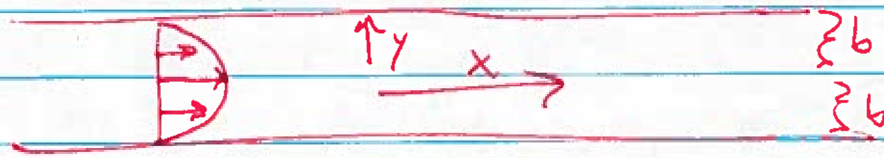
Taylor-Aris Dispersion:

Channel Flow



$$u = \frac{3}{2} U \left(1 - y^2/b^2\right)$$

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)$$

$$\left.\frac{\partial c}{\partial y}\right|_{y=0} = 0, \quad \left.\frac{\partial c}{\partial y}\right|_{y=\pm b} = 0 \quad \text{(no flux)}$$

Let $u^* = \frac{u}{U} = \frac{3}{2}\left(1 - y^{*2}\right)$; $y^* = y/b$

$$x^* = \frac{x}{U(b^2/D)} \qquad t^* = \frac{Dt}{b^2}$$

We have the integral condition:

$$\int_{-b}^{b}\int_{-\infty}^{\infty} c \, dy \, dx = I \quad \text{(total amount!)}$$

Thus: $c^* = \frac{c}{A}$

$$2A \int_0^1 \int_{-\infty}^{\infty} c^* \left(U \frac{b^3}{D}\right) dy^* dx^* = I$$

Let $A = \frac{I}{2 U b^3/D}$

So $$\int_0^1 \int_{-\infty}^{\infty} c^* dy^* dx^* = 1$$

Following Aris, we define the <u>moments</u>

$$c_p^* = \int_{-\infty}^{\infty} x^{*p} c^* dx^*$$

$$m_p^* = \int_0^1 c_p^* dy^*$$

In particular, we are interested in the growth of the <u>variance</u> of the distribution!

This variance is:

$$\sigma_x^2 = \frac{\int_{-\infty}^{\infty}\int_{-b}^{b} (x - \bar{x})^2 \, c \, dy \, dx}{\int_{-\infty}^{\infty}\int_{-b}^{b} c \, dy \, dx}$$

where $\bar{x}$ is the average position:

$$\bar{x} = \frac{\int_{-\infty}^{\infty}\int_{-b}^{b} x \, c \, dy \, dx}{\int_{-\infty}^{\infty}\int_{-b}^{b} c \, dy \, dx}$$

Now for a diffusion process

$$\frac{d\sigma_x^2}{dt} \sim 2D$$

For the dispersion problem, we have:

$$\frac{d\sigma_x^2}{dt} \sim 2K^d$$ dispersivity!

So:

$$\bar{x} = \frac{2Ab\left(\frac{Ub^2}{D}\right)^2 \int_{-\infty}^{\infty}\int_0^1 x^* c^* dy^* dx^*}{I}$$

$$= \left(\frac{Ub^3}{D}\right) m_1^*$$

Likewise,

$$\sigma_x^2 = \left(\frac{Ub^3}{D}\right)^2 \left(m_2^* - m_1^{*2}\right)$$

Thus:

$$2K = \frac{d\sigma_x^2}{dt} = \left(\frac{Ub^3}{D}\right)^2 \left(\frac{D}{b^2}\right) \frac{d}{dt^*}\left(m_2^* - m_1^{*2}\right)$$

or

$$\frac{K}{D} = \frac{1}{2}\left(\frac{Ub}{D}\right)^2 \left(\frac{dm_2^*}{dt^*} - 2m_1^* \frac{dm_1^*}{dt^*}\right)$$

So to get K/D, we need m_1^* and $\frac{dm_2^*}{dt^*}$!

Ok, so how do we get these moments?

Integrate the equations!

$$\frac{\partial c^*}{\partial t^*} + u^* \frac{\partial c^*}{\partial x^*} = \left(\frac{D}{Ub}\right)^2 \frac{\partial^2 c^*}{\partial x^{*2}} + \frac{\partial^2 c^*}{\partial y^{*2}}$$

we scaled w/ convection & y-diffusion! This is (usually) small!

Mult. by x^{*p} & integrate:

$$\frac{\partial c_p^*}{\partial t^*} + \int_{-\infty}^{\infty} x^{*p} u^* \frac{\partial c}{\partial x^*} dx^* = \left(\frac{D}{Ub}\right)^2 \int_{-\infty}^{\infty} x^{*p} \frac{\partial^2 c}{\partial x^{*2}} dx^* + \frac{\partial^2 c_p^*}{\partial y^{*2}}$$

We evaluate the integrals by parts:

$$\int_{-\infty}^{\infty} x^{*p} u^* \frac{\partial c^*}{\partial x^*} dx^* = \underbrace{\cancel{x^{*p} u^* c^*}\Big|_{-\infty}^{\infty}}_{\text{zero}} - p \int_{-\infty}^{\infty} x^{*p-1} u^* c^* dx^*$$

$$= -p\, u^* c_{p-1}^*$$

↳ not $f^n(x^*)$!

$$\int_{-\infty}^{\infty} x^{*p} \frac{\partial^2 c^*}{\partial x^{*2}} dx^* = p(p-1)\, c^*_{p-2}$$

So:

$$\frac{\partial c_p^*}{\partial t^*} = p\, u^* c^*_{p-1} + p(p-1) \overset{\left(\frac{D}{Ub}\right)^2}{\downarrow} c^*_{p-2} + \frac{\partial c_p^*}{\partial y^{*2}}$$

We have the boundary conditions for c_p^*:

$$\left.\frac{\partial c_p^*}{\partial y^*}\right|_{y^*=0,1} = 0 \qquad \left(\text{since } \left.\frac{\partial c^*}{\partial y^*}\right|_{y^*=0,1} = 0 \right)$$

Thus:

$$\frac{\partial m_p^*}{\partial t^*} = p \int_0^1 u^* c^*_{p-1}\, dy^* + \overset{\left(\frac{D}{Ub}\right)^2}{\downarrow} p(p-1)\, m^*_{p-2}$$

$$+ \underline{\underline{0}}$$

We get the sequence of problems:

$p=0$:

$$\frac{dm_0^*}{dt^*} = 0 \quad ; \quad \frac{\partial c_0^*}{\partial t^*} = \frac{\partial^2 c_0^*}{\partial y^{*2}}$$

$p=1$:

$$\frac{dm_1^*}{dt^*} = \int_0^1 u^* c_0^* \, dy^*$$

$$\frac{\partial c_1^*}{\partial t^*} = u^* c_0^* + \frac{\partial^2 c_1^*}{\partial y^{*2}}$$

$p=2$:

$$\frac{dm_2^*}{dt^*} = 2\int_0^1 u^* c_1^* \, dy^* + 2\left(\frac{D}{Ub}\right)^2 m_0^*$$

we don't need c_2^*!

Ok, now let's solve these problems!

m_0^* is the amount of solute in the system! It's not going anywhere, so just take

$$m_0^* = 1$$

Likewise, we anticipate that at long times the solute is uniformly distributed across the channel (y-dir)!

