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Modeling the powder roll compaction process: Comparison of 2-D finite element method and the rolling theory for granular solids (Johanson's model)

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ABSTRACT

This study compares the nip angle, normal stress at the roll gap, and the maximum material relative density computed from 2-D finite element method (FEM) simulations and the 1-D Johanson's model for roll compaction of powders. In general, the nip angles predicted from the Johanson model follow the same trends as those from the FEM model. Both predictions agree to within 25% using typical pharmaceutical material properties. However, the compact densities predicted by the Johanson model are greater than one regardless of the operating conditions or material parameters. As shown in the FEM model, this unrealistic result is due to a two-dimensional velocity gradient that is not accounted for in the Johanson model. Finally, the normal stresses in the roll gap predicted by the Johanson model are generally larger than those found using the FEM model. The two approaches agree better when the material is more compressible, has a lower effective internal friction angle, a larger roll-powder friction angle, and when the streamwise inlet normal stress decreases.

1. Introduction

Powder roll compaction is a dry granulation process used in a number of industries including those that process chemicals, pharmaceuticals, and food products. The product of a roll compaction process is an agglomerate strip, often referred to as a “ribbon,” which is ultimately milled to produce granules. In pharmaceutical solid dosage form manufacture, the granules are then compacted to form tablets. Owing to the granules' larger size, this process is more advantageous than direct compaction of powder blends in many respects, including a reduction in dusting and segregation, and improved flowability.

It is particularly useful to have analytical or computational models capable of accurately predicting significant parameters in a powder roll compaction process. Process parameters of interest typically include the forces and torques acting on the rolls, the “nip” angle (i.e., the angle at which the powder no longer slips against the rolls), and the final compacted ribbon mean density and density distribution. By understanding what factors influence these parameters and quantitatively predicting their values, engineers and operators can improve the design and operation of the process.

The focus of this work is to compare the predictions of powder roll compaction parameters using a commonly cited one-dimensional analytical model developed by Johanson [1] against two-dimensional finite element method (FEM) computer simulations. In addition to providing quantitative comparisons of results, explanations of model shortcomings and comparisons to relevant experimental data from the literature are presented.

2. Background

The development of powder roll compaction models began in the 1960s, with one of the earliest analytical models proposed by Johanson [1]. Additional models have since been proposed, including the slab method [2] and FEM computational models [3–6]. Since the present work focuses on comparisons between the Johanson [1] analytical model and an FEM model, the remainder of this section will focus on previous work concerning these two modeling approaches.

The Johanson [1] model is one of the most widely used analytical powder roll compaction models since it is straightforward to implement and computationally economical. Details concerning the Johanson model are provided in Section 3.1. Briefly, the Johanson model is a one-dimensional, continuum-level model that provides predictions of the stresses and powder relative density along the roll surface, as well as the roll force and torque. Inputs to the model include the inlet pressure acting on the powder, the inlet powder bulk relative density, the powder effective internal friction angle, the powder-wall friction angle, and the roll compactor geometry (e.g., roll diameter and gap width). Upstream of the nip angle, the powder is assumed to slip against the rolls and follow the Jenike-Shield yield criterion [7]. Downstream of the nip angle, the powder is assumed to no longer

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follow the Jenike-Shield yield criterion; instead, the stresses acting on the powder are found using a combination of the continuity equation and the powder bulk density-hydrostatic pressure relationship.

Despite its widespread use, only a few studies provide experimental validation for Johanson's model. Several examples include the work of Yusof et al. [8] and Bindhumadhavan et al. [9]. In the former investigation [8], the Johanson model-computed roll forces and torques were compared to experimentally measured ones for different values of the roll gap for a gravity-fed system. Reasonable agreement between measured and computed quantities was observed, but only for gap values smaller than 0.15 mm. The authors noted, however, that the Johanson analysis predictions were sensitive to the model input parameters. For example, the authors observed that a 10% increase in inlet powder bulk relative density doubled the predicted roll force values.

In the latter investigation [9], the Johanson model-computed roll normal stress distributions and nip angles were compared with experimentally measured ones for various roll gap widths. The authors found that the Johanson model-predicted nip angles agreed to within 15% of the experimentally measured ones. Comparisons of predicted and measured roll normal stress data, however, proved to be inconclusive as the former quantities were noted to be highly dependent on the normal stress at the nip angle, a quantity that the authors claimed could neither be computed from the Johanson analysis nor accurately measured from experimental data.

To gain further understanding of and more accurately model the roll compaction process, recent investigations have made use of finite element method (FEM) simulations. In an FEM model, the powder is treated as a continuum, but is divided into a number of deformable, connected elements (a mesh). Each of these elements deforms in response to applied stresses according to the powder's stress–strain constitutive relationship, such as the Drucker-Prager Cap (DPC) model [10]. As with the Johanson model, these constitutive material parameters must be provided to the model, along with the inlet pressure, inlet powder bulk relative density, and the roll compactor geometry.

