Investigating the effect of tablet thickness and punch curvature on density distribution using finite elements method

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\textbf{A B S T R A C T}

Finite elements method was used to study the influence of tablet thickness and punch curvature on the density distribution inside convex faced (CF) tablets. The modeling of the process was conducted on 2 pharmaceutical excipients (anhydrous calcium phosphate and microcrystalline cellulose) by using Drucker–Prager Cap model in Abaqus\textsuperscript{®} software. The parameters of the model were obtained from experimental tests.

Several punch shapes based on industrial standards were used. A flat-faced (FF) punch and 3 convex faced (CF) punches (BR11, BR8 and BR6) with a diameter of 8 mm were chosen. Different tablet thicknesses were studied at a constant compression force.

The simulation of the compaction of CF tablets with increasing thicknesses showed an important change on the density distribution inside the tablet. For smaller thicknesses, low density zones are located toward the center. The density is not uniform inside CF tablets and the center of the 2 faces appears with low density whereas the distribution inside FF tablets is almost independent of the tablet thickness.

These results showed that FF and CF tablets, even obtained at the same compression force, do not have the same density at the center of the compact. As a consequence differences in tensile strength, as measured by diametral compression, are expected. This was confirmed by experimental tests.

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1. Introduction

During the development of a pharmaceutical tablet, the choice of the shape is important. This choice can be esthetics and/or technical and has consequences in the coating and packaging processes and finally in all the handling steps. For example, to avoid high friability, beveled-edge or convex faced (CF) tablets are preferred. If coating is required, flat-faced (FF) and beveled-edge tablets should be discarded as they could stick together or twin during the coating process (Gad, 2008).

From an academic point of view, the study of the compaction of pharmaceutical powder is more easily performed on FF tablets. To study accurately the phenomena that occur during compaction, it is important to use an instrumented press, which gives access to the different compression parameters (stresses and displacements). It is difficult to precisely measure these parameters, especially the displacements, when using complex shaped punches. It is thus understandable that most of the published studies that deal with the characterization of powder compaction on instrumented presses are performed using FF punches.

Unfortunately, the results obtained using FF punches cannot always be generalized to the cases of more complex punch shapes. The phenomenon of capping is a good example. The term capping refers to the separation of the top layer of the tablet after ejection (Ritter and Sucker, 1980) and it is well-known that CF tablets are more prone to capping than FF tablets (Gad, 2008). Moreover, the capping tendency increases with the increase of the punch curvature. It was also mentioned in the literature that the thickness played a role in the capping phenomena of CF tablet, and that thinner CF tablets are more prone to capping than thicker ones (Sugimori et al., 1989).

To better understand the behavior of complex shape tablets, the study of the real compact geometry is required. Previous studies performed on tablets with convex shape for both experimental (Sinka et al., 2004) and numerical (Eilazadeh et al., 2004; Han et al., 2008; Kadiro and Michrafy, 2013; May et al., 2013) approaches
showed that the results obtained for convex shape, i.e., the density and stress distributions, are different from the ones obtained on FF tablets. In fact, these works pointed out that the density is not uniform inside the CF tablet. Thus, it would be interesting to perform further studies to better understand and control the effects of a convex shape on density distribution inside CF tablets. Nevertheless, at the moment, there is no experimental way to access to the behavior of the powder in the die during the compression in order to explain and anticipate the density distribution. After compaction, experimental characterizations can be done to access to the local distribution of the tablet properties (Busignies et al., 2006; Sinka et al., 2004) but these studies are often long and expensive.

To overcome these experimental problems, one solution is to use numerical modeling, especially using finite elements method (FEM). The application of FEM modelling to the compaction process has been widely developed in the last 15 years. It was found that, by using well calibrated models like Drucker–Prager Cap model, it was possible to simulate correctly the process of compaction. Comparison between experimental and simulated results demonstrated that this approach could be well suited to describe the phenomena occurring during powder compaction (Diarra et al., 2012, 2013; Han et al., 2008; Michrafy et al., 2011; Sinka et al., 2004).

In this study, FEM was used to investigate the local density distribution inside CF tablets in different conditions, i.e., using several punch curvatures and several tablet thicknesses. The relative density (RD) in different parts of the tablet was studied in order to understand the cohesion of CF tablets. In fact, the cohesion of the tablet is directly linked with its density. Consequently, changes in the density could explain differences in cohesion and thus in mechanical properties.

2. Materials and methods

Two powders were chosen and processed by die compaction in order to characterize the parameters of the numerical model.

2.1. Powders

Two pharmaceutical tableting excipients with different mechanical behaviors were used to conduct this study: anhydrous calcium phosphate (aCP) (ATAB®, Rhodia, France) which is a brittle material and microcrystalline cellulose (MCC) (Avicel® pH-200, FMC Biopolymer, Newark, Delaware) which has a ductile behavior. The powders were mixed with 1% (w/w) of magnesium stearate (MF3V®, Peter Greven, Bad Münstereifel, Germany) to reduce the frictions between powder and compaction tools. The mixture was performed in a turbula mixer (Type T2C, Willy A Bachofen, Muttenz, Switzerland) and the operating conditions were fixed at 50 rpm for 5 min.

2.2. Tableting press

To characterize the parameters of the numerical model, compaction experiments were performed using a Stylcam® 2008 compaction simulator (Medelpharm, Bourg en Bresse, France). This press performs symmetric compression. The pressure on the upper punch, the lower punch and the die wall and also the upper and lower punch displacements were measured. Further information concerning the experimental conditions for the running of this single station press can be found elsewhere (Mazel et al., 2012; Michaut et al., 2010). To characterize the model parameters (Section 2.3), pharmaceutical compacts were produced using standard euro B round flat-faced punches with a

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**Fig. 1.** Elastic parameters $E, v$ (A) and DPC model parameters: $d, R$ (B) and $P_b$ (C) obtained from experimental tests.