Flow Dynamics and Structure of solid pellets along the channel of a single screw extruder

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Abstract. Plasticating single screw extrusion involves the progressive compaction and heating of loose solid pellets that eventually melt, form a relatively homogenous stream and are subsequently pumped through a shaping tool. Traditional analyses of the solids conveying stage assume the sliding of an elastic solid plug due to differential wall friction coefficients. However, not only the corresponding predictions may fail considerably, but it is also well known that, at least in the initial screw turns, pellets are far from compact. This work follows previous efforts to model the flow of solids in the hopper and initial screw turns using the Discrete Element Method (DEM). The model considers the development of normal and tangential forces resulting from the inelastic collisions between the pellets and between them and the neighbouring metallic surfaces. As an example of the capability of the model to capture detailed features of granular flow, the effect of pellet size on flow is discussed.

Introduction

Many polymer processing technologies encompass a plasticating step, where the inward solid pellets are conveyed forward by gravity, followed by melting, melt conveying and pumping through a shaping tool. Given its practical importance, plasticating attracted extensive theoretical and experimental research. As a result, by the eighties the underlying thermal, physical and rheological phenomena were well identified and could be satisfactorily modelled from hopper to die exit (see, for example [1,2]). For this purpose, plasticating was analysed as a series of individual stages where distinct phenomena develop: gravity flow in the hopper, drag solids conveying, delay in melting, melting, melt conveying and die flow [3]. Generally, solids conveying is simply described as the drag flow of a cohesive elastic plug moving between flat walls with known friction coefficients, which may hinder the predictive capacities of the global model.

Research on the flow of granular materials is now quite active [4]. The first attempts to model granular flow in single screw extruders were made by Potente and Pohl [5] (2D approach) and Moysey and Thompson [6-8] (3D analysis), who used the Discrete Element Method (DEM) to predict the position and velocity of every pellet. In particular, Moysey and Thompson [6-8] elucidated the general pellet flow pattern, disclosed the influence of the screw flights on flow and demonstrated the potential of DEM to study and optimize this process step.

Thus, the present work aims at extending these efforts and investigates the role of operating, geometrical and material parameters on the flow characteristics. The algorithm developed computes velocities, coordination number, density/packing fractions and global output. After validating the model against the predictions of Moysey *et al*. [6,8], the effect of pellet size is studied.

Computational Model

Granular model. The model considers the flow of spherical particles whose resistance to overlap is expressed by a continuous potential function, following the approach of Walton and Braun (WB) [9]. Figure 1 illustrates a pair of spherical particles i and j, with radius R_i and R_j, respectively, that are in contact. The WB model is used to calculate the normal force ($\vec{F}_n$) by assuming the existence of two different spring constants, k_1 and k_2, for the loading and unloading forces during the contact, respectively:

$$\vec{F}_n = \begin{cases} k_1(\alpha - \alpha_0)\hat{n} & for \quad loading \\ k_2\alpha\hat{n} & for \quad unloading \end{cases} \qquad (1)$$

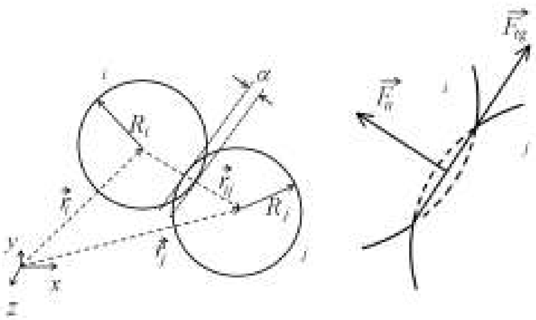

Fig. 1. Interaction between two particles i, j. (the overlap α is exaggerated for clearer perception).

