Numerical simulation of polymer blending in twin-screw extrusion: A computational primer for a digital twin

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The blending of homopolymers is commonly used to create polymeric materials with synergistic and tunable properties. Most polymer blends are immiscible, consequently this kind of system has a multiphase structure. The twin-screw extruder (TSE) is the most common device used for polymer compounding. To speed up the process design and optimization, a computational tool capable of predicting the final blend morphology by varying the processing parameters is desired. In this work, the evolution of the disperse polymer blend morphology in a twin-screw extruder is studied. Computational fluid dynamics simulations are employed along with a detailed model for blend morphology accounting for droplet coalesce, breakage, stretching and necking. The study is first carried out in a 2D planar TSE to validate the model. Our results are in a fair agreement with simulations available in the literature. The analysis is then extended to a real 3D geometry of a forward-conveying element of a corotating TSE. The flow fields as well as the evolution of the blend morphology within the extruder are analyzed by varying the relevant process parameters. This work represents the first step to build a digital twin of this process able to provide information on the blend microstructure evolution during compounding that would be impossible to obtain experimentally. Digital twining will facilitate human-machine relationships in order to optimize the characteristics of the final product, avoiding onerous trial-and-error procedures.

Keywords: *Polymer blends, Twin-screw extrusion, Morphology prediction, Digital twins*