The primary advantage of using an FEM model over the Johanson model is that the former requires fewer modeling assumptions than the latter. As an example, powder slip/no-slip behavior against the rolls occurs naturally in an FEM simulation. In contrast, the determination of the slip/no-slip region in the Johanson model relies on a priori assumptions (see Section 3.1.) More complex roll geometries and material stress–strain behaviors (i.e., material properties) can also be incorporated in an FEM model. In addition, an FEM model can be two- or three-dimensional, therefore giving additional process details that are not provided by the Johanson model.

Compared to Johanson's analysis, however, computation times for an FEM model are much longer. Whereas Johanson's model can generate data in a fraction of a second, FEM model computation times can range from hours to weeks depending on the model complexity. These long computation times restrict FEM use to engineering design rather than real-time process control. In addition, the implementation of an FEM model is also more challenging as it involves the use of a numerical solver to compute the equilibrium equations describing the stress and strain states of the deformable body (i.e., the powder). Although the user-friendliness of such software has improved significantly in recent years, the effort involved in using FEM software effectively is much greater than that required for the spreadsheet analysis typically involved in solving the Johanson model equations. Despite these disadvantages, FEM models are still valuable since, as mentioned previously, they provide greater detail and flexibility than the Johanson model.

Examples of powder roll compaction FEM studies include the work of Dec et al. [4], Zavaliangos et al. [3], Cunningham [5], and Michrafy et al. [6]. Three-dimensional FEM models providing ribbon density distributions along the roll surface were the focus of Michrafy et al.'s [6] study. Their model predictions show that roll-compacted ribbons are densest at their center and least dense at their sides. These observations qualitatively agree with experimentally measured compact density data using a mercury porosimeter. No quantitative comparisons were provided, however.

Cunningham [5] used two-dimensional FEM models to study the influence of inlet feed pressure and powder-roll friction on roll force, roll torque, nip angle, and material relative density at the roll gap. He found that the roll force, roll torque, and material relative density at the roll gap increase with increasing feed pressure or powder-roll friction coefficient. The nip angle, however, was largely unaffected by changes in feed pressure, but increased with an increase in powder-roll friction coefficient. Perhaps more importantly, Cunningham also observed a non-uniform velocity field in the span-wise direction at locations downstream of the nip angle, a result that the Johanson model cannot provide (similar observations were reported in Dec et al. [4] and Zavaliangos et al. [3]). Model validation in Cunningham [5] was provided by comparing the FEM-computed material relative density at different levels of roll force with corresponding experimental data. It was found that the two quantities agreed to within 15%. Such discrepancies were hypothesized to result from inaccurate inlet boundary conditions and from post-gap material expansion that was not accurately captured by the FEM simulations. Surprisingly, the literature contains no direct quantitative comparisons of the Johansson and FEM models.

The present work compares predictions from Johanson's model to those from two-dimensional FEM simulations. While it could be expected that the 1-D Johanson model will not agree exactly with a 2-D FEM model results, the comparative study presented in this work aims to determine and understand the impact of Johanson's simplifying assumptions on the model's predictions. The objective is to identify the conditions under which the computationally efficient and simple Johanson model may be used with sufficient accuracy in place of a more complex and time consuming FEM model.

3. Model descriptions

3.1. Johanson's model

The Johanson model is briefly outlined in this section. Note that only those portions of the model that are relevant to this study are discussed. More detailed derivations can be found in Johanson [1].

The geometry under consideration in Johanson's model is shown in Fig. 1. Johanson hypothesizes that during the roll compaction process, the powder slips along the roll surface near the inlet region. Closer to the narrowest gap region, the powder does not slip against

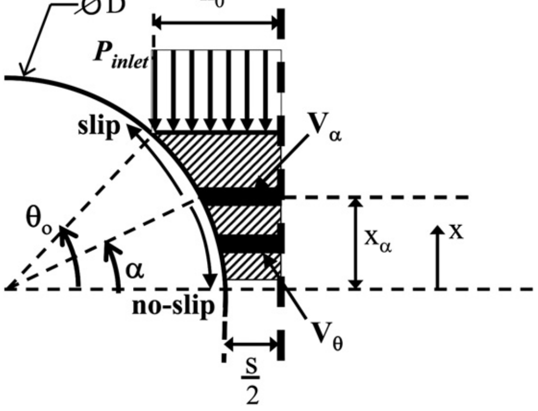

Fig. 1. Roll compaction geometry assumed in Johanson's model.