Thus, $c_0^* = 1$ too!

Now for $p = 1$:

$$\frac{dm_1^*}{dt^*} = \int_0^1 u^* \cdot (1)\, dy^* = 1$$

(since we normalized u w/ its avg!)

(in general, $\frac{dm_1^*}{dt^*} = \langle u^* \rangle = 1$)

We shall take the average x-position of the solute & at $t^* = 0$ to be zero

Thus:

$$m_1^* = t^* \qquad (\text{or } \langle u^* \rangle t^*)$$

Now for the only hard part:

$$\frac{\partial c_1^*}{\partial t^*} = u^* + \frac{\partial^2 c_1^*}{\partial y^{*2}}$$

we have that $\int_0^1 c_1^* \, dy^* = m_1^* = \langle u^* \rangle t^*$

Thus, we let:

$$c_1^* = \underbrace{\langle u^* \rangle t^*}_{m_1^*} + f(y^*)$$

So:

$$f'' = \langle u^* \rangle - u^*$$

$$f'(0) = f'(1) = 0$$

and, for consistency, $\int_0^1 f \, dy^* = 0$

Let's solve this:

$$f'' = 1 - \frac{3}{2}(1 - y^{*2})$$

$$= \frac{3}{2} y^{*2} - \frac{1}{2}$$

$$f' = \frac{1}{2} y^{*3} - \frac{1}{2} y^* + \cancel{c} \quad \text{as } f'(0) = 0$$

Note that $f'(1) = 0$ too...

$$\therefore f = \frac{1}{8} y^{*4} - \frac{1}{4} y^{*2} + c$$

$$\int_0^1 f \, dy^* = \frac{1}{40} - \frac{1}{12} + c = 0$$

$$\therefore c = \frac{1}{12} - \frac{1}{40} = \frac{7}{120}$$

So $f = \frac{1}{8} y^{*4} - \frac{1}{4} y^{*2} + \frac{7}{120}$

and

$$c_1^* = m_1^* + f(y^*)$$

Ok, now for $\frac{\delta}{\Delta}$!

$$\frac{dm_2^*}{dt^*} = 2 \int_0^1 u^* c_1^* \, dy^* + 2 \left(\frac{D}{Ub}\right)^2 m_0^*$$

$$= 2 m_1^* + 2 \left(\frac{D}{Ub}\right)^2 m_0^* + 2 \int_0^1 u^* f \, dy^*$$

But:

$$\frac{K}{D} = \frac{1}{2}\left(\frac{Ub}{D}\right)^2 \left(\frac{dm_2^*}{dt^*} - 2m_1^* \cancel{\frac{dm_1^*}{dt^*}} \right)$$

$$= \frac{1}{2}\left(\frac{Ub}{D}\right)^2 \left(\cancel{2m_1^*} + 2\left(\frac{D}{Ub}\right)^2 \cancel{m_0^*}^{\,1} + 2\int_0^1 u^* f\, dy^* \; \cancel{-2m_1^*} \right)$$

$$= 1 + \underbrace{\int_0^1 u^* f\, dy^* \left(\frac{Ub^2}{D}\right)}_{\text{dispersion}}$$

↑ molecular dif^n in x-dir

Evaluating the integral:

$$\int_0^1 u^* f\, dy^* = \int_0^1 \frac{3}{2}(1-y^{*2})\left(\frac{1}{8}y^{*4} - \frac{1}{4}y^{*2} + \frac{7}{120}\right) dy^*$$

$$= \int_0^1 (u^* - \langle u^* \rangle) f\, dy^* \quad \text{since} \quad \int_0^1 f\, dy^* = 0$$

Thus, since $f \sim u^* - \langle u^* \rangle$, the contribution is quadratic in Δu

So:

$$\int_0^1 \frac{3}{2}(1-y^{*2})\left(\frac{1}{8}y^{*4} - \frac{1}{4}y^{*2} + \frac{7}{120}\right) dy^*$$

$$= \frac{3}{2}\left[-\frac{1}{56} + \frac{1}{20} - \frac{7}{360}\right] = \frac{2}{105}$$

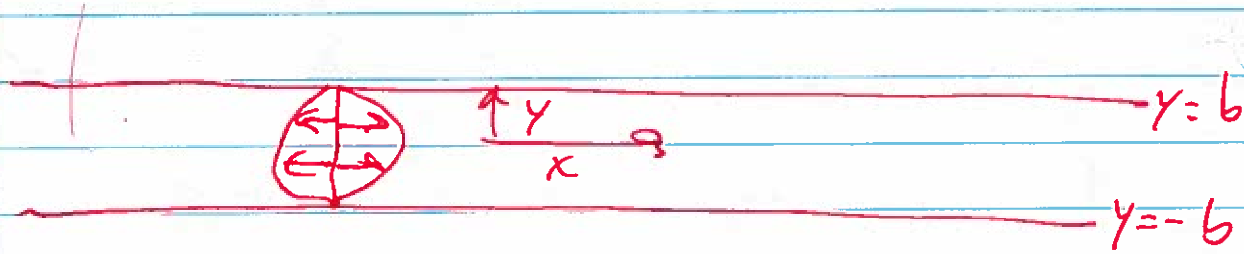
$$\text{So } \frac{K}{D} = 1 + \frac{2}{105}\left(\frac{Ub}{D}\right)^2$$

(for a tube, $\frac{K}{D} = 1 + \frac{1}{48}\left(\frac{Ua}{D}\right)^2$)

If you actually do the experiment in a wide aspect ratio channel, though, the meas. dispersivity is ~7.95 x higher! This is due to sidewalls!

Taylor-Aris Dispersion:

Oscillatory Channel flow



$$u = \frac{3}{2} U \left(1 - \frac{y^2}{b^2}\right) \cos \omega t$$

What is the stroke length?

$$2\Delta x = \int_{-\frac{\pi}{2\omega}}^{\frac{\pi}{2\omega}} U \cos \omega t \, dt$$

$$= \frac{U}{\omega} \left(\sin \omega t \right) \Big|_{-\frac{\pi}{2\omega}}^{\frac{\pi}{2\omega}} = \frac{2U}{\omega}$$

This, times the x-section area A, would be the volume of the tidal displacement!

Let's define $\Delta x = \frac{U}{\omega}$ - amplitude of tidal displacement.

We use Δx to render x dimensionless:

$$x^* = \frac{x}{\Delta x} = x\frac{\omega}{U}$$

So fluid moves $\pm \Delta x$ in x-direction.

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)$$

or, in dimensionless form,

$$\frac{\partial c^*}{\partial t^*} + u^*\frac{\partial c^*}{\partial x^*} = \left(\frac{D}{\omega b^2}\right)\left(\frac{\partial^2 c^*}{\partial y^{*2}} + \left(\frac{b}{\Delta x}\right)^2\frac{\partial^2 c^*}{\partial x^{*2}}\right)$$

So two dimensionless parameters appear:

$\frac{\Delta x}{b}$ = dimensionless amplitude of tidal displacement (or strain of motion)

$\frac{\omega b^2}{D} = \beta^2$ = dimensionless frequency — plays same role as Womersley # α for osc. unidirectional inertial flows.

