COMPARISON OF PORTER-GOULD CONSTITUTIVE MODEL WITH COMPRESSION TEST DATA FOR HTPB/SUGAR

R Cornish[1], D Porter[1], P Church[1], P Gould[1], T Andrews[1], B Proud[2], D Drodge[2], C Siviour[3]

[1]*QinetiQ Ltd, Fort Halstead, Sevenoaks, Kent, United Kingdom*
[2]*Physics & Chemical Solids Group, Cavendish Laboratory, Cambridge University, United Kingdom*
[3]*Engineering Department, Oxford University, Oxford, United Kingdom*

Abstract. We have been developing the physically based QinetiQ Porter-Gould (P-G) model for the mechanical response of PBXs over a number of years and applying it to the solution of real scenarios involving impact and blast. The main difficulty with these models is predicting the intermediate strain rate regime where the relaxation time for the polymer is of the same order as the duration of the loading (e.g. as in a Hopkinson bar test). The other main issue is the ability of the model to predict the stress/strain data as a function of temperature up to and through the glass transition temperature. The paper presents predictions from the QinetiQ P-G model compared to quasi-static compression and Hopkinson bar compression test data and discusses the results in terms of requirements for future developments of the model.

INTRODUCTION

The underlying assumption for the model is that the mechanical response of a PBX is determined by its behaviour as a composite material. To replicate this one has to know the properties of binder and energetic filler and then concentrate on the physics of binder-particle interaction in as simple a way as possible and then to see how good the predictions are. The properties of the polymeric binder and of the energetic filler can be either measured or predicted. The model should be simple to write down and be clear in order to make implementation into numerical codes as efficient as possible. This approach has already given good predictions for the equation of state of PBXs [1].

To illustrate the model development and to provide an easy route to understanding how the model works we shall first consider deformation at room temperature only. The PBXs we consider are of the order of 88% by mass energetic filler with particles ranging in size from <1μm to >1mm. This range of sizes allows an assumption of no particle-particle interactions. The binders that we use are plasticized HTPB with a glass transition very much lower than room temperature.

This implies, and is confirmed by Dynamic Mechanical Analysis (DMA) experiments, that the modulus of the binder varies only slightly with temperature in the region of 300K. Strain rate effects should only move the glass transition by 5–10° equivalent temperature per decade. We therefore make an initial assumption that, for deformation around room temperature we do not need to take any temperature or strain rate variation of the modulus into account.

If a full temperature and strain rate variation of binder modulus is required then the DMA curve can

be predicted using the Group Interaction Modelling (GIM) technique [2].

MODEL DEVELOPMENT

The model assumes that the material follows Hooke's Law but that the secant modulus is a function of damage in the composite. So the stress/strain curve is generated by:

$$\sigma = E_c \varepsilon \qquad (1)$$

The particles in the composite range in size from below 1μm to above 1mm so we split the particle size distribution into four mass fractions: of order 1μm, of order 10μm, of order 100μm and of order 1mm. The particle size distribution is known so these mass fractions can be calculated.

The composite modulus, E_c, is calculated by considering each length scale in turn. It is assumed that, at the 1μm length scale, the larger particles play no part in determining modulus. So, by denoting the particle modulus as E_p and binder modulus as E_b we calculate the composite modulus at this level as:

$$\frac{1}{E_{c,1}} = \frac{V_1}{E_p} + \frac{1 - V_1}{E_b} \qquad (2)$$

where V_1 is the volume fraction of particles at this length scale. This Reuss method is chosen because the binder is significantly more compliant than the particles. For temperatures nearer the glass transition the modulus is more likely to be represented by the Hill-Voight-Reuss method. At each length scale the particle fractions are found to be below the 55% level at which point particle-particle interactions must be considered [3]. This will not be the case for total composite filler loadings above 90%. At the 10μm length scale we assume that the smaller length scale is sufficiently small that it appears as a continuum and so calculate modulus at this scale in the same way. This is repeated at the higher levels using E_c from the lower lengthscale as E_b at the next.

