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Boundary element methods for 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 has been considered for which the correspondence principle applies. Two main BEM approaches are encountered in the literature. The first solves the problem in either Laplace or Fourier transformed domain and relies on numerical inversion for the determination for 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 benchmark problems. Scope for enhancing the potential of the method is identified by increasing the generality of material modelling and expanding its application to complex, industry-oriented problems.

Keywords: Polymers; Boundary element method; Viscoelastic materials

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 BEM analyses of 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

$$\sigma_{ij} = \int_{-\infty}^{t} G_{ijkl}(t-\tau)\frac{\partial \varepsilon_{kl}(\tau)}{\partial \tau}\mathrm{d}\tau \qquad (1)$$

where σ_{ij}, ε_{ij} are the stress and small strain tensors, respectively, and $G_{ijkl}(t)$ the relaxation moduli in the general case of an anisotropic medium. If the applied strain history begins at $t = 0$ with a non-zero initial value, relation (1) is written

$$\sigma_{ij} = G_{ijkl}(t)\varepsilon_{kl}(0) + \int_{0}^{t} G_{ijkl}(t-\tau)\frac{\partial \varepsilon_{kl}(\tau)}{\partial \tau}\mathrm{d}\tau \qquad (2)$$

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Integrating the second term of the right-hand side in Eq. (2) by parts yields the alternative form:

$$\sigma_{ij} = G_{ijkl}(0)\varepsilon_{kl}(t) + \int_0^t \frac{\partial G_{ijkl}(\tau)}{\partial \tau}\varepsilon_{kl}(t-\tau)\mathrm{d}\tau \tag{3}$$

The Stieltjes convolution of two functions ϕ and ψ is defined as [3]

$$\phi * \mathrm{d}\psi = \psi * \mathrm{d}\phi = \phi(t)\psi(0) + \int_0^t \phi(t-\tau)\frac{\partial \psi(\tau)}{\partial \tau}\mathrm{d}\tau \tag{4}$$

Using this notation, Eq. (2) or Eq. (3) can be more concisely written as

$$\sigma_{ij} = G_{ijkl} * \mathrm{d}\varepsilon_{kl} = \varepsilon_{kl} * \mathrm{d}G_{ijkl} \tag{5}$$

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, relation (5) becomes

$$\sigma_{ij} = \lambda(t) * \mathrm{d}\varepsilon_{kk}(t)\delta_{ij} + 2\mu(t) * \mathrm{d}\varepsilon_{ij}(t) \tag{6}$$

Defining the deviatoric stress and strain tensors by

$$s_{ij} = \sigma_{ij} - \tfrac{1}{3}\sigma_{kk}\delta_{ij}, \qquad e_{ij} = \varepsilon_{ij} - \tfrac{1}{3}\varepsilon_{kk}\delta_{ij} \tag{7}$$

an alternative form of the elasticity equations can be obtained

$$s_{ij} = 2\mu e_{ij}, \qquad \sigma_{kk} = 3K\varepsilon_{kk} \tag{8}$$

with the elastic bulk modulus K related to the Lamé constants λ and μ by

$$K = \lambda + \frac{2\mu}{3} \tag{9}$$

The viscoelastic relations corresponding to Eq. (8)

$$s_{ij} = 2\mu(t) * \mathrm{d}e_{ij}(t), \qquad \sigma_{kk} = 3K(t) * \mathrm{d}\varepsilon_{kk}(t) \tag{10}$$

have been frequently used instead of Eq. (6), particularly in modelling cohesive soils and soft rocks whose viscoelastic behaviour is markedly different under a purely deviatoric stress state from that due to hydrostatic pressure. In Eq. (10), the time-dependent relaxation moduli $\mu(t)$ and $K(t)$ characterise shear and dilatation behaviour, respectively. An alternative form of the linear viscoelastic constitutive equations for isotropic media is [3]

$$e_{ij} = J_1(t) * \mathrm{d}s_{ij}(t), \qquad \varepsilon_{kk} = J_2(t) * \mathrm{d}\sigma_{kk}(t) \tag{11}$$

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

Generalised standard linear solid (SLS) models are commonly used rheological models [4]. One SLS type consists of a Hookean spring and N Kelvin models, all connected in series, another type is made up of a spring and N Maxwell models, all connected in parallel. The constitutive equations governing the viscoelastic behaviour of such models are of the differential operator type

$$\begin{aligned} \sum_{n=0}^{N} p_n^{\mathrm{d}} D^n s_{ij} &= \sum_{n=0}^{N} q_n^{\mathrm{d}} D^n e_{ij}, \\ \sum_{n=0}^{N} p_n^{\mathrm{h}} D^n \sigma_{kk} &= \sum_{n=0}^{N} q_n^{\mathrm{h}} D^n \varepsilon_{kk} \end{aligned} \tag{12}$$

where D^n is an operator representing the nth time derivative and p_n^{d}, q_n^{d}, p_n^{h}, q_n^{h} are material constants with the superscripts d and h indicating association with the deviatoric and hydrostatic parts of stress and strain, respectively. These constants can be related to the moduli and viscosities of the spring and individual Kelvin or Maxwell elements [4] making up an SLS model.

