2015

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Petru S Fodor
Miron Kaufman

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Citation: AIP Conference Proceedings **1664**, 050010 (2015); doi: 10.1063/1.4918414
View online: http://dx.doi.org/10.1063/1.4918414
View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1664?ver=pdfcov
Published by the AIP Publishing

Moffatt Eddies in the Single Screw Extruder: Numerical and Analytical Study

Petru S. Fodor and Miron Kaufman

Physics Department, Cleveland State University, Cleveland, OH 44115

Abstract. A detailed analysis of the fluid flow in the single screw extruder is performed by combining numerical and analytical methods. While finite element analysis numerical models are used to extract the transversal velocity field, an analytical model in the limit of zero Reynolds numbers is used to determine the longitudinal component of the fluid velocities. The high resolution 3D model developed for the fluid flow in single screw extruders with aspect ratios (i.e. depth/width) ranging from 1 to 0.1, allows the identification of the position and extent of Moffatt eddies that impede the fluid mixing through the entire extruder's volume. This information is used to estimate the extent by which the Moffatt eddies formation affects the mixing in the extruder, and also to develop strategies to prevent their formation.

Keywords: Single-Screw Extruder; Corner/Moffatt Eddies; Particle Tracing.
PACS: 47.15.Rq; 47.85.md.

INTRODUCTION

As one of the fundamental processing tools in polymer engineering, single-screw extruders have been the scope of a sizable body of research in terms of optimization of their building blocks and flow modeling [1, 2]. While their basic design is quite simple, essentially an Archimedes' screw rotating inside a stationary cylindrical barrel, studies of the flows driven within them and similar cavity type systems have shown that the resulting fluid velocity fields are quite complex and difficult to model [3, 4]. Consequently, the geometrical parameters design of single-screw extruders relies heavily on empirical evidence and personal experience [5] besides the information provided by simple analytical models [6, 7] or direct visualization of the flow fields using imaging tracers [8].

In the single screw extruder, a particularly challenging task is to accurately map the flow field in the corners away from the moving boundary of the barrel and close to the screw flights. Seminal work by Moffatt [9], on the fluid flow close to a corner defined by rigid boundaries has shown that the general flow configuration in this type of region consists of series of eddies of decreasing spatial extent and intensity. Materials trapped in this type of eddies have both low longitudinal and low transversal velocity components. The associated long residence times in these regions can lead to polymer resin degradation. While the spatial extent of the Moffatt eddies is not large compared with the bulk of the extruder volume, the degradation products can eventually contaminate the batch of extruded polymer [5, 10]. Evaluating accurately the spatial extent of the corner eddies for specific processing parameters and screw dimensions in order to find ways to mitigate them, is however challenging. Experimental imaging of the fluid flow in this region is difficult and analytical models provide limited information due to the singularity imposed by the rigid boundaries defining it. As an alternative, numerical modeling has been quite successful in predicting the flow fields in the single-screw extruder system [11, 12]. Nevertheless, in order to visualize the corner eddies a purely numerical approach would require very fine meshing around the corners throughout the 3D geometry, which can be computationally expensive, if not prohibitive.

In this work we use a combined numerical and analytical approach, in which finite element analysis numerical simulations are used to determine the transversal velocity field. Taking advantage of the low Reynolds number applicable to the case of the single-screw extruder the longitudinal component of the fluid velocities are modeled using an analytical model. This approach permits sufficiently fine meshing of the cross section of the fluid stream, to locate up to three eddies in the Moffatt series, while limiting the necessary computational expense. The velocity fields are subsequently integrated in order to determine the trajectories of tracers released at the inlet of the extruder and evaluate the geometry of the corner eddies. Knowledge of the exact spatial extent of these eddies, is used to determine extent with which the corner regions can be rounded or filleted in order to suppress the formation of the Moffatt eddies.

Proceedings of PPS-30
AIP Conf. Proc. 1664, 050010-1–050010-5; doi: 10.1063/1.4918414

