Modeling Devolatilization in Single- and Multi-Screw Extruders

Vented single- and multi-screw extruders are widely used to remove undesirable residual volatile components from highly viscous polymer melts. To increase devolatilization efficiency, a thorough understanding of the transport phenomena governing the separation process is needed. A new modeling approach demonstrating the great influence of surface renewal on mass transport in vented extruders was developed. By increasing the general understanding of the problem, the new approach will help to meet the high demands in terms of melt quality.

**Devolatilization in Vented Extruders**

In the manufacturing process of most polymerization products, some undesirable volatile components such as unreacted monomers, water or other impurities remain in the polymer matrix. For both environmental and technological reasons, these low-molecular-weight components are usually separated from the bulk polymer in a post-reactor operation known as devolatilization. Employing vented single- and multi-screw extruders in particular provides a competitive solution, as they are able to devolatilize polymers with viscosities ranging across several orders of magnitude.

Only a few theoretical studies have examined devolatilization in vented extruders analytically. All of these analyses omitted the significant influence of surface renewal on mass transport, which provides the exposed surfaces with a continuous supply of fresh volatile component.

**A New Approach**

At low volatile levels, mass transport in polymers is controlled by molecular diffusion, where mass transfer is driven by a concentration gradient. In general, devolatilization in vented extruders is governed by two parallel mass transport mechanisms: evaporation from the circulating melt pool that develops in front of the active flight flank and from the wiped melt film deposited on the barrel surface.

![Fig. 1: Schematic diagram of a screw channel in the extraction zone of a vented extruder](image-url)
Previous studies ignored the influence of the circulatory motion of the polymeric material accumulated in front of the active flight flank of the screw, which provides the exposed surface with a continuous supply of fresh volatile component. To demonstrate the significance of surface renewal in the mass transport of volatiles, an approximate analytical solution for the circulatory flow in a partially filled screw channel is derived. The resulting velocity field is then applied to the governing conservation equation for the volatile concentration in the polymeric phase.

![Fig. 2: Vector plot of the flow field that develops in front of the active flight flank](image)

The resulting convection-diffusion equation, which is solved numerically using the finite-volume method, provides both qualitative and quantitative insights into how volatile depletion in the melt pool is related to the flow field developed. As a result, the new modeling approach shines light on the general understanding of the problem.

![Fig. 3: Volatile concentration distribution in the melt pool assuming a rotating screw](image)

Impact and Effects

The approximate solution for the cross channel flow in a partially filled channel provides a useful tool for in depth analysis of flow in vented extruders and other extruders where partial fill occurs. Furthermore, the new modeling approach clearly demonstrates that surface renewal considerably accelerates volatile depletion in the polymer melt even at low screw speeds, making it an effective means of improving devolatilization efficiency.

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