We also want to render c dimensionless.

As before,

$$\int_{-\infty}^{\infty}\int_{-b}^{b} c \, dy \, dx = I$$

Let $c^* = c/A$

$$\therefore 2Ab\Delta x \int_{-\infty}^{\infty}\int_{0}^{1} c^* \, dy^* \, dx^* = I$$

$$\therefore A = \frac{I}{2b\Delta X}$$

We have the moments:

$$c_p = \int_{-\infty}^{\infty} x^p c \, dx \quad , \quad m_p = \int_{-b}^{b} c_p \, dy$$

$$\therefore c_p = (\Delta x)^{p+1} \frac{I}{2b\Delta x} \int_{-\infty}^{\infty} x^{*p} c^* \, dx^*$$

$$\text{so} \quad c_p^* = \frac{c_p}{\Delta x^p \frac{I}{2b}}$$

$$m_p = \Delta x^p \frac{I}{\cancel{2b}} \cancel{2b} \int_0^1 c_p^* \, dy^*$$

so

$$m_p^* = \frac{m_p}{I \Delta x^p}$$

Now we have for σ_x^2:

$$\sigma_x^2 = \frac{\int_{-\infty}^{\infty}\int_{-b}^{b} (x-\bar{x})^2 c \, dy \, dx}{\int_{-\infty}^{\infty}\int_{-b}^{b} c \, dy \, dx} \quad = I$$

$$\bar{x} = \frac{\int_{-\infty}^{\infty}\int_{-b}^{b} x \, c \, dy \, dx}{\int_{-\infty}^{\infty}\int_{-b}^{b} c \, dy \, dx}.$$

$$\therefore \frac{d\sigma_x^2}{dt} = 2K \quad \text{at long times!}$$

(note - there is an osc. component too)

So:

$$K = \frac{1}{2}\frac{d\sigma_x^2}{dt} = \frac{1}{2}\Delta x^2\omega \cdot \left[\frac{dm_2^*}{dt^*} - 2m_1^*\frac{dm_1^*}{dt^*}\right]$$

$$\frac{K}{D} = \left(\frac{\Delta x}{b}\right)^2\left(\frac{\omega b^3}{D}\right)\left[\frac{1}{2}\frac{dm_2^*}{dt^*} - m_1^*\frac{dm_1^*}{dt^*}\right]$$

So we need equations for the moments!

$$\frac{\partial c^*}{\partial t^*} + u^*\frac{\partial c^*}{\partial x^*} = \left(\frac{D}{\omega b^2}\right)\left(\frac{\partial^2 c^*}{\partial y^{*2}} + \left(\frac{b}{\Delta x}\right)^2\frac{\partial^2 c^*}{\partial x^{*2}}\right)$$

$$\left.\frac{\partial c^*}{\partial y^*}\right|_{y^*=0,1} = 0$$

Multiply by x^{*p} & integrate:

$$\frac{\partial c_p^*}{\partial t^*} + \int_{-\infty}^{\infty} x^{*p} u^* \frac{\partial c^*}{\partial x^*}\,dx^* = \left(\frac{D}{\omega b^2}\right)\frac{\partial^2 c_p^*}{\partial y^{*2}}$$

$$+ \left(\frac{D}{\omega b^2}\right)\left(\frac{b}{\Delta x}\right)^2\int_{-\infty}^{\infty}\frac{\partial^2 c^*}{\partial x^{*2}}x^{*p}\,dx^*$$

As before:

$$\int_{-\infty}^{\infty} x^{*p} u^* \frac{\partial c^*}{\partial x^*} dx^* = -p\, u^* C^*_{p-1}$$

$$\int_{-\infty}^{\infty} \frac{\partial^2 c^*}{\partial x^{*2}} x^{*p} dx^* = p(p-1)\, C^*_{p-2}$$

So:

$$\frac{\partial C_p^*}{\partial t^*} = p^* u^* C^*_{p-1} + \left(\frac{D}{\omega b^2}\right)\frac{\partial^2 C_p^*}{\partial y^{*2}} + \left(\frac{D}{\omega b^2}\right)\left(\frac{b^*}{\Delta x}\right)^2 p(p-1)\, C^*_{p-2}$$

with $\left.\dfrac{\partial C_p^*}{\partial y^*}\right|_{y^*=0,1} = 0$

and we have the moment eq'n:

$$\frac{\partial M_p^*}{\partial t^*} = p^* \int_0^1 u^* C^*_{p-1}\, dy^* + \left(\frac{D}{\omega b^2}\right)\left(\frac{b^*}{\Delta x}\right)^2 p(p-1) M^*_{p-2}$$

The sequence of problems is:

$p=0$: $m_0^* = 1, \quad c_0^* = 1$

$p=1$:

$$\frac{\partial m_1^*}{\partial t^*} = \int_0^1 u^* c_0^* \, dy^* = \int_0^1 u^* \, dy^*$$

$$= \cos t^* \; ! \quad \text{(oscillatory)}$$

we thus take $m_1^* = \sin t^*$

(the slug moves back & forth & starts w/ avg. position $\bar{x} = 0$ at $t=0$)

$$\frac{\partial c_1^*}{\partial t^*} = u^* c_0^* + \left(\frac{D}{\omega b^2}\right) \frac{\partial^2 c_1^*}{\partial y^{*2}}$$

or
$$\frac{\partial c_1^*}{\partial t^*} - \left(\frac{D}{\omega b^2}\right) \frac{\partial^2 c_1^*}{\partial y^{*2}} = u^* = f^n(y^*, t^*) \, !$$

w/ B.C.
$$\left.\frac{\partial c_1^*}{\partial y^*}\right|_{y^*=0,1} = 0, \quad \int_0^1 c_1^* \, dy^* = \sin t^*$$

This is the hard problem!

What about m_2^* ?

$$\frac{dm_2^*}{dt^*} = 2\int_0^1 u^* c_1^* dy^* + 2\left(\frac{D}{\omega b^2}\right)\left(\frac{b}{\Delta x}\right)^2 m_0^*$$

$$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad 1$$

So:

$$\frac{K}{D} = \left(\frac{\Delta x}{b}\right)^2\left(\frac{\omega b^2}{D}\right)\left[\frac{1}{2}\frac{dm_2^*}{dt^*} - m_1^*\frac{dm_1^*}{dt^*}\right]$$

$$= \left(\frac{\Delta x}{b}\right)^2\left(\frac{\omega b^2}{D}\right)\left[\left(\frac{D}{\omega b^2}\right)\left(\frac{b}{\Delta x}\right)^2 + \int_0^1 u^* c_1^* dy^* - m_1^*\frac{dm_1^*}{dt^*}\right]$$

$$= 1 + \left(\frac{\Delta x}{b}\right)^2\left(\frac{\omega b^2}{D}\right)\left[\int_0^1 u^* c_1^* dy^* - \cos t^* \sin t^*\right]$$

molecular diffusion!

Ok, so now we need to get c_1^*!