The value of the overlap (α) can be defined as $\alpha = R_i - R_j - |\vec{r}_{ij}|$ where $\vec{r}_{ij} = |\vec{r}_{ij}|\hat{n}$ is the vector connecting the centres of the i^{th} and j^{th} particles and $\hat{n}$ is the unit vector in that direction. The tangential force ($\vec{F}_{tg}$) is defined as a function of the previous tangential force($\vec{F}^*_{tg}$) :

$$\vec{F}_{tg} = \vec{F}^*_{tg} + K_t \Delta\vec{s}_{\parallel} + k_0 \Delta\vec{s}_{\perp} \qquad (2)$$

where $\Delta\vec{s}_{\parallel}$ and $\Delta\vec{s}_{\perp}$ are the tangential displacements parallel and perpendicular to the tangential force, respectively, and K_t is the effective tangential stiffness in the parallel direction, given by:

$$K_t = \begin{cases} k_0\left(1 - \dfrac{F_{tg} - F^*_{tg}}{\mu F_n - F^*_{tg}}\right)^{\gamma} & when \quad F_{tg} \quad increases \\ k_0\left(1 - \dfrac{F^*_{tg} - F_{tg}}{\mu F_n + F^*_{tg}}\right)^{\gamma} & when \quad F_{tg} \quad deacreases \end{cases} \qquad (3)$$

Extruder Geometry. During flow it is necessary to consider the following boundary conditions, where contacts can/will take place: i) walls of the hopper; ii) edge between the hopper aperture and barrel, iv) internal barrel wall, v) screw flights, vi) flights crest (directly under the hopper aperture), vii) edge between screws flights and crest and viii) the screw root. No leakage flow between the screw crest and inner barrel wall exists, due to the small value of the gap in comparison with the size of the pellets.
Figure 2 illustrates the extruder geometry and shows the initial location of the pellets in the hopper. As the screw rotates and flow develops, new layers of pellets are appended to the hopper.

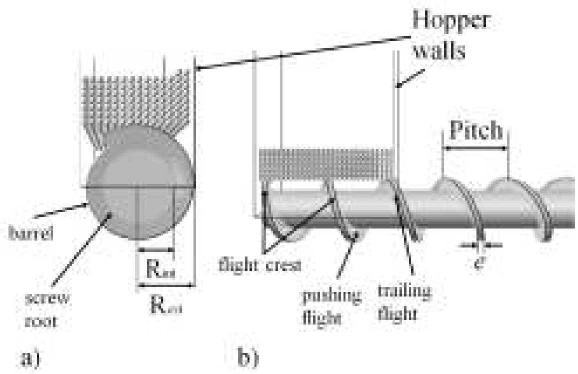

Fig. 2. Extruder geometry and initial pellets location. a) Front view; b) side view.

Model Validation. The assessment of the algorithm was performed by comparing the predictions of flow rate, coordination number and velocities with those of Moysey and Thompson [6,8] for the same problem.

Table 1 compares the predicted specific output with those determined using classical plug flow analytical models (Darnell and Mol [10] and Tadmor and Klein [11]), by the DEM approach of Moysey and Thompson [6, 8] and with the experimental value, according to these authors. The differences between the two DEM approaches are probably due to the difficulty in defining exactly the same initial conditions.

Table 1. Comparison of specific outputs.

Model	**Specific Output** [kg/h/rpm]
Darnell and Mol [10]	1.23
Tadmor and Klein [11]	0.93
Moysey and Thompson [7]	1.34
experimental [7]	1.36
present algorithm	1.31

The predictions of the cross-channel velocity (V_{sx}) at 100 rpm are compared in Figure 3. The profile is relatively flat. Conversely, the down-channel velocity profile (not represented) exhibits a significant gradient from the trailing to the pushing flight, with a nil velocity at the centre.

