Developments in boundary element applications to polymer analysis

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Abstract

The application of the boundary element method (BEM) to the stress analysis of polymers is reviewed. Since polymers are most often modelled as viscoelastic materials, formulations specifically developed for other such materials are also discussed. Essentially, only linear viscoelasticity, for which the correspondence principle applies, features in existing BEM formulations. One of the adopted BEM approaches solves the problem in either the Laplace or the Fourier transformed domain and relies on numerical inversion for the determination of the time-dependent response. The second solves directly in the time domain using appropriate fundamental solutions each depending on the viscoelastic model used. The developed algorithms have been validated through their application to a range of standard cases. Scope for enhancing the potential of the method to solve viscoelastic problems is identified. This can be achieved by increasing the generality of material modelling and expanding its application to complex, industry-oriented problems.

1 Introduction

Polymers have been modelled as viscoelastic materials for which a multiplicity of constitutive theories exists. Due to the complexity of such models, which include time as an independent variable, the available exact analytical solutions have been obtained for only a few simplified problems. Rigorous predictions of polymer behaviour usually rely on numerical approaches such as the finite difference method, the finite element method (FEM) and the boundary element method (BEM). BEM has the advantage of requiring only boundary data as input and, ideally, no division of the domain under consideration into elements. Its potential as an analytical tool in viscoelasticity has been demonstrated in the context of certain linear models for both quasi-static and dynamic problems.

The most commonly used constitutive equations have the form of convolution integrals leading to integro-differential field equations. The usual approach, originally adopted by Rizzo and Shippy [1], has been to formulate a BEM solution for the Laplace transforms of all variables, which satisfy an associated elastic problem, then obtain the solution in the time domain by numerical inversion. Incremental solutions in the time domain were first formulated by Shinokawa et al. [2]. Both techniques have been developed further through the creative work of many investigators.

The purpose of this paper is to give a comprehensive account of the BEM applications to polymers and then point to the direction for possible future developments. Viscoelastic models used in existing BEM formulations are described and the general principles of viscoelasticity presented. The transform and time domain solutions for both quasi-static and dynamic problems are explained. Finally, a brief account of applications is given focusing on those involving polymer materials.

2 Viscoelastic models

The linear viscoelastic model adopted in most BEM formulations is, in accordance with Boltzmann's principle, of hereditary integral type

$$\sigma_{ij} = c_{ijkl}(t)\varepsilon_{kl}(0) + \int_0^t c_{ijkl}(t-\tau)\frac{\partial \varepsilon_{kl}(\tau)}{\partial \tau}\,\mathrm{d}\tau \tag{1}$$

where σ_{ij}, ε_{ij} are the stress and small strain tensors, respectively, and $c_{ijkl}(t)$ the relaxation moduli in the general case of an anisotropic medium. Adopting the notation for the convolution of two functions, eqn (1) can be more concisely written

$$\sigma_{ij} = c_{ijkl} * \mathrm{d}\varepsilon_{kl} \tag{2}$$

In the case of an isotropic medium characterised by the moduli $\lambda(t)$ and $\mu(t)$, corresponding to the Lamé constants λ and μ in elasticity, relations (2) become

$$\sigma_{ij} = \lambda(t) * \mathrm{d}\varepsilon_{kk}(t)\delta_{ij} + 2\mu(t) * \mathrm{d}\varepsilon_{ij}(t) \tag{3}$$

An alternative form of the isotropic elasticity equations is

$$s_{ij} = 2\mu e_{ij}, \quad \sigma_{kk} = 3K\varepsilon_{kk} \tag{4}$$

where s_{ij} and e_{ij} are, respectively, the deviatoric stress and strain tensors and K the bulk modulus of elasticity. The viscoelastic equivalents to eqns (4):

$$s_{ij} = 2\mu(t) * \mathrm{d}e_{ij}(t), \qquad \sigma_{kk} = 3K(t) * \mathrm{d}\varepsilon_{kk}(t) \tag{5}$$

have been frequently used instead of eqn (3), particularly in soil mechanics applications where, as has been suggested [3], the viscoelastic behaviour of cohesive soils and soft rocks is markedly different under a purely deviatoric stress state from that due to hydrostatic pressure. In eqns (5), the time-dependent moduli $\mu(t)$ and $K(t)$ correspond to the elastic shear and bulk moduli. An alternative form to the constitutive equations (5) is [4]

$$e_{ij} = J_1(t) * \mathrm{d}s_{ij}(t), \qquad \varepsilon_{kk} = J_2(t) * \mathrm{d}\sigma_{kk}(t) \tag{6}$$

where J_1 and J_2 are, respectively, the shear and dilatation creep moduli.

