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A unified constitutive theory for paper

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Abstract

Paper is an orthotropic, rate sensitive material which makes modelling its stress–strain behaviour a difficult task. Classical methods are inadequate behaviour of paper and comparisons are made with previous experimental work for a particular paper. Comparisons between the two models are also made.

Introduction

With the advent of more powerful computers and new finite element methodologies, the amount of detail that can be included in a stress analysis is now much greater than ever before. The modelling of plastic deformations is almost a routine activity for some industries. However, to get realistic results, it is necessary to have a model which accurately reflects the structural behaviour of the material being modelled. Unfortunately, many of the standard material models are not really at the same level of sophistication as the finite elements methods themselves. A few finite element codes allow the user to define their own material models.

Current trends in paper modelling

Many material models have been suggested for the description of the structural response of paper. They fall into roughly three categories: network models [1,2], laminate models [3,4], and power law models [5]. The first two have some limited micro-mechanical basis.

Perkins & Sinha [2] described a micro-mechanically based network model. This model was based on monotonic data and was not tested for cyclic loading. It focused on the prediction of the rejsponse of a particular paper based on the fibre properties and the manufacturing processes that they have undergone rather than actually modelling the response of a paper structure. A randomly oriented fibre structure was generated and analysed, given certain fibre properties. This then allowed the effect of fibre properties to be analysed. However, fibre-to-fibre bonding also needs to be modelled. This was not very well understood at the time and, in our opinion, the overall usefulness of this kind of model is, as a result, limited. Network models generally focus on producing a model based on a network of fibres. At present, such approaches are generally confined to predicting the response in the elastic region.

Laminate models [3,4] are similar to network models but, starting with the properties of crystalline and amorphous cellulose, they try to predict the behaviour of paper based on classical laminate theory. Generlaly the results from this kind of model are also only good for predicting the elastic response.

There are also a number of models which use simple exponential rules to predict the behaviour under monotonic loading. One of these models is detailed in Barnes *et al.* [5] In this case [5] proposed a stress–strain relationship of the form

$$\sigma(\varepsilon) = A\varepsilon + B(1 - e^{-\alpha\varepsilon}) \tag{1}$$

This work also contained relationships for A, B and α which were based on the strain rate. However, these equations have not been experimentally validated.

None of these models were considered to be extremely useful in the structural modelling of the inelastic behaviour of paper structures. It was decided to evaluate the use of a 'unified constitutive theory' approach. The first model investigated arose out of work by Stouffer and co-workers [6].

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If paper behaved like most other materials, and showed little or no early reverse yielding, then there would be little difficulty in modifying such models to include the necessary elastic and plastic anisotropic effects. Unfortunately, as can be seen in Sawyer *et al.* [7], paper exhibits significant reverse yielding early in the unloading cycle. As a result, another model was developed based upon the results of creep presented by Padanyi [8]. This model was derived from a model designed specifically to exhibit this reverse yielding behaviour developed by McKinlay at AMCOR Research and Technology Centre. His original model is discussed in [9]. These material models were subsequently implemented into the finite element program ABAQUS, thereby enabling the applicability of the two models to be evaluated.

Unified constitutive modelling

In the classical approaches to plasticity it is useful to separate the strain tensor into elastic, plastic, creep and other inelastic components. However, in 'unified constitutive' approaches the strain is simply divided into elastic strain and inelastic strain components. Elastic strain is reversible and the inelastic strain is the irreversible strain. The elastic strain can be determined from the stress state by using Hooke's Law, and the inelastic strain is the remainder. This can, of course, be accomplished in the opposite manner using the strain and the inelastic strain to calculate the stress state.

In these approaches the inelastic strain is often modelled using an appropriate flow law together with various state variables. The flow law generally expresses the inelastic strain rate in terms of stress and these state variables, with the state variables being commonly evaluated via a set of evolution equations.

These state variables represent, in some way, the state of the microstructure of the material. In isotropic metals two state variables are frequently used, namely the 'drag stress' and the 'back stress'. The 'drag stress' is a scalar, and represents the piling up of dislocations around grain boundaries and imperfections. This results from the idea that the 'over stress', i.e. the difference between the deviatoric stress and the 'back stress', is believed to be the driving force of the deformation process. 'Drag stress', therefore, represents an isotropic hardening term and the 'back stress' an anisotropic hardening term. See Dame & Stouffer [6].

