ELSEVIER

International Journal of Pharmaceutics 105 (1994) 177–180

international journal of pharmaceutics

The Poisson's ratio of microcrystalline cellulose

R.J. Roberts [a,*], R.C. Rowe [a], P. York [b]

[a] *ZENECA Pharmaceuticals, Alderley Park, Macclesfield SK10 2NA, UK,*
[b] *Pharmaceutical Technology, The School of Pharmacy, University of Bradford, Bradford BD7 1DP, UK*

(Received 27 August 1993; Accepted 18 October 1993)

Abstract

The Poisson's ratio of microcrystalline cellulose has been found to be 0.30 (as determined by independent measurements of shear and Young's modulus). This value compares well to aspirin ($\nu = 0.29$ – calculated from single-crystal elastic constants), a material with similar yield and elastic properties to microcrystalline cellulose.

Key words: Poisson's ratio; Shear modulus; Young's modulus; Porous compacted specimen

1. Introduction

All materials when stressed under tension or compression undergo shrinkage or expansion, respectively, in the direction perpendicular to the applied stress. Both effects constitute a transverse strain, the ratio of which to the longitudinal strain is defined as the Poisson's ratio (ν) of the material. For an isotropic material ν will have an upper limit of 0.5 (equivalent to rubber which conserves its volume during deformation) while typical values of ceramics and metals range between 0.2 and 0.4 (Kaye and Laby, 1973).

In tabletting the Poisson's ratio of a material is specifically important, since it defines the relationship between the axial and radial pressures in the powder bed prior to yield. In fact, several authors (Long, 1960; Leigh et al., 1967; Summers et al., 1976) have attempted to calculate the Poisson's ratio of various materials from monitoring axial and radial pressures in a die during compaction. However, all appear to use different relationships in calculations and hence the results are inconclusive.

Direct measurement of Poisson's ratio involves measurement of very small strains and generally for specimens of pharmaceutical materials is experimentally difficult. Hence, little work has been done in this field, the majority of pharmaceutical scientists (e.g., Ridgway et al., 1970) assuming a global value of 0.3 when a figure is required. However, there are two notable exceptions; Church (1984) who used a biaxial flexure test on compacted cylindrical specimens to measure the Poisson's ratio of microcrystalline cellulose and starch and Sarumi (1987) who used uniaxial tension/compression testing of large cylindrical cylinders to measure the Poisson's ratio of directly compressible sugar.

* Corresponding author.

SSDI 0378-5173(93)E0335-N

Indirect measurement of Poisson's ratio from independent experimental measurements of Young's modulus, E, and shear modulus, G, is possible since all variables are related by the equation:

$$\nu = \frac{E}{2G} - 1 \quad (1)$$

This concept has been tested in this paper using literature data on microcrystalline cellulose measured using beam specimens.

2. Experimental

2.1. Determination of shear modulus, G

Radebaugh et al. (1989) have described a technique for directly measuring shear modulus using a small strain sinusoidal oscillation torsion of beam specimens of dimensions $122 \times 50 \times 2.8$ mm. Experiments performed on samples of microcrystalline cellulose (Avicel PH102) compressed to various porosities (Fig. 1) with the data fitted to a two-order polynomial of the form (Spinner et al., 1963):

$$G = G_0(1 - f_1 P + f_2 P^2) \quad (2)$$

where G is the measured shear modulus of the beams compared at porosities P and f_1 and f_2 are constants. This equation was chosen since Bassam et al. (1990) have found that it is the optimum describing the relationship between Young's modulus of elasticity and porosity for compacted beams of pharmaceutical materials of similar dimensions. In this case, the fit is remarkably good (a correlation coefficient and standard error of 0.9994 and 0.027, respectively) with values for f_1 and f_2 of 3.3006 and 2.7788, respectively. An extrapolation to zero porosity results in a value for the shear modulus of microcrystalline cellulose (Avicel PH102) of 3.49 GPa.

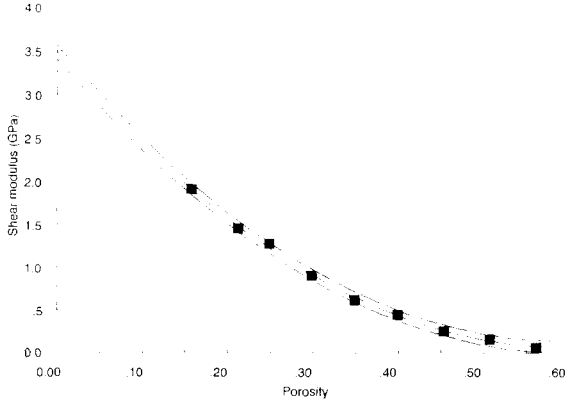

Fig. 1. Shear modulus vs porosity for microcrystalline cellulose (Avicel PH102 – adapted from Radebaugh et al. (1989). Continuous line represents the best fit for the data and the dotted lines are the 95% confidence limits for the data.

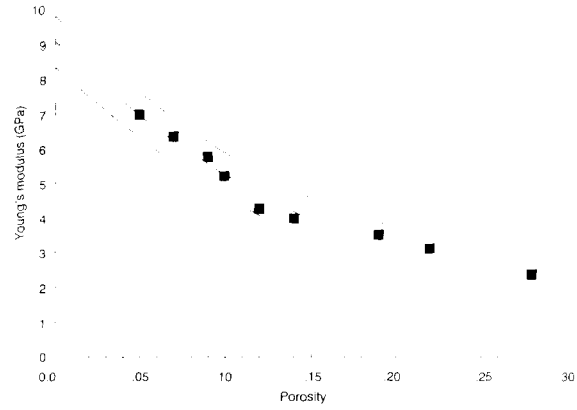

Fig. 2. Young's modulus vs porosity for microcrystalline cellulose (Avicel PH102 – data obtained from Bassam (personal communication)). Continuous line represents the best fit for the data and the dotted lines are the 95% confidence limits for the data.