A commonly used rheological model is the generalised standard linear solid (SLS) [3]. It consists of a Hookean spring and N Kelvin models, all connected in series. The resulting viscoelastic equations are of differential operator type,

$$\sum_{n=0}^{N} p_n \mathrm{D}^n s_{ij} = 2\sum_{n=0}^{N} \mu_n \mathrm{D}^n e_{ij}\,, \quad \sum_{n=0}^{N} q_n \mathrm{D}^n \sigma_{kk} = 3\sum_{n=0}^{N} K_n \mathrm{D}^n \varepsilon_{kk} \qquad (7)$$

where D^n is an operator representing the nth time derivative and p_n, q_n, λ_n, μ_n, are material constants, which can be related to the moduli and viscosities of the spring and individual Kelvin elements making up the SLS model [3]. The solution of the differential equations (7) under creep conditions leads to a series representation of the creep modulus [4].

The use of fractional-order time derivatives has been suggested as providing greater flexibility in fitting measured data [5,6]. Defining the fractional operator D^{γ} $(0 \le \gamma < 1)$ by the Riemann-Liouville integral

$$\mathrm{D}^{\gamma} f(t) = \frac{1}{\Gamma(1-\gamma)} \frac{d}{dt} \int_0^t \frac{f(t-\tau)}{\tau^{\gamma}} \mathrm{d}\tau$$

constitutive equations corresponding to eqns (5):

$$\sum_{n=0}^{N} p_n \mathrm{D}^{\alpha_n} s_{ij} = 2\sum_{n=0}^{M} \mu_n \mathrm{D}^{\beta_n} e_{ij}\,, \quad \sum_{n=0}^{N} q_n \mathrm{D}^{\alpha_n} \sigma_{kk} = 3\sum_{n=0}^{M} K_n \mathrm{D}^{\beta_n} \varepsilon_{kk} \qquad (8)$$

can be used where α_n, β_n are additional material constants.

3 Field equations

Introducing the small strain-displacement relations into the constitutive eqns (1) and substituting the latter into the stress equations of motion yields a system of integro-differential equations

$$c_{ijkl}(t) u_{k,lj}(0) + \int_0^t c_{ijkl}(t-\tau) \frac{\partial u_{k,lj}(\tau)}{\partial \tau} \mathrm{d}\tau + \rho b_i = \rho \ddot{u}_i \qquad (9)$$

where b_i is the body force and ρ the density of the material.

The problem is complemented by the initial conditions

$$u_i(0) = u_{i0}, \qquad \dot{u}_i(0) = \dot{u}_{i0} \qquad (10)$$

and the boundary conditions

$$u_i(t) = \bar{u}_i(t) \text{ on } \Gamma_1 \qquad \sigma_{ij}(t) n_j = \bar{p}_i(t) \text{ on } \Gamma_2 \qquad (11)$$

where $\mathbf{n}$ is the outward unit normal vector to the boundary $\Gamma = \Gamma_1 + \Gamma_2$. For exterior problems, that is, problems with boundaries extending to infinity, the radiation condition must also be satisfied. This physically means that waves cannot be reflected back from infinity.

Given two viscoelastic states (u_i, p_i, b_i) and (u_i^*, p_i^*, b_i^*), satisfying the boundary value problem described above, the reciprocity relation [7]

$$\int_{\Gamma} p_i * du_i^* d\Gamma + \int_{\Omega} \rho b_i * du_i^* d\Omega = \int_{\Gamma} u_i * dp_i^* d\Gamma + \int_{\Omega} \rho u_i * db_i^* d\Omega \qquad (12)$$

can be derived.