One particular model presented in Dame & Stouffer [6] can be expressed as

$$\dot{\varepsilon}^{\mathrm{I}}_{ij} = D \exp\left\{\frac{1}{2}\left(\frac{Z^2}{2K_2}\right)^n\right\}\frac{(S_{ij}-\Omega_{ij})}{\sqrt{K_2}} \tag{2}$$

$$\dot{\Omega}_{ij} = f_1\dot{\varepsilon}^{\mathrm{I}}_{ij} - \frac{3}{2} f_1 \frac{\Omega_{ij}}{\Omega_{\max}}\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}} + f_2\dot{S}_{ij} \tag{3}$$

$$Z = Z_1 - (Z_1 - Z_0)^{-mW_1} \tag{4}$$

$$S_{ij} = \sigma_{ij} - \frac{\sigma_{kk}}{3}\delta_{ij} \tag{5}$$

$$\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}} = \sqrt{\frac{2}{3}\dot{\varepsilon}^{\mathrm{I}}_{ij}\dot{\varepsilon}^{\mathrm{I}}_{ij}} \tag{6}$$

where $\dot{\varepsilon}^{\mathrm{I}}_{ij}$ is the inelastic strain rate, S_{ij} is the deviatoric stress, Z is the 'drag stress', Z_1, Z_2 are the initial and saturated values of Z, Ω_{ij} is the 'back stress', $\Omega_{\max}$ is the saturated 'back stress' $\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}}$ is the effective inelastic strain rate, W^{I} is the inelastic work, f_1 and f_2 are hardening parameters, D is a scaling parameter (and is usually 10^4), n is the strain rate sensitivity parameter and m is a parameter controlling work hardening.

Equation (2) represents the flow equation and eqns (3) and (4) are the evolution equations. K_2 is the second invariant of 'over stress' and was defined as

$$K_2 = \frac{1}{3}(\sigma_{ij} - \Omega_{ij})(\sigma_{ij} - \Omega_{ij}) \tag{7}$$

The modified Ramaswamy–Stouffer (MRS) model

An important factor in the previous model is the deviatoric stress S_{ij}, which is defined as the total stress tensor minus the hydrostatic stress. For isotropic materials the stress state is described by two quantities, *viz.* the hydrostatic stress (or pressure) which only induces a change of scale, and the deviatoric stress, which only induces a change of shape.

It is obvious that, for an orthotropic materials, this approach needs to be generalised, because a hydrostatic pressure applied to an anisotropic brick would result in different strains in each direction. This loading will not result in a change of scale only, as required by our generalised definition of 'pressure'.

Returning to the definition, and as a result of stating that the 'pressure' term should only produce a change of scale, then the strains in each direction must be the same. In turn, this should allow the calculation of the direct stress ratios that will produce only a change of scale. This now defines the 'direction' in stress space in which the pressure vector in stress space lies. Let us define α_{ij} such that the trace terms define the unit vector in this direction and the cross-terms are zero.

Now define the 'pressure' **P** as a constant times the unit vector in its direction

$$\mathbf{P}=A\cdot\alpha_{ij} \tag{8}$$

Then expressing the requirement that the deviatoric stress vector is independent of the 'pressure' term, i.e. their dot product is zero, gives

$$\mathbf{P}\cdot\mathbf{S}=0 \tag{9}$$

Equations (9) and (8) now yield the requirement that

$$\alpha_{ij}\cdot S_{ij}=0 \tag{10}$$

Then, following the traditional formulation, S_{ij} is defined as the stress minus the 'pressure'

$$S_{ij}=\sigma_{ij}-A\cdot\alpha_{ij} \tag{11}$$

Consequently, from eqns (10) and (11) we require that

$$0=\alpha_{ij}\cdot(\sigma_{ij}-A\alpha_{ij}) \tag{12}$$

and because α_{ij} is a unit vector and $\alpha_{ij}\alpha_{ij}=1$ we obtain

$$A=\alpha_{ij}\sigma_{ij} \tag{13}$$

and finally

$$S_{ij}=\sigma_{ij}-\alpha_{ij}\alpha_{kl}\sigma_{kl} \tag{14}$$

Having adopted the concept as outlined above it is now necessary to determine the values for α_{ij}. If it is assumed that 'pressure' does not induce inelastic flow, then α_{ij} can be determined from Hooke's Law. To do this we calculate the stress induced by applying the same elastic strain ε in each direction. The unit vector of pressure is then the unit vector along the direction of the stress vector found.

