with initial conditions, corresponding to $t = Z = 0$, $L = L_0$ and $n(L,0) = n_0(L_0)$. To obtain the dynamic evolution of the crystal size distribution, $n(L,0)$, eqn (2.59) and (2.60), with prescribed growth expressions, can be integrated repeatedly for different initial values $[L_0, n_0(L_0)]$.

For the expression of growth rate, the actual concentration is required. The accurate evaluation of the mass balance requires very fine CSD discretization, which degrades the simulation time. MOCH is often combined with the QMOM, where the QMOM provides the accurate concentration profile, which is then used as an input to the MOCH for growth rate calculation.[31] This elegantly and efficiently decouples the accuracy of the method from the calculation time.

The combined MOCH – QMOM is very efficient and accurate for growth-only problems. The implementation of nucleation, however reduces its efficiency. In addition, the implementation of secondary mechanisms (breakage, agglomeration) is possible, but complicated.

2.5.3 Finite Volume Methods

The finite volume method (FVM) is a standard approach for the numerical solution of hyperbolic partial differential equations,[32] which makes it well suited for the solution of PBEs. The FVM relies on the discretization of the crystal size domain and the finite volume approximation of the population density function on the defined grid. The method is demonstrated on the one dimensional PBE with nucleation and growth:

$$\frac{\partial n(L,t)}{\partial t} + G\frac{\partial n(L,t)}{\partial L} = B\delta(L - L_n) \tag{2.61}$$

Denoting with h the size and k the time interval, n_l^m is the approximate (discrete) population density function of the continuous $n(L,t)$, defined as:

$$n_l^m \approx \frac{1}{h}\int_{(l-1)h}^{lh} n(L,t)\,\mathrm{d}L \tag{2.62}$$

where m and l are integers such that $m \geq 0$ and $N \geq l \geq 1$. N stands for the mesh size (*i.e.* the number of discretization points). Then, the PBE reduces to a system of algebraic equations:

$$\begin{aligned} n_l^{m+1} &= n_l^m - \frac{k}{h}\left(G_l n_l^m - G_{l-1} n_{l-1}^m\right) \\ &- \begin{bmatrix} \dfrac{kG_l}{2h}\left(1 - \dfrac{kG_l}{h}\right)\left(n_{l+1}^m - n_l^m\right)\phi_l \\ -\dfrac{kG_{l-1}}{2h}\left(1 - \dfrac{kG_{l-1}}{h}\right)\left(n_l^m - n_{l-1}^m\right)\phi_{l-1} \end{bmatrix} + \frac{n_{l,f}^m - n_l^m}{\tau} + \varepsilon_\mathrm{b}\frac{k}{h}B \end{aligned} \tag{2.63}$$

ε_b is a binary existence variable with values $\{0, 1\}$: $\varepsilon_\mathrm{b} = 1$ if $l = 1$ (nucleon size) and is 0 otherwise. The second term in the right hand side of eqn (2.63) is the first order term. The FVM can also be solved using the first order term only,