Damage to the composite material is assumed to occur by a Griffith-type debonding process whereby work done to the material activates cracking in the binder. This cracking causes a loss of constraint and thereby reduces the modulus of the binder. We define two binder moduli, E_{dam}, the damaged modulus, and E_{undam}, the undamaged modulus. Each small local volume of binder is equally likely to crack and so we consider each to be a separate state. The fraction of failed states – that is the fraction of small local volumes that have cracked and thereby have E_{dam} rather than E_{undam} – is denoted "f". The binder modulus is therefore:

$$E_b = E_{undam} - f * \left(E_{undam} - E_{dam}\right) \qquad (3)$$

The work done on the binder is a function of the compliances. The "binder" at the highest length scale sees a fraction of the work done on the composite:

$$W_{c,100} = \frac{E_p}{E_p + E_{c,100}} W_c \qquad (4)$$

and so on at lower length scales.

The probability of cracking is an activation process. If W_0 is an energy density characteristic of failure in the binder then the fraction of failed states is:

$$f = \frac{2 * \exp\left(-\frac{W_0}{W_b}\right)}{1 + \exp\left(-\frac{W_0}{W_b}\right)} \qquad (5)$$

where W_0 is a material parameter which can, eventually, be calculated from theory. In the first instance, however, it is used as a fitting parameter.

The method is used here to predict the stress/strain behaviour of a HTPB/sugar composite. Sugar is used as an inert simulant as its mechanical properties are similar to RDX. A mixture of fine icing sugar and less fine caster sugar were used. The binder is the same as is used in normal PBXs: a plasticized HTPB.

RESULTS OF MODEL PREDICTION

The model, with binder moduli predicted by GIM, was used to predict stress/strain response at room temperature for low strain rate deformation

and for Hopkinson bar experiments. The same value for W_0 was used for both rates. The results are shown in Figure 1. The moduli predicted at both rates are very similar because the glass transition is at a significantly lower temperature than room temperature. The predicted stress/strain response for both rates in the model can thus be represented by a single curve. This can significantly underpredict the Hopkinson bar response as shown in Figure 1. The "updated prediction" curve is referred to later.

One can measure the moduli of the HTPB/sugar composite at Hopkinson bar rates by extracting the data from experimental stress/strain curves. They are compared over a range of temperatures with the predicted modulus variation in Figure 2. It can be seen that the glass transition is shifted to higher temperatures, as would be expected, but also that the transition occurs over a much wider temperature range than would be expected. The loss tangent associated with the glass transition is also lower than expected.
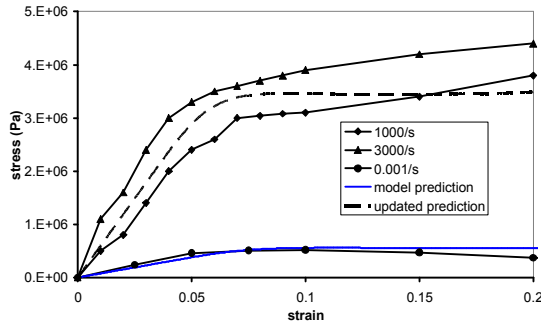

Figure 1: Comparison of model with data at low and high strain rate

DMA tests at rates equivalent to the Hopkinson bar loading rate do not show the effects seen here. The effect on the transition appears to be characteristic of the loading state. It could also be affected by the higher strains seen in the binder. Interactions between binder, plasticizer and filler may also play a role.

The issue of Hopkinson bar tests measuring stresses significantly higher than would be expected has been well documented [4]. Various mechanisms have been proposed for polymers [5] but the most compelling avenue for development appears to be that of Mullikan and Boyce [6]. The composite contains a number of different interactions that are

normally seen at low temperatures but that, under the influence of both high strain rate and high strain, move to a much higher temperature and also to different temperatures thereby widening the total transition curve.

