Chapter 8

STATISTICAL ASSESSMENT OF NUMERICAL DIFFUSION

The assessment of the performance of high-order numerical methods regarding the numerical diffusion introduced in the solution of the scalar transport equation is usually based on a comparative analysis of the results obtained for a set of numerical test problems. These problems are intended to show the distortion of an initially sharp scalar profile, e.g. step, square wave, cylinder, etc., consequence of numerical diffusion, as it is transported across a well defined test section. The comparison of the degree of distortion, thus, provides qualitative information about the relative performance of some methods with respect to others [50, 7, 82]. In addition, various mathematical parameters, such as error measures, maximum and minimum values, etc., are also calculated from the results of the test problems and used to give a quantitative estimate of the performance of a particular numerical scheme [66].

The implementation of high-order solute tracking in System Codes stems from the necessity of eliminating as much numerical diffusion as possible, so that the convective transport of a scalar is not artificially enhanced and real turbulent diffusion can be simulated without being overshadowed by the numerical one. For this reason, it is important to obtain a measure of the numerical diffusion that permits quantitative comparison of the method's diffusive character to the actual diffusion expected from the turbulence of the flow through nuclear system components.

Even though, as mentioned above, numerical test problems can be devised to compare the performance of different numerical methods against each other, it is important to determine how much false diffusion a numerical method introduces when simulating a particular flow configuration. For relatively simple numerical schemes, e.g. explicit and implicit Upwind, a mathematical expression for calculating the diffusion coefficient is available [60]. However, in case of more complex methods, or if non-linear numerical flux limiters are used, the task of obtaining a simple formula becomes much more difficult. Moreover, for the complex flow patterns and component noding schemes and configurations usually employed in simulations with System Codes, a formula to obtain the overall numerical diffusion may not be available.

A new statistical methodology was thus developed during the course of this work, aimed at obtaining a parameter which could be used to characterize the amount of false diffusion associated to a numerical method under different flow and noding configurations. An equivalent parameter can then be obtained from correlations for turbulent diffusion coefficients (available for one-dimensional flows), or
from the application of the statistical methodology to experimental results in case of multidimensional flows. Finally, the comparison of the values of the experimental and numerical parameters can be used in the assessment of the suitability of the numerical method to accurately model scalar transport for the flow under study.

8.1. The C-Curve Statistical Methodology

The purpose of the C-Curve methodology is to quantitatively characterize the diffusion associated with a particular numerical method when applied to the modeling of scalar transport in System Codes. 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 [56]. The C-Curve represents the normalized concentration vs. time response at the outlet of a vessel when an idealized instantaneous impulse of concentration (mathematically a Dirac $\delta$-function) is injected in the incoming flow at the inlet of that vessel. The normalization is based on the initial concentration of the injected tracer, $C_0$. As will be shown below, this curve is a statistical distribution related to the exit age distribution of the fluid leaving the vessel (known as E-Curve) [56]. It is necessary to point out that the term vessel as used here means closed flow path with an axially-dominant direction; although three-dimensional flow can also be expected, the cross-flow is small when compared to the flow in the axial direction. The main contribution of the cross-flow is then turbulent diffusion of the solute in a direction perpendicular to the main flow direction.

![Figure 8-1. Concept of C-Curve. Response to an Injection Impulse of Tracer](image)
Figure 8-1 shows a typical C-curve for arbitrary flow in the vessel. Since a $\delta$-function is a mathematical concept, the unit area instantaneous pulse is experimentally replaced by a square pulse of finite height, $C_0$, and a well defined time width.