The solutions of Eq. (12) under either creep or relaxation conditions yield explicit formulae for the respective moduli. For instance, the creep modulus derivable from a Kelvin generalised model comprising $N+1$ elastic springs with compliance J_n $(n = 0, 1, 2, \ldots, N)$ and N dashpots with viscosities η_n $(n = 1, 2, \ldots, N)$ is given by

$$J(t) = J_0 + \sum_{n=1}^{N} J_n\left[1 - \exp\left(-\frac{t}{\tau_n}\right)\right] \tag{13}$$

where $\tau_n = J_n\eta_n$ are the retardation times.

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

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

constitutive equations corresponding to Eq. (6)

$$\sum_{n=0}^{N} p_n D^{\alpha_n}\sigma_{ij} = \delta_{ij}\sum_{n=0}^{M}\lambda_n D^{\beta_n}\varepsilon_{kk} + 2\sum_{n=0}^{M}\mu_n D^{\gamma_n}\varepsilon_{ij} \tag{14}$$

or to Eq. (10)

$$\begin{aligned} \sum_{n=0}^{N} p_n^{\mathrm{d}} D^{\alpha_n} s_{ij} &= \sum_{n=0}^{M} q_n^{\mathrm{d}} D^{\beta_n} e_{ij}, \\ \sum_{n=0}^{N} p_n^{\mathrm{h}} D^{\gamma_n} \sigma_{kk} &= \sum_{n=0}^{M} q_n^{\mathrm{h}} D^{\delta_n} \varepsilon_{kk} \end{aligned} \tag{15}$$

can be used where α_n, β_n, γ_n and δ_n, are additional material constants. A special one-dimensional case of fractional operator constitutive equation

$$(1 + p_1 D^{\alpha_1})\sigma = (q_0 + q_1 D^{\beta_1})\varepsilon \tag{16}$$

was used to characterise a particular polymer and then applied to the axial transient BEM analysis of a viscoelastic column [5]. The parameters of the differential operator models of either integer or fractional type should satisfy certain restrictions so that non-negative internal work and rate of energy dissipation is predicted [7]. Such restrictions have been derived by Bagley and Torvic [7] in the case of the five-parameter uniaxial model given by Eq. (16). It is interesting to note, however, that the values of the parameters α_1 and β_1 obtained by Xie et al. [5] for a particular polymer by least square curve fitting did not satisfy the condition $\alpha_1 = \beta_1$ predicted by Bagley and Torvic.

3. Field equations

Introducing the small strain–displacement relations into the constitutive Eq. (2) and substituting the latter into the stress equations of motion yields a system of integro-differential equations

$$G_{ijkl}(t)u_{k,lj}(0) + \int_0^t G_{ijkl}(t-\tau)\frac{\partial u_{k,lj}(\tau)}{\partial \tau}\mathrm{d}\tau + \rho b_i = \rho \ddot{u}_i \quad (17)$$

where u_k and b_k $(k = 1,2,3)$ are the components of the displacement and body force, respectively, and ρ is the material density. A dot above a symbol indicates differentiation with respect to time. In the case of isotropic materials, Eq. (17) becomes

$$\begin{aligned}&[\lambda(t) + \mu(t)]u_{j,ji}(0) + \mu(t)u_{i,jj}(0) + \int_0^t [\lambda(t-\tau) \\ &+ \mu(t-\tau)]\frac{\partial u_{j,ji}(\tau)}{\partial \tau}\mathrm{d}\tau + \int_0^t \mu(t-\tau)\frac{\partial u_{i,jj}(\tau)}{\partial \tau}\mathrm{d}\tau \\ &+ \rho b_i = \rho \ddot{u}_i \end{aligned} \quad (18)$$

An alternative form of the field equations for isotropic materials, particularly suitable for harmonic vibration analysis, is [6]

$$\begin{aligned}&\int_{-\infty}^t E_\mathrm{D}(t-\tau)\frac{\partial u_{j,ji}(\tau)}{\partial \tau}\mathrm{d}\tau - \varepsilon_{ijk}\varepsilon_{klm} \\ &\times \int_{-\infty}^t \mu(t-\tau)\frac{\partial u_{m,lj}(\tau)}{\partial \tau}\mathrm{d}\tau + \rho b_i = \rho \ddot{u}_i \end{aligned} \quad (19)$$

where $E_\mathrm{D} = \lambda + 2\mu$ is the relaxation function for plane dilatation and ε_{ijk} is the permutation symbol.

The general dynamic boundary value problem is complemented by the initial conditions

$$u_i(0) = u_{i0}, \qquad \dot{u}_i(0) = \dot{u}_{i0} \quad (20)$$

and the boundary conditions

$$u_i(t) = \tilde{u}_i(t) \text{ on } \Gamma_1 \qquad \sigma_{ij}(t)n_j = \tilde{p}_i(t) \text{ on } \Gamma_2 \quad (21)$$

where **n** is the outward unit normal vector to the boundary $\Gamma = \Gamma_1 + \Gamma_2$ and $\tilde{u}_i(t)$, $\tilde{p}_i(t)$ are prescribed values of displacement and traction, respectively. 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.

