Towards simulation of compaction processes

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Abstract

A finite element modeling (FEM) method utilizing the axisymmetric capabilities of Comsol Multiphysics is presented. The model provides the possibility for evaluating both elastic and plastic deformation occurring during indentation experiment. The evaluation of the elastic and plastic deformation can be obtained from the calculated load displacement versus pressure profile that provides the maximum indentation depth at the highest load and the final indentation depth after unloading. Elastic recovery can, thus, be characterized by the ratio between the final indentation depth and the maximum indentation depth.

Introduction

Tablet compaction consists of several stages and is subsequently challenging to describe in simple mathematical equations.[1] Various numerical approaches have been applied to try and derive a more thorough understanding of the multiple interactions that occur during compaction.[2,3] A possible way to obtain insight into the behavior of solids during compression is to perform indentation load – displacement experiments and simulations[4].

Experimental

The FEM method was implemented using Comsol Multiphysics version 4.2a on a conventional Hewlett Packard ProBook 6550b laptop with a 2.4 GHz CPU processor and 4 GB RAM running on a 64-bit operating system.

Results and discussion

The sample and indenter is model in a cylindrical coordinate system (Figure 1, top). Due to the axis symmetry attributes of this system a mesh is only needed to be assigned to a 2D geometry that subsequently is revolved around the symmetry axis (Figure 1, bottom). A higher mesh density was assigned to the specimen area where the indentation contact occurred (Figure 1, bottom). The upper boundary, right hand side boundary and indenter boundaries are assigned with free conditions. The bottom boundary is supplied with roller conditions. The FEM is solving a partial differential equation for the balance of momentum (1) and the yield function (2):

$$-\nabla \cdot \sigma = F_v \qquad (1)$$

$$F = \sigma_{mises} - \sigma_{ys} \qquad (2)$$

Where $\nabla \cdot \sigma$ is the divergence of the stress, F_v is the volume forces, F is the yield function, σ_{mises} is the von mises stress and σ_{ys} is the yield stress.

The parameter values and parameters utilized for the simulation is listed in table 1.

Table 1

Parameter	Value
Young’s modulus	70 GPa
Poisson’s ratio	0.2
Density	200 kg/m^3
Initial yield stress	243 MPa
Isotropic tangent modulus	21.79 GPa

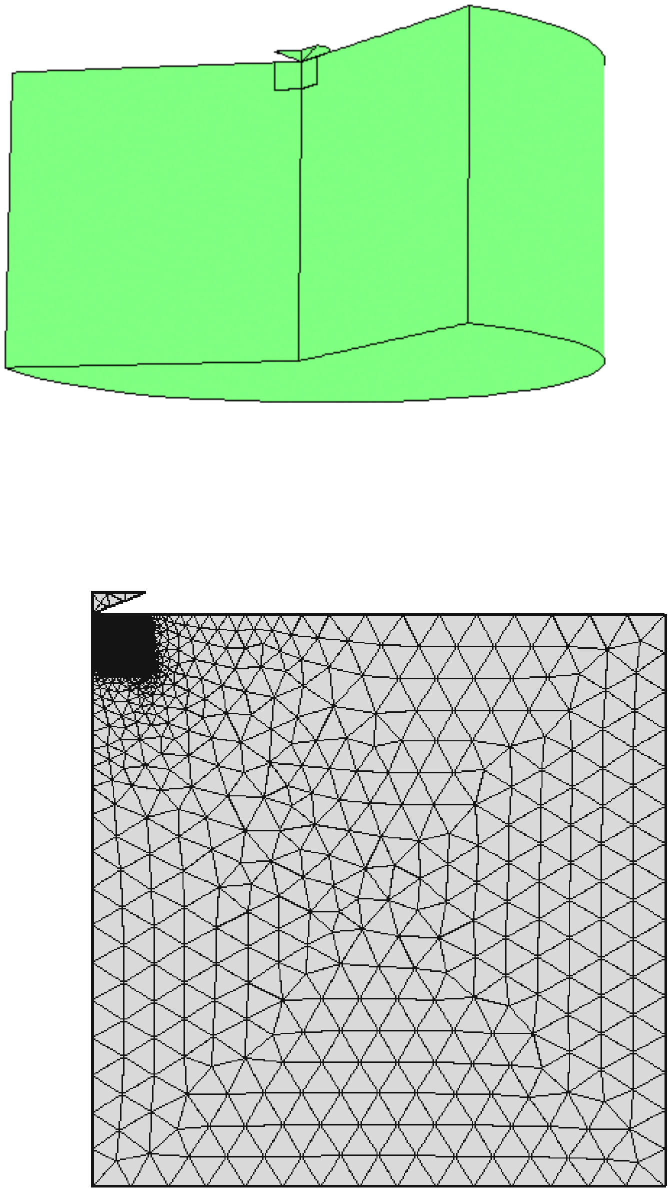

Figure 1 (top) schematic representation of the revolved 3D specimen and indenter geometry. (bottom) Meshed 2D geometry of the specimen and indenter.

The FEM method provides the possibility to obtain the indentation load – displacement curve. The form of this curve is dependent on the elastoplastic properties of the material. An example of such a curve is shown in Figure 2 where h_m depicts the maximum indentation depth at the highest load and h_f depicts the final indentation depth after unloading.