Recall that:

$$\frac{\partial c_1^*}{\partial t^*} - \left(\frac{D}{\omega b^2}\right)\frac{\partial^2 c_1^*}{\partial y^{*2}} = u^*$$

Let's subtract off m_1^*

$$c_1^* = m_1^* + g(y^*, t^*)$$

Note that $\frac{\partial m_1^*}{\partial t^*} = \langle u^* \rangle$ (spatial avg)

Thus

$$\frac{\partial g}{\partial t^*} - \left(\frac{D}{\omega b^2}\right)\frac{\partial^2 g}{\partial y^{*2}} = u^* - \langle u^* \rangle$$

and, plugging back in for $\frac{K}{D}$, we kill off the $m_1^* \frac{\partial m_1^*}{\partial t^*}$ term!

$$\frac{K}{D} = 1 + \left(\frac{\Delta x}{b}\right)^2 \left(\frac{\omega b^2}{D}\right) \int_0^1 u^* g(y^*, t^*)\, dy^*$$

So:

$$\frac{\partial g}{\partial t^*} - \left(\frac{D}{\omega b^2}\right)\frac{\partial^2 g}{\partial y^{*2}} = \cos t^* \left(\frac{1}{2} - \frac{3}{2} y^{*2}\right)$$

$$\left.\frac{\partial g}{\partial y}\right|_{y=0,1} = 0 \qquad \int_0^1 g\, dy = 0$$

Let's look at this behavior for <u>low</u> frequencies

Recall $\frac{\omega b^2}{D} \equiv \beta^2$

Let $\varepsilon = \beta^2$

Thus:

$$\varepsilon \frac{\partial g}{\partial t^*} - \varepsilon \cos t^* \left(\frac{1}{2} - \frac{3}{2} y^{*2}\right) = \frac{\partial^2 g}{\partial y^{*2}}$$

We let $g = g_0(y^*, t^*) + \varepsilon g_1(y^*, t^*) + \ldots$

$$\therefore \frac{\partial^2 g_0}{\partial y^{*2}} = 0 \qquad \left.\frac{\partial g_0}{\partial y^*}\right|_{y^*=0,1} = \int_0^1 g_0 \, dy^* = 0$$

$\therefore$ at $O(\varepsilon^0)$ $g_0 = 0$!

So at $O(\varepsilon^1)$:

$$\frac{\partial^2 g_1}{\partial y^{*2}} = \underbrace{\cancel{\frac{\partial g_0}{\partial t^*}}}_{0} - \cos t^* \left(\frac{1}{2} - \frac{3}{2} y^{*2}\right)$$

w/ same B.C.'s!

This yields :

$$g_1 = -\cos t^*\left(\frac{1}{4}y^{*2} - \frac{1}{8}y^{*4} + Ay^* + B\right)$$

but $g_1'\Big|_{y^*=0} = 0 \quad \therefore A = 0$

We automatically satisfy $g_1'(1) = 0$

Finally, $\int_0^1 g\, dy^* = -\cos t^*\left(\frac{1}{12} - \frac{1}{40} + B\right) = 0$

so $B = \frac{1}{40} - \frac{1}{12} = \frac{-7}{120}$

and $g = \varepsilon\left(\frac{1}{8}y^{*4} - \frac{1}{4}y^{*2} + \frac{7}{120}\right)\cos t^*$

$$+ O(\varepsilon^2)\ !$$

So :

$$\frac{K}{D} = 1 + \left(\frac{\Delta x}{b}\right)^2\left(\frac{\omega b^2}{D}\right)^2$$

$$\times \int_0^1 \cos^2 t^*\left(\frac{1}{2} - \frac{3}{2}y^{*2}\right)\left(\frac{1}{8}y^{*4} - \frac{1}{4}y^{*2} + \frac{7}{120}\right)dy^*$$

This can be evaluated:

$$\frac{K}{D} = 1 + \frac{2}{105}\cos^2 t^* \left(\frac{\Delta x}{b}\right)^2 \beta^4$$

remember this??

It's basically just steady flow T-A dispersion w/ time-dep. velocity!

Now we are interested in the average dispersion!

$$\langle \cos^2 t^* \rangle = \frac{1}{2}$$

So $\left\langle \frac{K}{D} \right\rangle = 1 + \frac{1}{105}\left(\frac{\Delta x}{b}\right)^2 \beta^4 + O(\beta^8)$

Note: β^6 term vanishes as $g_2 \sim \sin t^*$ and this is out of phase w/ u_0^*!

OK, now we look at high frequencies!

$$\frac{\partial \hat{g}}{\partial t^*} - \frac{1}{\beta^2}\frac{\partial^2 \hat{g}}{\partial y^{*2}} = e^{it^*}\left(\frac{1}{2} - \frac{3}{2}y^{*2}\right)$$

$g = Re\{\hat{g}\}$

Let $\hat{g} = e^{it} f(y^*)$

$$\therefore \; if - \frac{1}{\beta^2} f'' = \left(\frac{1}{2} - \frac{3}{2}y^{*2}\right)$$

$$f'(0) = f'(1) = \int_0^1 f \, dy^* = 0$$

We have $f = f_p + f_h$

$$f_p = Ay^{*2} + B$$

$$\therefore \; i(Ay^{*2} + B) - \frac{2A}{\beta^2} = \frac{1}{2} - \frac{3}{2}y^{*2}$$

$$\therefore \; iA = -\frac{3}{2} \qquad A = +\frac{3}{2}i$$

$$iB - \frac{2A}{\beta^2} = \frac{1}{2}$$

$$iB - \frac{3i}{\beta^2} = \frac{1}{2}$$

$$B = \frac{3}{\beta^2} - \frac{i}{2}$$

So:

$$f_p = \frac{3}{2} i y^{*2} + \frac{3}{\beta^2} - \frac{i}{2} = i\left(\frac{3}{2}y^{*2} - \frac{1}{2}\right) + \frac{3}{\beta^2}$$

f_h satisfies:

$$f_h'' - f_h^* \, i\beta^2 = 0$$

This has the solution:

~~$f_h = c \cosh$ (choose s.t. $f_h'(0)$~~

$\therefore$ ~~$f = c \cosh \frac{y^*}{\beta^2}$~~ $f_h = c \cosh \sqrt{i}\beta y^*$

where we keep the symmetric sol'n!

$$\therefore f = i\left(\frac{3}{2}y^{*2} - \frac{1}{2}\right) + \frac{3}{\beta^2} + C\cosh\sqrt{i}\beta y^*$$

Now $f'(1) = 0$

$$\therefore \; 3i + C\sqrt{i}\beta \sinh\sqrt{i}\beta = 0$$

$$C = \frac{-3\sqrt{i}}{\beta \sinh\sqrt{i}\beta}$$

and $$f = i\left(\frac{3}{2}y^{*2} - \frac{1}{2}\right) + \frac{3}{\beta^2} + \frac{-3\sqrt{i}\cosh\sqrt{i}\beta y^*}{\beta\sinh\sqrt{i}\beta}$$

Now we have:

$$g = \mathrm{Re}\{\hat{g}\} = \mathrm{Re}\left\{e^{i t^*} f(y^*)\right\}$$

$$= \mathrm{Re}\left\{\left[\cos t^* + i \sin t^*\right] f(y^*)\right\}$$

$$= \cos t^* \,\mathrm{Re}\{f\} - \sin t^* \,\mathrm{Im}\{f\}$$

only the $\cos t^*$ part of g will contribute, as the $\sin t^*$ part is out of phase with u^*!

