</tr>
</thead>
<tbody>
<tr>
<td>Araldite</td>
<td>1096</td>
<td>0.34</td>
<td>0.55e10</td>
<td>2.3e-8</td>
</tr>
<tr>
<td>Araldite/Tungsten</td>
<td>5766</td>
<td>0.34</td>
<td>1.05e10</td>
<td>1.5e-8</td>
</tr>
<tr>
<td>Nylon</td>
<td>1405</td>
<td>0.27</td>
<td>0.74e10</td>
<td>5e-9</td>
</tr>
<tr>
<td>Steel</td>
<td>7890</td>
<td>0.29</td>
<td>26.51e10</td>
<td>10e-8</td>
</tr>
</tbody>
</table>

TABLE 1. Material properties for transducer modeling.

FIGURE 1. (a) Case 1 - Aluminum block; (b) Case 2 - only water; (c) Case 3 - water-aluminum
The model consists of the piezoelectric and pressure acoustics modules as shown below:

The piezo element PZT-5A is one half wavelength ($\sim \lambda/2$) thick. The matching layer is a quarter wavelength ($\sim \lambda/4$). To provide a realistic dynamic response for the transducer, it is necessary to model a particularly backing layer, the insulating case, and outer body. The thickness of backing material in the current model is 10mm. The thickness of insulating case is 0.5mm while thickness of outer body steel casing is 1mm in the present model. These elements all contribute towards damping of the vibration of the active element. This damping reduces the mechanical quality factor $Q$ and thus increases the bandwidth [9]. Wide bandwidth is particularly necessary for NDT applications.

**BOUNDARY CONDITIONS**

It is necessary to couple the piezoelectric device module with the acoustics module to obtain the desired pattern of radiated waves. This is made possible by applying a boundary load in the piezoelectric device interface at a boundary common to both media. The same boundary is assigned a normal acceleration in the acoustics model. The acoustic analysis provides the acoustic load to the structural analysis while the structural analysis provides acceleration to the acoustic analysis. This couples the physics in the two modules. This is also achieved by applying continuity principle in the displacement field. A floating potential node is defined to give a pulse to the piezoelectric element and to receive echo response. This requires the excitation to have a potential defined in terms of charge. A zero charge node is defined for the boundary with null charge density. A rigid boundary node has been assigned to boundaries at which the normal acceleration is required to be zero [8].

Waves reflecting from the side walls of the model increase the degrees of freedom for the model [10]. Hence the model becomes computationally expensive and solution time increases. Absorbing boundaries reduce such reflections by allowing the outgoing wave to leave the computational domain with minimum reflections. This is necessary for the well posed solution of the partial differential equations.
FIGURE 4. Examples of time domain wave forms: (a) without absorbing boundaries and (b) with absorbing boundaries.

In a COMSOL time domain model, this can be achieved by using low reflecting boundaries, and cylindrical/spherical wave radiation nodes. Fig. 4a and Fig. 4b clearly show the differences seen in waveform at the boundary with and without an absorbing layer.

DISCRETIZATION

For the wave propagation model it is important to avoid aliasing and resolve the shortest wavelength and hence the highest frequency in the spectrum. For a structured mesh the average resolution differs significantly between the direction parallel to grid lines and directions rotated 45° to one of the axes. More importantly, the direction of wave propagation is not known in advance. Hence, an unstructured type of mesh is preferred over a structured mesh. The maximum element size in the mesh can be given by:

$$h = \frac{c}{F_0 N} = \frac{\lambda}{N}$$

Where
- $h$=maximum element size (m)
- $c$=speed of sound in wave propagating medium
- $F_0$=Highest frequency in the spectrum (Hz)
- $\lambda$= wavelength of medium, $N$= number of elements per wavelength

