5. THE AXIAL DISPERSION MODEL

The axial dispersion model can readily be extended to apply to turbulent flow conditions. Under such conditions the velocity profile is almost flat and averaging with respect to radial position is possible. The axial dispersion model for turbulent flow has the form as given before

$$\frac{1}{Pe_z}\frac{\partial^2 c}{\partial \xi^2} - \frac{\partial c}{\partial \xi} - Da_n c^n = \frac{\partial c}{\partial \theta} \tag{94}$$

$$\xi = 0 \quad ; \quad c - \frac{1}{Pe}\frac{\partial c}{\partial \xi} = c_o(\theta) \tag{95}$$

$$\xi = 1 \quad ; \quad \frac{\partial c}{\partial \xi} = 0 \tag{96}$$

$$\theta = 0 \quad ; \quad c = c^i(\xi) \tag{97}$$

with

$$Pe_z = \frac{\bar{u}\, L}{E_z} \tag{98}$$

where E_z is the axial dispersion coefficient.

Taylor suggested that the axial dispersion coefficient in fully turbulent flow should be proportional to the friction velocity u^*

$$E_z \propto d_t\, u^* \tag{99}$$

$$u^* = \sqrt{\frac{f}{2}}\,\bar{u} \tag{100}$$

where the friction factor f is given by

$$f = 0.0791\,\mathrm{Re}^{-0.25} \quad \text{(Blasius equation)} \tag{101}$$

Taylor suggested specifically:

$$E_z = 3.57\,\bar{u}\, d_t \sqrt{f} \tag{102}$$

An empirical correlation for the axial dispersion coefficient, E_z, in pipes, which includes the transition and fully developed turbulent flow, is:

$$\frac{E_z}{\bar{u}\, d_t} = \frac{3\,x\,10^7}{Re^{2.1}} + \frac{1.35}{Re^{1/8}} \tag{103}$$

with

$$Re = \frac{\bar{u}\, d_t}{\upsilon}$$

The axial dispersion coefficient in pipes can be also obtained from the enclosed graph (Figure 6). The effect of beads, constrictions, etc., has been described by Wen and Fan.

The reactor steady state problem now can be described as follows:

$$\frac{1}{Pe}\frac{d^2c}{d\xi^2} - \frac{dc}{d\xi} - Da_n c^n = 0 \tag{104}$$

$$\xi = 0 \quad , \quad c - \frac{1}{Pe}\frac{dc}{d\xi} = 1 \tag{105}$$

$$\xi = 1 \quad , \quad \frac{dc}{d\xi} = 0 \tag{106}$$

Caution should be taken in that the Peclet number is now properly interpreted as

$$Pe = \frac{\bar{u}\, L}{D_{app}} \quad for\ laminar\ flow \quad or \quad Pe = \frac{\bar{u}\, L}{E_z}\ for\ turbulent\ flow$$

while the correlations or graphs produce

$$\frac{\bar{u}\, d_t}{E_z} \quad so\ that \quad Pe = \frac{\bar{u}\, d_t}{E_z}\ x \left(\frac{L}{d_t}\right)$$

Analytical solution of eqs (104-106) has been found only for zeroth and first order reaction.

The solution for a first order reaction is:

$$1 - x_A = c(1) = \frac{4\sqrt{1+\frac{4Da_1}{Pe}}\ \exp\left\{\frac{Pe}{2}\left[1-\sqrt{1+\frac{4Da_1}{Pe}}\right]\right\}}{\left(1+\sqrt{1+\frac{4Da_1}{Pe}}\right)^2 - \left(1-\sqrt{1+\frac{4Da_1}{Pe}}\right)^2 \exp\left(-Pe\sqrt{1+\frac{4Da_1}{Pe}}\right)} \tag{107}$$

The limit as $Pe \to \infty$ becomes the solution for the PFR

$$\lim_{Pe \to \infty} c(1) = \underset{PFR}{c(1)} = e^{-Da_1} \tag{107a}$$

The other limit of $Pe \to 0$ is only of academic interest, and, indeed, it properly converges to the CSTR behavior

$$\lim_{Pe \to 0} c(1) = c_{CSTR} = \frac{1}{1 + Da_1} \tag{107b}$$

It should be remembered at all times that, due to the assumptions that led to the axial dispersion model, this model only makes physical sense at large Peclet numbers, or small dispersion numbers $N_D < 0.1$ ($Pe > 10$). At low Pe numbers representation of reality by the axial dispersion model is of doubtful accuracy and is ill founded.

The reader should derive the solution to the axial dispersion model in case of a zeroth order reaction.

For other reaction orders and for complex reaction schemes eqs. (104) - (106) must be solved numerically. Several approaches can be chosen:

- **Shooting method.** Create two 1st order equations equivalent to the original second order equation (104) by choosing $y_1 = c, y_2 = \frac{dc}{d\xi}$ and integrate them backwards from $\xi = 1, y_2 = 0, y_1 = y_{1i}$ where y_{1i} is the guessed value for $c(\xi = 1)$. See if condition (105) at $\xi = 0$ is met $y_1 - \frac{1}{Pe} y_2 = 1$ and if it is not, devise an algorithm for correcting y_{1i} at $\xi = 1$ until the condition is met.

- **Quasilinearization.** Linearize the equation around an assumed solution and obtain the answer by iteratively solving the linear equations.

- **Green's function.** Use the Green's function to convert the problem to an integral equation which is solved iteratively.

- **Finite differences.** Solve by standard finite difference schemes.

Details are left for the applied mathematics course.

Approximate solutions that rely on the perturbation theory are also quite useful in assessing dispersion effects and are described in the Appendix.

