The C-Curve Statistical Methodology

The purpose of the C-Curve (concentration curve) methodology is to quantitatively characterize the diffusion associated with a particular numerical method when applied to the modeling of scalar transport equations. It is based on experimental techniques developed to quantify the extent of non-ideal flow inside chemical reactor vessels by Levenspiel, Bishoff, Aris, and others. Given a known input pulse of material being tracked, and a measured output profile of that material’s concentration, this methodology permits calculation of a diffusion coefficient associated with the transport of the material.
The C-Curve

\[ C(t) \]

\[ \delta \text{-Function} \] (Input)

Unit Area

\[ t_{\text{lag}} \]

\[ t_{\text{mean}} \]

Time, \( t \)
Key Parameters

The *Mean Residence Time* of a small fluid element injected (with respect to the axially dominant flow direction) is given by:

\[ \bar{t} \equiv \frac{\text{Characteristic Axial Length}}{\text{Axial Velocity}}. \]

The *Mean Time* of the C-Curve distribution, \( t_C \).

\[ \bar{t}_C \equiv \frac{\int_0^\infty t \cdot C(t) \, dt}{\int_0^\infty C(t) \, dt} \approx \frac{\sum_i t_i \cdot C_i \cdot \Delta t_i}{\sum_i C_i \cdot \Delta t_i}, \]

This is calculated at a specific location in space (inlet of flow, outlet of flow)
From the *Mean Time*, the second moment of the distribution can be computed. This parameter, also known as the *Variance* of the distribution, measures the *spread* of the C-Curve in time about the mean, $t_C$.

$$
\sigma^2 = \frac{\int_0^\infty (t - \bar{t}_C)^2 \ C(t) \ dt}{\int_0^\infty C(t) \ dt} = \frac{\int_0^\infty t^2 \ C(t) \ dt}{\int_0^\infty C(t) \ dt} - \bar{t}_C^2 = \frac{\sum t_i^2 \ C_i \ \Delta t_i}{\sum C_i \ \Delta t_i} - \bar{t}_C^2.
$$

The value of the variance is *directly* related to the diffusive nature of the flow inside the flow region, and its value is often used to match experimental to theoretical curves. An impulse of concentration injected at the region inlet will be deformed and spread as a result of the diffusive character of the flow within the region. The variance of the exit concentration vs. time curve (C-Curve) will statistically measure the spread around the mean time.
Application

The Dispersion Model is applicable to flows whose characteristics are close to those of plug flow, that is, with a flat velocity profile across the flow area, low recirculation, and no stagnant pockets of fluid or large short-cutting of flow in the flow region. It relies on the fact that the standard diffusion equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2},$$

is obtained from statistically based processes (molecular or turbulent diffusion). We’re going to be dealing with the equation in the advection diffusion form:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2},$$
Non-Dimensional Form of the Equation

Let

\[ \theta \equiv \frac{t}{\text{Mean Residence Time}} = \frac{t}{t} \]

\[ z \equiv \frac{\text{distance from inlet}}{\text{Axial Length of flow}} = \frac{x}{L} \]

then the flow equation becomes:

\[
\frac{\partial C}{\partial \theta} = \left( \frac{D}{Lu} \right) \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z}
\]
Bounding Cases

The dimensionless parameter $D/Lu$, quantitatively characterizes the diffusion of the transport of the scalar $C$. This parameter is the reciprocal of the axial Péclet number for mass transfer.

$$\frac{D}{Lu} \rightarrow 0 \quad \text{Plug Flow. Little Diffusion}$$

$$\frac{D}{Lu} \rightarrow \infty \quad \text{Well Mixed Flow. Large Diffusion}$$

My experience is that when $D$ is associated with numerical diffusion, we are in the “Plug Flow” regime. In this case, for a delta function input, the shape of the outlet concentration curve (C-Curve) is close to a symmetric Gaussian curve (a normal distribution). Physically, the plug flow assumption requires that the diffusion at any point in the flow region be a function of local conditions only. In the case of numerical methods, numerical diffusion at a given computational cell is a function only of the conditions (velocity, time step size, cell size) at this cell (center and edges).
Additivity

One important property of the flows to which the dispersion model can be applied is the additivity of the variances of the C-Curve for different regions of the flow connected in series:

\[ \sigma_{\text{Outlet}}^2 = \sigma_{\text{Inlet}}^2 + \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_n^2. \]

The variance of the outlet curves can be computed as:

\[ \sigma_{\text{Outlet}}^2 = \sigma_{\text{Inlet}}^2 + \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_n^2. \]
Useful Results

First calculate the change in variance across a flow region:

\[ \Delta \sigma_{region}^2 = \sigma_{Outlet}^2 - \sigma_{Inlet}^2. \]

For moderate to small diffusion, the analytical C-Curve is a family of Gaussian curves whose variance change is given by:

\[ \Delta \sigma_{region}^2 = \frac{\Delta \sigma^2}{t^2} = 2 \frac{D}{uL}. \]

For large diffusion flows, the parameter is given by:

\[ \Delta \sigma_{region}^2 = \frac{\Delta \sigma^2}{t^2} = 2 \left( \frac{D}{Lu} \right) + 8 \left( \frac{D}{Lu} \right)^2. \]
Getting Useful Values

Having the formula and getting useful answers are two different things. You must construct carefully controlled numerical experiments that force dominantly 1-D flow on whatever mesh or portion of a mesh is important to you. If you apply this method to a region with large recirculation patterns or complex diverging and converging flow paths, the results that you get will reflect differences in transit times on different flow paths rather than a numerical (or physical) diffusion process.

Note that 1-D flow does not imply that the flow is always oriented along some favored direction parallel to dominant mesh lines. This information is valuable. However, you should also be looking at flow skewed relative to the mesh lines.