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\end{bmatrix}=\frac{1}{\beta}\begin{bmatrix}E_x(1-\nu_{yz}\nu_{zy}) & E_x(\nu_{yx}+\nu_{zx}\nu_{yz}) & E_x(\nu_{zx}+\nu_{yx}\nu_{zy})\\ E_y(\nu_{xy}+\nu_{xz}\nu_{zy}) & E_y(1-\nu_{xz}\nu_{zx}) & E_y(\nu_{zy}+\nu_{zx}\nu_{xy})\\ E_z(\nu_{xz}+\nu_{xy}\nu_{yz}) & E_z(\nu_{yz}+\nu_{xz}\nu_{yx}) & E_z(1-\nu_{xy}\nu_{yx})\end{bmatrix}\begin{bmatrix}\varepsilon\\ \varepsilon\\ \varepsilon\end{bmatrix} \tag{15}$$

where

$$\beta=1-\nu_{xy}\nu_{yx}-\nu_{xz}\nu_{zx}-\nu_{xy}\nu_{yz}\nu_{zx}-\nu_{xz}\nu_{yx}\nu_{zy}-\nu_{yz}\nu_{zy} \tag{16}$$

Hence

$$\frac{\sigma_{11}}{\sigma_{22}}=\frac{E_x(1-\nu_{yz}\nu_{zy}+\nu_{yx}+\nu_{zx}\nu_{yz}+\nu_{zx}+\nu_{yx}\nu_{zy})}{E_y(\nu_{xy}+\nu_{xz}\nu_{zy}+1-\nu_{xz}\nu_{zx}+\nu_{zy}+\nu_{zx}\nu_{xy})} \tag{17}$$

and

$$\frac{\sigma_{11}}{\sigma_{33}}=\frac{E_x(1-\nu_{yz}\nu_{zy}+\nu_{yx}+\nu_{zx}\nu_{yz}+\nu_{zx}+\nu_{yx}\nu_{zy})}{E_z(\nu_{xz}+\nu_{xy}\nu_{yz}+\nu_{yz}+\nu_{xz}\nu_{yx}+1-\nu_{xy}\nu_{yx})} \tag{18}$$

If we now define

$$\frac{\sigma_{11}}{\sigma_{22}}=\frac{1}{\lambda_1} \tag{19}$$

$$\frac{\sigma_{11}}{\sigma_{33}}=\frac{1}{\lambda_2} \tag{20}$$

The unit vector in the direction, described by the ratios above, and hence α_{ij} the unit pressure is as follows:

$$\alpha_{ij}=\frac{1}{1+\lambda_1^2+\lambda_2^2}\begin{bmatrix}1&0&0\\0&\lambda_1&0\\0&0&\lambda_2\end{bmatrix} \tag{21}$$

The orthotropic generalisation of the deviatoric stress is now completely defined. In an isotropic material $\lambda_1=\lambda_2=1$ and the proposed generalisation returns to the traditional isotropic case. As a note, it may seem that this cannot be correct as this allows the material to be inelastically compressible. This is perfectly allowable, however, because paper contains a large number of voids which can, of course, be permanently changed in volume.

Deviatoric stress is not the only concept that needs to be generalised. In the Ramaswamy–Stouffer formulation [6] the equations for the state variables have an isotropic form in that they have the same constants regardless of direction of flow. In this formulation the 'drag stress' was a scalar quantity, so only the 'back stress' equation detailed in eqn (3) needs to be generalised. This results in

$$\dot{\Omega}_{ij}=f_{1_{ijkl}}\dot{\varepsilon}^{\mathrm{I}}{}_{kl}-\frac{3}{2}g_{1_{ijkl}}\Omega_{kl}\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}}-f_{2_{ijkl}}\dot{S}_{kl} \tag{22}$$

where the trace elements of $g_{1_{ijkl}}$ are of the form f_1/Ω. This formulation has been previously suggested by Dame & Stouffer [6].

The experience gained in this work has shown that this level of generality may not be required. In this work it has been found that, in eqn (3), it was sufficient to have a different constant for each direction. As a result, this can be represented mathematically by using a vector representation, instead of the previous tensor representation, of the various stresses, strains and state variables. All this does is express the equations without some of the terms, which are zero due to a lack of cross-coupling of terms, of the flow law and state variable evolution equations. Of course these vectors, i.e. Ω_i, etc., only have six terms owing to the symmetric nature of the stress and strain tensors.

