Reactive extrusion: A computational approach. MANORANJAN
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Univeristy Eindhoven — Reactive extrusion is attractive for various reasons. One
of them is the flexibility of extruders for processing of polymers, but also the choice
of the scale of the operation that can be adjusted to the needs for research and
development or commercial production. We model reactive extrusion using a diffuse
interface modeling (DIM) approach. The problem is studied by dividing it into four
small/sub problems. First, the structure growth in case of homo-polymer blends was
studied with the effect of hydrodynamics. The logarithmic structure factor was found
to scale as $1/3$ with time for higher capillary numbers and $2/3$ for lower capillary
numbers. Second, the growth of structure for the block copolymer was studied for
the symmetric blocks, for which only micro phase separation was observed. Then,
the structure growth for the mixture of block copolymers and homo-polymers was
studied and both micro and macro phase separation can be observed. The final step
including the reaction kinetics of the formation of block copolymers from the homo-
polymer is studied. Results are mainly presented showing morphology development
and growth rates as a function of time.

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