Addenda: (Inversion of the Transfer Function for the Dispersion Model)

It might be instructive to show how to obtain the solution to eq (109) and the effect of B.C. on that solution.

By taking the Laplace transform of eq (109) we get

$$\frac{1}{Pe}\frac{d^2\bar{c}}{d\,\xi^2}-\frac{d\bar{c}}{d\xi}-s\bar{c}=0 \tag{A1}$$

where

$$\bar{c}=L\{c\}=\int_o^\infty e^{-s\theta}c(\theta)d\,\theta$$

We can rewrite this as:

$$\frac{d^2\bar{c}}{d\xi^2}-Pe\,\frac{d\bar{c}}{d\xi}-s\,Pe\,\bar{c}=0$$

The characteristic equation of the above ordinary differential equation is:

$$m^2-Pe\,m-s\,Pe=0$$

and the roots are

$$m_{1,2}=\frac{Pe\pm\sqrt{Pe+4s\,Pe}}{2}=\frac{Pe}{2}\left[1\pm\sqrt{1+\frac{4s}{Pe}}\right]$$

The solution in the Laplace domain is:

$$\bar{c}=Ae^{\left(\frac{Pe}{2}+\frac{Pe}{2}\sqrt{1+\frac{4s}{Pe}}\right)\xi}+Be^{\left(\frac{Pe}{2}-\frac{Pe}{2}\sqrt{1+\frac{4s}{Pe}}\right)\xi} \tag{A2}$$

The constants A and B have to be found by satisfying the boundary conditions. In case of conditions (110) and (111) required for the closed system this means

$$A+B-\frac{A}{Pe}\left(\frac{Pe}{2}+\frac{Pe}{2}\sqrt{1+\frac{4s}{Pe}}\right)-\frac{B}{Pe}\left(\frac{Pe}{2}-\frac{Pe}{2}\sqrt{1+\frac{4s}{Pe}}\right)=1$$

$$\frac{A}{Pe}\left(\frac{Pe}{2}+\frac{Pe}{2}\sqrt{1+\frac{4s}{Pe}}\right)e^{\frac{Pe}{2}\left(1+\sqrt{1+\frac{4s}{Pe}}\right)}+\frac{B}{Pe}\left(\frac{Pe}{2}-\frac{Pe}{2}\sqrt{1+\frac{4s}{Pe}}\right)e^{\frac{Pe}{2}\left(1-\sqrt{1+\frac{4s}{Pe}}\right)}=0$$

Solve for A and B, substitute into (A2) and show that when you evaluate $\bar{c}$ $at\ \xi=1$ eq (108) is obtained.

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

In contrast if eq (110) is replaced by the condition

$$\xi = 0,\ c = \delta(\theta)$$

the equations to be solved for A and B are

$$A + B = 1$$

$$A\left(1+\sqrt{1+\frac{4s}{Pe}}\right) e^{\frac{Pe}{2}\left(1+\sqrt{1+\frac{4s}{Pe}}\right)} + B\left(1-\sqrt{1+\frac{4s}{Pe}}\right) e^{\frac{Pe}{2}\left(1-\sqrt{1+\frac{4s}{Pe}}\right)} = 0$$

Now $\bar{c}\left(\xi = 1, s\right)$ is

$$\bar{c}(1,s) = \frac{2\sqrt{1+\frac{4s}{Pe}}\; e^{\frac{Pe}{2}}}{\left(1+\sqrt{1+\frac{4s}{Pe}}\right) e^{\frac{Pe}{2}\sqrt{1+\frac{4s}{Pe}}} - \left(1-\sqrt{1+\frac{4s}{Pe}}\right) e^{-\frac{Pe}{2}\sqrt{1+\frac{4s}{Pe}}}}$$

or

$$\bar{c}(1,s) = \frac{2\sqrt{1+\frac{4s}{Pe}}\; e^{\frac{Pe}{2}\left(1-\sqrt{1+\frac{4s}{Pe}}\right)}}{1+\sqrt{1+\frac{4s}{Pe}} - \left(1-\sqrt{1+\frac{4s}{Pe}}\right) e^{-Pe\sqrt{1+4s/Pe}}} \qquad (A3)$$

How do we invert forms like eq (108) or eq (A3) which are unlikely to be found in the pairs of transforms available in tables?

