Derivation and Analysis of Taylor Dispersion

Introduction

This paper derives and analyses the analytical solution Taylor got in his paper *Dispersion of soluble matter in solvent flowing slowly through a tube*. In his paper, Taylor injected a stream of solute, in this case a dye, into a tube with water already flowing with a fully developed profile. He used the apparatus shown in Figure 1 to measure the concentration profile of a solute across a horizontal length of tubing.

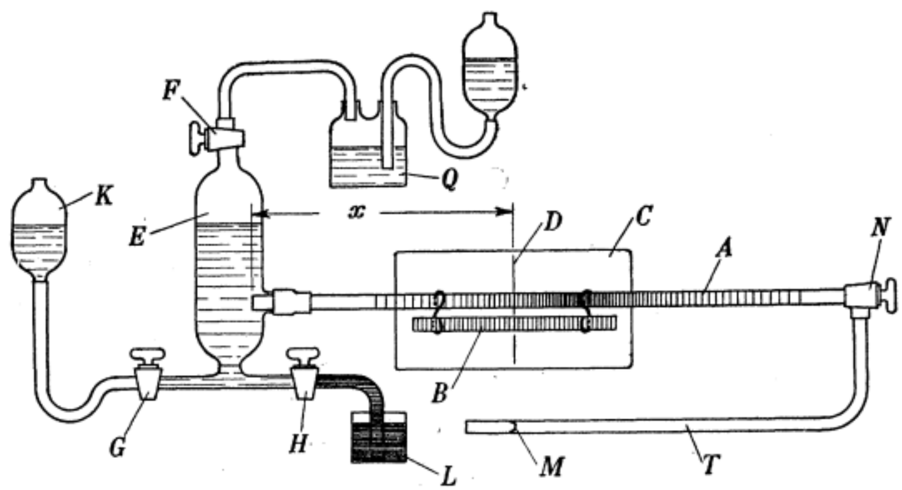

Figure 1: Experimental Apparatus

The phenomena that Taylor describes in his paper is that under certain conditions, the shear flow of the water causes non-molecular dispersion of the solute. This phenomenon is now referred to as Taylor dispersion. This work assumes that the solute has no molecular diffusion, and if Taylor dispersion were not a factor, a pulse of solute would move down the tube with an unchanging concentration profile. With Taylor dispersion, the parabolic velocity profile of the water will disperse the solute until it reaches a rough parabolic concentration profile.

While Taylor dispersion is only applicable under certain conditions, the impact of Taylor dispersion is significant in several areas. Taylor suggests that “The results may be useful to physiologists who may wish to know how a soluble salt is dispersed in blood streams.”. In their book *Transport Phenomena Revised Second Edition*, Bird, Stewart, and Lightfoot suggest that using Taylor’s analytical solution can be used to quickly measure liquid diffusivities.

Methods

Taylor developed several analytical solutions to the concentration profile of a tube with Taylor dispersion under several different conditions. The case I derived is for when at time = 0, solute is injected into the tube with flowing solvent at a constant rate. I used both Taylor's paper and Bird, Stewart, and Lightfoot's textbook as references.

My method starts with applying Taylor's simplifying assumptions to the diffusion equation that describes the mass fraction of the solute in the tube. I then change some coordinates and integrate to get an expression for the mass fraction as a function of a shifted axial coordinate. From this, I derive an expression for the average mass flux, which introduces the axial dispersion coefficient. I then substitute the average mass flux expression into the continuity expression, then use the Similarity Method to get an expression for the concentration profile across the tube.

Equation 1 shows the diffusion equation for Poiseuille flow assuming constant μ,ρ, and D_{AB}. The boundary conditions for this equation is that $\frac{dw_A}{dr} = 0$ for r = 0 and r = R.

$$\frac{dw_A}{dt} + v_{z,max}\left[1-\left(\frac{r}{R}\right)^2\right]\frac{dw_A}{dz} = D_{AB}\left(\frac{1}{r}\frac{d}{dr}\left(r\frac{dw_A}{dr}\right)+\frac{d{w_A}^2}{dz^2}\right) \qquad Equation\ 1$$

Where w_A is the mass fraction of the solute, t is the time, $v_{z,max}$ is the maximum velocity of the solvent (at the center of the tube), r is a portion of the radius, R is the value of the radius, z is a length across the horizontal tube, and D_{AB} is the diffusion coefficient for the solute and solvent.

