Evaluating and Modifying Johanson's Rolling Model to Improve its Predictability

MINGDA BI, FERNANDO ALVAREZ-NUNEZ, FRANCISCO ALVAREZ

Formulation Group, Pharmaceutical R&D, Amgen Inc., Thousand Oaks, California 91320

Received 20 October 2013; revised 16 March 2014; accepted 22 April 2014

ABSTRACT: The purpose of this study is to investigate if Johanson's rolling theory can correctly predict the maximum roll surface pressure during the roll compaction. Three model pharmaceutical formulations were roller compacted using the Gerteis Mini Pactor at multiple combinations of roll forces and roll gaps. The resultant ribbon density at each combination of roll force and roll gap was measured and the corresponding maximum roll surface pressure was predicted using Johanson's rolling model. The measured ribbon density and predicted maximum roll surface pressure from roller compactor was compared with the measured wafer density and maximum axial stress from die compression. The results indicate that predicted maximum roll surface pressure from roller compactor is higher than the axial stress from die compression to manufacture same density ribbons. The root cause of overprediction of maximum roll surface pressure from Johanson's model was found and corrected. The modified model offers reasonably accurate prediction of maximum roll surface pressure for all roller compaction experiments conducted in this study. © 2014 Wiley Periodicals, Inc. and the American Pharmacists Association J Pharm Sci 103:2062–2071, 2014

Keywords: roller compaction; die compression; material science; formulation; mechanical properties; modified Johanson's rolling model; powder technology; mathematical model

INTRODUCTION

Roller compaction (RC) process dates back to the 1800s when a roll type briquet machine was used to agglomerate coal screenings. Since then, different configurations of roller compactors were built and used in a variety of industries including: chemical, metals, pharmaceuticals, minerals, and recycling.

In the case of pharmaceutical rolling, RC of powder seems rather simple at first glance. However, it is a quite complex because of the nonlinear geometry around the feeding zone, compaction zone, and extrusion zone. In addition, the followings further complicate the powder rolling process including: (1) material constitutive and frictional properties are constantly changing during the rolling; (2) feeding angle, feeding stress, powder density in the feeding zone, roll surface pressure, and roll surface force are normally unknown; and (3) nonuniform powder feeding and nonuniform roll stress lead to nonuniform ribbon density and nonuniform ribbon tensile strength. Despite these challenges, several research groups have made significant contributions to the rolling theory. For example, Karman[1] formulated his rolling theory called slab model in 1925; Johanson[2] made significant contributions to the rolling theory for granular solids in 1965; Cunningham and Zavaliangos[3] also made significant contributions in modeling RC process using finite element method (FEM) in 2005.

Recently, the researchers in pharmaceutical field investigated the die compression and RC, and concluded that die compression can be used to simulate the RC.[4,5] However, it is known that stress path from die compression is different from that of RC.[3] Die compression has a stress path closer to hydrostatic stress, and RC has a stress path closer to the shear. It is believed that this stress path difference will lead to differences in ribbon density and tensile strength. Katashinskii and Vinogradov[6] and Mal'tsev[7] conducted a direct comparison of the maximum roll surface pressure in plane strain of RC versus the maximum axial stress in die compression using various metal powders and found that axial stress from die compression has to be larger in order to achieve the same ribbon density. The explanation is that larger shear stress during rolling enhanced the material consolidation and resulted in denser ribbons. Their experimental results are consistent with John Cunningham's finding[3] that the difference between maximum roll surface pressure and axial stress is about 2% at a relative ribbon density of 0.6 using microcrystalline cellulose PH102 (Avicel PH102) as a model material; however, the difference can be as much as 14% as the relative density of ribbons reaches 0.9. Fortunately, the target relative ribbon density in pharmaceutical rolling is generally less than 0.75, and the differences in the aforementioned two stresses is expected to be minimal. Therefore, it is possible to use the die compression to simulate compaction process in the compaction zone of a rolling press.

Because die compression is simple and die compression apparatus is normally available in most pharmaceutical laboratories, it will be very valuable if die compression can be used to simulate RC to derive the target ribbon density and the corresponding axial stress and then transfer this axial stress to roller compactor to manufacture the same density ribbons.

However, in practice, it is very difficult to transfer the derived axial stress from die compression to RC unless the counter-rotating rolls are instrumented. But this will increase the cost and complexity. One way to overcome the above issue is to evaluate existing RC models and calibrate it and then use the calibrated RC models to predict the conditions required to achieve the target stress derived from die compression. In this way, the ribbons with the target density can be manufactured by rolling

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Correspondence to: Mingda Bi (Telephone: +805-313-5194; Fax: +805-477-1986; E-mail: mbi@amgen.com)

Journal of Pharmaceutical Sciences, Vol. 103, 2062–2071 (2014)

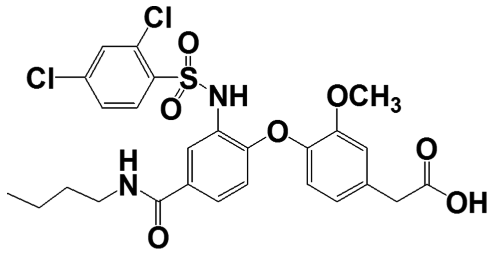

Figure 1. Chemical structure of AMG 009.

process. Thus, the objective of this study is to compare the die compression with Johanson's rolling model to evaluate if Johanson's model can be used to correctly predict the required maximum roll surface pressure (it should be approximately equal to the axial stress from die compression) to produce the ribbons with the same density as those from die compression. The reason to compare with Johnson's model is because Johanson's analytical model is easy to implement and computationally economical. In addition, previous studies have suggested that the Johanson rolling model provides reasonably accurate prediction with appropriate input values.[8–10]

AMG 009 is a small molecule that was investigated for its potential treatment for inflammatory diseases. Its chemical structure is shown in Figure 1. In this study, AMG 009 is used as the model compound to investigate the maximum roll pressure predictability of Johanson's model.

