POD 23:
Simulation of AF4 separation

Suppose we have the simple shear: $u_x = \dot{\gamma} y$ and we have a species which has diffusivity D. We have the convective diffⁿ eq'n:

$$\frac{\partial c}{\partial t} + \dot{\gamma} y \frac{\partial c}{\partial x} - u_0 \frac{\partial c}{\partial y} = D \frac{\partial^2 c}{\partial y^2}$$

scaling: $y^* = y/Y_c \quad Y_c = \frac{D}{u_0}$

$$t_c = \frac{Y_c^2}{D} = \frac{D}{u_0^2}, \quad x_c = \frac{\dot{\gamma} Y_c^3}{D} = \frac{\dot{\gamma} D^2}{u_0^3}$$

Recall we had the dimensionless dispersivity

$$\frac{K}{D} = 1 + 2\frac{x_c^2}{D t_c} = 1 + 2\left(\frac{\dot{\gamma} D^2}{u_0^3}\right)^2 \frac{u_0^2}{D^2} = 1 + 2\frac{\dot{\gamma}^2 D^2}{u_0^4}$$

obtained from method of moments.

In any event, we can simulate the dispersion!

Our Dimensionless eq'n is:

$$\frac{\partial c^*}{\partial t^*} + y^* \frac{\partial c^*}{\partial x^*} - \frac{\partial c^*}{\partial y^*} = \frac{\partial^2 c^*}{\partial y^{*2}}$$

Initially our distribution in the y direction is e^{-y^*}

We can get this by placing tracers s.t. $y = -\log(\text{rand}(n,1))$

At each time step we displace in the y direction $-dt^*$ and a random step $(2dt^*)^{1/2}\,\text{randn}(n,1)$. We integrate the velocity in the x direction and the dimensionless scaled dispersivity is just half the growth in the variance:

$$\sigma^{*2} \sim 2\, t^* \kappa^*$$

where $\kappa^* = \dfrac{\kappa}{\dfrac{\dot{\gamma}^2 D^3}{u_0^4}} = 2$

Thus σ^{*2} should increase as $4t^*$ at long times (e.g., in the Taylor limit).

What if we have a second species s.t. $D_2/D \equiv D_2^*$. We can simulate this by adding a random step $(2D_2^* dt^*)^{1/2}$ at each time. Our initial dist. should be

$$y^* = -D_2^* \log(\text{rand}(n,1)) \text{ as well.}$$

The two peaks should separate w/ velocity $D_2^* - 1$. If $D_2^* - 1$ is small then the variances should be similar.

Decent ~~[illegible]~~ separation would occur when

$$(D_2^* - 1)t^* > 4\,(4t^*)^{1/2}$$

$$\text{or} \quad t^{*1/2} > \frac{8}{D_2^* - 1} \quad \therefore t^* > \frac{64}{(D_2^* - 1)^2}$$

this is a pretty long time... (~~[illegible]~~ this!..)