Boundary integral equations are usually derived from reciprocity relations. The validity of such a relation has been proved for viscoelastic materials [3]. Given two viscoelastic states (u_i, p_i, b_i) and (u_i^*, p_i^*, b_i^*), satisfying the boundary value problem described above, then

$$\begin{aligned}&\int_\Gamma p_i * \mathrm{d}u_i^* \,\mathrm{d}\Gamma + \int_\Omega \rho b_i * \mathrm{d}u_i^* \,\mathrm{d}\Omega \\ &= \int_\Gamma u_i * \mathrm{d}p_i^* \,\mathrm{d}\Gamma + \int_\Omega \rho u_i * \mathrm{d}b_i^* \,\mathrm{d}\Omega \end{aligned} \quad (22)$$

where Ω is the domain of the viscoelastic continuum. The alternative form

$$\begin{aligned}&\int_\Gamma p_i * u_i^* \,\mathrm{d}\Gamma + \int_\Omega \rho b_i * u_i^* \,\mathrm{d}\Omega \\ &= \int_\Gamma u_i * p_i^* \,\mathrm{d}\Gamma + \int_\Omega \rho u_i * b_i^* \,\mathrm{d}\Omega \end{aligned} \quad (23)$$

involving Riemann instead of Stieltjes convolutions can also be shown to be valid.

4. Correspondence principle

The Laplace transform of a function $f(t)$ is defined by

$$\bar{f}(s) = \int_0^\infty f(t)\mathrm{e}^{-st}\,\mathrm{d}t \quad (24)$$

The transform of constitutive Eq. (2) is

$$\bar{\sigma}_{ij} = s\bar{G}_{ijkl}\bar{\varepsilon}_{kl} \quad (25)$$

By transforming also the equations of motion, the strain–displacement relations, as well as the initial and boundary conditions, a complete correspondence is established between the elastic and viscoelastic problem whereby the field variables are replaced by their Laplace transforms and the elastic constants G_{ijkl} are replaced by the functions $G^\mathrm{L}_{ijkl}(s) = s\bar{G}_{ijkl}$. When the material is isotropic, transforming Eq. (6) gives

$$\bar{\sigma}_{ij} = \lambda_\mathrm{L}(s)\bar{\varepsilon}_{kk}\delta_{ij} + 2\mu_\mathrm{L}(s)\bar{\varepsilon}_{ij} \quad (26)$$

In the case of constitutive equation (14)

$$\lambda_\mathrm{L} = s\bar{\lambda}(s) = \frac{\sum_{n=0}^M \lambda_n s^{\beta_n}}{\sum_{n=0}^N p_n s^{\alpha_n}} \quad (27)$$

and

$$\mu_\mathrm{L} = s\bar{\mu}(s) = \frac{\sum_{n=0}^M \mu_n s^{\gamma_n}}{\sum_{n=0}^N p_n s^{\alpha_n}} \quad (28)$$

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 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.

Taking the Laplace transform of both sides of Eq. (10) and introducing the Young's modulus E_L and Poisson's ratio ν_L in the transformed domain, the relations

$$2s\bar{\mu} = \frac{E_L}{1+\nu_L}, \qquad 3s\bar{K} = \frac{E_L}{1-2\nu_L}$$

are valid according to the correspondence principle. Thus, time-dependent uniaxial tension or compression modulus $E(t)$ and Poisson's ratio $\nu(t)$ can be obtained by finding the Laplace inverse transforms of the relations

$$E_L = s\bar{E} = \frac{9s\bar{\mu}\bar{K}}{(\bar{\mu}+3\bar{K})}, \qquad \nu_L = s\bar{\nu} = \frac{3\bar{K}-2\bar{\mu}}{2(3\bar{K}+\bar{\mu})} \tag{29}$$

In harmonic and transient dynamic analyses, the use of Fourier transforms has been found more appropriate. Applying the transformation

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(t)e^{i\omega t}\,dt$$

to Eq. (10) leads to relation of the form

$$\hat{s}_{ij} = 2\mu_F(i\omega)\hat{e}_{ij}, \qquad \hat{\sigma}_{kk} = 3K_F(i\omega)\hat{\varepsilon}_{kk} \tag{30}$$

where the complex, frequency-dependent complex moduli μ_F and K_F relate the Fourier transforms of stresses and displacements in exact correspondence with the elasticity relation (8). 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 (15), they are given by relations similar to Eqs. (27) and (28), that is, as ratios of complex polynomials.

For a harmonic analysis, the governing equations are derived from Eq. (18) and written in terms of the transformed displacements [8]

$$(\lambda_F + \mu_F)\hat{u}_{j,ji} + \mu_F\hat{u}_{i,jj} + \rho\hat{b}_i + \omega^2\rho\hat{u}_i = 0 \tag{31}$$

or alternatively using Eq. (19)

$$c_{1F}^2\hat{u}_{j,ji} - \varepsilon_{ijk}\varepsilon_{klm}c_{2F}^2\hat{u}_{i,jj} + \rho\hat{b}_i + \omega^2\rho\hat{u}_i = 0 \tag{32}$$

where c_{1F}, c_{2F}, are the complex velocities of dilatational and equivoluminal waves given by

$$c_{1F}^2 = \frac{E_D^F}{\rho}, \qquad c_{2F}^2 = \frac{\mu_F}{\rho} \tag{33}$$

The Fourier transformation is also applied to the boundary condition (21) 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

$$\kappa_{ij}\bar{u}_i = \int_\Gamma [\bar{p}_i(s)u_{ij}^*(s) - \bar{u}_i(s)p_{ij}^*(s)]d\Gamma + \rho\int_\Omega \bar{b}_i u_{ij}^*\,d\Omega \tag{34}$$

where $\kappa_{ij} = 0.5\delta_{ij}$ in the case of a smooth boundary, 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 Eqs. (25) or (26). If a particular solution to the transformed problem is known, the domain integral in Eq. (34) can be replaced by boundary integrals depending on that solution [9].