Taylor showed that if the Peclet number > 70 and if L >170R where L is the length of the tube, then the terms $\frac{dw_A}{dt}$ and $\frac{d{w_A}^2}{dz^2}$ can be neglected. Taylor introduced a shifted axial coordinate, $\acute{z} = z - \langle v_z\rangle t$, and a dimensionless radial coordinate, $\xi=\frac{r}{R}$. Making these substitutions to Equation 1 results in Equation 2.

$$\frac{1}{\xi}\frac{d}{d\xi}\left(\xi\frac{dw_A}{d\xi}\right) = \frac{R^2 v_{z,max}}{D_{AB}}\left(\frac{1}{2}-\xi^2\right)\frac{dw_A}{d\acute{z}} \qquad Equation\ 2$$

w_A can be expressed as $w_A(\xi, \acute{z}, t) = \langle w_A\rangle(\acute{z}, t) + w_A{}'(\xi, \acute{z}, t)$. Under the same conditions for the Peclet number and L, Taylor assumes that the $w_A{}'$ term is neglectable. This results in Equation 3,

$$\frac{1}{\xi}\frac{d}{d\xi}\left(\xi\frac{dw_A}{d\xi}\right) = \frac{R^2 v_{z,max}}{D_{AB}}[0.5-\xi^2]\frac{d\langle w_A\rangle}{d\acute{z}} \qquad Equation\ 3$$

which can then be integrated with the boundary conditions listed above to get an expression for the mass fraction of A as shown in Equation 4.

$$w_A(\xi,\acute{z}) = \frac{R^2 v_{z,max}}{8D_{AB}}\left[\xi^2-\frac{1}{2}\xi^4\right]\frac{d\langle w_A\rangle}{d\acute{z}} + w_A(0,\acute{z}) \qquad Equation\ 4$$

To get rid of the $w_A(0,\acute{z})$ term, we subtract $\langle w_A\rangle$ from w_A. $\langle w_A\rangle$ is calculated from Equation 5, and the resulting expression is shown as Equation 6.

$$\langle w_A \rangle = \frac{\int_0^1 w_A \xi d\xi}{\int_0^1 \xi d\xi} \qquad \text{Equation 5}$$

$$w_A - \langle w_A \rangle = \frac{R^2 \langle v_z \rangle}{4D_{AB}} \frac{d\langle w_A \rangle}{d\acute{z}} \left(-\frac{1}{3} + \xi^2 - \frac{1}{2}\xi^4 \right) \qquad \text{Equation 6}$$

The mass flow of the solute through a plane of constant $\acute{z}$ can be found as shown in Equation 7.

$$\Pi R^2 \rho \langle w_A (v_z - \langle v_z \rangle) \rangle = -\frac{\Pi R^4 \rho \langle v_z \rangle^2}{48 D_{AB}} \frac{d\langle w_A \rangle}{d\acute{z}} \qquad \text{Equation 7}$$

We assume that the solute and solvent are moving at the same axial speed. Because the density is assumed to be constant, we can assume that $\rho \langle w_A \langle v_z \rangle \rangle = \langle \rho_A \rangle \langle v_z \rangle$ and that $\rho \langle w_A v_z \rangle \sim \langle \rho_A v_{Az} \rangle = \langle n_{AZ} \rangle$ where n_{AZ} is the mass flux of the solute. Using these assumptions, we divide Equation 7 by ΠR^2 to get an expression for the average mass flux as shown in Equation 8.

$$\langle n_{AZ} \rangle = \langle \rho_A \rangle \langle v_z \rangle - K \frac{d\langle \rho_A \rangle}{d\acute{z}} = \langle \rho_A \rangle \langle v_z \rangle - K \frac{d\langle \rho_A \rangle}{dz} \qquad \text{Equation 8}$$

Where K is the axial dispersion coefficient, which essentially describes how strong the influence of Taylor dispersion is. Equation 9 gives the expression for K

$$K = \frac{R^2 \langle v_z \rangle^2}{48 D_{AB}} = \frac{1}{48} D_{AB} Pe^2 \qquad \text{Equation 9}$$

where Pe is the Peclet number. The continuity equation averaged over the cross section of the tube is shown in Equation 10. Substituting Equation 8 into Equation 10 gives Equation 11. Equation 11 can then be solved using the Similarity Method to give the final analytical solution shown in Equation 12. Because this Similarity Method is nearly identical to what was done in class, this paper won't discuss how to use this method. Attached to this paper will be an appendix with my hand-written calculations if the reader is interested in seeing how the Similarity Method was used.