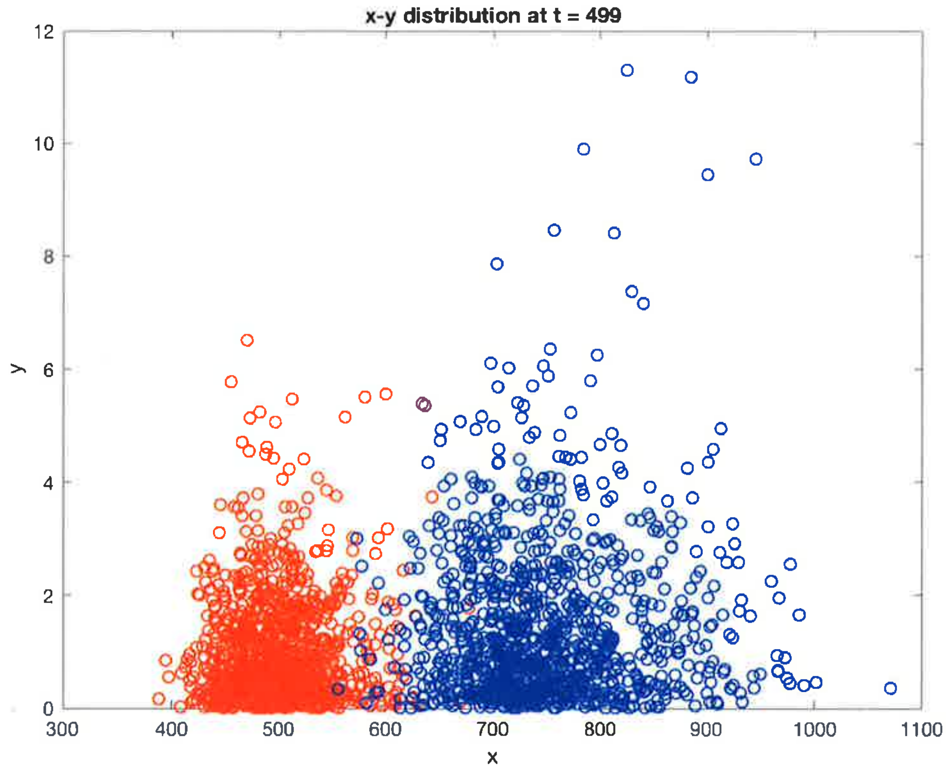
Contents

POD 23: MC Simulation of Taylor Dispersion in AF4

We construct a simple Monte Carlo simulation of dispersion in a asymmetric flow field flow fractionation device. The distribution is exponential in y, and there is a simple shear flow in the x direction. We add in a second species to see separation based on the diffusivity.

```
n= 1000;

Dastar = 1.5; % A second species with a different diffusivity.
% We distribute them randomly.

y = -log(rand(n,1));
x = zeros(n,1);

ya = -Dastar*log(rand(n,1));
xa = zeros(n,1);

dt = 0.001; %Our time step
tquit = 500;
t = [dt:dt:tquit]'; %Our times

ux = @(y) y; %our velocity profile

varx = zeros(1/dt,1); %we keep track of the variance.
varxa = zeros(1/dt,1); %we keep track of the variance.

for i=1:tquit/dt-1
    dx1 = ux(y);
    y = y - dt+ randn(n,1)*(2*dt)^.5; %Updating y
    y = abs(y); %Reflection from the accumulating wall
    dx2 = ux(y);
    x = x + (dx1+dx2)/2*dt; %We update the velocity

    varx(i) = var(x);

    % Now we repeat for the second type of particle.

    dxa1 = ux(ya);
    ya = ya - dt+ randn(n,1)*(2*Dastar*dt)^.5;
    ya = abs(ya);
    dxa2 = ux(ya);
    xa = xa + (dxa1+dxa2)/2*dt; %We update the velocity

    varxa(i) = var(xa);

    % We plot up the distributions every thousand iterations.
    if i/1000==round(i/1000)
      figure(1)
      plot(x,y,'or',xa,ya,'ob')
      xlabel('x')
      ylabel('y')
      title(['x-y distribution at t = ',num2str(t(i))])
```

```
      drawnow
    end

end

figure(2)
plot(t(1:i),varx(1:i),'r',t(1:i),varxa(1:i),'b')
xlabel('t')
ylabel('x variance')
title('variance in the x direction')
legend('unit diffusivity',['diffusivity = ',num2str(Dastar)])

figure(3)
histogram([x,xa])
xlabel('x')
ylabel('frequency')
title(['Particle Locations at t = ',num2str(tquit)])
```


