A NUMERICAL STUDY ON THE MECHANICAL BEHAVIOUR OF PHARMACEUTICAL POWDERS DURING COMPRESSION

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Introduction

Tablets are the most common and popular dosage form for administering drugs via an oral route due to their various advantages over other dosage forms, such as chemical and physical stability, acceptable shelf time, accurate dosage of the drug and ease of controlling drug release. For patients, tablets are convenient to be handle since they are portable, easy to administer, and sweeteners or coatings can be used to mask any unpleasant tastes. From the manufacturing point of view, tablets can be mass-produced with high production rates. The process of tabletting can be divided into three distinct stages [1]: 1) die filling, 2) compression, and 3) ejection. The powder behaviour during each of these stages influences the properties of the final compact. Therefore, understanding the mechanical behaviour of powders during compaction is very important.

In this study, the finite element method (FEM) is employed to analyse the compression behaviour of pharmaceutical powders. The effects of kinematics of punch movements and the friction between powder and die wall is explored.

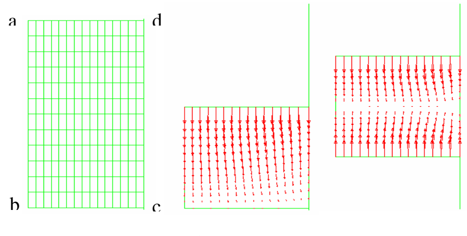
Finite element analysis of pharmaceutical powder compaction

Finite element methods (FEM) have been widely used for modelling the compaction of metallic and ceramic powders, and have recently been used for analysing pharmaceutical powder compaction [2, 3]. In FEM, powders are modelled as continuum media and the compaction behaviour is analysed by solving boundary value problems. Powders are generally assumed to be elastic-plastic materials with proper yield surfaces to represent the yield behaviour of the materials. The most widely used yield surface in modelling powder compaction is Drucker-Prager-Cap model [4], which also is chosen in this study.

A commercial package, ABAQUS [4], was used to simulate the compaction process with the Drucker-Prager-Cap model implemented. User subroutines were developed to determine the relative density distribution and the average density of the compact. The evolution of density during compression was analysed using the Heckel function, which was developed to characterise the compressibility of powders. Lactose powder is considered and corresponding material properties given by Michrafy *et al.* [2] were used. The influence of die-wall friction was investigated by varying the friction coefficients, which were set to 0.06 and 0.3 in this study.

We considered a typical case to make a cylindrical tablet of 10mm in diameter and 5mm in height. The initial height of the powder bed was 10mm. Two types of processes were considered: 1) Single Ended Compression (SEC): where the powder is compressed by the upper punch only; 2) Double Ended Compression (DEC): where the powder is compressed by both the upper and lower punches simultaneously. Since both cases are axisymmetric, they can be analysed with a 2-dimensional finite element model.

Figure 1a shows the FE mesh before compaction, which consists of 180 four-node axisymmetric continuum elements. The die-wall, upper and lower punches were modelled as rigid bodies. The interaction between the powder and die-wall and punches are modelled by master-slave contacts with finite sliding. The nodes on the symmetrical axis (ab) are restricted to move in horizontal direction.

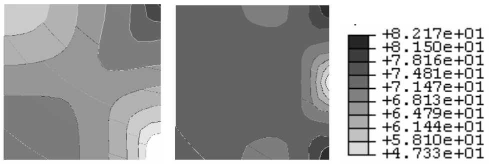


a) b) SEC c) DEC

Fig. 1 a) Finite element meshes; b) and c) displacement distributions

Results and discussion

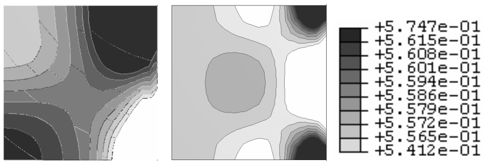
During compression, the motion of the powder bed is driven by the moving punches. Figures 1a and 1b show the displacement of the powder bed during compression under SEC and DEC, respectively. It is clear that the displacement gradually decreases towards the stationary punch for SEC and the mid-height of the powder bed in DEC. A significant reduction in displacement can be clearly observed at the die-wall boundary; this is due to the presence of friction that inhibits the movement of powders near the die wall. Consequently, the powder close to the junction of the moving punch and die-wall is highly compressed, as shown in Fig. 2 in which the stress distribution during compression is presented.



a) SEC b) DEC

Fig. 2 The effective stress distribution during compression ($\mu = 0.06$).

a) SEC ($\mu = 0.06$) b) DEC ($\mu = 0.06$)



c) SEC($\mu = 0.3$) d) DEC ($\mu = 0.3$)

Fig. 3 The density distribution during compression.

As the powder bed is not compressed uniformly, a non-uniform density distribution is produced. Figure 3 shows density distributions obtained for SEC and DEC with different die-wall frictions. It can be seen that a high density zone is developed around the top corner, and a low density zone near the bottom corner for SEC (Figs. 3a and 3c), while for DEC, high density zones are developed near both the top and bottom corner, and a low density zone is found located at the mid-height of the compacts. It appears that, at low wall friction, DEC (see Fig. 3b) has certain advantages over SEC (Fig. 3a), since a more uniform density distribution is obtained in DEC. However, at high wall friction, potential defects such as chipping around the edge could be produced in both SEC and DEC (Figs.3c &3d).

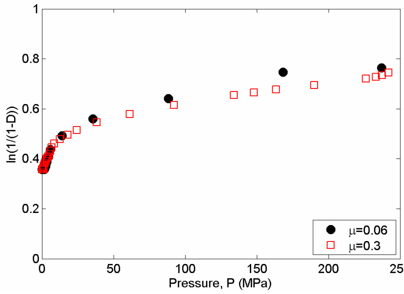


Fig. 4 Variation of density with pressure as defined by Heckel function.

The average density of the powder bed is dependent upon the applied pressure during compression. The correlation can be analysed in terms of Heckel function [5]. Figure 4 shows the Heckel plot of FEA data for SEC at different frictions, in which only data points for the pressures less than the maximum calibration pressure (ca. 250Mpa, [2]) are shown. It can be seen that a curved section is visible at low pressure (<50MPa) and at high pressure a linear relation is obtained, which is due to the different dominant compression mechanisms [6]: particle rearrangement and fragmentation at low pressure and plastic deformation at high pressure. The FEA results are hence consistent with the published data. In addition, it can be seen from Fig.4 that the die wall friction has only limited effects on the variation of density with pressure.

Conclusion

Mechanical behaviour of lactose powder during compression was analysed using FEM. The effects of two different compaction schemes and the friction between powder and die wall were explored. It was found that a significant density variation during compression is induced due to die wall friction, which has potentially detrimental effects on the properties of the final compacts. The variation of average density with applied pressure is analysed in terms of Heckel function. It is demonstrated that FEA can capture the essential aspects of the behaviour of pharmaceutical powders during compression.

Acknowledgements

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