Conditional moment closure model

The full equations that govern $F + O \to P$ are

$$\frac{\partial Y_F}{\partial t} = D\nabla^2 Y_F - (u\cdot\nabla)Y_F - A Y_F Y_O$$

$$\frac{\partial Y_O}{\partial t} = D\nabla^2 Y_O - (u\cdot\nabla)Y_O - rA Y_F Y_O$$

If we evolve a z-scalar by

$$\frac{\partial z}{\partial t} = D\nabla^2 z - (u\cdot\nabla) z$$

and initialize z appropriately then $z = \dfrac{rY_F - Y_O + Y_{O,\emptyset}}{rY_{F,\emptyset} + Y_{O,\emptyset}}$

If we assume that $Y_{O,\emptyset} = Y_{F,\emptyset} = 1$ then:

$$z = \frac{rY_F - Y_O + 1}{r+1}$$

Now define $Q_F(n,t) = \langle Y_F \mid z = n \rangle_t$

$Q_O(n,t) = \langle Y_O \mid z = n \rangle_t$

⇝ conditional averages of Y_F, Y_O for $z = n$ at time t.

The actual values $Y_F(\vec{x},t)$ are distributed around $Q_F(z(\vec{x},t),t)$ with a "small" deviation. We write then:

$$Y_F(\vec{x},t) = Q_F(z(\vec{x},t),t) + y_F(\vec{x},t)$$

$$Y_O(\vec{x},t) = Q_O(z(\vec{x},t),t) + y_O(\vec{x},t).$$

The CMC model wants to describe the behaviour of Q_F and Q_O. To do that we substitute these equations to the full PDEs for Y_F and Y_O.

$$\frac{\partial Y_F}{\partial t} = \frac{\partial y_F}{\partial t} + \frac{\partial Q_F}{\partial z}\frac{\partial z}{\partial t} + \frac{\partial Q_F}{\partial t}$$

$$\frac{\partial Y_O}{\partial t} = \frac{\partial y_O}{\partial t} + \frac{\partial Q_O}{\partial z}\frac{\partial z}{\partial t} + \frac{\partial Q_O}{\partial t}.$$

Also, for x, y, z derivatives:

$$\frac{\partial Y_F}{\partial x} = \frac{\partial y_F}{\partial x} + \frac{\partial Q_F}{\partial z}\frac{\partial z}{\partial x}$$

$$\frac{\partial Y_F}{\partial y} = \frac{\partial y_F}{\partial y} + \frac{\partial Q_F}{\partial z}\frac{\partial z}{\partial y}.$$

$$\frac{\partial Y_F}{\partial z} = \frac{\partial y_F}{\partial z} + \frac{\partial Q_F}{\partial z}\frac{\partial z}{\partial z}$$

In vector notation:

$$\nabla Y_F = \nabla y_F + \frac{\partial Q_F}{\partial z}\nabla z \qquad \text{and} \qquad \nabla Y_O = \nabla y_O + \frac{\partial Q_O}{\partial z}\nabla z .$$

For second derivatives:

$$\frac{\partial^2 Y_F}{\partial x^2} = \frac{\partial^2 y_F}{\partial x^2} + \frac{\partial}{\partial x}\left(\frac{\partial Q_F}{\partial z}\frac{\partial z}{\partial x}\right) =$$

$$= \frac{\partial^2 y_F}{\partial x^2} + \frac{\partial^2 z}{\partial x^2}\frac{\partial Q_F}{\partial z} + \frac{\partial z}{\partial x}\frac{\partial}{\partial x}\left(\frac{\partial Q_F}{\partial z}\right) =$$

$$= \frac{\partial^2 y_F}{\partial x^2} + \frac{\partial^2 z}{\partial x^2}\frac{\partial Q_F}{\partial z} + \left(\frac{\partial z}{\partial x}\right)^2 \frac{\partial^2 Q_F}{\partial z^2} .$$

and likewize for the y, z derivatives. Then:

$$\nabla^2 Y_F = \nabla^2 y_F + \frac{\partial Q_F}{\partial z}\nabla^2 z + (\nabla z \cdot \nabla z)\frac{\partial^2 Q_F}{\partial z^2} .$$

$$\nabla^2 Y_O = \nabla^2 y_O + \frac{\partial Q_F}{\partial z}\nabla^2 z + (\nabla z \cdot \nabla z)\frac{\partial^2 Q_F}{\partial z^2} .$$