x-y distribution at t = 499
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x
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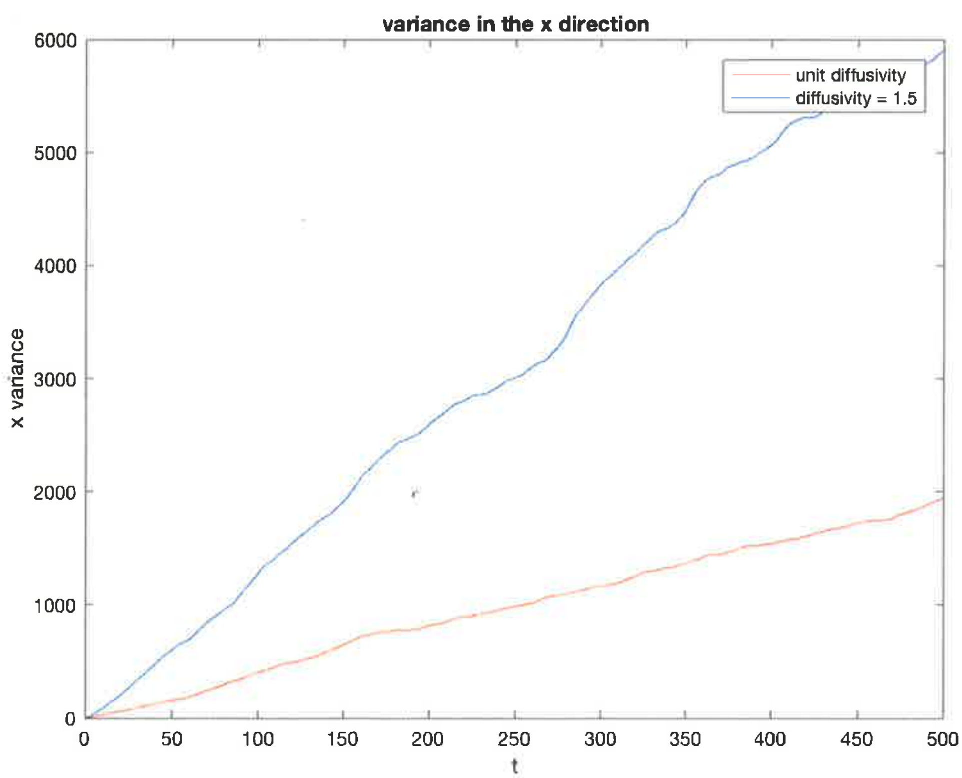
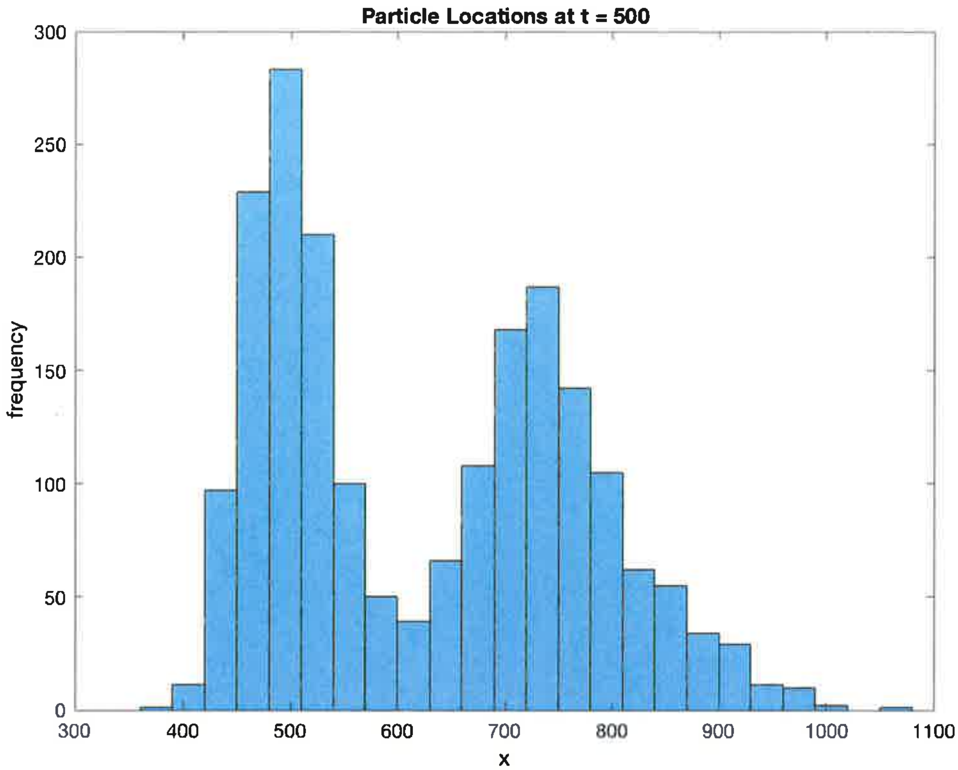
2
4
6
8
10
12
300
400
500
600
700
800
900
1000
1100


variance in the x direction
unit diffusivity
diffusivity = 1.5
x variance
t
0
1000
2000
3000
4000
5000
6000
0
50
100
150
200
250
300
350
400
450
500



Conclusion

As can be seen, the variance of the distribution with the higher diffusivity is much larger (going as D^3). This actually degrades the separation significantly requiring a greater simulation time for complete separation. The scalings are correct, however. There is also considerable skewness to the distributions resulting from the shear flow.

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