A second order triangular Lagrange element is used for meshing in COMSOL. The finite element mesh represents solution field of the problem. This solution field is computed at the nodal points and then interpolated using a polynomial basis function. In such a case, the second order element gives better accuracy for the solution, when compared to a first order element, due to use of a greater number of nodal points. Apart from spatial discretization, temporal discretization is also important for the stability of numerical method and hence the convergence of the solution. COMSOL time dependent simulation by default use an implicit time method to solve the partial differential equations. Generalized-$\alpha$ [11, 12] is the implicit method used in which the $\alpha$ parameter controls the numerical dissipation at higher frequencies. It provides relatively less dissipation as compared to a Backward Differentiation formula (BDF) which severely dissipates energy at higher frequencies [8]. The degree of dissipation can inversely affect the accuracy of solution at the higher frequency. The absolute and relative tolerances defined in COMSOL control the error at each integration step. Moreover, for the stability of the algorithm using the generalized-$\alpha$ method, it is necessary for the error growth rate to be constant. This can be achieved be defining the Courant-Friedrichs-Lewy (CFL) number [13] for the time step as shown below:

$$CFL = \frac{c \Delta t}{h}$$

Where $\Delta t$ the time step (sec), c and h are as defined in equation (11).

Hence the time step can be defined as

$$\Delta t = \frac{h \times CFL}{c}$$

Where
- $0 < CFL \leq 1$
For the stability of the algorithm, the distance travelled by a wave in one time step should not exceed the length of one spatial step h as defined in Equations (11) and (13). For applications where all shape functions are quadratic, the CFL is taken as approximately 0.2 [6]. But to calculate an optimum CFL for specific cases that are being simulated, iterations have been performed by varying element size and time step. Using the data book value of speed of sound in the medium [14], the percentage difference (%D) has been calculated for the data book speed and computed speed of wave in the medium. The solution time (T) is recorded against N and CFL to estimate computation expense. These iterations can also help in developing a combination of different time step and element size which can give preliminary results within acceptable tolerance and more importantly in shorter solution times.

For the case-1, waves in an Aluminum block with a 3mm side drilled hole, the following is data obtained from a series of model:

**FIGURE 5.** Investigation of computational efficiency. (a) Difference vs. number of element per wavelength (N) and (b) solution time (T) vs. N.

From Fig. 5a, it can be seen that with an increased number of elements per wavelength and reduction in CFL, the percentage difference between theoretical wave speed and computed wave speed reduces. Less than 5% difference is considered to be the acceptable result for the all the cases that are simulated. Hence CFL<0.4 is observed to give acceptable values for result. From Fig. 5b for CFL<0.4, the solution time seems to follow an exponential form with increase in the number of elements. Hence, a tradeoff is needed between number of elements and time step which is the basic purpose of performing these iterations. To determine this trade off, we also plot the percentage difference (%D) between the data book wave speed and computed wave speed, with change in CFL. This is represented as:

**FIGURE 6.** Investigation of computational efficiency- (a) Percentage difference vs CFL and (b) Solution time vs CFL

From Fig. 6a, it is seen that at CFL=0.2, the percentage difference (%D) seems to converge irrespective of the number of elements. Hence, by considering the data from Fig. 5a through (6b), N=8 and CFL=0.2 is used for running the simulation for validation with the experimental data in all three cases discussed in the current work. The data in Table 2 can be used to plot Figs. 5a through 6b:
TABLE 2. Percentage difference and solution for varying element size and time step.

<table>
<thead>
<tr>
<th>CFL</th>
<th>C theory*</th>
<th>C computed (m/s)</th>
<th>%Difference</th>
<th>Computation time(sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/s</td>
<td>N= 6</td>
<td>8</td>
<td>10</td>
<td>N= 6</td>
</tr>
<tr>
<td>1</td>
<td>6420</td>
<td>5673.8</td>
<td>5755.4</td>
<td>5818.2</td>
</tr>
<tr>
<td>0.8</td>
<td>6420</td>
<td>5776.2</td>
<td>5839.4</td>
<td>5860.8</td>
</tr>
<tr>
<td>0.6</td>
<td>6420</td>
<td>5818.2</td>
<td>5860.8</td>
<td>6106.7</td>
</tr>
<tr>
<td>0.4</td>
<td>6420</td>
<td>6106.7</td>
<td>6106.7</td>
<td>6130.3</td>
</tr>
<tr>
<td>0.2</td>
<td>6420</td>
<td>6153.8</td>
<td>6177.6</td>
<td>6177.6</td>
</tr>
<tr>
<td>0.1</td>
<td>6420</td>
<td>6225.6</td>
<td>6225.6</td>
<td>6374.5</td>
</tr>
</tbody>
</table>