Based on the physical nature of the problems we know that there should not be any branch cuts in the complex plane and that the residue theorem can be used. Then if

$$\bar{f}(s) = \frac{P(s)}{Q(s)}$$

is the Laplace transform of $f(t)$ i.e

$$\bar{f}(s) = \int_o^\infty e^{-st} f(t)dt$$

and s_n are the poles of $\bar{f}(s)$ i.e the roots of $Q(s)$

$$Q(s_n) = 0, \; n = 1,2...$$

then the inverse Laplace transform is obtained by:

$$f(t) = \sum_{n=1}^{\infty} \frac{P(s_n)}{Q'(s_n)} e^{s_n t}$$

Let us apply this to eq (108)

$$P(s) = \sqrt{1+\frac{4s}{Pe}} \; exp\left\{\frac{Pe}{2}\left[1-\sqrt{1+\frac{4s}{Pe}}\right]\right\}$$

$$Q(s) = \left(1+\sqrt{1+\frac{4s}{Pe}}\right)^2 - \left(1-\sqrt{1+\frac{4s}{Pe}}\right)^2 e^{-Pe\sqrt{1+\frac{4s}{Pe}}} = 0$$

Let $\sqrt{1+\frac{4s}{Pe}} = z$

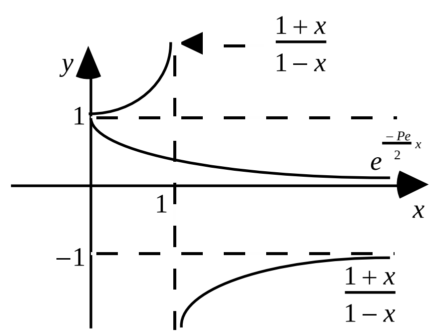
where z is a complex number $z = x + i\,y$

Then from the equation that identifies the poles i.e., $Q(s) = 0$ it follows

$$\left(\frac{1+z}{1-z}\right)^2 = e^{-Pez}$$

or

$$\left(\frac{1+z}{1-z}\right) = e^{-\frac{Pe}{2}z}$$



If $z = x$ is real the above equation has only one root at $x = 0$ as shown on the sketch above. (Figure A).

If z is complex, $z = x + i\,y$, then

$$\frac{1+x+iy}{1-x-iy} = e^{-\frac{Pe}{2}x}\, e^{-\frac{Pe}{2}iy}$$

$$\frac{1-x^2-y^2+2iy}{(1-x)^2+y^2} = e^{-\frac{Pe}{2}x}\, e^{-\frac{Pe}{2}iy}$$

$$\frac{\sqrt{\left(1-x^2-y^2\right)+4y^2}}{(1-x)^2+y^2}\, e^{i\,arctan\left(\frac{2y}{1-x^2-y^2}\right)} = e^{-\frac{Pe}{2}x}\, e^{-\frac{Pe}{2}iy}$$

This requires

$$\frac{\sqrt{\left(1-x^2-y^2\right)^2+4y^2}}{(1-x)^2+y^2} = e^{-\frac{Pe}{2}x}$$

$$arc\,tan\left(\frac{2y}{1-x^2-y^2}\right) = -\frac{Pe}{2}y$$

This is satisfied when $x = 0$ and

$$\frac{2y}{1-y^2} = -\,tan\left(\frac{Pe}{2}y\right)$$

Let $\frac{Pe}{2}y = \omega \rightarrow y = \frac{2}{Pe}\,\omega$. The above equation becomes:

$$-\frac{\frac{4}{Pe}\,\omega}{1-\frac{4}{Pe^2}\,\omega^2} = tan\,\omega$$

Thus

$$tan\;\omega_n = \frac{4Pe\,\omega_n}{4\,\omega_n^2 - Pe^2} = \frac{4\frac{\omega_n}{Pe}}{4\frac{\omega_n^2}{Pe^2}-1} \qquad (115)$$

which is given as eigenvalue equation (115) in the notes.