To obtain the CMC equations compare

$$\frac{\partial Y_F}{\partial t} = \frac{\partial y_F}{\partial t} + \frac{\partial Q_F}{\partial z}\frac{\partial z}{\partial t} + \frac{\partial Q_F}{\partial t}$$

$$\frac{\partial Y_F}{\partial t} = D\nabla^2 Y_F - (u\cdot\nabla)Y_F - A Y_F Y_O$$

using the substitutions:

$$\frac{\partial z}{\partial t} = D\nabla^2 z - (u\cdot\nabla) z$$

$$\nabla^2 Y_F = \nabla^2 y_F + \frac{\partial Q_F}{\partial z}\nabla^2 z + \frac{\partial^2 Q_F}{\partial z^2}(\nabla z \cdot \nabla z).$$

$$(u\cdot\nabla)Y_F = \frac{\partial Q_F}{\partial z}(u\cdot\nabla)z + (u\cdot\nabla)y_F .$$

If we do that we obtain:

$$\frac{\partial y_F}{\partial t} + \frac{\partial Q_F}{\partial z}\left(\cancel{D\nabla^2 z} - \cancel{(u\cdot\nabla)z}\right) + \frac{\partial Q_F}{\partial t} = D\left[\nabla^2 y_F + \cancel{\frac{\partial Q_F}{\partial z}\nabla^2 z} + \frac{\partial^2 Q_F}{\partial z^2}(\nabla z\cdot\nabla z)\right]$$

$$- \left[\frac{\partial Q_F}{\partial z}\cancel{(u\cdot\nabla)z} + (u\cdot\nabla)y_F\right] - A(Q_F + y_F)(Q_O + y_O).$$

$$\frac{\partial y_F}{\partial t} + \frac{\partial Q_F}{\partial t} = \left[D\nabla^2 y_F - (u\cdot\nabla)y_F - A(Q_F + y_F)y_O - A(Q_O + y_O)y_F\right]$$

$$+ D(\nabla z\cdot\nabla z)\frac{\partial^2 Q_F}{\partial z^2} - A Q_F Q_O .$$

Define the conditional dissipation $N(\vec{x},t) = D(\nabla Z \cdot \nabla Z)$.
and define the conditional average:
~~$N(\vec{x},t)$~~

$$\tilde{N}(\eta) = \langle N \mid Z = \eta \rangle.$$

and expand

$$N(\vec{x},t) = \tilde{N}(Z(\vec{x},t)) + \eta(\vec{x},t).$$

Then the CMC equation becomes:

$$\cancel{\frac{\partial y_F}{\partial t} + \frac{\partial Q_F}{\partial t} = (N+\eta)\frac{\partial^2 Q_F}{\partial Z^2} - AQ_F Q_0 + [D\nabla^2 y_F - (u\nabla)y_F - A(Q_F + y_F)y.}$$

$$\frac{\partial y_F}{\partial t} + \frac{\partial Q_F}{\partial t} = (\tilde{N}+\eta)\frac{\partial^2 Q_F}{\partial Z^2} - AQ_F Q_0 + [D\nabla^2 y_F - (u\cdot\nabla)y_F - 2Ay_F y_0 - A(Q_F y_0 + Q_0 y$$

This is an equation true to every point of our volume.
If we take a conditional average accross the volume on Z then those quantities that are indepedent of $\vec{x} = (x,y,z)$ will remain invariant. So:

$$\langle \frac{\partial Q_F}{\partial t} \mid Z \rangle = \frac{\partial Q_F}{\partial t}$$

$$\langle \tilde{N} \frac{\partial^2 Q_F}{\partial Z^2} \mid Z \rangle = \tilde{N} \frac{\partial^2 Q_F}{\partial Z^2}$$

$$\langle A Q_F Q_0 \mid Z \rangle = A Q_F Q_0$$

A few other quantities will vanish:

$$\langle \frac{\partial y_F}{\partial t} \mid Z \rangle = \frac{\partial}{\partial t} \langle y_F \mid Z \rangle = 0$$

