

and the QMOM was successfully extended to aggregation-breakage problems.¹⁵ Generally speaking, the QMOM provides high accuracy even with reduced number of points (i is generally < 5).

A major common limitation of all moment based methods is that they are not able to accurately calculate the CSD. If accurate CSD calculation is required, another numerical solution technique has to be applied. In addition, the implementation of dissolution is difficult because of the zeroth moment (crystal number): the zeroth moment is decreasing only if there are crystals at the left boundary of the crystal size domain, which can disappear from the system. This information is however not available, since the CSD cannot be exactly reconstructed from the moments.

2.5.2 Method of Characteristics

The method of characteristics (MOCH) provides an elegant way to determine the evolution of the crystal size distribution for crystallization processes.²⁹ The MOCH for first order PDEs determines lines, called characteristic lines, along which the PDE degenerates into a set of ODEs.³⁰ The MOCH is demonstrated through the pure size independent growth batch PBE:

$$\frac{\partial n(L,t)}{\partial t} + G \frac{\partial n(L,t)}{\partial L} = 0 \quad (2.55)$$

MOCH finds curves in the $(L-t)$ plane, which reduces the PBE to a system of ODEs. The $(L-t)$ plane can be expressed in a parametric form by $L = L(Z)$ and $t = t(Z)$, where the parameter Z gives the measure of distance along the characteristic curve. Then, the population density function can be redefined as:

$$n(L,t) = n(L(Z),t(Z)) \quad (2.56)$$

Applying the chain rule on we can obtain:

$$\frac{dn(L,t)}{dZ} = \frac{dt}{dZ} \frac{\partial n(L,t)}{\partial t} + \frac{dL}{dZ} \frac{\partial n(L,t)}{\partial L} \quad (2.57)$$

Comparing the coefficients of eqn (2.55) and (2.57), it can be concluded that:

$$\frac{dt}{dZ} = 1 \Rightarrow dt = dZ \quad (2.58)$$

$$\frac{dL}{dZ} = G \Leftrightarrow \frac{dL}{dt} = G \quad (2.59)$$

$$\frac{dn(L,t)}{dZ} = 0 \Leftrightarrow \frac{dn(L,t)}{dt} = 0 \quad (2.60)$$