2.2. Determination of Young's modulus, E

Data from four-point flexure testing of beams of $100 \times 10 \times h$ mm (h varying with porosity) on microcrystalline cellulose (Avicel PH102) are shown in Fig. 2 (Bassam et al., 1990). As with shear modulus the data have been fitted to a second order polynomial (Eq. 3).

$$E = E_0(1 - f_1 P + f_2 P^2) \quad (3)$$

where E is the measured Young's modulus of the beams compared at porosities P and f_1 and f_2 are constants. In this case the fit is not as good as that for shear modulus (a correlation coefficient and standard error of 0.9887 and 0.269, respectively) with values for f_1 and f_2 of 5.1193 and

9.1224, respectively. An extrapolation to zero porosity results in a value of the Young's modulus of 9.08 GPa.

2.3. Determination of Poisson's ratio, ν

Using Eq. 1 and substituting values for the shear and Young's modulus of microcrystalline cellulose (Avicel PH102) of 3.49 and 9.08 GPa respectively, results in a value of Poisson's ratio of 0.30. This compares with values of between 0.24 and 0.38 (dependent on specimen) reported by Church (1984). Unfortunately, Church (1984) did not extrapolate any data to zero porosity, preferring to work over a small range of porosities of 0.16–0.20.

2.4. Calculation from single crystal elastic constants

In a recent paper, Roberts et al. (1991) have demonstrated that knowing the single-crystal elastic constants of various materials it is possible to calculate values of both shear and Young's modulus comparable to those measured by flexure testing. Of pharmaceutical interest in this respect is aspirin where it is possible using literature data on single-crystal elastic constants (Kim et al., 1985) to calculate values of shear modulus and Young's modulus of 3.3 and 8.5 GPa, respectively. Substitution of these values into Eq. 1 results in a Poisson's ratio of 0.29 for aspirin. The similarity of the two values for the two materials microcrystalline cellulose and aspirin is not surprising, since both have similar yield stresses (49 MPa – Roberts and Rowe, 1986; 25 MPa – Humbert-Droz et al., 1983; respectively) and Young's modulus (9.08 GPa – this work; and 7.45 GPa – Roberts et al., 1991; respectively) and can be regarded as plastic deforming ductile materials.

3. Conclusion

It is possible to determine Poisson's ratio of microcrystalline cellulose indirectly from experimental measurements of shear and Young's modulus of elasticity on compacted beams. The data are reasonable in light of known values of other similar materials. It would appear that taking a value of Poisson's ratio of 0.3 for pharmaceutical materials is justifiable. However, this may not be the general rule, since Roberts et al. (1991) have shown that hexamine has a Poisson's ratio of 0.18. With care compacted beams can be produced fairly easily for a wide variety of drugs and excipients used in tabletting (Roberts et al., 1991), and therefore it should be now possible to accurately measure Poisson's ratios for such materials. This will enable predictions to be made regarding the relative build up of die wall stresses during tabletting resulting in more optimal tablet formulations.

4. References

Bassam, F., York., Rowe, R.C. and Roberts, R.J., Young's modulus of powders used as pharmaceutical excipients, *Int. J. Pharm.*, 64 (1990) 55–60.

Church, S.C., Mechanical characterisation of pharmaceutical powder compacts, Ph.D. Thesis, Nottingham (1984).

Humbert-Droz, P., Gurny, R., Mordier, D. and Doekler, E., Densification behaviour of drugs presenting availability problems, *Int. J. Pharm. Tech. Prod. Mfr.* 4 (1983) 29–35.

Kaye, G.W.C. and Laby, T.H., Tables of physical and chemical constants: and some mathematical functions, 14th Ed., Longman, London, 1973.

Kim, Y., Machida, K., Taga, T. and Osaki, K., Structure redetermination and packing analysis of aspirin crystal, *Chem. Pharm. Bull.*, 33 (1985) 2641–2647.

Leigh, S., Carless, J.E. and Burt, B.W., Compression characteristics of some pharmaceutical materials. *J. Pharm. Sci.*, 56 (1967) 888–892.

Long, W.M., Radial pressures in powder compaction. *Powder Metall.*, 6 (1960) 73–86.

Radebaugh, G.W., Babu, S.R. and Bondi, J.N., Characterisation of the viscoelastic properties of compacted pharmaceutical powders by a novel nondestructive technique. *Int. J. Pharm.*, 57 (1989) 95–105.

Ridgway, K., Aulton, M.E. and Rosser, P.H., The surface hardness of tablets. *J. Pharm. Pharmacol.*, 22 (1970) 70S–78S.

Roberts, R.J. and Rowe, R.C., The effect of the relationship between punch velocity and particle size on the compaction behaviour of materials with varying deformation mechanisms. *J. Pharm. Pharmacol.*, 36 (1986) 567–571.

Roberts, R.J., Rowe, R.C. and York, P., The relationship between Young's modulus of elasticity of organic solids

and their molecular structure. *Powder Technol.*, 65 (1991) 139–146.

Sarumi, M., Compaction of pharmaceutical powders, M.Sc. Thesis, UMIST, 1987.

Spinner, S., Knudsen, F.P. and Stone, L., Elastic constant porosity relations for polycrystalline thoria. *J. Res. Nat. Bur. Stand. (Eng. Instr.)*, 1 (1963) 39.

Summers, M.P., Enever, R.P. and Carless, J.E., The influence of crystal form on the radial stress transmission characteristics of pharmaceutical materials. *J. Pharm. Pharmacol.*, 28 (1976) 89–99.