Chemical Engineering Science ∎ (∎∎∎∎) ∎∎∎–∎∎∎

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Co-rotating twin-screw extruders: Detailed analysis of conveying elements based on smoothed particle hydrodynamics. Part 1: Hydrodynamics

Andreas Eitzlmayr[a], Johannes Khinast[a,b,*]

[a] Institute for Process and Particle Engineering, Graz University of Technology, Inffeldgasse 13, 8010 Graz, Austria
[b] Research Center Pharmaceutical Engineering, Inffeldgasse 13, 8010 Graz, Austria

HIGHLIGHTS

- We applied SPH to study the flow in a co-rotating twin-screw extruder.
- A new model which accounts for the flow in unresolved clearances was presented.
- We showed detailed results for pressure drop, flow rate and power consumption.
- We achieved excellent agreement with CFD data for the completely filled state.
- Detailed results for the partially filled state are included.

ARTICLE INFO

Article history:
Received 5 November 2014
Received in revised form
15 April 2015
Accepted 23 April 2015

Keywords:
Smoothed particle hydrodynamics
SPH
Co-rotating twin-screw extruder
Complex geometry
Partially filled
Flow

ABSTRACT

Due to the complex geometry of the rotating screws and, typically, free surface flows in partially filled screw sections, first principles simulations of the flow in co-rotating intermeshing twin-screw extruders using the well-established, mesh-based CFD (computational fluid dynamics) approaches are highly challenging. These issues can be resolved via the smoothed particle hydrodynamics (SPH) method thanks to its meshless nature and the inherent capability to simulate free surface flows. In our previous work, we developed a novel method for modeling the boundary conditions with complex wall geometries, under which SPH could be efficiently applied to complex surfaces of typical screw geometries of extruders. In this work, we employed SPH and our boundary method to study the flow in a conveying element in detail. To address unresolved clearances, we developed a new model that is coupled to SPH and can correctly account for the flow through unresolved clearances. A validation of our approach using CFD data from the literature for a completely filled conveying element indicated excellent agreement. Consequently, we studied the flow in a partially filled conveying element and obtained results for the flow rate, the power input and the axial force with variable filling ratio. A detailed analysis of the corresponding mixing phenomena is presented in Part 2. Our results show that the proposed method is a comprehensive approach to study the flow in different types of screw elements in detail, providing an excellent basis for further development of simplified models of entire extrusion processes.

1. Introduction

Developed in the 1940s and 1950s, intermeshing extruders have been widely used in different industries for many decades, for example, to manufacture polymers, chemicals and foodstuffs. The most common type is the co-rotating, intermeshing twin-screw extruder. Its advantages include good mixing performance, self-cleaning screws, short residence time and good product quality. Single-screw extruders are primarily used for melting and pressure build-up and do not have superior mixing properties. Other types of extruders, such as counter-rotating twin-screw, multi-screw or ram extruders, are designed for more specialized applications. (Kohlgrüber, 2008)

In recent years, extrusion has become increasingly attractive to the pharmaceutical industry with regard to manufacturing of solid drug products (Ghebre-Sellassie and Martin, 2003). Depending on the materials involved, there are several types of pharmaceutical

---

Abbreviations: 1D, one-dimensional; 3D, three-dimensional; CAD, computer aided design; CFL, Courant–Friedrichs–Lewy; FEM, finite element method; FVM, finite volume method; SPH, smoothed particle hydrodynamics; STL, surface tessellation language

[*] Corresponding author at: Institute for Process and Particle Engineering, Graz University of Technology, Inffeldgasse 13, 8010 Graz, Austria.
Tel.: +43 316 873 30400.
E-mail address: khinast@tugraz.at (J. Khinast).

http://dx.doi.org/10.1016/j.ces.2015.04.055
0009-2509/© 2015 Elsevier Ltd. All rights reserved.

Please cite this article as: Eitzlmayr, A., Khinast, J., Co-rotating twin-screw extruders: Detailed analysis of conveying elements based on smoothed particle hydrodynamics. Part 1: Hydrodynamics. Chem. Eng. Sci. (2015), http://dx.doi.org/10.1016/j.ces.2015.04.055

extrusion processes, such as hot melt extrusion (HME), hot melt granulation, wet extrusion and solid lipid extrusion (Kleinebudde, 2011). HME is particularly promising for pharmaceutical applications in terms of increasing the bioavailability of poorly soluble drug molecules and forming solid solutions and amorphous solid dispersions (Breitenbach, 2002; Repka et al., 2005). Moreover, since HME is solvent-free, it does not involve costs associated with the solvent, separation, recovery and disposal. Due to its variety of individual screw elements (e.g., conveying elements, kneading elements and mixing elements), the typical modular screw design of co-rotating, intermeshing twin-screw extruders offers almost unlimited options with regard to the actual screw configuration design. Although this allows high operational flexibility, developing an appropriate screw configuration to accommodate the actual process requirements is highly challenging and normally requires extensive experience and/or experimental and empirical work.

In experiments, an extruder is essentially a black box, and accurate measurements of process variables such as the filling ratio and the melt temperature are difficult to achieve. Modeling and simulation methods can provide an understanding of the complex flow and mixing phenomena associated with the interaction between the rotating screw geometry, material properties and operation conditions, potentially leading to effective scale-up approaches.

However, extruders are highly complex, witnessed by the fact that no fully-resolved first-principles simulations of entire twin-screw extruders have been reported to date. There are several reasons: first, free-surface flows, which are difficult to model, occur in the partially filled screw sections. Second, the flow behavior of the processed material mixtures is typically complex, mostly non-Newtonian, which requires an extensive amount of measurements for a complete description of the macroscopic properties of the material mixtures. Third, extruders are highly non-isothermal, requiring the coupling between mass, momentum and energy balances. Fourth, due to the small gap between the screws and between the screws and the barrel, the flow needs to be highly resolved. Moreover, a fully resolved simulation of the transition from the granular to the molten state is currently infeasible.