Since the dispersion model with B.C. (105) and (106) is a closed system, then eq (107) represents the Laplace transform of $E_\theta(\theta)$ when s is substituted for Da_1.

$$L\{E_\theta(\theta)\} = \bar{c}(1,s) = \frac{4\sqrt{1+\frac{4s}{Pe}}\exp\left\{\frac{Pe}{2}\left[1-\sqrt{1+\frac{4s}{Pe}}\right]\right\}}{\left(1+\sqrt{1+\frac{4s}{Pe}}\right)^2 - \left(1-\sqrt{1+\frac{4s}{Pe}}\right)^2\exp\left(-Pe\sqrt{1+\frac{4s}{Pe}}\right)} \tag{108}$$

where $E_\theta(\theta)$ is the solution of the following transient problem:

$$\frac{1}{Pe}\frac{\partial^2 c}{\partial \xi^2} - \frac{\partial c}{\partial \xi} = \frac{\partial c}{\partial \theta} \tag{109}$$

$$\xi = 0 \quad , \quad c - \frac{1}{Pe}\frac{\partial c}{\partial \xi} = \delta(\theta) \tag{110}$$

$$\xi = 1 \quad , \quad \frac{\partial c}{\partial \xi} = 0 \tag{111}$$

$$\theta = 0 \quad , \quad c = 0 \tag{112}$$

Then

$$c(\xi = 1, \theta) = E_\theta(\theta) \tag{113}$$

Inversion of eq (108) gives:

$$E_\theta(\theta) = e^{\frac{Pe}{2}} \sum_{n=1}^{\infty} \frac{2\,\omega_n \sin\omega_n \left[Pe^2 + 4\,\omega_n^2\right] exp\left\{-\frac{Pe^2 + 4\,\omega_n^2\,\theta}{4\,Pe}\right\}}{Pe\left[Pe^2 + 4\,Pe + 4\,\omega_n^2\right]} \tag{114}$$

where ω_n are the positive roots of:

$$tan\ \omega_n = \frac{4\,\omega_n\,Pe}{4\,\omega_n^2 - Pe^2} \tag{115}$$

Unfortunately, expression (114) is not convenient for calculations. It converges very slowly at small θ and alternative functional forms are needed for evaluation of $E_\theta(\theta)$ at small θ. It also requires extra caution in calculations for $Pe > 16$ to prevent overflow of exponential terms.

An approximate expression can be derived by replacing B.C. (110) with

$$\xi = 0 \quad , \quad c = \delta(\theta) \tag{110a}$$

It turns out that, although this makes the system open, the differences in the response are small, and the result is:

$$E_\theta(\theta) \approx \sqrt{\frac{Pe}{4\,\pi\theta}}\; exp\left[-\frac{Pe(1-\theta)^2}{4\,\theta}\right] \tag{116}$$

This result is a good approximation at $Pe > 16$.

Since at $Pe > 16$ the $E_\theta(\theta)$ becomes quite narrow, the details of micromixing should not affect reactor performance by much. Therefore, if one wants to avoid solving a nonlinear boundary value problem given by eqs (104-106) for reaction orders not equal to one, one can obtain an approximate solution by using the segregated flow concept

$$C_{exit} = \int_o^\infty C_b(\theta) E_\theta(\theta)\, d\theta \tag{117}$$

where eq (116) is used for the $E_\theta(\theta)$. Please nota bene, that eq (117) does not represent the physical reality of the axial dispersion model but is based on the fact that for narrow RTD's micromixing effects cannot be very large except at very high conversions closing in on 1.

One should establish, as an exercise, that the moments of $E_\theta(\theta)$ given by eq (114) can readily be obtained from its Laplace transform, i.e eq (108) and are:

$$\begin{aligned} &\mu_0 = 1 \\ &\mu_1 = 1 \quad \text{(recall this is } \theta \text{ scale } \theta = t/\bar{t}) \\ &\sigma_D^2 = \frac{2}{Pe} - \frac{2}{Pe^2}\left(1 - e^{-Pe}\right) \end{aligned} \tag{118}$$

For reasonable values of Pe ($Pe > 10$) the second term in the expression for the dimensionless variance is negligible

$$\sigma_D^2 \approx \frac{2}{Pe} \tag{118a}$$

Thus, the dimensionless variance of the impulse tracer response can be interpreted in terms of the Peclet number of the axial dispersion model.

For other details of tracer studies and their interpretation see Levenspiel or Wen and Fan.

Recall now the Tanks in Series model for which the E-curve and variance are:

$$E_\theta(\theta) = \frac{N^N \theta^{N-1}}{(N-1)!} e^{-N\theta} \qquad \overline{\sigma}_D^2 = \frac{1}{N} \tag{119}$$

By using the equality of variance for the axial dispersion and the tanks in series model the two models can be related:

$$\overline{\sigma}^2 = \frac{2}{Pe} = \frac{1}{N} \qquad N = \frac{Pe_{app}}{2} \tag{120}$$

This allows us to extend the form of the E-curve for N-CSTRs to a case when N is a non integer <u>i.e</u> for an arbitrary value of the variance.

$$\begin{aligned} E_{ax.disp}(\theta) &= \frac{\left(\frac{Pe}{2}\right)^{\frac{Pe}{2}} \theta^{\left(\frac{Pe}{2}-1\right)}}{\Gamma\left(\frac{Pe}{2}\right)} e^{-\frac{Pe}{2}\theta} \\ &= \frac{\left(\frac{1}{\overline{\sigma}^2}\right)^{\frac{1}{\overline{\sigma}^2}} \theta^{\frac{1}{\overline{\sigma}^2}-1}}{\Gamma\left(\frac{1}{\overline{\sigma}^2}\right)} e^{-\theta/\overline{\sigma}^2} \end{aligned} \tag{121}$$

where σ^2 is the dimensionless variance.