THEORETICAL BACKGROUND

In 1965, Johanson published his rolling theory for granular solids.[2] In this paper, he proposed that there are two rolling regions between the counter-rotating rolls. One is slip region, where the roll speed is faster than that of powder. The other is nonslip region, where the roll speed is same as the powder moving speed. The transition from slip to nonslip region defines the nip angle. He further proposed that in the slip region, the shear stress and normal stress at roll surface is dictated by the roll-material friction angle or wall friction angle of the material against the roll surface. As a result, he combined two differential equations of equilibrium with the equations of two-dimensional field of limiting stresses and used method of characteristics together with finite difference approach[11] to derive pressure gradients along the rolling direction at the slip region. Eq. (1) shows the results.

$$\frac{d\sigma}{dx}\,|\text{slip} = \frac{4\sigma(\pi/2-\theta-\nu)\tan\delta}{(D/2)(1+S/D-\cos\theta)(\cot(A-\mu)-\cot(A+\mu))} \tag{1}$$

where $2\nu = \pi - \phi - \arcsin\left(\frac{\sin\phi}{\sin\delta}\right)$, $\mu = \frac{\pi}{4} - \frac{\delta}{2}$, and $A = \frac{\left(\frac{\pi}{2}+\theta+\nu\right)}{2}$.

In the nonslip region, Johanson assumes continuity transport theorem is valid and the flow of powders between the rolls is laminar and there is no velocity gradient along the transverse direction or through the ribbon thickness direction (Axial direction in Fig. 2). This assumption has been proposed by the previous researchers and claimed it is appropriate.[12,13] As a result, Johanson assumes that powder mass entered into the nip region (upstream) will be 100% delivered to downstream between the rolls. Then, Eq. (2) was derived, which satisfies his continuity assumption.

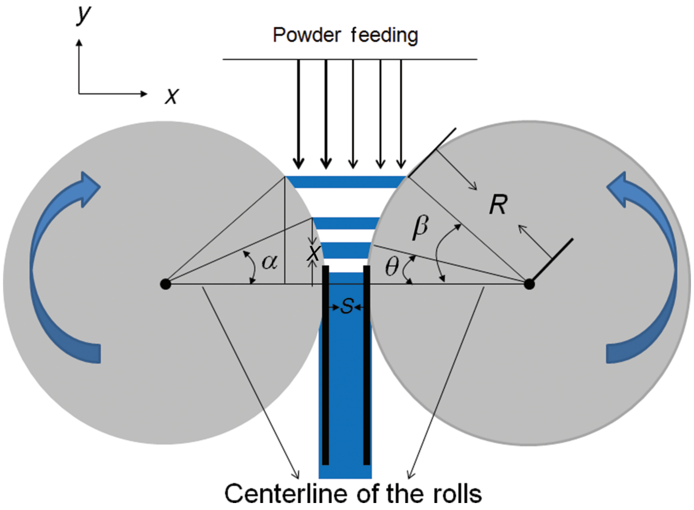

Figure 2. Region of nip in a roller compactor.

$$\frac{\rho_\alpha}{\rho_\theta} = \frac{V_\theta}{V_\alpha} \tag{2}$$

Next, Johanson related the density from Eq. (2) with the stress according to empirical observation that log density is a linear function of log stress. Therefore, Eq. (3) was derived.

$$\frac{\sigma_\alpha}{\sigma_\theta} = \left(\frac{\rho_\alpha}{\rho_\theta}\right)^k = \left(\frac{V_\theta}{V_\alpha}\right)^k \tag{3}$$

Using the geometric relationship from Figure 2, Johanson derived Eq. (4).

$$\left(\frac{V_\alpha}{V_\theta}\right)^k = \left[\frac{(1+S/D-\cos\alpha)\cos\alpha}{(1+S/D-\cos\theta)\cos\theta}\right]^k \tag{4}$$

By combining Eqs. (3) and (4), Eq. (5) was derived.

$$\sigma_\theta = \sigma_\alpha\left[\frac{(1+S/D-\cos\alpha)\cos\alpha}{(1+S/D-\cos\theta)\cos\theta}\right]^k \tag{5}$$

Pressure gradient in the nonslip region (Eq. (6) was derived by differentiating Eq. (5) with respect to x, where $x = D/2\sin\theta$.

$$\frac{d\sigma}{dx}\bigg|\text{nonslip} = \frac{k\sigma(2\cos\theta-1-S/D)\tan\theta}{(D/2)(1+S/D-\cos\theta)\cos\theta} \tag{6}$$

Johanson proposed that pressure gradients from slip region and nonslip region should be equal at nip angle. Therefore, by equating Eqs. (1) and (6), nip angle can be determined. This can be performed graphically by plotting the pressure gradients from both slip and nonslip region in the same plot. The nip angle is derived from the intersection point of two gradients. Johanson also derived the relationship between total roll force and maximum roll surface pressure according to studies by Blake et al. and Kurtz and Barduhn.[12,13] Eq. (7) shows the