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 [8,10]

$$\kappa_{ij}\hat{u}_j(\omega) = \int_\Gamma [\hat{p}_i(\omega)u_{ij}^*(\omega) - \hat{u}_i(\omega)p_{ij}^*(\omega)]d\Gamma + \rho\int_\Omega u_{ij}^*(\omega)\hat{b}_j\,d\Omega \tag{35}$$

with the fundamental solution of the elastic harmonic problem in which the elastic wave speeds have been substituted by the viscoelastic ones. Eq. (35) 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 Eq. (35) 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, Eq. (22) [11,12]. Both approaches lead to

$$\kappa_{ij}u_i(t) = \int_\Gamma (u_{ij}^* * dp_i - p_{ij}^* * du_i)d\Gamma + \rho\int_\Omega b_i * du_{ij}^*\,d\Omega \tag{36}$$

where the time-dependent fundamental solution $u_{ij}^*(\mathbf{x}-\xi, t)$ satisfies Eq. (17) or (18) in an infinite domain with the acceleration term removed and the body force given by

$$\rho b_i^* = \delta_{ij}\delta(\mathbf{x}-\xi)H(t) \tag{37}$$

where δ_{ij} is the Kronecker delta, $\delta(\mathbf{x}-\xi)$ the delta function and $H(t)$ the Heaviside step function. Applying the correspondence principle, $u_{ij}^*(\mathbf{x}-\xi, t)$ is obtained as the inverse Laplace transform of the corresponding elastic fundamental solution in the transformed space divided by the Laplace parameter s. Such an operation has been carried out in several special cases. Shinokawa 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. [13]. Carini and De Donato [4] obtained expressions of the fundamental solutions due to unit force, displacement and strain discontinuities for the general viscoelastic model of differential operator type, Eq. (12). The general procedure for deriving the time-dependent fundamental solution and results in some special cases are given in Appendix A.

Integrating by parts, the boundary integral in Eq. (36) can be transformed to

$$\int_{\Gamma} (p_i * \mathrm{d}u_{ij}^* - u_i * \mathrm{d}p_{ij}^*)\mathrm{d}\Gamma \tag{38}$$

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 [13].

Uniform temperature variations can be accounted for by replacing real time t in Eq. (36) by a reduced time ζ given by [14–16]

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

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

This approach has been demonstrated in the context of a geomechanics problem involving a cavity subjected to known tractions $\tilde{p}_i(t)$ [17]. A number of fictitious loads $f_i^{(r)}$ are assumed applied at source points distributed just outside the domain, opposite to an equal number of boundary elements. These fictitious forces produce, in the infinite domain, the stresses

$$\sigma_{kj}^{\prime} = \sum_r f_i^{(r)} \sigma_{ijk}^{(r)*} \tag{39}$$

where $\sigma_{ijk}^*(t)$ is the stress fundamental solution. For the stress field given by Eq. (39) to be an approximate solution, the tractions due to $f_i^{(r)}$ on the entire boundary Γ

$$p_j^{\prime} = n_k \sigma_{kj}^{\prime} = n_k \sum_r f_i^{(r)} \sigma_{ikj}^{(r)*} = \sum_r f_i^{(r)} p_{ij}^{(r)*} \tag{40}$$

should be as close as possible to the actual tractions $\tilde{p}_i(t)$. This can be achieved by minimising the mean square value of the error

$$\int_{\Gamma} (p_j^{\prime} - \tilde{p}_j)(p_j^{\prime} - \tilde{p}_j)\mathrm{d}\Gamma \tag{41}$$

The contour integral (41) can be written as a summation of integrals over individual elements the derivatives of which with respect to each $f_i^{(r)}$ should vanish. This leads to a consistent and symmetric system of equations for the determination of the fictitious loads. Alternative indirect BEM formulations for solving elastic problems can be found in the literature.

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 [18]. 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

$$\kappa_{ij}(t) * u_j(\mathbf{x}, t) \tag{42}$$

Using the Maxwell model, the fundamental solution in the time domain was obtained by inverse Laplace transform [14,19]. 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.

A procedure has been developed based on the corresponding BEM formulation of the elastodynamic problem [19,20]. 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 yields the kernels for the viscoelastic boundary integral formulation. It is clear that the final form of the kernels depends on the choice of the material model. Explicit expressions have been obtained for the special case of the Maxwell model [20].

5.6. Mixed formulation—dynamic problems

A particular mixed scheme [18] was based on the boundary integral equation

$$\kappa_{ij} * u_i(t) = \int_{\Gamma} (u_{ij}^* * p_i - p_{ij}^* * u_i)\mathrm{d}\Gamma + \rho \int_{\Omega} b_i * u_{ij}^* \mathrm{d}\Omega \tag{43}$$

which can be obtained from the reciprocity relation (23) if the fundamental solution $u_{ij}^*(\mathbf{x}-\xi,t)$, $p_{ij}^*(\mathbf{x}-\xi,t)$, due to the body force

$$\rho b_i^* = \delta_{ij}\delta(\mathbf{x}-\xi)\delta(t) \quad (44)$$

is used as the second viscoelastic state. If time t is divided into N equal intervals Δt so that $t = N\Delta t$, the convolution integrals in Eq. (43) may be performed by the convolution quadrature method proposed by Lubich [21,22]. This quadrature formula allows the numerical approximation of these convolution integrals by the finite sums

