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The Young's modulus of pharmaceutical materials

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Summary

Currently available data on the Young's modulus of elasticity of a number of pharmaceutical materials used in tabletting are reviewed and compared with those predicted using the equation given by Marsh (1964) relating the Young's modulus of a material to its indentation hardness and yield pressure. There is very good agreement for the softer materials but anomalies exist for the harder materials.

Introduction

If an isotropic body is subjected to a simple tensile stress in a specific direction it will elongate in that direction while contracting in the two lateral directions, its relative elongation being directly proportional to the stress. The ratio of the stress to the relative elongation (strain) is termed the Young's modulus of elasticity of the material. It is a fundamental property of the material, a measure of its stiffness directly related to its interatomic bonding energy. It is an important property with respect to tabletting not only in determining compaction behaviour but also in governing the mechanical properties of the resultant compact.

The Young's modulus of elasticity of a material can be determined by many techniques several of which have been used in the study of pharmaceutical materials viz. flexure testing of beam specimens (Church, 1984; Church and Kennerley, 1984), compression of cylindrically shaped specimens (Kerridge and Newton, 1986) and indentation of crystals (Ridgway et al., 1969). While the methods may be regarded as direct measurements since the modulus is determined from actual stress/strain data, it is also possible to calculate the modulus from equations relating it to other mechanical properties more easily determined experimentally. An equation shown by Tabor (1970) to be of almost universal applicability is that of Marsh (1964):

$$\frac{H}{P_y} = 0.07 + 0.6 \ln \frac{E}{P_y} \quad (1)$$

where E is the Young's modulus of elasticity of the material, H is its indentation hardness and P_y its yield pressure. Although P_y in this equation is the yield pressure under the indenter and hence difficult to measure, recent data by Roberts and Rowe (1987) collated for a wide variety of materials, e.g. iron, copper, polyethylene, and polytetra-

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TABLE 1

A comparison of the Young's modulus of elasticity of pharmaceutical materials, determined from different techniques

Young's modulus of elasticity (GPa)						
Material	Flexure testing		Compressive testing	Indentation	Predicted	Literature values
	Eqn. 2	Eqn. 3				
Aspirin	–	–	2.3	0.1	1.3	–
Sodium Chloride	19.1	14.3	–	1.9	15.9	35.5–336.0 [1]
Potassium Chloride	–	–	9.2	–	–	21.2–25.6 [1]
Paracetamol D.C.	–	–	–	–	5.7	–
Lactose (spray-dried)	13.5	7.6	–	–	–	–
Lactose (anhydrous)	–	–	–	–	53.0	–
Sucrose	–	–	–	2.2	–	–
Mannitol	–	–	–	–	24.2	–
Cellulose (microcrystalline)	9.7	8.3	4.7	–	13.2	10.0–16.0 [2]
Cellulose (microfine)	8.6	6.7	–	–	–	–
Dicalcium phosphate dihydrate	181.5	16.3	–	–	7.0	–
Maize starch (modified)	6.1	3.1	–	–	–	–

[1] Simmons and Wang (1971)
[2] Atkins and Mai (1985).

fluoroethylene, have shown that it is numerically equal to the yield pressure determined from compaction experiments performed at very low speeds (0.033 mm/s). Hence, by using recently generated yield pressure data (Roberts and Rowe, 1985) and indentation hardness measurements (Jetzer et al., 1983), it is possible to calculate Youngs' modulus of a wide range of pharmaceutical materials.

Data from all the various techniques in addition to that given in the engineering literature are summarised in Table 1. One of the problems associated with the comparison of data for specimens prepared from particulate solids is in the definition of the porosity at which the comparisons should be made. While the data from Kerridge and Newton (1986) and that used in Eqn. 1 had already been extrapolated to zero porosity, that from Church (1984) had not. In this case two equations were used, Eqn. 2 (Spriggs, 1961) equivalent to that used by Kerridge and Newton (1986) and Eqn. 3 recommended by Wachtman (1969), for low porosities:

$$E = E_0 \exp(-b\epsilon) \quad (2)$$

$$E = E_0(1 - a\epsilon) \quad (3)$$

where E is the Young's modulus of the specimen of porosity ϵ, E_0 is the Young's modulus at zero porosity and b and a are constants. It is interesting to note that whereas Eqn. 2 is a purely empirical one, Eqn. 3 is a simplified form of that derived by Hashin (1962) from a consideration of the fundamental fluid mechanics of heterogeneous systems. In this case the constant, a, is related to the shape of the pores within the compacted specimen ranging from 2 for specimens with spheroidally shaped pores (predicted theoretically by Mackenzie (1950) and Hashin (1962) and determined experimentally using glass by Hasselman and Fulrath (1964) to 3 for specimens with cylindrically shaped pores of circular cross section (as reported by Bert (1985) and to 4 for specimens with ellipsoidal shaped pores (predicted theoretically by Rossi (1968)). High-correlation coefficients were obtained for the data using both equations' values for the constant, a, ranged from 2.97 for the microfine cellulose (Elcema) to 3.34 for the microcrystalline cellulose (Avicel) to 4.0 for the sodium chloride and to 4.15 for the starch. These are reasonable values in the light of what is generally known about the pore structure of compacts prepared from these materials (Ritter and Sucker;

1980; DeBoer et al., 1978; Paronen and Juslin, 1983).

With the exception of the dicalcium phosphate dihydrate (Emcompress) the values of E_0 from both equations are comparable and similar to those calculated using Eqn. 1. The reason for the anomalies in the data for the Emcompress is not fully understood and may well be due to the fact that this material is difficult to compact to low porosities and hence the extrapolation of indentation hardness H to zero porosity may not be valid in this case. It is interesting to note that the values for sodium chloride are a factor of 2 lower than the engineering literature values on single crystals whereas those for microcrystalline cellulose are comparable with the engineering literature values for coniferous pine wood, the pulp of which is similar to that used in the manufacturing process (Lamberson and Raynor, 1976) of microcrystalline cellulose.

The moduli from compression testing are lower than those from both flexure testing and prediction using Eqn. 1. This is surprising since generally compressive moduli are higher than tensile moduli. The data from indentation measurements are extremely low but it is interesting to note that the ratio between the values for sodium chloride and aspirin are similar to that between the predicted values for the same materials.

In conclusion it can be seen that for the softer materials there is reasonably good agreement between the predicted values and those from direct measurement. However, despite this proviso, the data generated are useful in distinguishing between materials in terms of their resistance to deformation.

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