$$\langle \eta \frac{\partial^2 Q_F}{\partial Z^2} \mid Z \rangle = \frac{\partial^2 Q_F}{\partial Z^2} \langle \eta \mid Z \rangle = 0$$

$$\langle A(Q_F y_0 + Q_0 y_F) \mid Z \rangle = AQ_F \langle y_0 \mid Z \rangle + AQ_0 \langle y_F \mid Z \rangle = 0 + 0 = 0$$

and a few others will not vanish:

$$\langle \nabla^2 y_F \mid Z \rangle, \quad \langle (u\cdot\nabla) y_F \mid Z \rangle, \quad \langle y_F y_0 \mid Z \rangle.$$

It follows that:

$$\frac{\partial Q_F}{\partial t} = \tilde{N} \frac{\partial^2 Q_F}{\partial Z^2} - AQ_F Q_0 + \langle D\nabla^2 y_F - (u\cdot\nabla) y_F - 2Ay_F y_0 \mid Z \rangle$$

In a similar manner we obtain:

$$\frac{\partial Q_0}{\partial t} = \tilde{N} \frac{\partial^2 Q_0}{\partial Z^2} - rAQ_F Q_0 + \langle D\nabla^2 y_0 - (u\cdot\nabla) y_0 - 2Ay_F y_0 \mid Z \rangle.$$

A critical assumption here is that the conditional average terms are negligible. Then we obtain:

$$\boxed{\begin{aligned}\frac{\partial Q_F}{\partial t} &= \tilde{N}(z)\frac{\partial^2 Q_F}{\partial z^2} - A Q_F Q_0 \\ \frac{\partial Q_0}{\partial t} &= \tilde{N}(z)\frac{\partial^2 Q_0}{\partial z^2} - rA Q_F Q_0\end{aligned}}$$

The critical assumption is that

$$\varepsilon_F(n,t) = \langle D\nabla^2 y_F - (u\cdot\nabla)y_F - 2Ay_F y_0 \,|\, z = n\rangle_t$$

and

$$\varepsilon_0(n,t) = \langle D\nabla^2 y_0 - (u\cdot\nabla)y_0 - 2Ary_F y_0 \,|\, z = n\rangle_t$$

are negligible. This should be verified numerically.

<u>Boundary conditions</u>

These equations are valid for $0 \leq z \leq 1$, therefore we need boundary conditions for

$$Q_F(0,t) = \langle Y_F \,|\, z = 0\rangle$$
$$Q_F(1,t) = \langle Y_F \,|\, z = 1\rangle$$

and

$$Q_0(0,t) = \langle Y_F \,|\, z = 0\rangle \quad , \quad Q_0(1,t) = \langle Y_F \,|\, z = 1\rangle$$

Recall that

$$z = \frac{rY_F - Y_0 + 1}{r+1}$$

and $0 \leq Y_F \leq 1$ and $0 \leq Y_0 \leq 1$

a) Suppose that $z = 0$. Then

$$\frac{rY_F - Y_0 + 1}{r+1} = 0 \Leftrightarrow Y_0 = rY_F + 1.$$

$$\left.\begin{array}{l} Y_0 \leq 1 \Rightarrow rY_F + 1 \leq 1 \Rightarrow Y_F \leq 0. \\ \text{Moreover } \ Y_F \geq 0 \end{array}\right\} \Rightarrow Y_F = 0.$$

and $Y_0 = r\cdot 0 + 1 = 1$.

Therefore $(z = 0 \Rightarrow Y_F = 0 \wedge Y_0 = 1) \Rightarrow \begin{cases} Q_F(0,t) = 0 \\ Q_0(0,t) = 1. \end{cases}$

b) Suppose that $Z=0$. Then,

$$\frac{rY_F - Y_O + 1}{r+1} = 1 \Leftrightarrow rY_F - Y_O = r \Leftrightarrow \underline{Y_O = r(Y_F - 1)}$$

$$\left.\begin{array}{l} Y_F \leq 1 \Rightarrow Y_O = r(Y_F - 1) \leq 0 \\ \quad \text{but also } \; Y_O \geq 0 \end{array}\right\} \Rightarrow Y_O = 0.$$

It follows that $r(Y_F - 1) = 0 \Leftrightarrow Y_F = 1$.