$$\sum_{k=0}^{n} \omega_{n-k}(u_{ij}^*, \Delta t) p_i(k\Delta t), \qquad \sum_{k=0}^{n} \omega_{n-k}(p_{ij}^*, \Delta t) u_i(k\Delta t) \quad (45)$$

for $n = 1,2,\ldots,N$ with the integration weights ω_n calculated using the approximations

$$\omega_n(u_{ij}^*, \Delta t) \approx \frac{1}{L}\sum_{l=0}^{L-1} \bar{u}_{ij}^*\left(\frac{\gamma(z_l)}{\Delta t}\right) z_l^{-n}$$

and

$$\omega_n(p_{ij}^*, \Delta t) \approx \frac{1}{L}\sum_{l=0}^{L-1} \bar{p}_{ij}^*\left(\frac{\gamma(z_l)}{\Delta t}\right) z_l^{-n}$$

where $\gamma(z)$ is a well-defined polynomial in the complex variable z according to the quadrature method and

$$z_l = R\,\mathrm{e}^{\mathrm{i}l2\pi/L}$$

R being the radius of a circle in the domain of analyticity of $\bar{u}_{ij}^*(z)$ or $\bar{p}_{ij}^*(z)$. The characteristic advantage of the quadrature rule (45) is that only the Laplace transformed functions $\bar{u}_{ij}^*$ and $\bar{p}_{ij}^*$ are used. Thus a time stepping procedure directly in the time domain can be formulated, although only the Laplace transforms of the fundamental solutions are used, that is, a viscoelastic boundary element formulation in the time domain is achieved without requiring the knowledge of the time-dependent fundamental solutions.

6. BEM modelling

Initial numerical implementations of BEM formulations in the transformed domain were based on constant boundary elements [1,23,24] leading to simple integration schemes and algebraic equations for the discrete values of the field variables. Higher-order one-dimensional [8,12] and two-dimensional [18] elements were introduced in later, more advanced formulations.

Time domain formulations based on integral equations (36) or (43) require boundary modelling in both space and time dimensions. If the boundary surface Γ is discretised in E isoparametric elements Γ_e, where F polynomial shape functions $N_e^f(\mathbf{x})$ are defined, the following representation can be adopted

$$u_j(\mathbf{x},t) = \sum_{f=1}^{F} N_e^f(\mathbf{x}) u_j^{ef}(t) \qquad p_j(\mathbf{x},t) = \sum_{f=1}^{F} N_e^f(\mathbf{x}) p_j^{ef}(t) \quad (46)$$

where $u_j^{ef}(t)$ and $p_j^{ef}(t)$ are the time-dependent nodal values of displacement and traction, respectively. Using constant time interpolation [12], 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 [15].

Inserting the boundary model (46) in Eq. (43) with body forces neglected results in

$$\kappa_{ij} * u_i(t) = \sum_{e=1}^{E}\sum_{f=1}^{F}\left\{\int_{\Gamma_e} u_{ij}^*(\mathbf{x},\xi;t) * p_j^{ef}(t) N_e^f(\mathbf{x})\mathrm{d}\Gamma_e - \int_{\Gamma_e} p_{ij}^*(\mathbf{x},\xi;t) * u_j^{ef}(t) N_e^f(\mathbf{x})\mathrm{d}\Gamma_e\right\} \quad (47)$$

Applying the quadrature formula (45) to the integral Eq. (47) results in the following boundary element time-stepping formulation for $n = 0,1,\ldots,N$

$$\sum_{k=0}^{n} c_{ij}(\mathbf{x}) u_j(\xi, k\Delta t) = \sum_{e=1}^{E}\sum_{f=1}^{F}\sum_{k=0}^{n}\{\omega_{n-k}(\bar{u}_{ij}^*, \xi, \Delta t) p_j^{ef}(k\Delta t) - \omega_{n-k}(\bar{p}_{ij}^*, \xi, \Delta t) u_j^{ef}(k\Delta t)\} \quad (48)$$

with the spatial integration incorporated into the weights ω_n which are now given by

$$\omega_{n-k}(\bar{u}_{ij}^*, \xi, \Delta t) = \frac{1}{L}\sum_{l=0}^{L-1}\left[\int_{\Gamma_e} \bar{u}_{ij}^*\left(\mathbf{x}, \xi, \frac{\gamma(z_l)}{\Delta t}\right) N_e^f(\mathbf{x})\mathrm{d}\Gamma\right] z_l^{-n}$$

$$\omega_{n-k}(\bar{p}_{ij}^*, \xi, \Delta t) = \frac{1}{L}\sum_{l=0}^{L-1}\left[\int_{\Gamma_e} \bar{p}_{ij}^*\left(\mathbf{x}, \xi, \frac{\gamma(z_l)}{\Delta t}\right) N_e^f(\mathbf{x})\mathrm{d}\Gamma\right] z_l^{-n}$$

Thus an algebraic system of equations for the discrete nodal values $p_j^{ef}(k\Delta t)$ and $u_j^{ef}(k\Delta t)$ is formed with coefficients depending on the Laplace transforms of the fundamental solutions $u_{ij}^*(\mathbf{x}, \xi, t)$ and $p_{ij}^*(\mathbf{x}, \xi, t)$.