4 Correspondence Principle

Taking the Laplace transform of both sides of constitutive eqns (1) gives

$$\bar{\sigma}_{ij} = s\bar{c}_{ijkl}\bar{\varepsilon}_{kl} = c^{v}_{ijkl}\ \bar{\varepsilon}_{kl} \qquad (13)$$

By transforming also the equations of motion (9), the strain-displacement relations, as well as the initial conditions (10) and the boundary conditions (11), a complete correspondence is established between the elastic and viscoelastic problem. Thus a linear viscoelastic problem can be solved in the transformed domain for any range of values of the transform variable s by the same methods as those applicable to the corresponding elasticity problem in which the field variables are replaced by their Laplace transforms and the elastic constants c_{ijkl} are replaced by the functions $c^{v}_{ijkl}(s)$. In the end, it is, of course, necessary to obtain the solution in real time through inversion of the transform so obtained. This, so called, correspondence principle has been applied directly to generate BEM solutions of the transformed physical problem but also to obtain the fundamental solutions for particular viscoelastic models, which are then used in time domain BEM formulations.

In harmonic and transient dynamic analyses, the use of Fourier transforms has been found more appropriate. Applying this transformation to eqns (5) leads to relations of the form

$$\hat{s}_{ij} = 2\mu_v(\mathrm{i}\omega)\,\hat{e}_{ij}\,, \quad \hat{\sigma}_{kk} = 3K_v(\mathrm{i}\omega)\,\hat{\varepsilon}_{kk} \qquad (14)$$

where the complex, frequency-dependent complex moduli μ_v and K_v relate the Fourier transforms of stresses and displacements in exact correspondence with the elasticity relations (4). The viscoelastic moduli are given in terms of the Fourier transforms of the corresponding time-dependent properties. In the particular case of the differential operator model (8), they are obtained as ratios of complex polynomials involving fractional powers of $\mathrm{i}\omega$.

For a harmonic isotropic analysis, the governing equations are written in terms of the transformed displacements as [6]

$$c_{v1}^2 \hat{u}_{j,ji} - \varepsilon_{ijk}\varepsilon_{klm} c_{v2}^2 \hat{u}_{i,jj} + \rho\hat{b}_i + \omega^2 \rho\hat{u}_i = 0 \qquad (15)$$

where c_{v1}, c_{v2}, are the complex velocities of dilatational and equivoluminal waves given by

$$c_{v1}^2 = \frac{\lambda_v + 2\mu_v}{\rho}\,, \qquad c_{v2}^2 = \frac{\mu_v}{\rho} \qquad (16)$$

The Fourier transformation is also applied to the boundary conditions (11) so that a complete correspondence is established between a harmonic elastic and viscoelastic problem.

5 BEM formulations

5.1 Laplace transform domain

If the correspondence principle is applied to the quasi-static problem, the relevant boundary integral equation in the Laplace transformed domain is written

$$\kappa_{ij}\bar{u}_i = \int_{\Gamma}[\bar{p}_i(s)u^*_{ij}(s) - \bar{u}_i(s)p^*_{ij}(s)]\mathrm{d}\Gamma + \rho\int_{\Omega}\bar{b}_i u^*_{ij}\mathrm{d}\Omega \qquad (17)$$

where $\kappa_{ij} = 0.5\delta_{ij}$ in the case of a smooth boundary, and $(u^*_{ij},\ p^*_{ij})$ is the elastic fundamental solution for displacements and tractions in which however the elastic constants have been replaced by the corresponding functions in the transformed space according to eqns (13). If a particular solution to the transformed problem is known, the domain integral in eqn (17) can be replaced by boundary integrals depending on that solution [8].

Laplace transforms of boundary or domain variables can be numerically converted back into time-dependent functions. Schapery's inversion method [9] was the earliest one to be used [1,4] and its collocation procedure improved [10]. Piessens's method [11] was applied to a 3-D BEM solution of the quasi-static problem [8]. Durbin's inversion method [12] was used in a BEM formulation of the 3D dynamic problem [5].