Thus at the roots of $Q\,(s\,) = 0$

$$\sqrt{1+\frac{4\,s_n}{Pe}} = i\,\frac{2}{Pe}\,\omega_n$$

and so the roots s_n are

$$s_n = -\frac{Pe}{4}\left(1+\frac{4}{Pe^2}\omega_n^2\right)$$

Now

$$Q'(s)=\left[2\left(1+\sqrt{1+\frac{4s}{Pe}}\right)+2\left(1-\sqrt{1+\frac{4s}{Pe}}\right)e^{-Pe\sqrt{1+\frac{4s}{Pe}}}+Pe\left(1-\sqrt{1+\frac{4s}{Pe}}\right)^2 e^{-Pe\sqrt{1+\frac{4s}{Pe}}}\right]$$

$$x\,\frac{\frac{4}{Pe}}{2\sqrt{1+\frac{4s}{Pe}}}$$

$$Q'(s)=\frac{2}{Pe\sqrt{1+\frac{4s}{Pe}}}\left[2\left(1+\sqrt{1+\frac{4s}{Pe}}\right)+e^{-Pe\sqrt{1+\frac{4s}{Pe}}}\left(1-\sqrt{1+\frac{4s}{Pe}}\right)\left[2+Pe\left(1-\sqrt{1+\frac{4s}{Pe}}\right)\right]\right]$$

$$Q'(s_n)=\frac{2}{Pe\,i\frac{2}{Pe}\omega_n}\left[2\left(1+i\frac{2}{Pe}\omega_n\right)+e^{-iPe\frac{2}{Pe}\omega_n}\left(1-i\frac{2}{Pe}\omega_n\right)\left[2+Pe-i2\omega_n\right]\right]$$

$$Q'(s_n)=-\frac{i}{\omega_n}\left[2+i\frac{4\omega_n}{Pe}+e^{-i2\omega_n}\left(1-i\frac{2\omega_n}{Pe}\right)\left(2+Pe-i2\omega_n\right)\right]$$

$$P(s_n)=i\,4\frac{2}{Pe}\omega_n e^{\frac{Pe}{2}}e^{-i\omega_n}$$

$$\frac{P(s_n)}{Q'(s_n)}=-\frac{8\omega_n^2 e^{\frac{Pe}{2}}}{Pe\left\{\left(2+i\frac{4\omega_n}{Pe}\right)e^{i\omega_n}+e^{-i\omega_n}\left(2+Pe-\frac{4\omega_n^2}{Pe}-i\left(4\omega_n+\frac{4\omega_n}{Pe}\right)\right)\right\}}$$

$$\frac{P(s_n)}{Q'(s_n)}=-\frac{8\omega_n^2 e^{Pe/2}}{Pe\left[\left(4+Pe-\frac{4\omega_n^2}{Pe}\right)\cos\omega_n-4\omega\left(1+\frac{2}{Pe}\right)\sin\omega_n\right]}$$

Thus one could write the inversion formula as:

$$c(1,\theta) = \sum_{n=1}^{\infty} \frac{8\omega_n^2 e^{Pe/2} e^{-\frac{Pe}{4}\left(1+\frac{4}{Pe^2}\omega_n^2\right)\theta}}{Pe\left[4\omega_n\left(1+\frac{2}{Pe}\right)\sin\omega_n - \left(4+Pe-\frac{4\omega_n^2}{Pe}\right)\cos\omega_n\right]}$$

$$= \sum_{n=1}^{\infty} \frac{8\omega_n^2 exp\left\{\frac{Pe}{2}\left[1-\frac{1}{2}\left(1+\frac{4\omega_n^2}{Pe^2}\right)\theta\right]\right\}}{4\omega_n(Pe+2)\sin\omega_n - \left(Pe^2+4Pe-4\omega_n^2\right)\cos\omega_n} \quad \text{(A4)}$$

We can get this into the form of eq (114) by using various algebraic manipulations and trigonometric identities as shown below and by invoking eq (115).