7. Numerical inversion of Laplace transforms

Laplace transforms of boundary or domain variables can be numerically converted back into time-dependent functions. Schapery's inversion method [25] was the earliest one to be used [1,23]. It is based on the argument that displacements or stresses may be approximated by a function in the form

$$f(t) = A + Bt + \sum_{r=1}^{M-2} a_r\,\mathrm{e}^{-b_r t} \quad (49)$$

Transforming both sides of Eq. (48) gives

$$s\bar{f}(s) = A + \frac{B}{s} + \sum_{r=1}^{M-2} \frac{a_r}{1 + b_r/s} \tag{50}$$

The BEM solution is obtained for M discrete values of the transform variable s_ρ, $\rho = 1,2,\ldots,M$. Eq. (50) is then applied for each s_ρ choosing b_r to be the first $M-2$ values of s_ρ. Thus a consistent system of equations is generated for the unknowns A, B and a_r leading to evaluation of the inverse transform of the solution at any time through the use of Eq. (49). An alternative collocation procedure was proposed by Kusama and Mitsui [24] who represented the transient part of the response function $f(t)$ as a sum of orthogonal functions.

Bellman's inversion technique [26] introduces the new variable $x = \mathrm{e}^{-t}$ in Eq. (24) which then becomes

$$\bar{f}(s) = \int_0^1 f(-\ln x)x^{s-1}\,\mathrm{d}x \tag{51}$$

Integral (51) is approximated by the Gauss–Legendre quadrature formula

$$\bar{f}(s) = \sum_{i=1}^{N} w_i x_i^{s-1} f(-\ln x_i) \tag{52}$$

where x_i are the roots of the Legendre polynomials of order N and w_i the corresponding weights. By setting s equal to N distinct values $1,2,\ldots,N$, a consistent linear system of equations

$$\sum_{i=1}^{N} w_i x_i^k f(-\ln x_i) = \bar{f}(k+1) \tag{53}$$

is obtained which can be inverted to yield $f(t)$ at N distinct times $t_i = -\ln x_i$. This method was used in the viscoelastic plate analysis by Ding et al. [27] who proposed a refinement allowing for the evaluation of $f(t)$ at any time. Other numerical inversion methods mentioned in BEM literature are Piessens's [28], applied to the three-dimensional quasi-static problem [9] and Durbin's [29] which was used in a formulation of the three-dimensional dynamic problem [5].

8. Applications

8.1. Benchmark problems

Most benchmark problems involved a cylindrical cavity in a viscoelastic medium subjected to a uniform pressure $p(t) = p_0 H(t)$ where $H(t)$ is the Heaviside step function. Since these problems have exact analytical solutions, several authors have used them for validating their formulations. A hole in an infinite viscoelastic space, modelled as SLS, has been analysed in both the Laplace transformed [23,24] and time domain [2,12]. A particular case of a cylindrical 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 [12,15] but also on a more general n-parameter Maxwell model [13].

Rizzo and Shippy [1] considered the case of a cylinder constrained over its outer boundary by a thin elastic ring. They adopted SLS in shear as the material model and a BEM formulation in the Laplace transform domain with the solution inverted by Schapery's method. Plots of time variations of radial and hoop stress at various radial distances from the centre were found in good agreement with the exact analytical solution. The time domain solution of this problem has also been treated with a similar degree of accuracy [12].

Three-dimensional analyses of rectangular blocks were performed in the Laplace transformed domain under both quasi-static [9] and transient [5,18] conditions with time domain responses obtained by numerical inversion. In the former case, a cubical and a prismatic block were 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 values of the parameters were estimated by curve fitting and then found to represent fairly accurately the experimentally determined complex moduli [5]. 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 [14].

8.2. Plates

The applicability of BEM to viscoelastic plate analyses would be practically useful since polymers are quite often used as thin-walled elements. Such a formulation was developed for the dynamic problem in the Laplace transform domain [27]. The governing equation was derived as

$$D_\mathrm{L}\nabla^4\bar{w} + \rho h s^2\bar{w} = \bar{q} \tag{54}$$

where w is the plate deflection, h the plate thickness, q the applied dynamic pressure and D_L the plate rigidity in the transformed domain given by

$$D_\mathrm{L} = \frac{s\bar{E}h^3}{12(1 - s^2\bar{\nu}^2)}$$

The knowledge of the fundamental solution for the differential operator in the left-hand side of Eq. (54) leads to the derivation of the standard pair of boundary integral equations for a thin plate in the Laplace domain. Ding et al. [27] derived two approximate forms of such a fundamental solution and used an improved version of Bellman's inversion technique to obtain the time history of the plate response to sinusoidal lateral pressure.

8.3. Fracture

An early attempt to introduce BEM analysis to polymer fracture concerned the prediction of stress and displacement fields in the neighbourhood of a crack filled with failed, so-called craze material [23]. The craze was represented by a slit of length $2a$ in a plate of finite width subjected to a step far field tension. Accounting for symmetry relative to two orthogonal axes, the problem was modelled as shown in Fig. 1. The effect of the craze on the linear viscoelastic material was modelled as a time-dependent stiffness $k_c(x_1, t)$ and the boundary conditions along the crack surface ($0 \leq x_1 \leq a$) were

$$p_1 = 0, \qquad p_2 = -k_c u_2$$

A non-linear finite element analysis, validated by experimental data, provided the initial stiffness $k_c(x_1, 0)$. Its time-dependence was assumed to be the same as that of the relaxation modulus of the analysed polymer. The BEM solution was based on a SLS Kelvin creep model and performed in the Laplace transformed domain.

