

To calculate recycles their parameters are initially estimated and based on these estimations new values are computed. From these calculated values better estimations could be obtained. The process continues iteratively until convergence is reached. The convergence here is the minimization of residual between calculated and previously estimated values of tear streams.

$$|Y_{calc} - Y_{est}| > |Y_{calc}| \cdot R_{tol} + A_{tol}$$

where Y_{calc} – calculated values; Y_{est} – estimated values; R_{tol} – relative tolerance; A_{tol} – absolute tolerance.

Estimation algorithm significantly affects the convergence rate and thereby the performance of the whole simulation system.

The simplest method, applied in Dyssol system is the **direct substitution**, which uses values calculated on the previous iteration as the initial data for the next iteration:

$$x_{k+1} = F(x_k)$$

This method is the least computationally intensive, but has slow convergence rate.

To increase the convergence rate results of the several previous iterations should be used for data estimation. It could be done by providing direct substitution method with the relaxation parameter λ :

$$x_{k+1} = (1 - \lambda)F(x_{k-1}) + \lambda F(x_k)$$

If $\lambda = 1$ it transforms to the direct substitution method.

Other methods are more computationally intensive but can provide faster convergence.

Wegstein's method uses results of two previous iterations:

$$X_{k+1} = qX_k + (1 - q)F(X_k)$$

where q is an acceleration parameter:

$$q = \frac{s}{s - 1}$$

$$s = \frac{F(X_k) - F(X_{k-1})}{X_k - X_{k-1}}$$

Convergence is possible if the parameter q is in range $[-5; 1]$ and accelerates with a decreasing of its value. So for the greater control over the convergence process the acceleration parameter can be additionally bounded on a smaller range.

Steffensen's method uses current and two previous iterations:

$$X_{k+3} = X_k - \frac{(X_{k+1} - X_k)^2}{X_{k+2} - 2X_{k+1} + X_k}$$