VALIDATION PROCEDURE

To validate the computed data, experimental data is required for all three cases. Hence, simple pulse-echo measurements were made using a 2.2 MHz transducer with nominal diameter of 13mm for the active element (Olympus V306). The data is normalized for the ease of comparison with the computed data. For case-1 with an aluminum block, Sonotech gel is used as couplant. Case 2 consists of the pulse-echo response in water, while case 3 is the response in water and with a 6.5 mm thick aluminum plate, set as a reflector. The set up for experiments can be seen in Fig. 7:

FIGURE 7. Experimental configurations for validation. (a) Case 1 – Aluminum block; (b) Case 2 – water; Case 3 – Aluminum plate immersed in water

RESULTS

The normalized pulse echo experimental and computed data for all three cases can be compared.

Case 1: Wave propagation in a 50mm thick aluminum block with 3mm diameter side drilled hole

FIGURE 8. (a) Experimental data and (b) Computed data

The pulse-echo response is measured at peak amplitude of the wave for the experimental and computed data. As shown in Fig.8a, the first echo is received from waves reflected from the cylindrical defect (side drilled hole - SDH).
The second echo is due to the waves reflected back from bottom surface of the aluminum. The third echo is also from the SDH. The amplitude of the waves reflected from the SDH reduce significantly between the first and last pulse. This can be seen in Fig. 8a) and 8b). Figure 9a shows plane wave and edge wave which are due to the edges of the transducer. Fig. 9b through 10b shows the wave fields due to the cylindrical reflector.

Case 2: Wave propagation in water

Figure 11 a) through 12b) shows, pulse-echo response for measurements in water. The wave arrival time measured at the peak amplitude for the experiment and the simulation shows a difference of less than 2%. For the case 3, a 6.5mm thick aluminum plate is immersed in water. The wave arrival time and peak amplitude time are considered to calculate the difference between the experimental and computed data.
Case 3: Wave propagation in water and aluminum plate

Since there is the possibility of variation in peak amplitude time, the wave arrival time is also observed. The wave arrival times differ by less than 1% for case 3 between the experimental and simulation data. For cases 2 and 3, in the models, unlike the experimental data, a pulse is reflected off the one of the boundaries after the incidence pulse, and this is shown in the computed data waveform in Fig.11b and 13b. This anomaly is currently being investigated.

DISCUSSIONS

The percentage difference for the pulse-echo response between experimental and computed data is tabulated for all three cases:

**TABLE 3.** Difference in pulse echo response between experimental and computed data.

<table>
<thead>
<tr>
<th>Case</th>
<th>% maximum Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1-Aluminum block</td>
<td>2.4</td>
</tr>
<tr>
<td>Case 2-water</td>
<td>1.6</td>
</tr>
<tr>
<td>Case 3-Aluminum and water</td>
<td>3.2</td>
</tr>
</tbody>
</table>

As seen from the Table 3, the computational model is validated by the experimental data to within 5% of difference in the wave arrival and wave peak amplitude times. Element size and time step are varied for specific model to determine optimum element size in the mesh and time step. These iterations can also help in developing a combination of different time step and element size which can give preliminary results within acceptable tolerance and more...
importantly in less solution time. It can make the design cycle more efficient. The present work uses mesh size of 8 elements per wavelength and time step at CFL = 0.2. Absorbing boundaries can further be explored for effective damping of outgoing waves at the side walls of computational geometry. By adding external electric circuit to the transducer model, voltage source can be accurately modelled.

CONCLUSIONS

Thus, the new computational model can now be developed in near future for added complexity such as modelling temperature dependency on performance parameters of active element of transducer. This will help to address the issues of degradation of transducer performance parameters which is has been critical for inspection capabilities in nuclear reactors.

ACKNOWLEDGEMENT

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