$$\frac{d}{dt} \langle \rho_A \rangle = -\frac{d}{dz} \langle n_{AZ} \rangle \qquad \text{Equation 10}$$

$$\frac{d}{dt} \langle \rho_A \rangle = K \frac{d^2}{dz^2} \langle \rho_A \rangle \qquad \text{Equation 11}$$

$$\frac{\rho_A}{\rho_{A,0}} = 1 - erf\left(\frac{z}{2\sqrt{Kt}} \right) \qquad \text{Equation 12}$$

Results and Discussion

Table 1 shows the parameters given by Taylor that was used in Equation 12 to generate a plot of the concentration profile. This plot is shown below as Figure 2.

Table 1: Parameters used by Taylor

t (seconds)	11000
L (m)	1.52
Maximum velocity (m/s)	0.002625
R (m)	0.000252
D_{AB} (m^2/s)	7E-10

Assuming that the same equipment is used and that the solute and solvent remain the same, the only variable we can adjust is the velocity of the solvent. Figure 3 shows the impact the velocity has on the axial dispersion coefficient and Figure 4 shows how the velocity impacts the concentration profile. It is readily seen that an increasing velocity increases the effect of Taylor dispersion, which also makes sense conceptually.

While Taylor used a time of 11000 seconds in his paper, I wanted to see how time influences the concentration profile. Figure 5 shows the concentration profile at different times. It is interesting that even though 11000 seconds seems like a sufficiently large amount of time for this experiment, the concentration profile changes significantly at much larger times.

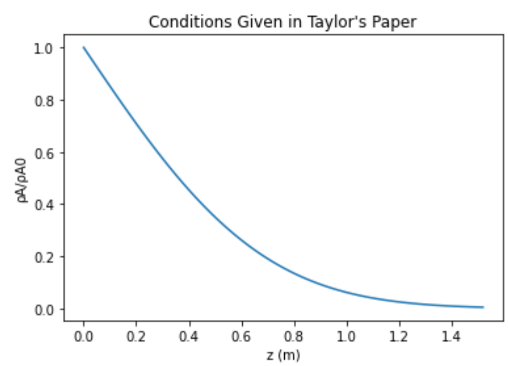

Figure 2: Concentration Profile using Taylor's Parameters

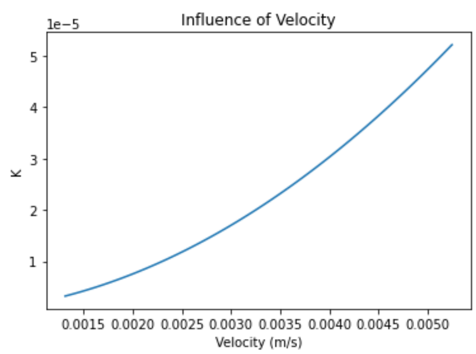

Figure 3: Influence of velocity on the axial dispersion coefficient

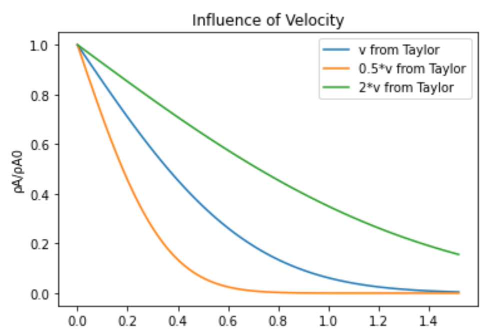

Figure 4: Influence of velocity on the concentration profile

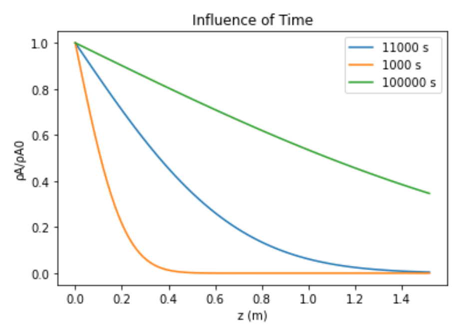

Figure 5: Influence of time on the concentration profile.

Conclusion

Taylor’s work on Taylor dispersion shows how at high Peclet numbers and at large times, the shear flow of a solvent can has a significant impact on the concentration profile of a non-molecular diffusing solute. An understanding of Taylor dispersion has multiple applications, but one worth highlighting is the ability to quickly experimentally determine the diffusivity of liquids.