5.2 Fourier transform domain

In the case of harmonic vibrations, the boundary integral equation has the same form as that of the corresponding elastic problem in the frequency domain [13,14]

$$\kappa_{ij}\hat{u}_j(\omega) = \int_{\Gamma}[\hat{p}_i(\omega)u^*_{ij}(\omega) - \hat{u}_i(\omega)p^*_{ij}(\omega)]\mathrm{d}\Gamma + \rho\int_{\Omega}u^*_{ij}(\omega)\hat{b}_j\mathrm{d}\Omega \qquad (18)$$

with the fundamental solution of the elastic harmonic problem in which the elastic wave speeds have been substituted by the viscoelastic ones as given by eqns (16). Eqn (18) provides the BEM solution to a harmonic excitation at a particular ω. The time-dependent response to a transient excitation can be found by solving eqn (18) for a sufficient number of ω.

5.3 Time domain - quasi-static problems

The boundary integral equation can be obtained by either taking the inverse Laplace transform of that equation for the corresponding elastic problem [2] or directly from the reciprocal theorem of linear viscoelasticity (12) [7,15]. Both approaches lead to

$$\kappa_{ij}u_i(t) = \int_{\Gamma}(u^*_{ij} * dp_i - p^*_{ij} * du_i)\mathrm{d}\Gamma + \rho\int_{\Omega}b_i * du^*_{ij}\mathrm{d}\Omega \qquad (19)$$

The inverse Laplace transform of the elastic fundamental solution in the transformed space is required in the above time domain formulation. Such an operation has been carried out in several special cases. Shinikawa *et al.* [2] obtained the inverse in the case of an SLS shear relaxation model combined with elastic volumetric behaviour. An elaborate scheme, generating the time domain fundamental solution in a more general case, was developed by Lee *et al.* [16]. An alternative approach adopted by Carini and De Donato [17] yielded the fundamental solutions for a wide range of linear viscoelastic models.

Integrating by parts, the boundary integral in eqn (19) can be transformed to

$$\int_{\Gamma} (p_i * du_{ij}^* - u_i * dp_{ij}^*) d\Gamma \qquad (20)$$

which does not involve time derivatives of the unknown boundary displacements and tractions. Thus no smoothness restrictions need to be imposed on the respective shape functions while the time derivatives of the kernels can be evaluated exactly [15].

Uniform temperature variations can be accounted for by replacing real time t in eqn (19) by a reduced time ζ given by [18,19,20]

$$\zeta = \int_0^t \frac{d\tau}{a_T[T(\tau)]}$$

where a_T is a shift parameter depending on the temperature history. The thermo-viscoelastic BE equation should account for thermal expansion by including the appropriate boundary traction term.

5.4 Time domain - indirect BEM

An indirect BEM approach has been demonstrated in the context of a geomechanics problem involving a cavity subjected to known tractions [3]. A number of fictitious loads are assumed applied at source points distributed just outside the domain, opposite to an equal number of boundary elements. The total stresses due to the fictitious forces can be found in terms of the stress fundamental solution. For these stresses to constitute an approximate solution, the tractions due to fictitious loads on the entire boundary Γ should be as close as possible to the actual tractions. This can be achieved by minimising the mean square value of the error and leads to a consistent and symmetric system of equations for the determination of the fictitious loads.

5.5 Time domain - dynamic problems

In this case, a BEM formulation can be based on a boundary integral equation, identical in form with that of the corresponding elastodynamic problem [21]. If the Poisson's ratio is time-dependent, then the coefficients κ_{ij} are also functions of time and the right hand side of the integral equation becomes the convolution integral.

Using the Maxwell model, the fundamental solution in the time domain was obtained by inverse Laplace transform [18,22]. This is a closed form solution of considerable complexity. In view of the limitations of the Maxwell model, it would be preferable to retain the versatility of the general constitutive equations, including those with fractional differential operators. The inversion however of the fundamental solution would then require numerical integration.

An alternative procedure has been developed based on the corresponding BEM formulation of the elastodynamic problem [22,23]. A modelling scheme is adopted in the time domain and convolutions are explicitly integrated over time steps. The resulting expressions, as functions of the current solution time, can be transformed to Laplace domain. The transition to viscoelastic solution takes place at that stage when the elastic material properties are replaced by the corresponding viscoelastic ones expressed in terms of the transformed space variable s. Then, the inversion of these expressions results in the kernels for the viscoelastic boundary integral formulation. Explicit expressions for the inverted kernels were obtained for the special case of the Maxwell model [23].