Until such time as we understand the physics at intermediate rate and can predict both the DMA curve and how its component transition losses are affected by temperature, rate and strain we will not be able to produce a more physically real prediction. We are forced to use empirical fits to data in the interim.

We have taken an empirical fit to the binder behaviour in an attempt to retain as much composite materials physics as possible. This fit is then used in the model described above to reproduce the experimental results, Figures. 3 and 4 and the "updated prediction" in figure 1.
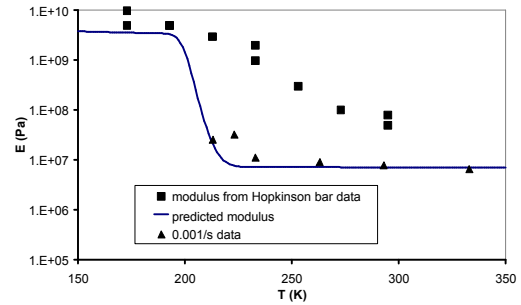

Figure 2: Comparison of predicted initial modulus with that measured from data

As would be expected from an empirical fit the initial modulus is well described as is the peak stress. This gives confidence that, should an accurate physical description of the binder properties in the intermediate strain rate regime be developed, the model would be a good predictor of general behaviour in these composites.

The manner in which the curve turns over – which depends upon the manner in which the particle size distribution is implemented – is too sharp. At the moment damage affects the composite modulus by changing the binder modulus. The model should include other indirect effects of damage such as changing the local transitions and thereby the modulus. Isolation of particles by debonding should remove them from influencing the shear modulus and the model should take this into

account by an evolution of the particle size distribution during deformation. This latter need not be empirical as it is generally understood that the largest particles will debond first. Thus the number of failed states could be converted into a surface area of debonding and thereby into how many of the particles, largest first, have debonded.
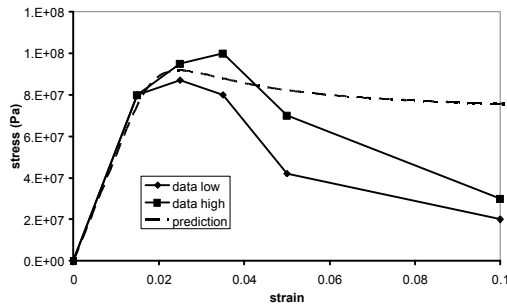

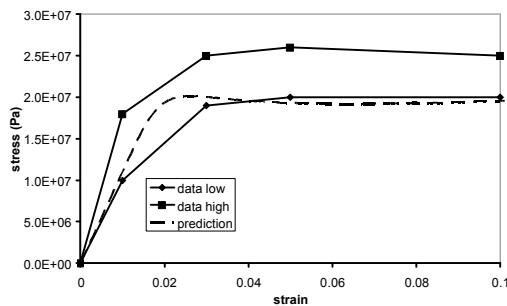**Figure 3:** Prediction using empirical fit to binder properties at 193K, 2000/s

Figure 4: Prediction using empirical fit to binder properties at 233K, 2000/s

The evolution post peak is also not well reproduced. This is, in part, due to an inability of the model to include large scale cracking; implementation into a numerical code could remedy this. There is also an effect of the damaged modulus. This modulus includes a number of complex local effects but is represented by a single global number. Such local effects include local relaxation on debonding and the manner in which a locally relaxed volume will then resist relaxation of neighbouring volumes when they, in turn, try to relax on debonding.

CONCLUSIONS

What we have tried to present is a continuum approach that takes into account microstructure of PBXs using composite materials science. Whilst the model is simple it provides a physically based framework into which the detailed mechanisms of the composite mechanical response can be inserted. There is every reason to believe that the interactions can be described in a physical manner without recourse to empiricism although that goal is still some way off. It is also clear that the main challenge to be overcome to achieve this goal is a truly physically based description of the intermediate strain rate behaviour.

ACKNOWLEDGMENT

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