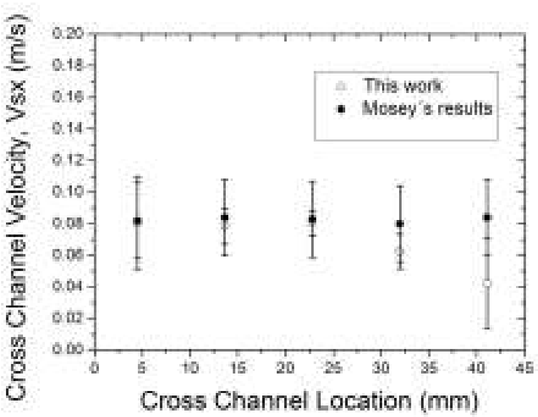

Fig. 3. Cross-channel velocity profile.

Density profiles

Figure 4 shows the cross-channel variation of the packing fraction at 2.5L/D for 100 rpm, after 2.55s of flow. A maximum is reached at the core of the channel, as the contacts with the flights drive the pellets towards the centre.

Figure 5 displays the evolution of the packing fraction along the screw channel, again at 100 rpm, for different flow times. No relevant fluctuations take place under the aperture of the hopper, probably due to the local vertical hydrostatic pressure. Downstream, cyclic fluctuations develop with a frequency matching the screw rotation. These fluctuations are due to gravity: higher packing fractions occur at the bottom of the channel. Also, the fluctuations decrease with increasing flow time and range approximately between 0.7 and 0.5, i.e., between close and loose packing, respectively.

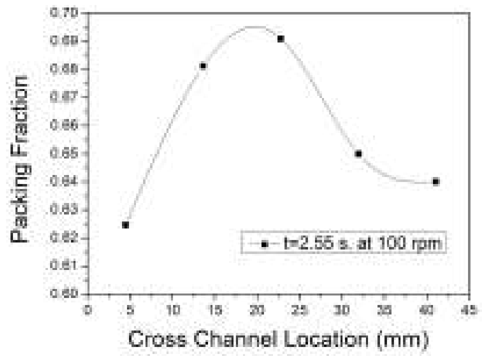

Fig. 4. Packing fraction at 2.55 s, for 100 rpm.

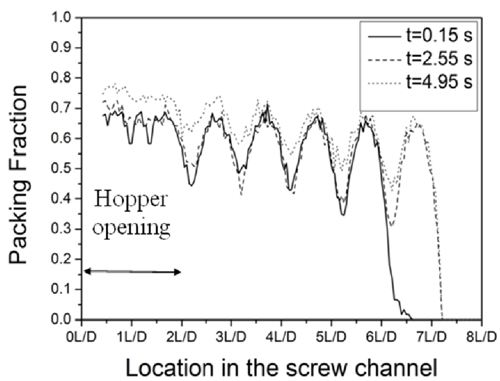

Fig. 5. Packing fraction along the channel at different times, for 100 rpm.

Effect of pellet size

Computational runs with pellets of different sizes showed that this variable has an effect on the flow characteristics. The flow of pellets with a bimodal size distribution (see Figure 6, where the black and the grey pellets have a diameter of 2 and 3 mm, respectively) reveal that the smaller pellets accumulate to some extent at the bottom of the channel.

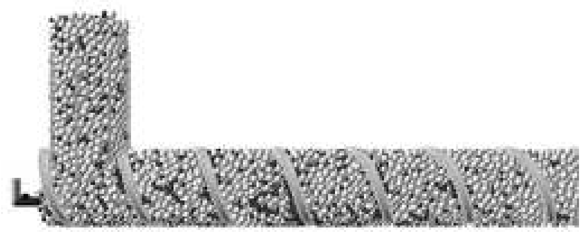

Fig. 6. Transport of pellets with a bimodal size distribution.

Conclusions

The solids conveying analysis using DEM seems to be able to capture the features of granular flow in single screw extruders. For example, at a given channel cross-section, the down-channel velocity profile exhibits a significant gradient from the trailing to the pushing flight, while the cross-channel velocities are positive and change little. Density fluctuations along of the channel set in instantly, even if they become less intense.

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