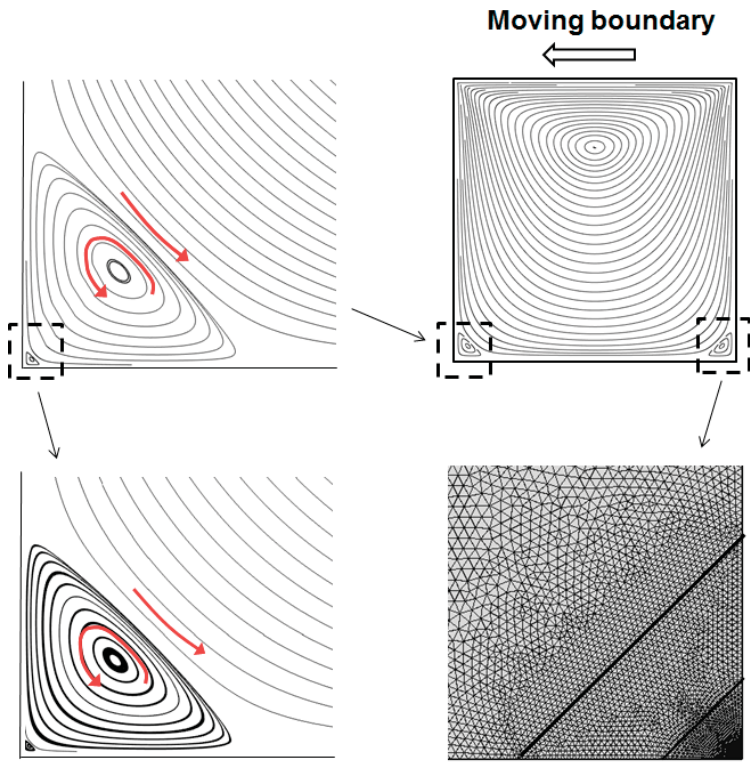

FIGURE 1. Streamlines in the longitudinal cross section of the extruder (Aspect ratio = 1; Reynolds number Re = 0.02). High resolution meshing (lower right figure) of the corner regions is needed to reveal the formation of the corner eddies.

MODELING AND DISCUSSION

Under normal operation conditions, i.e. low Reynolds number, the helical geometry of the single-screw extruder can be analyzed from the point of view of fluid mechanics as a channel with the upper boundary moving diagonally at an angle determined by the pitch of the screw [2,3]. Within this model the axial component of the boundary velocity is responsible for the drag flow that conveys the fluid along the channel. In the same time, the drag associated with the transversal component of the boundary motion, induces a transversal flow within the extruder and thus is responsible for its mixing action.

Within the above approximation, we use finite element analysis simulations to solve the Navier-Stokes equations for the transversal flow field. For all the simulations described in this work we use the computational package COMSOL Multiphysics and its Computational Fluid Dynamics/Chemical Engineering module. The accuracy of the numerical work employed for this type of flows has been previously validated against well described cavity flows [13]. For this specific situation, the typical values used for the density and the viscosity are 0.9×10^3 kg/m^3 and 100 Pa·s, respectively. For simplicity, all the solutions presented here are for an incompressible Newtonian fluid, although a non-Newtonian model using the strain dependence of viscosity for polyethylene was also developed. Nevertheless, for the strain rates investigated the results of the two models are similar. The depth D of the single-screw is set to 2.5×10^{-2} m while its width W is changed from 2.5 to 25×10^{-2} m, setting a range for the aspect ratio (=depth/width) from 1 to 0.1. The top boundary of the cross-section of the screw is moving at speeds v_{bxy} from 0.005 to 0.5 m/s. For typical pitch angles this implies that the flow regime corresponds to low Reynolds numbers (<1). The flow equations are solved in the steady state with non-slip boundary conditions imposed at all the walls, using a generalized minimal residual method (GMRES) iterative solver with a geometrical multigrid pre-conditioner and a Vanka algorithm for the pre- and post-smoothing. A free triangular mesh is used for the entire cross-section. For the bulk of the extruder the maximum element size in the mesh is 1.5×10^{-3} of the depth D. As shown in Fig. 1 the mesh is made progressively finer at the corners of the geometry in order to accurately map the Moffatt eddies induced by the disturbance associated with the movement of the top boundary. In the region occupied by the series of three