Time domain formulations require boundary modelling in both space and time dimensions. Using constant time interpolation [15], displacements and tractions can be represented by simple expressions leading to analytical evaluation of time integrals over each time step. Higher order quadrature rules for convolution integration have also been successfully applied [19]. A particular such scheme uses the Laplace transform of one of the functions involved which can be the fundamental solution in the transformed domain [21]. Thus no knowledge of the time-dependent fundamental solution is required.

6 Applications

Most benchmark problems involved a hole subjected to a uniform pressure $p(t)=p_oH(t)$ where $H(t)$ is the Heaviside step function. Since these problems have exact analytical solutions, they have been used by several authors for validating their formulations. A hole in an infinite viscoelastic space, modelled as SLS, has been analysed in both the Laplace transformed [4, 10] and time domain [2,15].

A particular case of a hole in a finite space is the thick-walled cylinder, which has also been analysed by several authors for validation purposes. Time domain solutions were based on the SLS model [15,19] but also on a more general model [16]. The case of a cylinder constrained over its outer boundary by a thin elastic ring was also analysed in the Laplace transform domain adopting SLS in shear as the material model [1]. The time domain solution of this problem has also been treated with a similar degree of accuracy [15].

Three-dimensional analyses of rectangular blocks were performed in the Laplace transformed domain under both quasi-static [8] and transient [5,21] conditions. In the former case, a cubical and a prismatic block was subjected to gravity body force and the material was assumed to behave according to Maxwell viscoelastic model.

In the latter case, a block with square cross-section and a length to width ratio equal to 3, was fixed at one end and subjected to an axial step load at the free end. Its relaxation properties were deduced from a fractional operator constitutive model. The predicted responses were in good agreement with an analytical solution. A similar application involved a cylindrical elastomer isolator analysed in the frequency domain assuming a modified, fractional order, Kelvin model [18].

Assessment of polymer crazing was an early application of practical importance. The craze was represented by a slit in a plate of finite width subjected to a step far field tension [4]. The transformed domain BEM solution, based on a SLS creep model, provided information on quasifracture opening displacement as well as envelop stress development with time.

A composite material was analysed as two perfectly bonded regions, a viscoelastic one representing the polymer matrix and an elastic one representing the fibre or particle reinforcement [19]. The discretised algebraic problems were formulated for each zone and then coupled through the displacement compatibility and traction equilibrium conditions over the interfaces. The scheme was extended to account for uniform temperature fluctuations by introducing the effects of thermal expansion and temperature dependent viscoelastic properties. It was then validated through an example involving a composite sphere with inner elastic and outer viscoelastic layer under uniform temperature change [19].

The two-dimensional viscoelastic rolling contact with Coulomb's dry friction was considered for steady-state rolling of two cylinders [24]. This problem was solved using a special boundary element formulation, based on the SLS model, and one-dimensional Green's functions for the surface displacement. Numerical results included the stress distribution at the contact surfaces and in viscoelastic bodies as well as rolling resistance. The contact between a viscoelastic body and an elastic one covered by a thin viscoelastic boundary film has also been studied by the same method [25].

7 Conclusions

Two main approaches have been adopted for linear viscoelasticity. The first has the advantage of being directly applicable to any generally acceptable constitutive model but requires numerical inversion of the Laplace or Fourier transform. This not only increases the amount of computations but its accuracy and efficiency also depends on the choice of the range and distribution of the transform variables. The second method requires the derivation of the relevant fundamental solution for each constitutive model as well as discretization in the time domain.

The validity and effectiveness of both approaches has been demonstrated through the solution of simple examples. Most problems solved by BEM were essentially validation exercises. The majority of other existing practical BEM solutions were obtained in the field geomechanics. There is therefore considerable scope for extending the use of BEM to industrial applications of polymers.

There is also scope for generalising material modelling. Temperature variations have a strong influence on viscoelastic properties, they should be therefore routinely accounted for in any BEM formulation. Anisotropy may also be present and methods for generating fundamental solutions in both transformed and time domains have been suggested in the literature [26]. Widening the applicability of viscoelastic plate or shell analyses [27,28] would also be useful since polymers are quite often used as thin-walled elements. Finally, an important development would be to account for material non-linearity, which has been observed to be strong in the case of long term viscoelastic responses.

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