While the PDE portion of this derivation was straight forward, working on the derivation and analysis of Taylor’s paper reinforced several key principles in transport phenomena. I had to revisit dimensionless coordinates, shifted coordinates, applying the continuity equation, and the method of similarity and changing boundary conditions to a new set of variables.

Most importantly, this analysis taught me about taylor dispersion and the strong impact it can have on mass and momentum transport of a substance we’d normally consider non-diffusing.

Assume constant μ, ρ, D_{AB}

$$\frac{\partial w_A}{\partial t} + v_{z,max}\left[1-\left(\frac{r}{R}\right)^2\right]\frac{\partial w_A}{\partial z} = D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial w_A}{\partial r}\right) + \frac{\partial^2 w_A}{\partial z^2}\right) \quad (20.5\text{-}1)$$

No analytical Solution.
Taylor gave approximate analyses.

B.C.

$$\left.\frac{\partial w_A}{\partial r}\right|_{r=0} = 0 \qquad \left.\frac{\partial w_A}{\partial r}\right|_{r=R} = 0$$

radial symmetry — no transfer across pipe wall

Taylor

- neglect axial molecular diffusion term $\left(\frac{\partial^2 w_A}{\partial z^2}\right)$ $\quad \frac{L}{v_{z,max}} \gg \frac{R^2}{(3.8)^2 D_{AB}}$ (20.5-4)
  - Valid if $Pe \gtrsim 70$ and $L \gtrsim 170R$
- $\langle v_z \rangle = \frac{1}{2} v_{z,max}$

$t \begin{cases} \text{long} \\ \text{mass} \end{cases}$

estimated validity of his results.

Shifted axial coordinates

$\bar{z} = z - \langle v_z \rangle t \xrightarrow{\text{into}} 20.5\text{-}1$

$\bar{z} = z - \frac{1}{2} v_{z,max} t$

$$\frac{\partial w_A}{\partial t} + v_{z,max}\left(\frac{1}{2} - \xi^2\right)\frac{\partial w_A}{\partial \bar{z}} = \frac{D_{AB}}{R^2}\frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi\frac{\partial w_A}{\partial \xi}\right) \quad (20.5\text{-}6)$$

where $\xi = \frac{r}{R}$

under conditions of 20.5-4, $\frac{\partial w_A}{\partial t} \ll$ radial diffusion term

$$\frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi\frac{\partial w_A}{\partial \xi}\right) = \frac{R^2 v_{z,max}}{D_{AB}}\left(\frac{1}{2} - \xi^2\right)\frac{\partial w_A}{\partial \bar{z}} \quad (20.5\text{-}7)$$

$$w_A(\xi, \bar{z}, t) = \langle w_A \rangle(\bar{z}, t) + w_A'(\xi, \bar{z}, t) \qquad \text{where } |w_A'| \ll \langle w_A \rangle$$

RHS, neglect w_A'

$$\frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi\frac{\partial w_A}{\partial \xi}\right) = \frac{R^2 v_{z,max}}{D_{AB}}\left(\frac{1}{2} - \xi^2\right)\frac{\partial \langle w_A \rangle}{\partial \bar{z}} \quad (20.5\text{-}9)$$

B.C.

$$\left.\frac{\partial w_A}{\partial r}\right|_{r=0} = 0, \quad \left.\frac{\partial w_A}{\partial r}\right|_{r=R} = 0 \qquad \xi = \frac{r}{R} \rightarrow \left.\frac{1}{R}\frac{\partial w_A}{\partial \xi}\right|_{\xi=0} = 0, \quad \left.\frac{1}{R}\frac{\partial w_A}{\partial \xi}\right|_{\xi=1} = 0$$

$w_A(0, \bar{z}) = 1$

$$\int \partial\left(\xi\frac{\partial w_A}{\partial \xi}\right) = \int \frac{R^2 v_{z,max}}{D_{AB}}\frac{\partial \langle w_A \rangle}{\partial \bar{z}}\left(\frac{1}{2}\xi - \xi^3\right)\partial \xi$$

$$\xi\frac{\partial w_A}{\partial \xi} = \frac{R^2 v_{z,max}}{D_{AB}}\frac{\partial \langle w_A \rangle}{\partial \bar{z}}\left(\frac{1}{4}\xi^2 - \frac{1}{4}\xi^4\right) + C_1$$