Several simulation approaches for twin-screw extruders exist today, which are mainly divided into one-dimensional (1D) and three-dimensional (3D) methods. The computationally less expensive 1D approach yields an approximate description of the process variables along the screw axes (e.g., filling ratio, pressure, and temperature) while neglecting their distributions in radial and azimuthal direction. Here, the flow around the screw geometry is not fully resolved, thus, the 1D approach depends on simplified models (based on first principles), which account for the impact of the actual screw geometry by correlating integral properties of the flow field (for example the flow rate, the axial pressure gradient or the power input). This usually involves parameters which are characteristic for the considered screw element geometries. For specific types of screw elements (e.g., conveying elements) these parameters can be determined based on analytical equations. Beyond that, the characteristic screw parameters can also be determined by experiments or fully resolved simulations, which can particularly be important for complex (real) materials and more complex geometries. Since the averaging over the cross section involves also the spatial distribution of material properties, e.g., the viscosity, the characteristic screw parameters can also depend on the considered material. However, this simplified method often yields sufficiently accurate predictions that contribute to process understanding and significantly reduce experimental effort. Due to its comparably low computational expense, it is still the only way to develop a simulation of the entire extrusion process. For more detailed information about 1D modeling, please refer to the literature, e.g., (White and Chen, 1994; Potente and Hanhart, 1994; Vergnes et al., 1998; Potente et al., 1999; White et al., 2001; Potente and Kretschmer, 2002; Prat et al., 2002; Choulak et al., 2004; Vergnes and Berzin, 2006; Bahloul et al., 2011; Teixeira et al., 2012; Eitzlmayr et al., 2014b).

For first principles simulations of the flow in co-rotating twin-screw extruders, mainly mesh-based CFD (computational fluid dynamics) methods, such as the FEM (finite element method) and FVM (finite volume method), have been used (e.g., Ishikawa, 2001; Bertrand et al., 2003; Malik and Kalyon, 2005; Ficarella et al., 2006a; Ficarella et al., 2006b; Kalyon and Malik, 2007; Barrera et al., 2008; Bierdel, 2008; Conzen, 2008; Rodríguez, 2009; Haghayeghi et al., 2010; Vyakaranam et al., 2012; Sarhangi Fard et al., 2012a; Sarhangi Fard et al., 2012b; Sarhangi Fard and Anderson, 2013; Hétu and Ilinca, 2013; Rathod and Kokini, 2013; Sobhani et al., 2013; Durin et al., 2014). FEM was also used to simulate complex fluids in extruders including wall slip phenomena, (e.g., Kalyon et al., 1999; Lawal et al., 1999; Malik et al., 2014). However, simulating free-surface flows in partially filled screw sections remains extremely challenging. To address this issue, Pokriefke (2005), for example, used FVM with an Eulerian multiphase model and applied a sophisticated mesh refinement at the free surfaces.

Being mesh-free, the smoothed particle hydrodynamics (SPH) method may be used to simulate partially filled extruders: achieving partial filling requires the same effort as complete filling and mixing phenomena can be observed by tracking tracer particles without additional modeling work. Cleary and Robinson (2011) applied SPH to study mixing in a co-rotating twin-screw extruder using boundary particles to model the screw and barrel surfaces.

In this work, we applied SPH to study the hydrodynamics (Part 1) and mixing (Part 2) in a conveying element of a co-rotating twin-screw extruder in completely- and partially-filled states. For the boundary conditions at the wall surfaces, we used a new approach proposed in our previous work (Eitzlmayr et al., 2014a). Instead of the classical method of modeling walls in SPH based on particles (e.g., boundary particles and ghost particles), we determined polynomial fits to calculate the interaction of a solid wall with adjacent fluid particles directly from the distances between the wall and the fluid particles. This can be efficiently applied to complex geometries in the STL (surface tessellation language) format generated by commonly used CAD (computer aided design) software and, thus, allows a practicable pre-processing strategy for complex geometries in SPH simulations.

2. Dimensionless groups

Pawlowski (1971) introduced dimensionless groups to describe the flow in screw machines and, specifically, single-screw extruders. Kohlgrüber (2008) applied them to twin-screw extruders based on the assumption that the relevant flow parameters of a completely filled screw element were the barrel diameter D as the measure of the length scale, the fluid viscosity η, the fluid density ρ, the screw speed n, the achieved flow rate $\dot{V}$, the axial pressure drop Δp over the considered length L, the screw driving power P and the axial force F exerted on the screws. By means of dimensional analysis, these nine parameters can be reduced to six dimensionless groups. One of them is the simplex L/D, which is usually neglected by considering an infinitely extended system ($L/D \to \infty$). The remaining five dimensionless groups are the Reynolds number $Re = nD^2\rho/\eta$, the dimensionless flow rate $\dot{V}/nD^3$, which can be viewed as throughput per screw revolution (using the screw speed n) relative to the volume of the extruder (represented by the cubed barrel diameter D), the dimensionless axial pressure drop $\Delta pD/\eta nL$ (based on viscosity η and the

Please cite this article as: Eitzlmayr, A., Khinast, J., Co-rotating twin-screw extruders: Detailed analysis of conveying elements based on smoothed particle hydrodynamics. Part 1: Hydrodynamics. Chem. Eng. Sci. (2015), http://dx.doi.org/10.1016/j.ces.2015.04.055