With formulation we obtain

$$\dot{\Omega}_i=f_{1_{ij}}\dot{\varepsilon}^{\mathrm{I}}{}_j-\frac{3}{2}g_{1_{ij}}\Omega_j\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}}-f_{2_{ij}}\dot{S}_j \tag{23}$$

where the translation from tensor to vector notation is as below

$$\Omega^{\mathrm{T}}{}_i=[\Omega_{11}\quad\Omega_{22}\quad\Omega_{33}\quad\Omega_{12}\quad\Omega_{13}\quad\Omega_{23}] \tag{24}$$

and, similarly, for all other variables that were expressed in tensorial form.

In a two-dimensional case, where there are of course, only three terms in the strain or stress vector, the hardening constant can be expressed as

$$f_{1_{ij}}=\begin{bmatrix}f_{1_1}&0&0\\0&f_{1_2}&0\\0&0&f_{1_3}\end{bmatrix},\ f_{2_{ij}}=\begin{bmatrix}f_{2_1}&0&0\\0&f_{2_2}&0\\0&0&f_{2_3}\end{bmatrix},\ g_{1_{ij}}=\begin{bmatrix}\frac{f_{1_1}}{\Omega_{\max_1}}&0&0\\0&\frac{f_{1_2}}{\Omega_{\max_2}}&0\\0&0&\frac{f_{1_3}}{\Omega_{\max_3}}\end{bmatrix} \tag{25}$$

The effective inelastic strain-rate defined in eqn (6) is only valid when isotropic assumptions are used. Therefore, it is also necessary to use a more general form for the inelastic effective strain rate $\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}}$, see Tay [10] (p. 94). To wit:

$$\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}}=\frac{\dot{\varepsilon}_{ij}S_{ij}}{\bar{S}} \tag{26}$$

where

$$\bar{S}=\sqrt{\frac{3}{2}S_{ij}S_{ij}} \tag{27}$$

This has now completely defined a potential MRS.

A general unified viscosity (GUV) model

The next model to be considered was based on similar principals to those discussed above, with a flow law, 'back stress' and some evolution equations for the state variables. The governing equations for this model are

$$\dot{\varepsilon}^{\mathrm{I}}_{ij}=D\exp\{eK_2\}\sinh\{EK_2\}\frac{(S_{ij}-\Omega_{ij})}{\sqrt{K_2}} \tag{28}$$

$$\Omega_{ij}=F_{ij}+g_{ij}\varepsilon^{\mathrm{I}}_{\mathrm{eff}} \tag{29}$$

$$F_{ij}=k_{ijkl}(\varepsilon^{\mathrm{I}}_{kl}-x_{kl}) \tag{30}$$

$$\dot{x}_{ij}=A_{ij}\exp\{b_{ijkl}F_{kl}\}\sinh\{c_{ijkl}F_{kl}\} \tag{31}$$

$$K_2=\sqrt{\frac{3}{2}(S_{ij}-\Omega_{ij})(S_{ij}-\Omega_{ij})} \tag{32}$$

$$\bar{S}=\sqrt{\frac{3}{2}S_{ij}S_{ij}} \tag{33}$$

$$\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}}=\frac{\dot{\varepsilon}^{\mathrm{I}}_{ij}S_{ij}}{\bar{S}} \tag{34}$$

where

$$\exp(A_{ij})=\begin{bmatrix}\exp(A_{11}) & \exp(A_{12}) & \dots\\ \exp(A_{21}) & \exp(A_{22}) & \dots\\ \vdots & \vdots & \dots\end{bmatrix} \tag{35}$$

Here D, E, E, G_{ij}, k_{ijkl}, A_{ij}, b_{ijkl} and c_{ijkl} are material constants and Ω, S, $\bar{S}$, $\dot{\varepsilon}^{\mathrm{I}}$ and $\varepsilon^{\mathrm{I}}_{\mathrm{eff}}$ are the back stress, the effective deviatoric stress, the inelastic strain rate and the inelastic strain respectively. F and x are additional state variables.