$$4\omega_n(Pe+2)\sin\omega_n - \left(Pe^2+4Pe-4\omega_n^2\right)\cos\omega_n$$

$$= \cos\omega_n\left[4\omega_n(Pe+2)\tan\omega_n - Pe^2 - 4Pe + 4\omega_n^2\right]$$

$$= \frac{\cos\omega_n}{4\omega_n^2 - Pe^2}\left[16\,Pe\,\omega_n^2(Pe+2) - \left(4\omega_n^2 - Pe^2\right)\left(Pe^2+4Pe-4\omega_n^2\right)\right]$$

$$= \frac{\sin 2\omega_n}{2\sin\omega_n\left[4\omega_n^2 - Pe^2\right]}\left[16\,Pe\,\omega_n^2(Pe+2) - \left(4\omega_n^2 - Pe^2\right)\left(Pe^2+4Pe-4\omega_n^2\right)\right]$$

$$= \frac{2\tan\omega_n\left[16\,Pe\,\omega_n^2(Pe+2) - \left(4\omega_n^2 - Pe^2\right)\left(Pe^2+4Pe-4\omega_n^2\right)\right]}{2\sin\omega_n\left[1+\tan^2\omega_n\right]\left[4\omega_n^2 - Pe^2\right]}$$

$$= \frac{4Pe\,\omega_n\left[16\,Pe\,\omega_n^2(Pe+2) - \left(4\omega_n^2 - Pe^2\right)\left(Pe^2+4Pe-4\omega_n^2\right)\right]}{\sin\omega_n\left[4\omega_n^2 - Pe^2\right]^2\left[1+\frac{16Pe^2\omega_n^2}{\left(4\omega_n^2-Pe^2\right)^2}\right]}$$

$$= \frac{4Pe\,\omega_n\left[16Pe\,\omega_n^2(Pe+2) - 4\omega_n^2\left(Pe^2+4Pe\right) + 16\omega_n^4 + Pe^2\left(Pe^2+4Pe\right) - 4\omega_n^2 Pe^2\right]}{\sin\omega_n\left[4\omega_n^2 + Pe^2\right]^2}$$

$$= \frac{4\,Pe\,\omega_n\left[8\,Pe^2\omega_n^2 + 16\,Pe\,\omega_n^2 + 16\omega_n^4 + Pe^2\left(Pe^2+4Pe\right)\right]}{\sin\omega_n\left[4\omega_n^2 + Pe^2\right]^2}$$

$$= \frac{4Pe\,\omega_n\left[4\omega_n^2\left(2Pe^2+4Pe+4\omega_n^2\right) + Pe^2\left(Pe^2+4Pe\right)\right]}{\sin\omega_n\left[4\omega_n^2 + Pe^2\right]^2}$$

$$= \frac{4\,Pe\,\omega_n\left[4\omega_n^2(Pe^2+4Pe) + 4\omega_n^2\left(Pe^2+4\omega_n^2\right) + Pe^2\left(Pe^2+4Pe\right)\right]}{\left[4\omega_n^2 + Pe^2\right]^2\sin\omega_n}$$

$$= \frac{4Pe\,\omega_n \left[(Pe^2 + 4Pe)\left(4\omega_n^2 + Pe^2\right) + 4\omega_n^2\left(Pe^2 + 4\omega_n^2\right)\right]}{\left[4\omega_n^2 + Pe^2\right]^2 \sin\omega_n} = \frac{4Pe\omega_n\left(Pe^2 + 4Pe + 4\omega_n^2\right)}{\left(4\omega_n^2 + Pe^2\right)\sin\omega}$$

Finally, we have shown that

$$4\,\omega_n\,(Pe + 2)\sin\omega_n - \left(Pe^2 + 4Pe - 4\omega_n^2\right)\cos\omega_n$$
$$= \frac{4\,Pe\,\omega_n\left(Pe^2 + 4Pe + 4\omega_n^2\right)}{\left(4\omega_n^2 + Pe^2\right)\sin\omega_n}$$

Then, substituting the above in eq (44) we get

$$c(1,\theta) = \sum_{n=1}^{\infty} \frac{2\,\omega_n \sin\omega_n \left(4\omega_n^2 + Pe^2\right) e^{\frac{Pe}{2}}\, e^{-\frac{Pe}{4}\left[1 + \frac{4\omega_n^2}{Pe^2}\right]\theta}}{Pe\left[Pe^2 + 4Pe + 4\omega_n^2\right]} \qquad \text{(A4a)}$$

which is equation (114) in the notes.

For an exercise one should be able to develop the response to a unit impulse injection for a model whose transfer function is given by eq (A3). This model would be valid for a fairly long reactor where the exactness of the inlet condition is not that important.