$$\int w_A = \int \frac{R^2 v_{z,max}}{D_{AB}}\frac{\partial \langle w_A \rangle}{\partial \bar{z}}\left(\frac{1}{4}\xi - \frac{1}{4}\xi^3\right) + \frac{C_1}{\xi}\, \partial \xi$$

$$w_A(\xi, \bar{z}) = \frac{R^2 v_{z,max}}{8 D_{AB}}\frac{\partial \langle w_A \rangle}{\partial \bar{z}}\left(\xi^2 - \frac{1}{2}\xi^4\right) + w_A(0, \bar{z}) \quad (20.5\text{-}10)$$

$$\langle w_A \rangle = \frac{\int_0^1 w_A \xi\, \partial \xi}{\int_0^1 \xi\, \partial \xi} = \frac{R^2 v_{z,max}}{24 D_{AB}}\frac{\partial \langle w_A \rangle}{\partial \bar{z}} + w_A(0, \bar{z}) \quad (20.5\text{-}11)$$

$v_{z,max} = 2\langle v_z \rangle$

$$w_A - \langle w_A \rangle = \frac{R^2 \langle v_z \rangle}{4 D_{AB}}\frac{\partial \langle w_A \rangle}{\partial \bar{z}}\left(-\frac{1}{3} + \xi^2 - \frac{1}{2}\xi^4\right) \quad (20.5\text{-}12)$$

Taylor, Part 2

total mass A through constant z

$$\pi R^2 \rho \langle w_A (v_z - \langle v_z \rangle)\rangle = \frac{\pi R^4 \rho \langle v_z\rangle^2}{D_{AB}} \frac{d\langle w_A\rangle}{dz} \int_0^1 \left(-\frac{1}{3} + \xi^2 - \frac{1}{2}\xi^4\right)\left(\frac{1}{2} - \xi^2\right)\xi \, d\xi$$

$$= \frac{-\pi R^4 \rho \langle v_z\rangle^2}{48 D_{AB}} \frac{d\langle w_A\rangle}{dz} \qquad (20.5\text{-}13)$$

ρ = const.

$\rho\langle w_A \langle v_z\rangle\rangle = \langle \rho_A\rangle\langle v_z\rangle$

$\rho\langle w_A v_z\rangle \approx \langle \rho_A v_{Az}\rangle = \langle n_{Az}\rangle$ with axial diffusion neglected, A and B move with same speed

$\div \pi R^2 \rightarrow \langle n_{Az}\rangle = \langle \rho_A\rangle\langle v_z\rangle - K\frac{d\langle \rho_A\rangle}{dz} = \langle \rho_A\rangle\langle v_z\rangle - K\frac{d\langle \rho_A\rangle}{dz} \qquad (20.5\text{-}14)$

axial diffusion coefficient

$K = \frac{R^2\langle v_z\rangle^2}{48 D_{AB}} = \frac{1}{48} D_{AB} Pe^2 \qquad (20.5\text{-}15) \qquad K = f(R, \langle v_z\rangle, D_{AB})$

Cont. averaged over tube cross section

$\frac{\partial}{\partial t}\langle \rho_A\rangle = \frac{-\partial}{\partial z}\langle n_{Az}\rangle \qquad$ (20.5-16, from 19.1-6)

$$\boxed{\frac{\partial}{\partial t}\langle \rho_A\rangle = K\frac{\partial^2\langle \rho_A\rangle}{\partial z^2}}$$

Similarity method

$\phi = \frac{\rho_A}{\rho_{A0}}, \quad \tilde{z} = \frac{z}{L}, \quad \tilde{t} = \frac{t}{\tau}$

B.C.
$\rho_A(0,t) = \rho_{A0}$
$\rho_A(\infty,t) = 0$
$\rho_A(z,0) = 0$

$\frac{\partial(\rho_{A0}\phi)}{\partial(\tau\tilde{t})} = \frac{K\partial^2(\rho_{A0}\phi)}{\partial(L\tilde{z})^2} \rightarrow \frac{\rho_{A0}}{\tau}\frac{\partial\phi}{\partial\tilde{t}} = K\frac{\rho_{A0}}{L}\frac{\partial\phi}{\partial\tilde{z}}$

$\frac{\partial\phi}{\partial\tilde{t}} = \frac{\tau K}{L^2}\frac{\partial\phi}{\partial\tilde{z}}$

\# dim: len, mass, time (3)
\# var: $\rho_A, \rho_{A0}, z, K, t$ (5) $\quad > 2$ dim. groups