Again, experience has shown that this level of complexity was not required. The equations could be simplified by reducing the tensor forms down to equivalent vector terminology as follows:

$$\dot{\varepsilon}^{\mathrm{I}}_{i}=D\exp\{eK_2\}\sinh\{EK_2\}\frac{(S_{i}-\Omega_{i})}{\sqrt{K_2}} \tag{36}$$

$$\Omega_{i}=F_{i}+\tilde{g}_{i}\varepsilon^{\mathrm{I}}_{\mathrm{eff}} \tag{37}$$

$$F_{i}=\tilde{k}_{ij}(\varepsilon^{\mathrm{I}}_{j}-x_{j}) \tag{38}$$

$$\dot{x}_{i}=\tilde{A}_{i}\exp\{\tilde{b}_{ij}F_{j}\}\sinh\{\tilde{c}_{ij}F_{j}\} \tag{39}$$

where

$$\exp(A_i)=[\exp(A_1)\quad \exp(A_2)\quad \dots] \tag{40}$$

Even in this case the material constant tensors $\tilde{k}_{ij}$, $\tilde{b}_{ij}$, $\tilde{c}_{ij}$ are such that they only have trace elements. The vector $\tilde{g}_i$ is also a material constant. Of course the effecvtive terms K_2 and $\dot{\varepsilon}^{\mathrm{I}}_{\mathrm{eff}}$ are still calculated as before.

This formulation arose from an investigation of distributed viscosity and has therefore been termed a GUV model. The exponential multiplied the hyperbolic sine flow law, eqn (28), is similar to that presented in [11].

Finite element implementation

These models were subsequently implemented into the ABAQUS finite element code using the 'user material subroutine' facility. The rate equations presented above can be solved by writing them in the correct order and using the powerful LSODE package available from the Lawrence Livermore Laboratory and is documented in Hindmarsh [12]. To validate these material models, their predicted uniaxial stress–strain behaviour was compared with the results in Sawyer *et al.* [7].

To provide a computationally efficient solution ABAQUS requires that a consistent Jacobean be provided. This is defined as

$$J_{ij}=\frac{\partial\Delta\sigma_i}{\partial\Delta\varepsilon_j} \tag{41}$$

and is the change in the resulting stress increments given a change to one of the elements of the input strain increment vector. This was calculated using the perturbation method outlined in Trippit & Jones [13].

The major difficulty in this approach is the calculation of the size of the perturbation. If it is too small

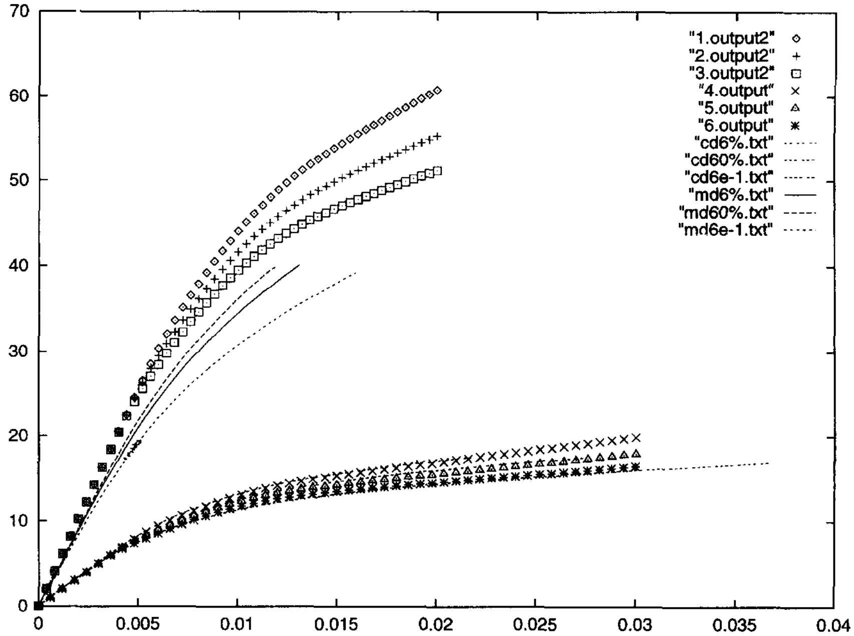

Fig. 1. The comparison of experimental machine direction and cross-direction stress–strain response with the predictions of the MRS model.

