Efficient Calculation of Molecular Weight Distribution in the Presence of Non-ideal Mixing

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The polymer is composed of various macromolecules, and its mechanical properties are determined by the molecular weight distribution (MWD). However, few models could predict detailed MWD in the presence of non-ideal mixing, due to computational complexity and calculation load; The non-ideal mixing effect should be analyzed by the computational fluid dynamics (CFD) runs, and detailed MWD calculation involves the infinite number of differential equations. In this study, two efficient approximations were proposed to mitigate the complexity.

1) CFD-compartments method: CFD result was simplified into a network of several CSTRs where local hydrodynamics were averaged.

2) Z- transformation: The infinite number of differential equations were projected into the z-domain where the selected number of equations were specified to efficiently calculate the MWD in the virtual domain. Then, the solution was reverse-transformed into the original domain to recover the actual MWD.

The developed dynamic model was shown to be faster than the real physics. The model was also validated with industrial LDPE reactor and could successfully predict the detailed shape of MWD.