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Mechanistic modeling of modular co-rotating twin-screw extruders

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ABSTRACT

In this study, we present a one-dimensional (1D) model of the metering zone of a modular, co-rotating twin-screw extruder for pharmaceutical hot melt extrusion (HME). The model accounts for filling ratio, pressure, melt temperature in screw channels and gaps, driving power, torque and the residence time distribution (RTD). It requires two empirical parameters for each screw element to be determined experimentally or numerically using computational fluid dynamics (CFD). The required Nusselt correlation for the heat transfer to the barrel was determined from experimental data. We present results for a fluid with a constant viscosity in comparison to literature data obtained from CFD simulations. Moreover, we show how to incorporate the rheology of a typical, non-Newtonian polymer melt, and present results in comparison to measurements. For both cases, we achieved excellent agreement. Furthermore, we present results for the RTD, based on experimental data from the literature, and found good agreement with simulations, in which the entire HME process was approximated with the metering model, assuming a constant viscosity for the polymer melt.

1. Introduction

Developed in the 1940s and 1950s, intermeshing extruders have been firmly established in various industries for many decades. Examples include the manufacture of polymers, chemicals and foodstuffs. The most common type of extrusion devices is the co-rotating twin screw extruder, specifically for the purpose of mixing of highly viscous materials. Single-screw extruders are typically used as a melting device in injection molding machines. Other types of extruder, such as counter-rotating twin-screws, multi-screws or ram-extruders are preferred for more specific applications (Kohlgrüber, 2008).

In recent years, co-rotating twin-screw extruders have attracted increasing interest in the pharmaceutical industry, mainly for wet extrusion, solid lipid extrusion, hot melt granulation and hot melt extrusion (HME) processes (Kleinebudde, 2011). The latter, in particular, is used for the preparation of solid solutions and amorphous solid dispersions for improving the bioavailability of poorly water-soluble drugs (Breitenbach, 2002; Repka et al., 2005). For this and other pharmaceutical applications, the good mixing performance, the self-wiping properties, the short residence time and the resulting product quality and yield of the co-rotating intermeshing twin-screws are a major advantage (Ghebre-Sellassie and Martin, 2003). In addition, the process is solvent-free, which is highly beneficial in day-to-day manufacturing as costs associated with solvent use, recovery, separation and disposal are high. Furthermore, the commonly used modular screw design provides high operational flexibility. However, a major challenge is the complexity of developing an appropriate screw configuration to accommodate the actual process requirements. This task usually requires extensive experience and/or experimental (and mostly empirical) work.

Modeling and simulation methods can help increase the understanding of the complex interaction between screw geometry, material properties and the operating conditions. In experimental studies, extruders are essentially black-box systems, since detailed measurements of the filling ratio, the pressure distribution and the local material temperature along the screws are very difficult to achieve. A simulation has the potential to provide

Abbreviations: 1D, one-dimensional; 3D, three-dimensional; CFD, computational fluid dynamics; DEM, discrete element method; HME, hot melt extrusion; HTC, heat transfer coefficient; LDPE, low density poly-ethylene; ODE, ordinary differential equation; RTD, residence time distribution.