A series of statistical parameters can then be computed based on the information obtained from the flow characteristics and the C-Curve associated to the transport of the solute field by the flow. Thus, for constant velocity flow, the Mean Residence Time of a small fluid element injected in the vessel (with respect to the axially dominant flow direction) is given by:

$$t = \frac{\text{Characteristic Axial Length}}{\text{Axial Velocity}}.$$  

(8-1)

The Mean Residence Time is a crude measure of the dispersion of a tracer signal injected in the vessel. A better parameter obtained from the C-Curve is the first moment of the distribution with respect to the origin of times, $t=0$, that is, the Mean Time of the C-Curve distribution, $t_C$. When the concentration, $C(t)$, is a continuous function of time, this parameter can be computed by the integral shown in Eq. (8-2). If, on the other hand, the C-Curve has been obtained from experimental measurements at sampling time intervals, $\Delta t_i$, the discrete approximation of Eq. (8-2) can be used to estimate the value of the Mean Time. Obviously, the shorter the sampling time the more accurate the value of $t_C$.

$$t_C = \frac{\int_0^\infty t C(t) dt}{\int_0^\infty C(t) dt} \approx \frac{\sum_i t_i C_i \Delta t_i}{\sum_i C_i \Delta t_i},$$  

(8-2)

where $C(t)$ represents the concentration measured at the vessel outlet. The Mean Time is also known as the location parameter of the distribution, in this case, the location in time of the C-Curve with respect to the initial time of injection.

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, $t_C$, and it is equivalent to the square of the radius of gyration of the distribution. Equation (8-3) shows the expression for a continuous function together with the approximation for the case of discrete sampling.
The value of the variance is directly related to the diffusive nature of the flow inside the vessel, and its value is often used to match experimental to theoretical curves [56]. An impulse of concentration injected at the vessel inlet will be deformed and spread as a result of the diffusive character of the flow within the vessel. The variance of the exit concentration vs. time curve (C-Curve) will statistically measure the spread around the mean time.

The methodology described in this Chapter is based on the Dispersion Model introduced by Levenspiel [56]. This model was originally used to characterize non-ideal flow patterns within vessels, and is based on the analogy of the turbulent mixing in actual flows with a diffusive process. Its use in order to characterize numerical diffusion is a new application introduced in this thesis, and will be based on the analogy between the turbulent diffusive process and the false diffusion introduced by a numerical method when solving the scalar transport equation.

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 vessel. On top of the plug flow, a certain degree of turbulent mixing is superimposed, whose magnitude is independent of the position within the vessel, and only depends on the local flow conditions. As is well known, turbulent mixing, resulting from small turbulent velocity fluctuations, is statistical in nature. The mixing process occurs as a result of a redistribution of matter by eddies, whose behavior and distribution within a turbulent flow can be considered statistical. Therefore, turbulent diffusion can be approximated by models used to treat other statistical transport phenomena such as conductive heat transfer or molecular diffusion. In particular, diffusive transport can be expressed in general as a function of the gradient of the scalar being transported. For instance, for molecular diffusion Fick’s Law can be written for axially dominant diffusion along the x-axis as:

\[
\frac{\partial C}{\partial t} = D_{mol} \frac{\partial^2 C}{\partial x^2}.
\]  

(8-4)

The analogy of diffusion caused by turbulent eddies to molecular diffusion yields then:
\[ \frac{\partial C}{\partial t} = D_{\text{mol}} \frac{\partial^2 C}{\partial x^2} + D_{\text{turb}} \frac{\partial^2 C}{\partial x^2}. \]  
\hspace{1cm} (8-5)

\( D_{\text{mol}} \) and \( D_{\text{turb}} \) are the coefficients of molecular and turbulent diffusion respectively.

The statistical basis of the original experimental methodology stems from the hypothesis that physical turbulent diffusion is a statistical process similar to molecular diffusion. The independence of the local turbulent transport on the rest of the system conditions makes it possible to apply statistical tools to analyze the diffusion process. In this regard, the C-Curve is a distribution of the exit age of the particles of tracer injected in the vessel, since it records when these particles leave the vessel by measuring the exit concentration. As such, it has a mean time and variance associated as discussed above, and the variance is directly related to the degree of dispersion inside the vessel.

The ultimate purpose of the experimental methodology is to determine the diffusion present in the flow by matching experimentally obtained C-Curves to a family of theoretical curves obtained from the analytical solution of the dimensionless axial transport equation for a specific flow configuration and boundary conditions. The basic equation for axially dominant transport is:

\[ \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2}, \]  
\hspace{1cm} (8-6)

where the velocity \( u \) is the axially dominant velocity in the \( x \) direction.