then the round-off errors tend to dominate. If it is too large then the detail can be lost. In Trippit & Jones [13] the equation

$$\Delta\varepsilon_{\text{pert}_{ij}} = 10^{n}|(\varepsilon_{\text{relative}}\varepsilon^{\text{I}}{}_{ij} + \varepsilon_{\text{absolute}})|\text{sign}\{\Delta\varepsilon_{ij}\} + \Delta\varepsilon_{ij} \tag{42}$$

was presented for determining the perturbation size, where $\Delta\varepsilon_{\text{pert}_{ij}}$ is the new strain increment for this perturbation in direction ij, $\Delta\varepsilon_{ij}$ is the strain increment for the step in direction ij, $\varepsilon_{\text{relative}}$ is the relative tolerance of the solver for $\varepsilon^{\text{I}}{}_{ij}$, $\varepsilon_{\text{absolute}}$ is the absolute tolerance of the solver for $\varepsilon^{\text{I}}{}_{ij}$, n is the number of significant figure required in the solution and sign(x) is given as $|x|/x$

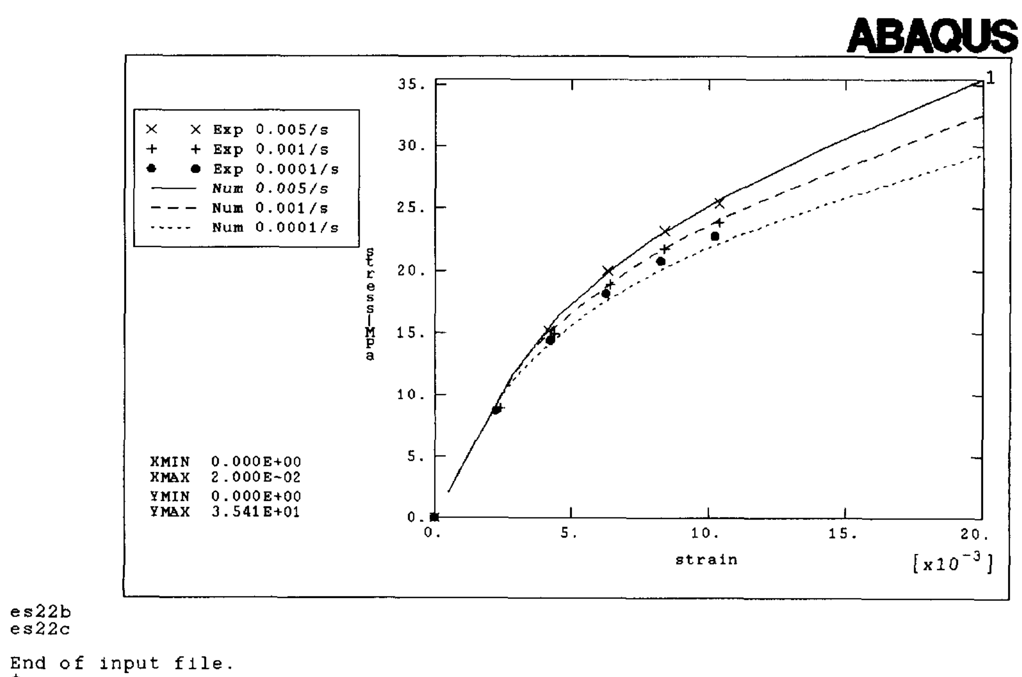

Fig. 2. The comparison of experimental response for samples cut at 32° from the machine direction with the predictions from the MRS model.

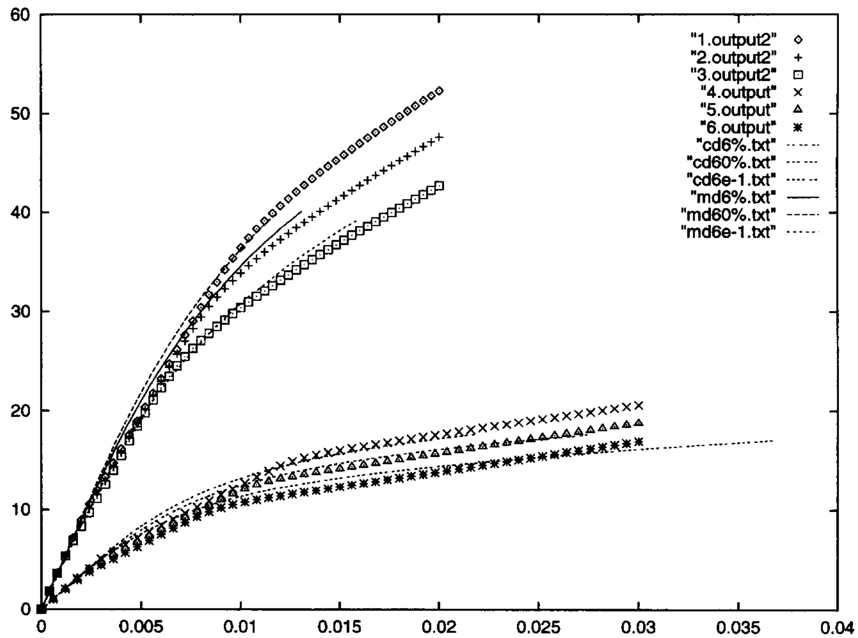

Fig. 3. The comparison of experimental machine direction and cross-direction stress–strain response with the predictions of the GUV model.