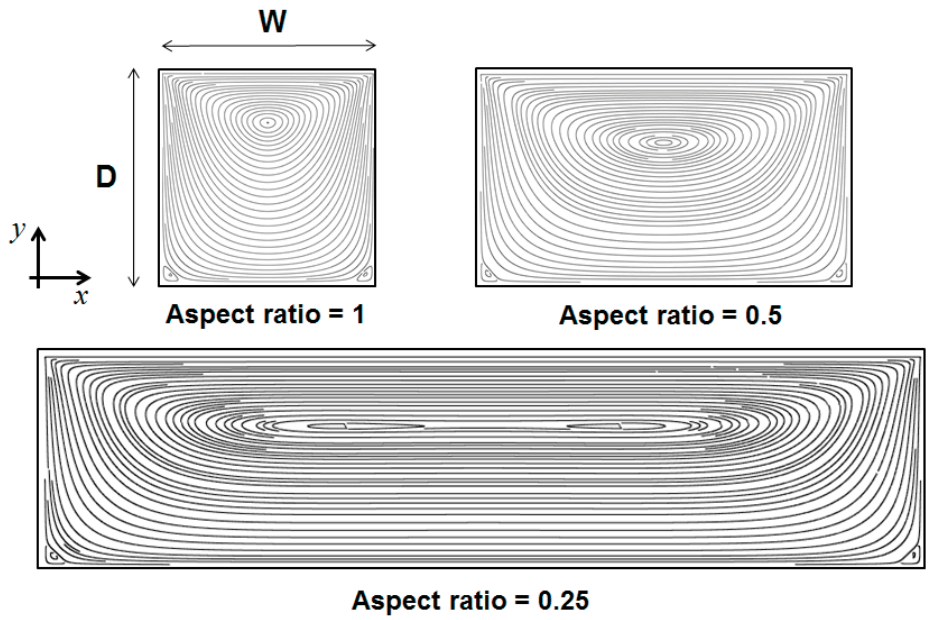

FIGURE 2. Field line for three different aspect ratios at a Reynolds number of 0.2. In all cases the top boundary is moving at a constant speed towards right.

corner eddies the maximum mesh element size is decreased to 0.3×10^{-4}, then 0.1×10^{-4}, and then 0.1×10^{-5} of the depth D, respectively. Typically, to avoid overmeshing, a simulation is done with a rougher mesh in order to identify the basic outline of the corner flows. In any case, it is quite clear that the small mesh size required to map the corner features would make a complete 3D numerical modeling of the geometry exceedingly computationally expensive.

Figure 2 shows the simulated cross-sectional flow fields for various aspect ratios. Similar results have been obtained for aspect ratios down to 0.1. For all the aspect ratios and Reynolds numbers investigated the flow fields show common features. Besides the primary vortex which is responsible for the bulk mixing in the single-screw extruder, all the simulations show the presence of corner eddies.

While the transversal components of the velocity field u_x and u_y are extracted from the numerical simulations, its longitudinal component u_z is determined analytically assuming a pressure and drag driven flow [2]:

$$\frac{u_z(x,y)}{v_{bz}} = \frac{4}{\pi}\sum_{i=1,3,5}^{\infty}\frac{\sinh\left(i\pi\frac{D}{W}\frac{y}{D}\right)}{i\sinh\left(i\pi\frac{D}{W}\right)}\sin\left(i\pi\frac{x}{W}\right) + \\ +\left(\frac{D^2}{2\mu v_{bz}}\frac{\partial P}{\partial z}\right)\left(\frac{y^2}{D^2}-\frac{y}{D}+\frac{8}{\pi^3}\sum_{i=1,3,5}^{\infty}\frac{\cosh\left[i\pi\left(\frac{x}{W}-0.5\right)/\left(\frac{D}{W}\right)\right]}{i^3\cosh\left[i\pi/\left(2\frac{D}{W}\right)\right]}\sin\left(i\pi\frac{y}{D}\right)\right) \tag{1}$$

where v_{bz} is the speed of the moving wall in the axial direction.

Based on the complete description of the flow field the paths of the material advected through the volume of the single-screw extruder can be determined. To this end we use massless particle tracers that are released at the inlet of the extruder and their trajectory is calculated by solving their equation of motion:

$$\frac{d\vec{r}}{dt} = u(\vec{r}) \tag{2}$$

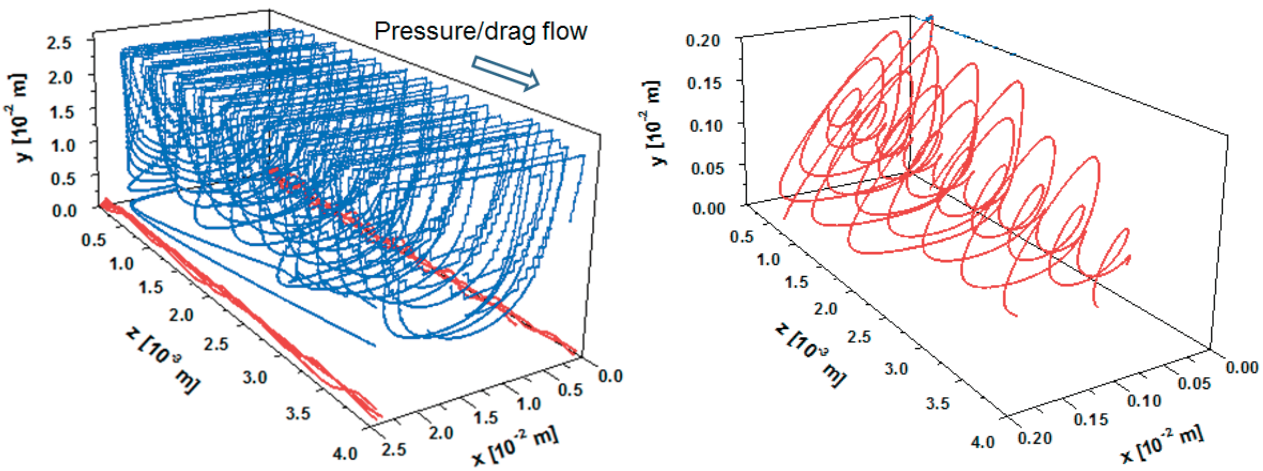

FIGURE 3. (left) Particle trajectories for particles released within the primary vortex of the extruder (blue) and within the corner eddies region (red). (right) Close up on particle trajectories within the Moffatt eddies region.

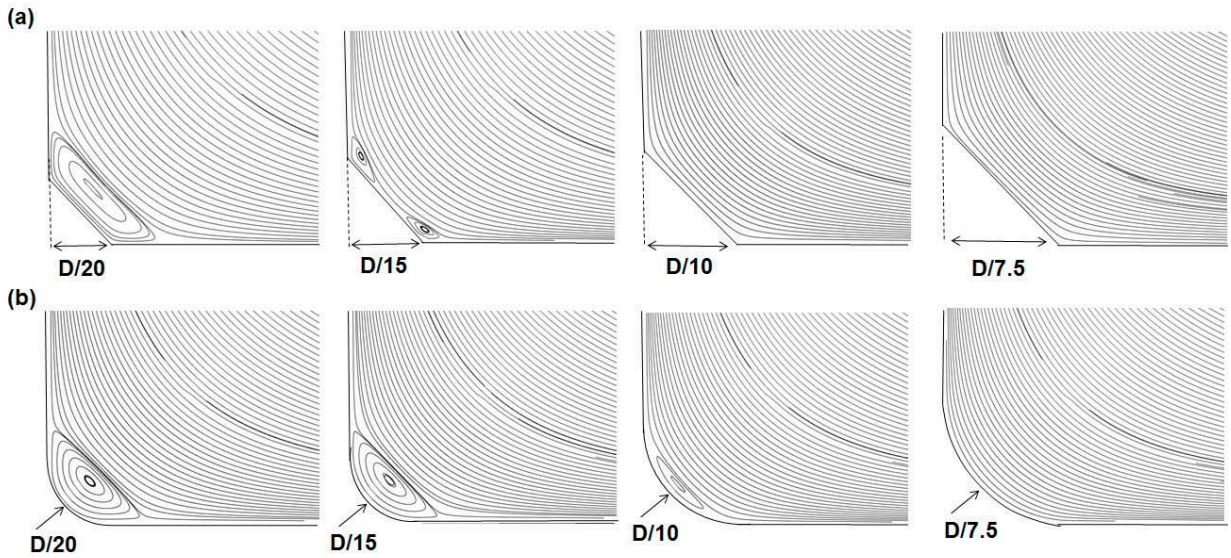

FIGURE 4. Streamlines for modified cross sections in which geometrical features such as (a) fileted and (b) rounded corners are used to eliminate the eddies.

The time evolution of typical trajectories is shown in Fig. 3. It is immediately apparent that particles released in the corner eddies mix very poorly while in the melt with the bulk of the material driven by the primary vortex. Also the stagnation regions associated with the long residence time in the corner eddies can lead to material degradation and process failure [5, 10].

Knowledge of the location of the Moffatt eddies as a function of the speed of the extruder, Reynolds number and screw depth, allows for mitigation strategies to be developed, such as geometrically modifying the corners. The effect of the flight radius of the screw extruder on the quality of the extruded polymer has been documented [10]. However, in this case we benefit from accurate information on the extent of the corner eddies, allowing an optimal determination of the extent by which the geometry has to be modified to eliminate the eddies. Figure 4 shows results for cross-sections in which the corners have either been fileted or rounded. The transition between flow patterns with or without corner eddies can be easily determined enabling the determination of the minimum flight radius needed, so that the optimal throughput of the extruder can be preserved.

SUMMARY

Information from numerical simulations and from an analytical model is used to describe the flow field in the single screw extruder in the low Reynolds number regime. The combined approach allows accurate mapping of the eddies formed at the corners of the extruding channel, while limiting the computational resources needed. Knowledge of the position and spatial extent of these stagnant regions allows for the geometrical parameters of the extruder to be optimally chosen to eliminate them. In particular a quantitative assessment of distributive and species mixing using entropic measures [14, 15] is planned.

ACKNOWLEDGMENTS

This work is partially supported by the National Science Foundation under Grant No. 1126126. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

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