Therefore $(Z = 1 \Rightarrow Y_F = 1 \wedge Y_O = 0) \Rightarrow \left\{\begin{array}{l} Q_F(0,t) = 1 \\ Q_O(1,t) = 0 \end{array}\right.$

We obtain then the following boundary conditions:

$$Q_F(0,t) = 0 \qquad \text{and} \qquad Q_O(0,t) = 1$$
$$Q_F(1,t) = 1 \qquad \qquad \qquad Q_O(1,t) = 0.$$

Remark.

If we solve the equation

$$\frac{\partial Z}{\partial t} + (u \cdot \nabla) Z = D \nabla^2 Z$$

for "counterflow" we obtain

$$\tilde{N}(Z) = N_0 \exp\left\{-2\left[\operatorname{erf}^{-1}(2Z-1)\right]^2\right\}$$

What does this mean?

Derivation of the product CMC equation.

The CMC equation for fuel + oxidizer is:

$$\frac{\partial Q_F}{\partial t} = \tilde{N}(z,t)\frac{\partial^2 Q_F}{\partial z^2} - A Q_F Q_o$$

$$\frac{\partial Q_o}{\partial t} = \tilde{N}(z,t)\frac{\partial^2 Q_o}{\partial z^2} - rA Q_F Q_o$$

where $Q_F(n,t) = \langle Y_F | z = n \rangle_t$ $\quad \tilde{N}(z,t) = \langle N | z = n \rangle_t$

$Q_o(n,t) = \langle Y_o | z = n \rangle_t$

with boundary conditions

$Q_F(0,t) = 0 \qquad Q_o(0,t) = 1$

$Q_F(1,t) = 1 \qquad Q_o(1,t) = 0$

Fact 1 : Q_F, Q_o are related by $\frac{rQ_F - Q_o + 1}{r+1} = z$.

Solve for $Q_o = rQ_F + 1 - (r+1)z$

Fact 2 : The conditional average of the product is

$Q_P = 1 - Q_F - Q_o$

We express Q_F, Q_o in terms of Q_P:

$$Q_F + Q_o = 1 - Q_P \Leftrightarrow Q_F + rQ_F + 1 - (r+1)z = 1 - Q_P \Leftrightarrow$$

$$\Leftrightarrow (r+1)Q_F + \cancel{1} - (r+1)z = \cancel{1} - Q_P \Leftrightarrow$$

$$\Leftrightarrow (r+1)Q_F = (r+1)z - Q_P \Leftrightarrow \boxed{Q_F = z - \frac{Q_P}{r+1}}$$

and

$$Q_o = rQ_F + 1 - (r+1)z = r\left[z - \frac{Q_P}{r+1}\right] + 1 - (r+1)z =$$

$$= \cancel{rz} - \frac{rQ_P}{r+1} + 1 - \cancel{rz} - z =$$

$$= (1-z) - \frac{rQ_P}{r+1}$$

Putting these together:

$$\boxed{Q_F = z - \frac{Q_P}{r+1}} \qquad \boxed{Q_o = (1-z) - \frac{rQ_P}{r+1}.}$$

To rewrite in terms of Z_{st} use $\frac{1}{r+1} = Z_{st}$ and $r = \frac{1-Z_{st}}{Z_{st}}$

$$\boxed{\begin{aligned} Q_F &= Z - Z_{st}\, Q_P \\ Q_O &= (1-Z) - (1-Z_{st})\, Q_P. \end{aligned}}$$

Now note that

$$\frac{\partial Q_F}{\partial t} = -Z_{st} \frac{\partial Q_P}{\partial t}$$

and $$\frac{\partial^2 Q_F}{\partial Z^2} = \frac{\partial^2}{\partial Z^2}\left[Z - Z_{st}\, Q_P\right] = -Z_{st} \frac{\partial^2 Q_P}{\partial Z^2}.$$

We substitute to the CMC equation for the fuel:

$$\frac{\partial Q_F}{\partial t} - \tilde{N} \frac{\partial^2 Q_F}{\partial Z^2} = \dot{w}_F \Leftrightarrow$$

$$\Leftrightarrow -Z_{st}\left[\frac{\partial Q_P}{\partial t} - \tilde{N} \frac{\partial^2 Q_P}{\partial Z^2}\right] = \dot{w}_F$$

$$\Leftrightarrow \frac{\partial Q_P}{\partial t} = \tilde{N} \frac{\partial^2 Q_P}{\partial Z^2} - \frac{\dot{w}_F}{Z_{st}}$$

where $\dot{w}_F = -A\, Q_F Q_O = -A\left(Z - Z_{st} Q_P\right)\left[(1-Z) - (1-Z_{st}) Q_P\right]$.