More recently [30], a BEM formulation closer to classical fracture mechanics concepts concerned the evaluation of the energy release rate with respect to crack growth. The viscoelastic problem shown in Fig. 1 was again considered for which the path-independent J-integral is equal to the energy release rate and can be derived analytically for simple viscoelastic models. An appropriate expression for the potential energy was identified and converted to a boundary integral. The energy release rate was then calculated as a numerical approximation of the derivative of the potential energy relative to the crack length. The time history of the energy release rate obtained from a time domain BEM formulation was shown to be in close agreement with the analytically predicted J-integral.

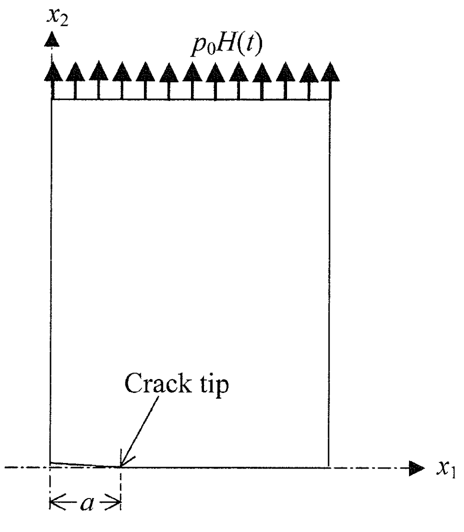

Fig. 1. Analysed quarter of centre-cracked plate under tension.

8.4. Composites

The composite material was considered consisting of two perfectly bonded regions, a viscoelastic one representing the polymer matrix and an elastic one representing the fibre or particle reinforcement [15]. 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 [15].

8.5. Rolling contact

The simulation of rolling contact between two viscoelastic solids is a geometrically non-linear problem combining a BEM formulation with an iterative scheme modelling the contact conditions. Solutions of the two-dimensional problem can be found in the literature based on time domain fundamental solutions obtained through the application of correspondence principle. These solutions lead to steady-state fundamental solutions, which have been used in BEM formulations of steady-state rolling contact. One such two-cylinder application [31] used the half-space Green's function as the fundamental solution with the SLS model characterising the viscoelastic material behaviour in tension or compression. Coulomb's dry friction was incorporated in the contact algorithm. The contact between a viscoelastic body and an elastic one covered by a thin viscoelastic boundary film has been analysed using the Kelvin fundamental solution for the two-dimensional domain [32]. Numerical results included the stress distribution at the contact surfaces and within the viscoelastic bodies as well as rolling resistance. A practical application of this problem is the numerical simulation of self-lubricating polymer transfer film in gears or bearing systems.

9. 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. A recently proposed mixed method solving the problem directly in the time domain but using the Laplace transform of the fundamental solution has only been tried on dynamic problems. Its applicability to quasi-static problems should be tested and its performance compared with that of the other methods.

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.

One particular field where BEM applications have been so far limited is fracture mechanics. Interest in polymer fracture has prompted considerable theoretical and numerical work, which can be the basis of various BEM formulations. Further research can focus on refined approaches to identify stress intensity factors, strain energy release rates and even the crack propagation velocity in highly stressed polymers. Other developments may concern the introduction of fundamental solutions specific to cracked geometries or the consideration of cracks along interfaces of bi-material continua.

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 [33] although such techniques should be re-examined because of the unrealistic behaviour of the adopted material models. 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 and high stress concentrations.

Appendix A

The Laplace transform of the viscoelastic time-dependent fundamental solution of the quasi-static problem can be written in the general form

$$\bar{u}^*_{ij}(s) = \bar{A}(s)f_{ij}(\mathbf{x}-\xi) + \bar{B}(s)g_{ij}(\mathbf{x}-\xi) \tag{A1}$$

The functions f_{ij} and g_{ij} are obtained from the corresponding elasticity solutions. For two-dimensional problems, they are given by

$$f_{ij} = -\frac{\delta_{ij}\ln r}{8\pi} \tag{A2}$$

$$g_{ij} = \frac{r_{,i}r_{,j}}{8\pi} \tag{A3}$$

where $r = |\mathbf{x}-\xi|$. The functions $\bar{A}(s)$ and $\bar{B}(s)$ correspond to constant coefficients in the elastic solutions usually expressed in terms of the shear modulus and Poisson's ratio. If isotropic viscoelastic behaviour is characterised by the shear and bulk relaxation moduli, the effective Young's modulus and Poisson's ratio in the Laplace transformed domain are given by Eq. (29). Typical expressions for $\bar{A}(s)$ and $\bar{B}(s)$ are given below.

(i) Plane strain

$$\bar{A} = \frac{2(3\bar{K}+7\bar{\mu})}{s^2\bar{\mu}(3\bar{K}+4\bar{\mu})} \tag{A4}$$

$$\bar{B} = \frac{2(3\bar{K}+\bar{\mu})}{s^2\bar{\mu}(3\bar{K}+4\bar{\mu})} \tag{A5}$$