Equation (8-6) is similar to the one-dimensional solute transport equation with an additional diffusive term, which can be associated with the false diffusion introduced by a numerical method in the convective solution. Equation (8-6) can be made dimensionless, rendering:

\[
\frac{\partial C}{\partial \theta} = \frac{\partial C}{\partial \theta} \equiv \left( \frac{D}{L u} \right) \frac{\partial^2 C}{\partial z^2} \]  
\hspace{1cm} (8-7)

Only for small extents of diffusion has the solution for this equation been found for different boundary conditions. According to these boundary conditions, a vessel can be considered:

- *Closed*, if no diffusion is assumed at the inlet or outlet points and the diffusion is constant throughout the vessel.
- *Open*, when there is no discontinuity at the inlet or outlet regions, i.e. diffusion is possible in these regions.

In case of highly diffusive flows, the solution of Eq. (8-7) is only available for open vessels. Nevertheless, means and variances can be obtained for all cases.

The dimensionless parameter $D/Lu$, called the vessel dispersion number, quantitatively characterizes the diffusion of the transport of the scalar $C$. This parameter is the reciprocal of the axial Péclet number for mass transfer. Its value determines the degree of diffusivity of the flow compared to the convective transport represented by $u$, and $t$ defines the flow as *Plug Flow*, when there is very little diffusion, and the convective transport dominates the flow, and as *Well Mixed Flow*, where the turbulent diffusion is the most active transport mechanism.

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

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

From the analytical solution of Eq. (8-7), a series of C-Curves can be obtained for different flow conditions. The value of $D/Lu$ calculated for the theoretical curve that most closely fits the experimental C-Curve is then used to predict the behavior of the vessel as a chemical reactor. In a real vessel, the value of $D/Lu$ would depend mainly on the degree of turbulent diffusion in the flow; in a numerical solution, this parameter can be associated to the numerical diffusion (note that vessel is used here in a general sense; it can be a one-dimensional model, but also a three dimensional model with predominantly axial flow).

The dispersion model satisfactorily represents flows close to *Plug Flow* conditions, with relatively low diffusion ($D/Lu$ about 0.025). In such cases, the distortion of injected tracer profiles is relatively small, and the shape of the C-Curve is close to a symmetric Gaussian curve, a normal distribution or an error function, and is not sensitive to the boundary conditions imposed on the vessel. For highly diffusive flows ($D/Lu$ about 0.2), however, the C-Curve becomes increasingly asymmetric as the diffusion grows, and its shape is sensitive to inlet and exit boundary conditions. For flows with large backmixing at the inlet and outlet regions, i.e. recirculation and large diffusion at measurement points, the Dispersion Model’s accuracy decreases with increasing diffusion.

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, or different vessels, connected in series:
Figure 8-2. Additivity of Variances For Regions or Vessels Connected in Series

Figure 8-2 shows an example of the additivity of the variances for different flow regions or vessels connected in series. The variance of the outlet curves can be computed as:

$$\sigma_{\text{Outlet}}^2 = \sigma_{\text{Inlet}}^2 + \sigma_{1}^2 + \sigma_{2}^2 + \cdots + \sigma_{n}^2,$$

for \(n\) regions or vessels connected in series.

The additivity property is important because it allows the use of any tracer input signal, regardless of its shape, e.g. a square impulse. The variance of the C-Curve associated to the flow in a given vessel, which may consist of a number of regions with different flow characteristics, can be found, once the variances of the tracer signal at the inlet and outlet are known, from the following equation:

$$\Delta \sigma_{\text{Vessel}}^2 = \sigma_{\text{Outlet}}^2 - \sigma_{\text{Inlet}}^2.$$

The solution of the dimensionless transport equation, Eq. (8-7), for flows to which the dispersion model described above is applicable, provides relationships between the parameter \(D/Lu\) and the variance obtained from Eq. (8-10) (see Ref. [62, 56]).