It follows that

$$\boxed{\frac{\partial Q_P}{\partial t} = \tilde{N} \frac{\partial^2 Q_P}{\partial Z^2} + \dot{w}_P}$$

where $\dot{w}_P = +\frac{A}{Z_{st}}\left(Z - Z_{st} Q_P\right)\left[(1-Z) - (1-Z_{st}) Q_P\right]$

Numerical solution of the CMC equation

We want solver for problems of the form

$$\frac{\partial u}{\partial t} = b(x,t)\frac{\partial^2 u}{\partial x^2} + w(x,t,u) \quad , x \in [a_0, a_1].$$

with Dirichlet boundary conditions.
Use a split scheme
- diffusion term $\longrightarrow$ Crank-Nicolson scheme
- inhomogeneity $\longrightarrow$ Runge-kutta

Let $x_m = a_0 + (a_1 - a_2)m/M = a_0 + (a_1 - a_0)hm$

$u_m^n = u(x_m, nk)$

$b_m^n = b(x_m, nk)$ where $h = 1/M$

$w_m^n = w(x_m, nk, u_m^n)$. k = timestep.

Also define $\mu = k/h^2$

Crank-Nicolson step

$$A_m^n u_{m-1}^{n+1} + B_m^n u_m^{n+1} + C_m^n u_{m+1}^{n+1} = D_m^n \quad , \forall m \in \{1, 2, \dots, M-1\}$$

where

$$A_m^n = -b_m^n \mu/2 \quad , \forall m \in \{2, \dots, M-1\}$$
$$B_m^n = 1 + b_m^n \mu \quad , \forall m \in \{1, \dots, M-1\}$$
$$C_m^n = -b_m^n \mu/2 \quad , \forall m \in \{1, \dots, M-2\}$$

~~Taking boundary conditions~~

$$D_m^n = u_m^n + \frac{1}{2} b_m^n \mu \left(u_{m-1}^n - 2u_m^n + u_{m+1}^n\right).$$

Taking boundary conditions into account:

$$\begin{bmatrix} B_1^n & C_1^n & 0 & 0 & 0 \\ A_2^n & B_2^n & C_2^n & 0 & 0 \\ 0 & A_m^n & B_m^n & C_m^n & 0 \\ 0 & 0 & A_{M-2}^n & B_{M-2}^n & C_{M-2}^n \\ 0 & 0 & 0 & A_{M-1}^n & B_{M-1}^n \end{bmatrix} \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ u_m^{n+1} \\ u_{M-2}^{n+1} \\ u_{M-1}^{n+1} \end{bmatrix} = \begin{bmatrix} D_1^n - u_0^n A_1^n \\ D_2^n \\ D_m^n \\ D_{M-2}^n \\ D_{M-1}^n - u_M^n C_{M-1}^n \end{bmatrix}$$

To solve the tridiagonal system with Thomas algorithm the matrix must be diagonally dominant.

$$|B_m^n| \geqslant |A_m^n| + |C_m^n| \Leftrightarrow |1+b_m^n\mu| \geqslant |-b_m^n\mu/2| + |-b_m^n\mu/2| \Leftrightarrow$$

$$\Leftrightarrow |1+b_m^n\mu| \geqslant |b_m^n\mu| \Leftrightarrow (1+b_m^n\mu)^2 \geqslant (b_m^n\mu)^2 \Leftrightarrow 1+2b_m^n\mu \geqslant 0$$

$$\Leftrightarrow b_m^n\mu \geqslant -\frac{1}{2}.$$

The requirement will be true if $b(x,t) \geqslant 0$ as it is expected in a parabolic system.