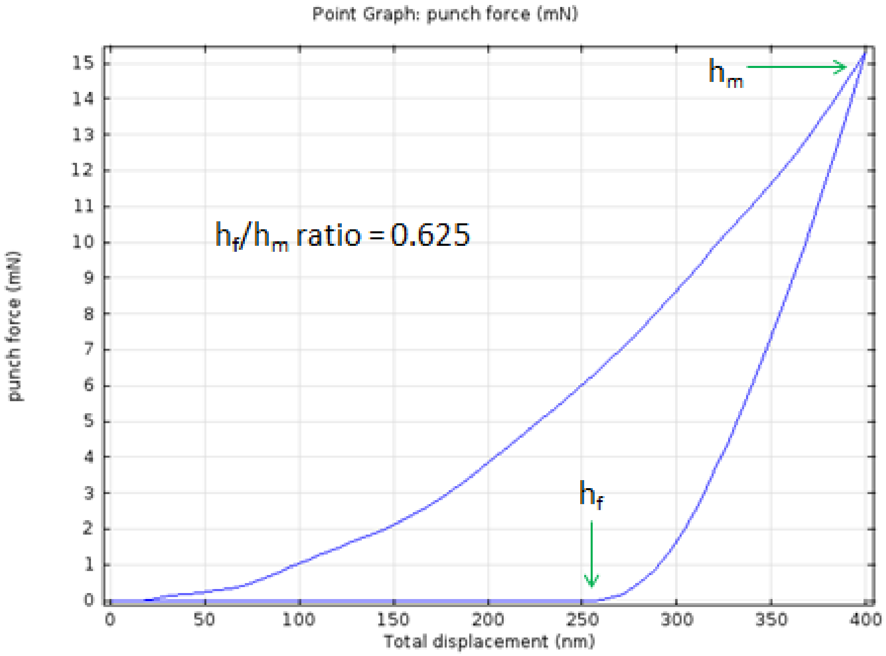

Figure 2 FEM simulated indentation load – displacement curve for an elastoplastic material with high yield stress and high tangent modulus from table 1.

If material properties such as yield stress and isotropic tangent modulus are changed to 200 MPa and 2.71 GPa respectively different indentation depths (h_f) and maximum loads (h_m) can be obtained. These changes also affect the h_f/h_m ratio (Figure 3). Therefore, it is suggested that it may be possible to obtain essential powder characteristics from fitting FEM simulations to atomic force microscopy (AFM) measurements[5,6]. These obtained powder characteristics could subsequently be employed for further optimization of the tablet compaction process.

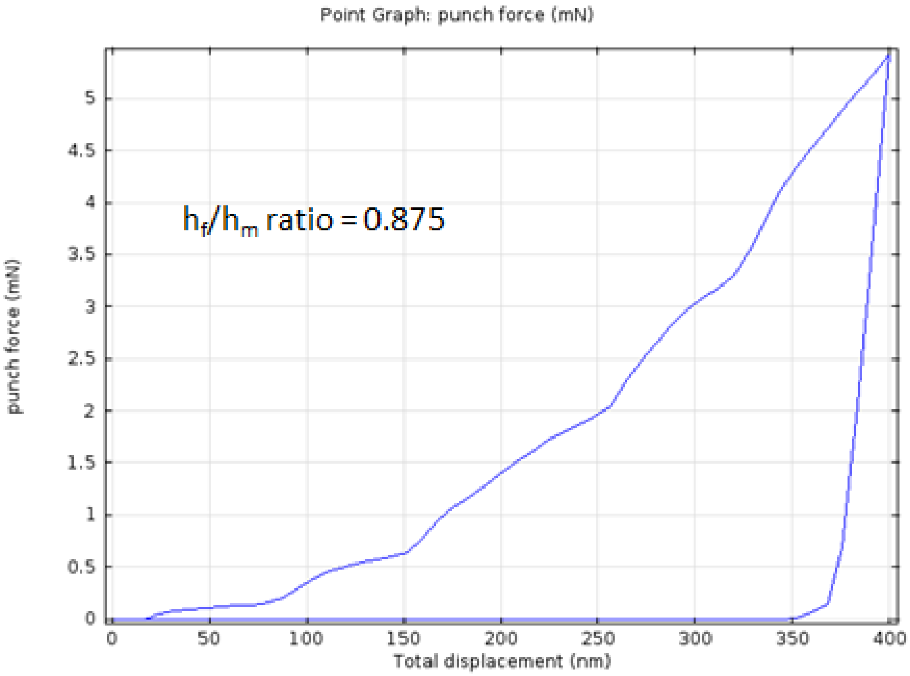

Figure 3 FEM simulated indentation load – displacement curve for an elastoplastic material with low yield stress (200 MPa) and low tangent modulus (2.71 GPa).

Conclusion

The finite element modeling (FEM) method was shown to be capable of simulating indentation load - displacement curves that differed in indentation depth after unloading, highest load at maximum indentation depth and h_f/h_m ratios when the material parameters were altered. It is therefore suggested that the FEM method could be used to extract material parameters from experimentally obtained indentation load – displacement curves. These material parameters could subsequently be used to deepen our understanding of tablet compression processes.

References

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