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Notation

Latin symbols

A_0	Screw parameter for non-conveying elements [−]
A_1, A_2	Screw parameters for conveying elements [−]
A_3	Empirical shear rate parameter [−]
A_b, A_s	Cross-section area of barrel and screws [m^2]
A_{bm}, A_{sm}	Heat exchange area barrel/melt and screws/melt [m^2]
A_e	Barrel/environment surface area [m^2]
A_{cr}	Free cross-section area of the twin-screw [m^2]
$A_{s,ch}$	Screw channel surface area [m^2]
$A_{s,tip}$	Screw tip surface area [m^2]
A_{surf}	Total screw surface area [m^2]
a_T	Temperature shift factor (Carreau model, WLF equation) [−]
C	Coefficient in the Nusselt correlation [−]
C_1, C_2	Parameters of the WLF equation [−, °C]
C_L	Centerline distance [m]
c_p^b, c_p^m, c_p^s	Heat capacity of the barrel, melt, screws [J/kgK]
D	External screw diameter [m]
D_B	Barrel diameter [m]
D_C	Screw core diameter [m]
d	Die diameter [m]
$E(t)$	Pulse response (RTD density function) [s^{-1}]
$F(t)$	Step response (cumulative RTD) [−]
f	Filling ratio [−]
H	Channel depth [m]
h	Gap distance [m]
K_1, K_2, K_3, K_4	Parameters of the Menges model [Pa × m^3/kg, Pa × m^3/kgK, Pa, Pa]
K_b, K_f	Screw conveying parameter [−]
K_p	Screw pressure parameter [−]
k	Reynolds exponent in the Nusselt correlation [−]
L_{Die}	Die length [m]
L_D	Disc length of kneading elements [m]
L_{off}	Offset length of kneading elements [m]
m	Carreau index [−]
m_b, m_s	Mass of barrel and screws [kg]
$\dot{m}$	Mass flow rate [kg/s]
$\dot{m}_f, \dot{m}_b$	Forward or backward screw-driven mass flow rate [kg/s]
$\dot{m}_p$	Pressure-driven mass flow rate [kg/s]
N	Number of numerical elements [−]
Nu	Nusselt number [−]
n	Screw speed [s^{-1}]
n_F	Number of flights [−]
n_D	Kneading element disc number [−]
P_{heat}	Barrel heating/cooling power [W]
P_{pump}	Pumping power [W]
P_{screw}	Screw driving power [W]
Pr	Prandtl number [−]
p	Pressure [Pa]
$\dot{Q}$	Heat flux [W]
$\dot{Q}_e$	Heat loss to the environment [W]
$\dot{Q}_{bm}, \dot{Q}_{sm}$	Heat fluxes barrel/melt and screws/melt [W]
$\dot{q}$	Volume-specific heat source [W/m^3]
Re	Reynolds number [−]
T	Temperature [°C]
T^e	Environment temperature [°C]
T^b, T^m, T^s	Temperature of barrel, melt, screws [°C]
ΔT_{ga}	Temperature increase in the gap [°C]
T_r	Reference temperature (WLF equation) [°C]
T_s	Screw pitch [m]
T_{screw}	Screw torque [Nm]
T_{trans}	Transition temperature (Menges model) [°C]
t	Time [s]
V	Volume [m^3]
$\dot{V}$	Volumetric throughput [m^3/s]
$\dot{V}^*$	Dimensionless volumetric throughput [−]
v	Specific volume [m^3/kg]
w	Species mass fraction [−]
x	Axial coordinate [m]

Greek symbols

α	Tip angle [°]
α_b, α_s	HTC barrel/melt and screws/melt [W/m^2K]
α	HTC barrel/environment [W/m^2K]
$\dot{\gamma}$	Shear rate [s^{-1}]
$\dot{\gamma}_{crit}$	Critical shear rate (Carreau model) [s^{-1}]
$\dot{\gamma}_r$	Representative shear rate [s^{-1}]
$\dot{\gamma}_w$	Wall shear rate [s^{-1}]
ε	Volume fraction [−]
η	Dynamic viscosity [Pas]
η_o	Zero-shear-rate viscosity (Carreau model) [Pas]
η_r	Representative viscosity [Pas]
κ	Kneading element offset angle [°]
λ_b, λ_m, λ_s	Thermal conductivity of the barrel, melt, screws [W/mK]
ρ	Density [kg/m^3]
σ	Standard deviation of the residence time [s]
τ	Mean residence time [s]
τ_W	Wall shear stress [Pa]
ψ	Angle in the screw cross-section [°]

Indices

ax	Axial
ch	Channel
circ	Circumferential
diss	Viscous dissipation
ga	Gap
i	Element i
off	Offset

complete access to critical parameters in a twin screw extrusion process. This is a particularly powerful approach for scaling-up the process. However, it is still not possible to develop a comprehensive HME model (Kohlgrüber, 2008). In part, this arises from the complex behavior of the processed materials, which are, typically, polymers. Although adequate models have been developed for pure polymers, most applications of HME involve the mixture of two, three or even more components. In these cases, the actual values of the macroscopic material properties (e.g., viscosity, density) depend on the degree of mixing. Due to dissipative heating in small gaps, flows are non-isothermal with the associated effect on the local viscosity. A further challenge is that for the detailed simulation of the flow in partially filled screw sections, well-established methods are currently not available. Similarly, a detailed simulation of the transition from granular to molten state has not yet been developed.

Computational methods for the three-dimensional (3D) simulation of screw sections are available, e.g., the discrete element method (DEM) for the granular flow in the intake zone and computational fluid dynamics methods (CFD, mainly finite element and finite volume methods) for the simulation of viscous