So:

$$\langle \cos^2 t^* \rangle$$

$$\frac{K}{D} = 1 + \left(\frac{\Delta x}{b}\right)^2 \beta^2 \int_0^1 \left(\frac{1}{2} - \frac{3}{2} y^{*2}\right) \mathrm{Re}\{f\}\, dy^*$$

Now as $\beta \to \infty$, we need to look at the asymptotic form of f:

$$\cosh \sqrt{i}\, \beta y^* = \cosh \frac{1+i}{\sqrt{2}} \beta y^*$$

$$=$$

pulled out of f (β^{-2} factored out too)

So

$$\frac{K}{D} = 1 + \frac{3}{2}\left(\frac{\Delta x}{b}\right)^2 \underbrace{\int_0^1 \left(\frac{1}{2} - \frac{3}{2}y^{*2}\right) Re\left\{1 - \frac{\beta\sqrt{i}\cosh\sqrt{i}\beta y^*}{\sinh\sqrt{i}\beta}\right\} dy^*}$$

factor from $\langle \cos^2 t^* \rangle$

this integrates to one as $\beta \to \infty$!

For a tube, get

involves Bessel f^n of complex arg.

$$\frac{K}{D} = 1 + 4\left(\frac{\Delta x}{a}\right)^2 \cdot f^n(\beta)$$

$$\text{or } 1 + \left(\frac{2\Delta x}{a}\right)^2$$

We could get the same result by examining the strain & using the

$$\frac{K}{D} = 1 + \frac{1}{2}\left(\frac{\dot{\gamma}}{\omega}\right)^2$$ formula for unbounded domains.

$\Delta x = \frac{U}{\omega}$

$$\frac{\dot{\gamma}}{\omega} = \left(\frac{\Delta x}{b}\right) 3y^* \quad \therefore \quad \left\langle \left(\frac{\dot{\gamma}}{\omega}\right)^2 \right\rangle = \left(\frac{\Delta x}{b}\right)^2 \int_0^1 (3y^*)^2 dy^*$$

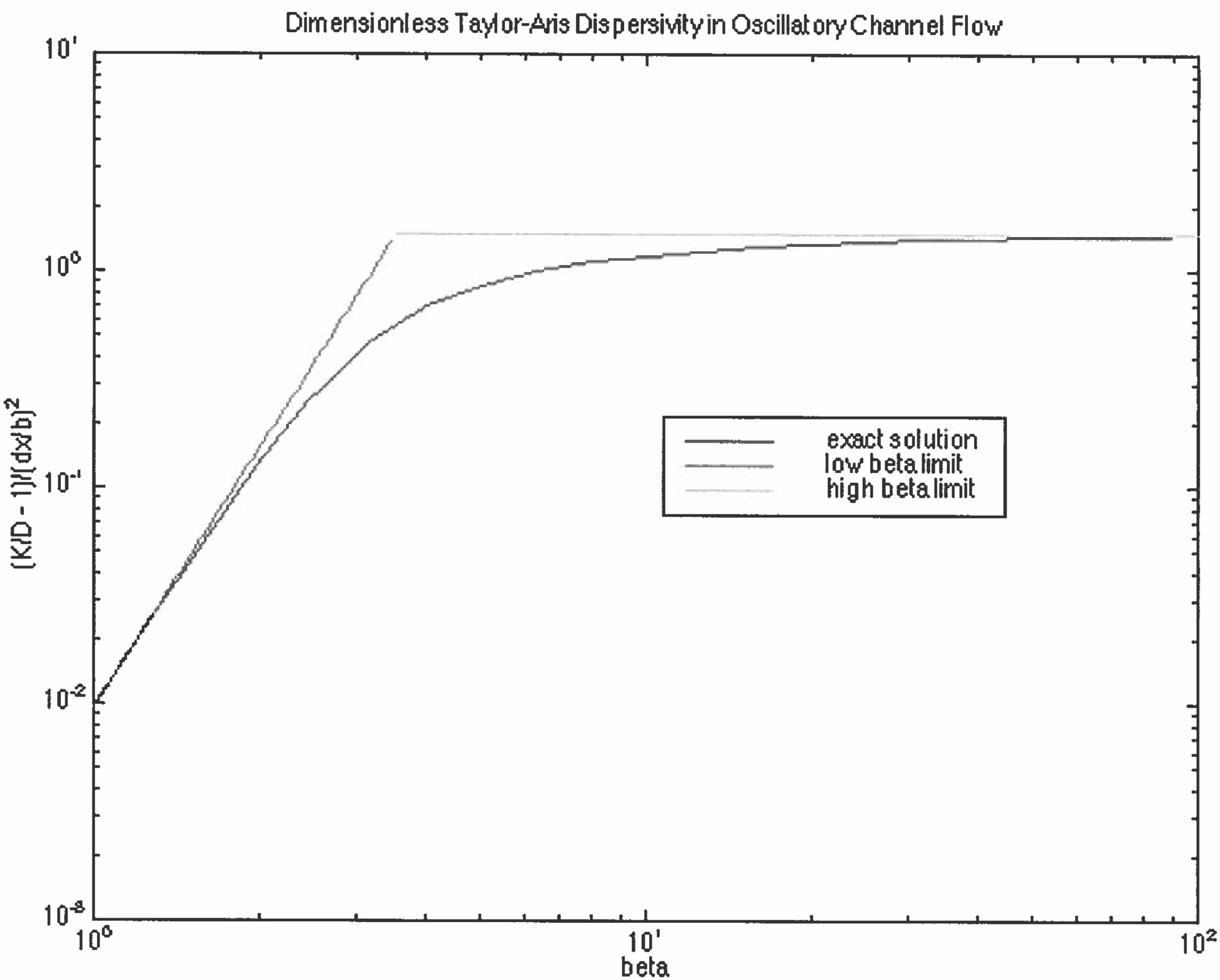
$$= 3\left(\frac{\Delta x}{b}\right)^2$$

```
%This script plots up the dispersivity for oscillatory flow in a channel
%dx is taken as the amplitude of the stroke length (total travel is twice
%this value!).

clear
betaall=10.0.^[0:.1:2];
for kk=1:length(betaall);
beta=betaall(kk);
dy=.001;
y=[0:dy:1];
f=1-beta*i^.5*cosh(i^.5*beta*y)/sinh(i^.5*beta);
f=real(f);
ig=(0.5-1.5*y.^2).*f;
n=length(y);
result(kk)=1.5*(sum(ig)-.5*ig(1)-.5*ig(n))*dy;
end
figure(1)
loglog(betaall,result)

lowbetalim=(1.5*105)^.25;
lowbeta=10.0.^[0:.01:log10(lowbetalim)];
highbeta=10.0.^[log10(lowbetalim):.01:2];
hold on
plot(lowbeta,lowbeta.^4/105,'r',highbeta,1.5*ones(size(highbeta)),'g')
hold off

title('Dimensionless Taylor-Aris Dispersivity in Oscillatory Channel Flow')
xlabel('beta')
ylabel('(K/D - 1)/(dx/b)^2')
legend('exact solution','low beta limit','high beta limit')
```