except when x is zero then $\mathrm{sign}(0) = 0$. This formula was based on an error analysis of the problem. The work of Trippit & Jones [13] suggested that n should be approximately 3.

Comparison with experimental results

The experimental results presented in Sawyer *et al.* [7] were used in conjunction with some off-axis test data

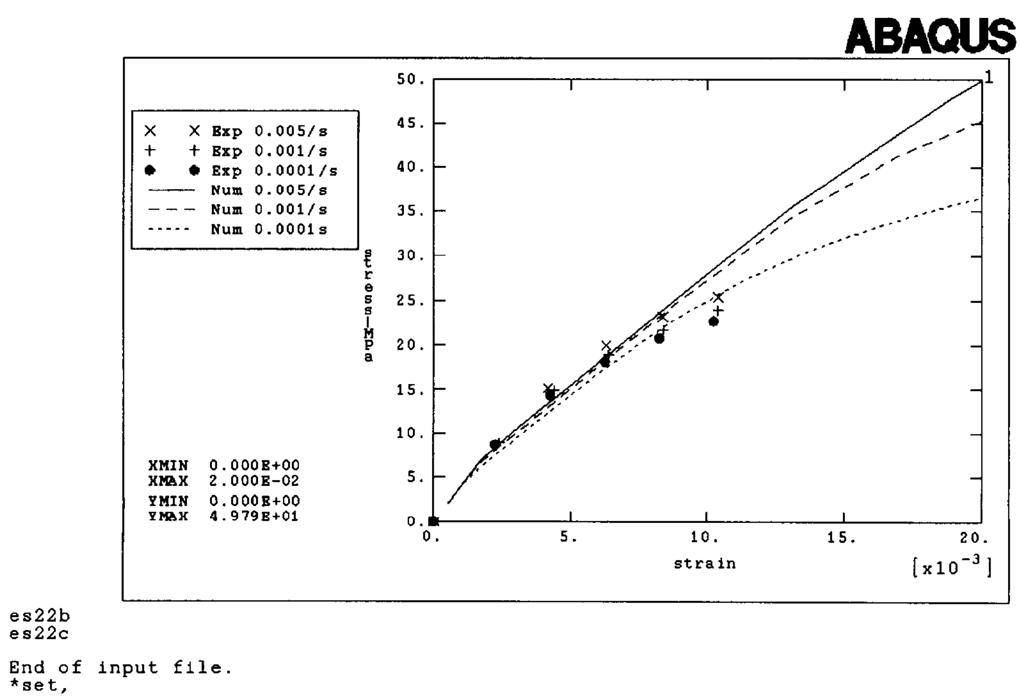

Fig. 4. The comparison of experimental response for samples cut at 32° from the machine direction with the predictions of the GUV model.

to deduce acceptable constants for this particular paper. The first was used to determine the constants necessary to model direct stresses and the off-axis tests were used to extract constants for the shear behaviour. The off-axis tests were performed using the test methodology described in Sawyer *et al.* [7], with the samples cut at 32° from the machine direction.

The results for the machine directions and the cross-direction for the first model can be seen in Fig. 1. The results for the off-axis test can be seen in Fig. 2. A similar set of results for the second model can be seen in Figs 3 and 4.

The results for the MRS model were not as good as for the machine direction, but the accuracy of this model for the cross-direction and off-axis tests were very good.

The predictions of the GUV model described above were excellent in both the machine direction and cross-direction the off-axis response was not as good. However, this model is believed to be the more appropriate approach.

Conclusions

This paper has presented two potential constitutive models for the structural response of paper. Both approaches are capable of accurately representing the monotonic response of paper. Work on the cyclic response, stress relaxation and environmental effects is continuing and will be reported in a subsequent paper. This latter work suggests that the 'unified viscosity' model may be a more appropriate approach.

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