(ii) Plane stress

$$\bar{A} = \frac{15\bar{K}+8\bar{\mu}}{2s^2\bar{\mu}(3\bar{K}+\bar{\mu})} \tag{A6}$$

$$\bar{B} = \frac{9\bar{K}}{2s^2\bar{\mu}(3\bar{K}+\bar{\mu})} \tag{A7}$$

As mentioned in Section 5.3, Carini and De Donato [4] performed the required inversions of Laplace transforms in both two and three dimensions for n-parameter standard linear solid models of Kelvin or Maxwell type. Their general expressions can be specialised to simple cases but this process was found to be cumbersome and hampered by errors in some key formulae. In such cases, it may be faster and safer to invert Eqs. (A4)–(A7). A common viscoelastic model in the BEM literature combines elastic dilatation $K = K_0$ with the simplest, three-parameter SLS for shear relaxation

$$\mu(t) = \frac{\mu_0}{\mu_2}(\mu_1 + \mu_0\,\mathrm{e}^{-\lambda t}), \qquad \lambda = \frac{\mu_2}{\eta} \text{ (Kelvin model)}$$

or

$$\mu(t) = (\mu_0 + \mu_1\,\mathrm{e}^{-\lambda t}), \qquad \lambda = \frac{\mu_1}{\eta} \text{ (Maxwell model)}$$

with $\mu_2 = \mu_0 + \mu_1$, where μ_0 and μ_1 are the elastic shear moduli and η the viscosity of the models. In this case, $\bar{A}$ and $\bar{B}$ were found to have the common form

$$\frac{c(s+\lambda)(s+\alpha)}{s(s+\lambda_1)(s+\lambda_2)}$$

so that their inverse transforms are given by

$$a_0 + a_1\,\mathrm{e}^{-\lambda_1 t} + a_2\,\mathrm{e}^{-\lambda_2 t}$$

where

$$a_0 = \frac{c\alpha\lambda}{\lambda_1\lambda_2}, \qquad a_1 = \frac{c(\lambda-\lambda_1)(\lambda_1-\alpha)}{\lambda_1(\lambda_2-\lambda_1)},$$

$$a_2 = \frac{c(\lambda-\lambda_2)(\lambda_2-\alpha)}{\lambda_2(\lambda_1-\lambda_2)}$$

In the case of plain strain, the fundamental solution is given by

$$u_{ij}^*(t) = (b_{01} - b_1\,\mathrm{e}^{-\lambda_1 t})(f_{ij} + g_{ij}) + (b_{02} - b_2\,\mathrm{e}^{-\lambda_2 t})(f_{ij} - g_{ij}) \tag{A8}$$

where for the Kelvin model

$$\lambda_1 = \frac{\mu_1}{\mu_2}\lambda, \quad \lambda_2 = \frac{3K_0\mu_2 + 4\mu_0\mu_1}{(3K_0 + 4\mu_0)\mu_2}\lambda$$

$$b_{01} = \frac{2\mu_2}{\mu_0\mu_1}, \quad b_{02} = \frac{6\mu_2}{3K_0\mu_2 + 4\mu_0\mu_1},$$

$$b_1 = \frac{2}{\mu_1}, \quad b_2 = \frac{24\mu_0^2}{(3K_0 + 4\mu_0)(3K_0\mu_2 + 4\mu_0\mu_1)}$$

and the Maxwell model

$$\lambda_1 = \frac{\mu_0}{\mu_2}\lambda, \quad \lambda_2 = \frac{3K_0 + 4\mu_0}{3K_0 + 4\mu_2}\lambda$$

$$b_{01} = \frac{2}{\mu_0}, \quad b_{02} = \frac{6}{3K_0 + 4\mu_2},$$

$$b_1 = \frac{2\mu_1}{\mu_0\mu_2}, \quad b_2 = \frac{24\mu_1}{(3K_0 + 4\mu_0)(3K_0 + 4\mu_2)}$$

For plane stress

$$u_{ij}^*(t) = (b_{01} - b_1\,\mathrm{e}^{-\lambda_1 t})(5f_{ij} + 3g_{ij}) + (b_{02} - b_2\,\mathrm{e}^{-\lambda_2 t})(f_{ij} - g_{ij}) \tag{A9}$$

with

$$\lambda_1 = \frac{\mu_1}{\mu_2}\lambda, \quad \lambda_2 = \frac{3K_0\mu_2 + \mu_0\mu_1}{(3K_0 + \mu_0)\mu_2}\lambda$$

$$b_{01} = \frac{\mu_2}{2\mu_0\mu_1}, \quad b_{02} = \frac{3\mu_2}{2(3K_0\mu_2 + \mu_0\mu_1)},$$

$$b_1 = \frac{1}{2\mu_1}, \quad b_2 = \frac{3\mu_0^2}{2(3K_0 + \mu_0)(3K_0\mu_2 + \mu_0\mu_1)}$$

for the Kelvin model, and

$$\lambda_1 = \frac{\mu_0}{\mu_2}\lambda, \quad \lambda_2 = \frac{3K_0 + \mu_0}{3K_0 + \mu_2}\lambda$$

$$b_{01} = \frac{1}{2\mu_0}, \quad b_{02} = \frac{3}{2(3K_0 + \mu_0)},$$

$$b_1 = \frac{\mu_1}{2\mu_0\mu_2}, \quad b_2 = \frac{3\mu_1}{2(3K_0 + \mu_0)(3K_0 + \mu_2)}$$

for the Maxwell model.

As mentioned in Section 5.5, a time domain fundamental solution for the dynamic problem in three dimensions has been presented for the Maxwell model, that is, a spring and dashpot in series. The material was assumed to behave in both shear and bulk deformation according to this model but with a common decay time constant, it is therefore characterised by only three parameters. The fundamental solution has been obtained by applying the correspondence principle to the corresponding elastodynamic solution and is given in full by Gaul et al. [19].

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