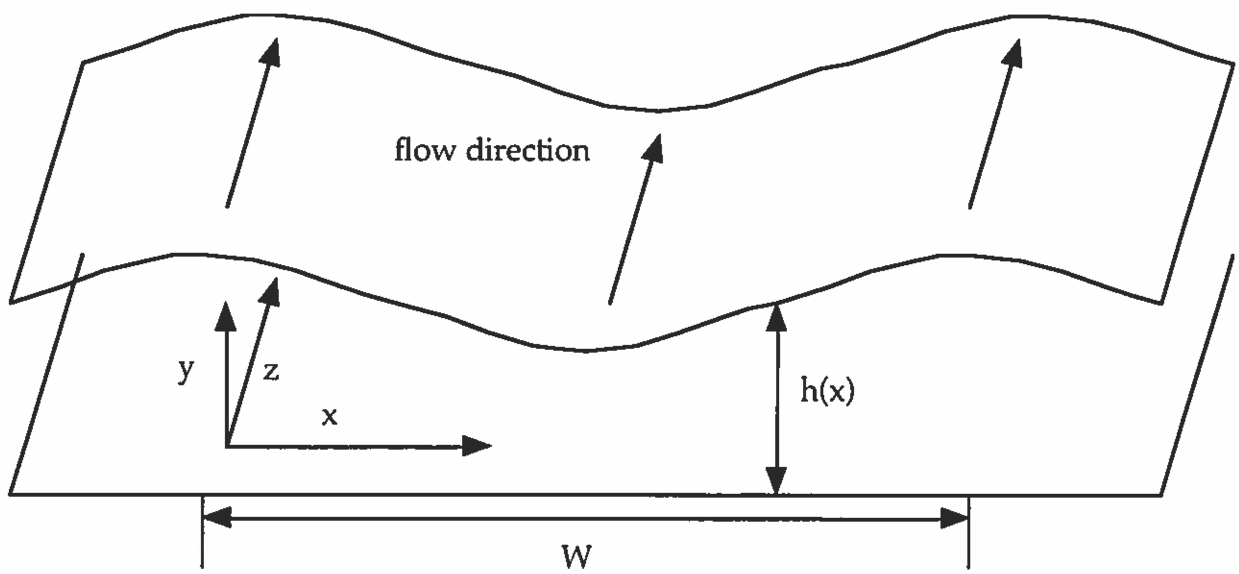

Dimensionless Taylor-Aris Dispersivity in Oscillatory Channel Flow
exact solution
low beta limit
high beta limit
(K/D - 1)/(dx/b)^2
beta
10^1
10^0
10^-1
10^-2
10^-3
10^0
10^1
10^2

CBE 20258 Project 11

Due in class 4/17/14

Taylor Dispersion in Microchannels

A classic problem in mass transfer is the phenomenon of Taylor dispersion: the spread of a solute as it travels down a conduit such as a tube or channel. This is the same phenomenon that leads to peak spreading in chromatography: an initially focused slug of solute (e.g., what you inject onto a column) spreads out in the flow direction because not all solute molecules of the same type move with the same velocity all the time, but rather have a velocity which fluctuates about an average. In a conduit, this fluctuation is due to a non-uniform velocity profile. Typically, the fluid velocity is zero at the walls, and is a maximum in the middle, thus solute molecules move with different speeds depending on where they happen to be in the conduit cross-section at any instant. Eventually the solute molecules just move with the average velocity as they diffuse back and forth across the conduit, but while this diffusion process takes place the slug spreads out in the flow direction. This phenomenon is called Taylor dispersion, and is a big problem in designing microfluidic analysis systems (e.g., lab-on-a-chip systems). The geometry we will look at in this project is depicted below:



As you will learn next year, the concentration distribution of a solute flowing through a channel is governed by the *convective diffusion equation:*

$$\frac{\partial c}{\partial t} + u_z \frac{\partial c}{\partial z} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)$$

where we have ignored diffusion in the direction of fluid motion (the z-direction), as this is usually negligible relative to the much larger convection term. The diffusion coefficient characterizes the random motion of the solute across the channel, and is given by D. The quantity u_z is the velocity in the flow direction (z direction) which, for the conduit depicted above is approximately given by:

$$u_z \approx \frac{6U}{h_0^2} y(h-y)$$

where the wavy upper wall is described by:

$$h = h_0 + \Delta h \cos\left(2\pi \frac{x}{W}\right)$$

This expression for the velocity is only correct if either $\Delta h = 0$ or if $W >> h_0$.
The *boundary condition* associated with the convective diffusion equation for this problem is that the normal derivative of the concentration is zero at the wall (this is called the no-flux condition):

$$\vec{\nabla} c \cdot \vec{n}\big|_{\partial D} = 0$$

where ∂D is the boundary and $\vec{n}$ is the unit normal. At the bottom wall this condition just reduces to:

$$\left.\frac{\partial c}{\partial y}\right|_{y=0} = 0$$

while the condition at the wavy top wall is more complex.

This set of equations is difficult to solve for the transient injection of a slug of solute for anything but the simplest geometry. An appealing alternative numerical approach is to solve the equation by performing a Brownian Dynamics simulation: we simulate the evolution of the concentration distribution by tracking the motion of a large number of tracer particles. The position of the particles is obtained by integrating the *Langevin Equations:* the particles follow along with the fluid velocity in the z direction, and at each time step we add in a random motion in the x and y directions proportional to $(2\, D\, \Delta t)^{1/2}$ times a normally distributed random number with zero mean and standard deviation of one. The distribution of these particles (for large numbers of them, and small time steps) is identical to the solution of the convective diffusion equation. Such Brownian Dynamics simulations are easy to code up, but take a lot of computer power - which fortunately we now have!