The application of the experimental methodology described above in order to characterize numerical diffusion is based on the assumption that purely convective transport of solute (with no physical diffusion added) can be assimilated to plug flow conditions: a perfect convective solution without numerical diffusion would move the solute as a perfect plug; the numerical diffusion acts as the superimposed turbulent diffusion in the plug flow model discussed above.

Physically, the plug flow assumption requires that the diffusion at any point in the vessel be a function of local conditions only. In the case of numerical methods solving purely convective problems,
one can maintain that the 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), and does not depend on the overall flow configuration. In addition, since numerical diffusion appears at every computational cell, the flow modeled in numerical experiments can be assumed to satisfy the open vessel conditions.

The loss of accuracy of the dispersion model with large diffusion flows is based on the possibility of backmixing and recirculation at the injection and measurement points. This can usually be avoided in numerical experiments by appropriately designing the configuration of the tests problems. The statistical analysis of the C-Curves obtained from numerical experiments for the convective transport of a “plug” of solute, permits the computation of the diffusion parameter, $D/Lu$, cases where the numerical diffusion introduced is not excessively large. Hence, the application of the C-Curve methodology to numerical diffusion analysis is based on the characterization of the parameter $D/Lu$ for the numerical method employed and the flow configuration being modeled. The value of this parameter can be calculated from the variance of the C-Curve associated with the flow under study. This approach permits the design of numerical experiments in order to obtain the extent of diffusion introduced by the numerical method for a specific geometry or flow configuration. The additivity property of the variances permits the use of any tracer input signal (with known variance), to extract the variance of the C-Curve from Eq. (8-10). By using the dispersion model and the assumption of open vessel discussed above for numerical tests, the parameter $D/Lu$ characterizing the false diffusion introduced by the numerical method can then be obtained from the variance of the C-Curve. The parameter $D/Lu$ defines the analytical solution of the dimensionless transport equation, Eq. (8-7). For moderate to small diffusion, the analytical C-Curve is a family of Gaussian, normal or error curves whose variance is given by:

$$
\Delta \sigma_{\text{Vessel}}^2 = \Delta \sigma_t^2 = 2 \frac{D}{uL},
$$

(8-11)

and for large diffusion flows, (available only for open vessels, i.e. undisturbed flow at boundaries of vessel), the parameter is given by:

$$
\Delta \sigma_{\text{Vessel}}^2 = \frac{\Delta \sigma_t^2}{t^2} = 2 \left( \frac{D}{Lu} \right) + 8 \left( \frac{D}{Lu} \right)^2.
$$

(8-12)

These expressions, valid for flows that can be described by the dispersion model, were obtained by Levenspiel and Smith (1957) and Aris (1959) [54].

Knowledge of the parameter $D/Lu$ will also allow the comparison between the amount of false diffusion introduced by a numerical method and the turbulent diffusion expected from the flow.
characteristics. The real turbulent diffusion can be obtained directly as an experimental parameter from correlations for one-dimensional pipe flow [62], or from concentration curves obtained from experimental facilities. In this latter case, an equivalent $D/Lu$ parameter can be computed by calculating the variance of the experimentally obtained curve. In both cases, a quantitative assessment of the numerical diffusion relative to the expected turbulent diffusion can then be made. Finally, the value of the parameter $D/Lu$ for different numerical methods can also be used to compare their performances, and to obtain an estimate of the numerical diffusion coefficient in cases where a mathematical formula for this parameter is not available.

The application of the methodology to multidimensional flows would only be justified in cases where the flow were markedly axial. In such cases, an equivalent $D/Lu$ parameter can be obtained to represent the predominant axial diffusion. If the flow under study presents cross flow of the same magnitude as the axial one, the dispersion model, as described above, may not be satisfactory.

In any case, the comparison of the variances obtained from Eq. (8-10), for numerical or experimental tests, can always be used to compare the degree of diffusion of any flow or vessel configuration provided the inlet and outlet measurement points are well defined. This can be justified because the spread of the concentration curves measured at the outlet is directly correlated to the degree of turbulent diffusion inherent to the flow.