Startup of fReactors



With batch reactors, the composition of the reactors changes with time until a steady state is reached. With flow reactors, once these have been running for long enough, the composition of the outgoing product is constant. During the initial phase of running a flow reactor, the conditions take some time to equilibrate and for this steady state to be reached.

A useful parameter in estimating the time it takes to reach steady state is to express the cumulative flow through the reactor in terms of (flowed) reactor volumes.

(Flowed) reactor volumes (RV) = $\frac{\text{Total flowrate of incoming streams (ml/min)}}{\text{Reactor volume (ml)}} \times \text{time (min)}$

By monitoring the output of the reactor and plotting an indicator of the reaction (for example the yield or concentration of one of the products) as a function of reactor volumes allows the time taken to reach steady state to be established and confirmation that the reactor and reaction is running in this way.

By expressing behaviour in terms of reactor volumes allows a wide range of data to be used to give a rule-of-thumb for how many reactor volumes are required to reach steady state. Figure 1 shows the data from 2 example reactions¹. The total fReactor classic volume is ~10ml, so 1 reactor volume is simply 10ml of total flow. After 10ml of flow has passed through the reactor, a small sample is taken, the composition measured and the instantaneous yield calculated. Steady state in these two cases has been achieved after ~2 reactor volumes. The big advantage of this approach is that you can have a low flowrate (a long mean residence time) or a high flowrate (a short mean residence time) and still know that you need to flow 2 to 2.5 x the reactor volume (20-25ml for the fReactor classic) of fluid before steady state is reached.



¹ Orange curve is Scheme 4 and blue curve is Scheme 2 from Chapman MR, Kwan MH, King G, Jolley KE, Hussain M, Hussain S, Salama IE, Gonzalez Nino C, Thompson LA, Bayana ME, Clayton AD, Bao NN, Turner NJ, Kapur N, Blacker JA. Simple and Versatile Laboratory Scale CSTR for Multiphasic Continuous-Flow Chemistry and Long Residence Times. Organic Process Research & Development. 2017 Jul 20;21(9):1294-301 https://pubs.acs.org/doi/pdf/10.1021/acs.oprd.7b00173

NOTE: This information is intended for guideline purposes only.