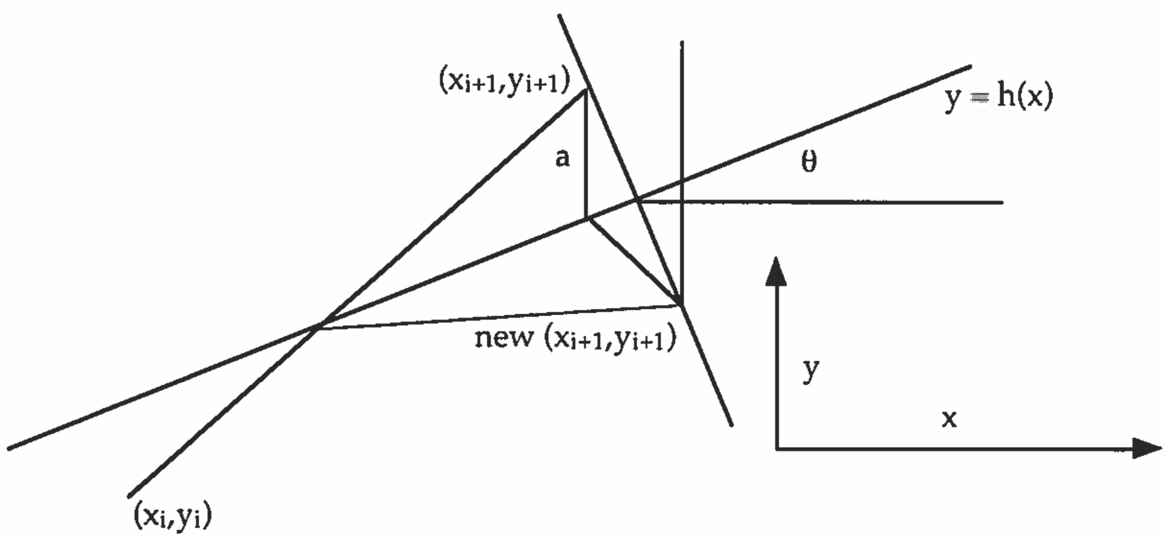
Your goal is to use Brownian Dynamics to calculate the Taylor dispersion coefficient K for this geometry. This is quite easy: if you have simulated the z-position of all the particles, you can calculate the variance in the z-direction σ_z^2. The dispersion coefficient is just:

$$\lim_{t \to \infty} \frac{d\sigma_z^2}{dt} = 2K$$

e.g., after some initial transient has passed.

OK, how do we do such a simulation? First, you set up an initial distribution. You take the particles to be initially in the plane z=0, but distributed uniformly in the x & y directions. For a non-uniform geometry such as we are looking at here it is convenient to distribute them over a rectangular box that contains the conduit (or the unit cell of the conduit in this case) and just keep the ones that are inside using the "find" command. The "rand" command which gives a uniformly distributed random number between 0 and 1 is useful here! The integration process is simple: at each time step you give the particles a random step in the x direction and the y direction (a different random number for each - use the "randn" command!) and update the z position by integrating the position-dependent z-velocity using the trapezoidal rule (or, just as easily, Simpson's rule for higher accuracy: the midpoint is just the average of new and old x and y locations). You keep track of the variance in the z-direction, and let the simulation run sufficiently long that the growth becomes linear. You then calculate the slope of this growth, and half that value gives you K!

Boundary Reflections:
The only hard part of the simulation is getting the boundary conditions right. The no-flux condition for the differential equation corresponds to a reflection condition in the simulation: if the random step places you outside the boundary, simply reflect the particle back inside. For the bottom wall this is easy: identify all particles such that $y < 0$ and place them at $y=|y|$. For the top wall it is a bit harder. The wall location is at $y = h(x)$, with derivative $h'(x)$. Because of the slope of the wall, the reflection actually shifts the particle in both the x and y directions. We have the following picture:



From the geometry depicted above we get the sequence of problems for figuring out the new x and y positions:

1. calculate Δx (the random displacement in x) and x_{i+1} for all particles
2. calculate Δy (the random displacement in y) and y_{i+1} for all particles

3. find the indices of particles for which $y_{i+1} < 0$ and reflect them to $|y_{i+1}|$ (this is the bottom wall reflection)
4. find the indices of particles for which $a = y_{i+1} - h(x_{i+1}) > 0$
5. calculate the local slope of the wall $\theta = \text{atan}(h'(x_{i+1}))$
6. correct the y position $y_{i+1} = h(x_{i+1}) - a\cos(2\theta)$
7. correct the x position $x_{i+1} = x_{i+1} + a\sin(2\theta)$

To get higher accuracy in updating the z position, you also need to modify the integration rule for the particles interacting with either wall. Since they are bouncing off the wall, they spend part of this time step with velocity $u_z = 0$. You can easily correct for this by determining the fraction of the time step dt it spends going from (x_i, y_i) to the wall (call this f), and then the rest of the time step it is bouncing off to the new position. For the upper wall, a little work with similar triangles and geometry produces:

$$f = \frac{h(x_i) - y_i}{\Delta y - \left(h(x_i) - h(x_i + \Delta x)\right)}$$

This works for the lower wall too, only there h(x) is just zero. The velocity at either wall is zero, so integration of these two segments via the trapezoidal rule is done by:

$$\Delta z = \frac{1}{2} dt \left(f\, u_z(x_i, y_i) + (1-f)\, u_z(x_{i+1}, y_{i+1}) \right)$$

For this problem, reflection from the sides is not an issue as the domain is periodic in the x-direction. Particles which leave the central cell $[0 < x < W]$ are simply moved to the appropriate value of x in the replicated cell (e.g., if x>W move them to x-W, and if x<0 move them to W+x). Again, the "find" command is useful here!

Non-Dimensionalization:

In solving a problem on a computer, it is very useful to render the problem dimensionless analytically first. This way you can see how varying parameters such as h_0 and U affect the dispersivity without having to re-run your computer code! For this problem we define the following dimensionless variables and parameters:

$$x^* = \frac{x}{h_0} \quad ; \quad y^* = \frac{y}{h_0} \quad ; \; z^* = \frac{z}{\left[\frac{Uh_0^2}{D}\right]} \quad ; \; t^* = \frac{t}{\left[\frac{h_0^2}{D}\right]}$$

$$h^* = \frac{h}{h_0} = 1 + \frac{\Delta h}{h_0}\cos\left(2\pi \frac{h_0}{W} x^*\right) \quad ; \quad u_z^* = \frac{u_z}{U} = 6y^*\left(h^* - y^*\right)$$

This non-dimensionalization results in the dimensionless problem:

$$\frac{\partial c}{\partial t^*} + u_z^* \frac{\partial c}{\partial z^*} = \left(\frac{\partial^2 c}{\partial x^{*2}} + \frac{\partial^2 c}{\partial y^{*2}} \right)$$

where the dimensionless Taylor dispersivity is just:

$$K^* = \frac{K D}{(U h_0)^2} = \lim_{t^* \to \infty} \frac{1}{2} \frac{d\sigma_z^{*2}}{dt^*}$$

and it is a function only of the two dimensionless parameters:

$$\varepsilon = \frac{\Delta h}{h_0} \quad \text{and} \quad W^* = \frac{W}{h_0}$$

The dimensionless displacement in the x* and y* directions thus scales as $(2\Delta t^*)^{1/2}$, and the z* position is updated with the appropriate position dependent dimensionless velocity u_z^*. You need to pick a time step Δt^* so that particles only move a relatively small distance across the channel in each jump - but making it too small means a really large amount of computing time!

The Problem:

1. Write a simulation code that can track the motion of tracer particles for arbitrary W* and ε. Plot the initial x-y particle positions up together with the boundaries to be sure that you have a uniform distribution across the cross-section for the wavy wall case. During the simulation it is fun to plot up the x-z distribution using the "drawnow" command - you can get a nice movie out of it and see the dynamics. These graphics take a long time, though, so you will want to comment them out later!