$\phi, \tilde{t}, \tilde{z}, \underbrace{\frac{\tau K}{L^2}}_{1} \rightarrow L = \sqrt{\tau K}$

$\eta = \frac{z}{\sqrt{tK}}$

$\frac{\partial\langle \rho_A\rangle}{\partial t} = \frac{\partial(\rho_{A0}\phi)}{\partial t} = \rho_{A0}\frac{d\phi}{d\eta}\left(\frac{\partial\eta}{\partial t}\right) = \rho_{A0}\frac{d\phi}{d\eta}\left(\frac{\partial}{\partial t}\left(\frac{z}{\sqrt{tKz}}\right)\right) = \underline{\frac{-\rho_{A0}\eta}{2t}\frac{d\phi}{d\eta}}$

$\frac{\partial(\rho_A)}{\partial z} = \rho_{A0}\frac{d\phi}{d\eta}\left(\frac{\partial\eta}{\partial z}\right) = \rho_{A0}\frac{d\phi}{d\eta}\left(\frac{1}{\sqrt{tKt}}\right)$

$\frac{\partial^2\langle\rho_A\rangle}{\partial z^2} = \frac{\partial}{\partial z}\left(\frac{\partial\rho_A}{\partial z}\right) = \frac{\partial}{\partial\eta}\left(\frac{\partial\rho_A}{\partial z}\right)\frac{\partial\eta}{\partial z} = \frac{\partial}{\partial\eta}\left(\rho_{A0}\frac{d\phi}{d\eta}\left(\frac{1}{\sqrt{tKt}}\right)\right)\left(\frac{1}{\sqrt{tKt}}\right) = \underline{\frac{\rho_{A0}}{tKt}\frac{d^2\phi}{d\eta^2}}$

$\frac{-\rho_{A0}\eta}{2t}\frac{d\phi}{d\eta} = K\frac{\rho_{A0}}{tKt}\frac{d^2\phi}{d\eta^2} \rightarrow \frac{d^2\phi}{d\eta^2} + \frac{t\eta}{2}\frac{d\phi}{d\eta} = 0$

B.C.
$\rho_A(0,0) = \rho_{A0} \rightarrow \phi(0) = 1$
$\rho_A(\infty,t) = 0 \rightarrow \phi(\infty) = 0$
$\rho_A(z,0) = 0$

$Pe = Re\,Sc$
$= \frac{Lv\rho}{\mu}\left(\frac{\mu}{\rho D_{AB}}\right)$.

$\left(\frac{Lv}{D_{AB}}\right)^2$

$\frac{1}{48}\frac{D_{AB}L^2v^2}{D_{AB}^2}$

$\frac{1}{48 D_{AB}}L^2v^2$

let $\psi = \frac{d\phi}{d\eta}$

$$\frac{d\psi}{d\eta} + \frac{c\eta}{2}\psi = 0$$

$$\int \frac{1}{\psi}\, d\psi = \int \frac{-c\eta}{2}\, d\eta$$

$$\ln(\psi) = \frac{-c\eta^2}{4} + K_1$$

$$\psi = K_1 \exp\left(\frac{-c\eta^2}{4}\right)$$

$$\int d\phi = \int K_1 \exp\left(\frac{-c\eta^2}{4}\right) d\eta$$

$$\phi = \int_0^\eta K_1 \exp\left(\frac{-c\bar{\eta}^2}{4}\right) d\bar{\eta} + K_2 \qquad \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-x'^2)\, dx'$$

$$\phi(0) = 1 \rightarrow K_2 = 1$$

$$\phi(\infty) = 0 = \int_0^\infty K_1 \exp\left(\frac{-c\bar{\eta}^2}{4}\right) d\bar{\eta} + 1$$

$$K_1 = -\left[\int_0^\infty \exp\left(\frac{-c\bar{\eta}^2}{4}\right) d\bar{\eta}\right]^{-1}$$

$$K_1 = -\sqrt{\frac{c}{\pi}}$$

$$\phi = 1 - \sqrt{\frac{c}{\pi}} \int_0^\eta \exp\left(\frac{-c\bar{\eta}^2}{4}\right) d\bar{\eta} \qquad \text{let } c = 4$$

$$\phi = 1 - \mathrm{erf}(\eta)$$

$$\boxed{\frac{\rho_A}{\rho_{A0}} = 1 - \mathrm{erf}\left(\frac{z}{2\sqrt{\kappa t}}\right)}$$