2. For the case $\varepsilon = 0$, the dispersion is not a function of W*. For this case, plot up σ_z^{*2} as a function of time. Using the last third of your values of σ_z^{*2} as a function of time, determine K* (e.g., do a linear fit to these points to get the slope and intercept) and graphically compare the asymptotic linear result for the variance to the simulation values for all the times. About how long do you need to wait for the variance to approach a linear growth rate? (Hint: for a uniform initial distribution it is pretty fast - everything is over long before you reach t* = 1) This time scale is the time necessary to reach the Taylor limit.

3. Examine random error for the case $\varepsilon = 0$ by repeating the calculation a number of times, and determining the standard deviation of the mean value. Take this script and turn it into a function of Δt^* and the stopping point, returning the average K* and its standard deviation. Examine algorithm error by plotting up the calculated value of K* for different Δt^* (keeping the stopping point constant, and reasonably long) and different stopping points (keeping Δt^* constant, and reasonably short). Based on these calculations, determine the best value of K* for the $\varepsilon = 0$ case, as well as its uncertainty. Does it match the theoretically predicted value of K* = 1/210?

4. Now explore the effect of wavy walls. By plotting up σ_z^{*2} as a function of t* for $\varepsilon = 0.2$ and W*=5, show that the variance is much larger than the $\varepsilon = 0$ case and that it takes much longer to approach the Taylor limit (it will scale as W^{*2} as the tracers have to diffuse much farther in the x-direction). What is the value of K* for this case? Print out the x-y and x-z distributions at the end of your simulation of the wavy wall case.

```
%This script calculates the Taylor dispersivity due to flow through a wavy
%channel.  The lower wall is at y=0 and the upper wall is at
%h=1+e*cos(2*pi*x/w) where e is the amplitude of the waviness and w is the
%width of the unit cell.

e=.2;
w=5;

%We begin by introducing all of our particles:

n=20000;

nstart=round(n*(1+2*e));  %A bit more than n particles, as some are discarded.

x=w*rand(nstart,1); %The x locations
y=(1+e)*rand(nstart,1); %The y locations

%Now we need to determine the values which are inside our domain:

i=find(y<(1+e*cos(2*pi*x/w)));

x=x(i);
y=y(i);

%These are all the valid particles.  We really only want n of them:

x=x(1:n);
y=y(1:n);

%We can plot this up:
figure(1)
xp=w*[0:.01:1];
plot(w*[0,1],[0,0,],'k',xp,1+e*cos(2*pi*xp/w),'k',x,y,'ob')
xlabel('x')
ylabel('y')
axis('equal')
title('Initial distribution')
drawnow

%Now for the simulation:

tlim=0.3*w^2;
dt=0.001;

t=[dt:dt:tlim]'; %We have a column vector of times
varz=zeros(size(t));
zbar=zeros(size(t));

z=zeros(size(x));  %We start the particles at zero...

for j=1:length(t)
    %We have the random steps:
    dx=randn(n,1)*(2*dt)^.5;
    dy=randn(n,1)*(2*dt)^.5;

    xt=x+dx;
    yt=y+dy;

    %Now we check to see if particles have bounced out:

    ilow=find(yt<0); %the particles below the bottom wall
    ihigh=find(yt>(1+e*cos(2*pi*xt/w))); %the particles above the top wall

    yt(ilow)=abs(yt(ilow)); %Reflect those back!

    a=yt(ihigh)-(1+e*cos(2*pi*xt(ihigh)/w));
    theta=atan(-e*2*pi/w*sin(2*pi*xt(ihigh)/w));
    yt(ihigh)=(1+e*cos(2*pi*xt(ihigh)/w))-a.*cos(2*theta);
```

```
    xt(ihigh)=xt(ihigh)+a.*sin(2*theta);

    %Now for getting dz.  We use simpson's rule:
    h=1+e*cos(2*pi*x/w);
    ht=1+e*cos(2*pi*xt/w);

    %We calculate the midpoint of the jump:
    xm=(x+xt)/2;
    ym=(y+yt)/2;
    hm=1+e*cos(2*pi*xm/w);

    %and we get dz via Simpson's rule:
    dz=1/6*(6*y.*(h-y)+24*ym.*(hm-ym)+6*yt.*(ht-yt))*dt;

    %Now we deal with the change in z for particles bouncing off the walls:
    f=-y(ilow)./dy(ilow);
    dz(ilow)=0.5*dt*(f.*6.0.*y(ilow).*(h(ilow)-y(ilow))+(1-f)*6.0.*yt(ilow).*(ht(ilow)-
yt(ilow)));

    f=(h(ihigh)-y(ihigh))./((h(ihigh)-y(ihigh))+a); %The value of a was calculated
before!
    dz(ihigh)=0.5*dt*(f.*6.0.*y(ihigh).*(h(ihigh)-y(ihigh))+(1-f)*6.0.*yt(ihigh).*(ht
(ihigh)-yt(ihigh)));

    %Move x values back into the unit cell:
    ileft=find(xt<0);
    xt(ileft)=w+xt(ileft);
    iright=find(xt>w);
    xt(iright)=xt(iright)-w;

    %We update z and get the statistics:
    z=z+dz;
    x=xt;
    y=yt;

    %now we populate the columns of zbar and varz:
    zbar(j)=mean(z);
    varz(j)=var(z);

    %We do a little plotting to see what is going on: comment this out
    %later to speed things up!

%      figure(1)
%      xp=w*[0:.01:1];
%      plot(w*[0,1],[0,0,],'k',xp,1+e*cos(2*pi*xp/w),'k',x,y,'ob')
%      axis('equal')
%      xlabel('x')
%      ylabel('y')
%      title(['x and y positions for t = ',num2str(t(j))])
%
%      figure(2)
%      plot(x,z,'o')
%      xlabel('x')
%      ylabel('z')
%      title(['x and z positions for t = ',num2str(t(j))])
%      drawnow

end

%and we get the value of the Taylor dispersivity from the slope of the
%variance.  We fit the last 1/3 of the values:
ifit=[round(length(t)*2/3):length(t)];
tfit=t(ifit);
varzfit=varz(ifit);

xx=[ones(size(tfit)),tfit]\varzfit;

k=xx(2)/2; %The Taylor dispersivity
```

```
disp('The ratio of the Taylor dispersivity to that of a channel with no side-walls is:')
out=k*210  %The ratio to the channel theoretical result

figure(2) %We can comment this out if we wish.
plot(t,varz,t,[ones(size(t)),t]*xx,t,t/105)
legend('simulation','linear fit','e=0 theory','Location','NorthWest')
xlabel('t')
ylabel('variance in z')
title(['Variance for e = ',num2str(e),' and W = ',num2str(w)])
grid on
drawnow

    figure(3)
    xp=w*[0:.01:1];
    plot(w*[0,1],[0,0,],'k',xp,1+e*cos(2*pi*xp/w),'k',x,y,'ob')
    axis('equal')
    xlabel('x')
    ylabel('y')
    title(['x and y positions for t = ',num2str(t(j))])

    figure(4)
    plot(x,z,'o')
    xlabel('x')
    ylabel('z')
    title(['x and z positions for t = ',num2str(t(j))])
    drawnow
```