- <u>Runge-kutta step for the inhomogeneity.</u>

Define:
$$\begin{aligned}
K_1 &= k\,w(x_m, nk, u_m^n)\\
K_2 &= k\,w(x_m + h/2, nk, u_m^n + K_1/2)\\
K_3 &= k\,w(x_m + h/2, nk, u_m^n + K_2/2)\\
K_4 &= k\,w(x_m + h, nk, u_m^n + K_3).
\end{aligned}$$

and then:
$$u_m^{n+1} = u_m^n + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4).$$

Test cases

To test the reliability of the solver one can use the following test cases:

a) Simple diffusion:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad \text{with} \quad u(x,0) = \sin(2\pi x) \quad , \forall x \in [0,1]$$

has solution $u(x,t) = \sin(2\pi x)e^{-4\pi^2 t}$

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - u \quad \text{with} \quad u(x,0) = \sin(2\pi x) \quad , \forall x \in [0,1]$$

has solution $u(x,t) = \sin(2\pi x)e^{-(4\pi^2+1)t}$

b) Diffusion with variable diffusion coefficient

i) $$\frac{\partial u}{\partial t} = x(1-x)\frac{\partial^2 u}{\partial x^2} \quad \text{with} \quad u(x,0) = x(1-x)$$

has solution $u(x,t) = x(1-x)e^{-2t}$

$$\frac{\partial u}{\partial t} = x(1-x)\frac{\partial^2 u}{\partial x^2} + (2-\lambda)u \quad \text{with} \quad u(x,0) = x(1-x)$$

has solution $u(x,t) = x(1-x)e^{-\lambda t}$

$$\frac{\partial u}{\partial t} = x(1-x)\frac{\partial^2 u}{\partial x^2} + [x(1-x) + u]$$

has solution $u(x,t) = x(1-x)(1-e^{-t})$

c) The boundary value problem:

$$x(1-x)\frac{\partial^2 u}{\partial x^2} = x(1-x) + u$$

with $u(0) = u(1) = 0$

has solution $u(x) = x(1-x)$.

Counterflow problem

Suppose that $\vec{u} = (u, v, w)$ is given by

$$u = ax \;,\; v = -ay \;,\; w = 0$$

and that at $t = 0$

$$z(x, y, t=0) = \begin{cases} 0 & y > 0 \\ 1 & y < 0 \end{cases}$$

The evolution equation for z is:

$$\frac{\partial z}{\partial t} + (u \cdot \nabla) z - D \nabla^2 z = 0 \Leftrightarrow$$

$$\Leftrightarrow \frac{\partial z}{\partial t} + ax \frac{\partial z}{\partial x} - ay \frac{\partial z}{\partial y} - D\left(\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2}\right) = 0$$

Suppose we ignore the x dependence. Then:

$$\boxed{\frac{\partial z}{\partial t} - ay \frac{\partial z}{\partial y} - D \frac{\partial^2 z}{\partial y^2} = 0.}$$

with boundary condition $z(y, 0) = \begin{cases} 0 & y > 0 \\ 1 & y < 0 \end{cases}$

and $z(+\infty, t) = 1$, $z(-\infty, t) = 0$.

$$N(y, t) = D(\nabla z \cdot \nabla z) = D\left(\frac{\partial z}{\partial y}\right)^2$$

To solve the PDE let

$$z(y, t) = c_1 + c_2 \operatorname{erf}\left(\frac{y}{\delta(t)}\right)$$

where $\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \rightsquigarrow$ error function.

Note that $\frac{d}{dx} \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \frac{d}{dx} \int_0^x e^{-t^2} dt = \frac{2 e^{-x^2}}{\sqrt{\pi}}$

It follows that

$$\frac{\partial z}{\partial t} = c_2 \frac{\partial}{\partial t} \operatorname{erf}\left(\frac{y}{\delta(t)}\right) = c_2 \frac{2}{\sqrt{\pi}} \exp\left(-\frac{y^2}{\delta^2(t)}\right) \frac{\partial}{\partial t}\left(\frac{y}{\delta(t)}\right) =$$

$$= \frac{2c_2}{\sqrt{\pi}} e^{-y^2/\delta^2} \frac{-y}{\delta^2(t)} \frac{d\delta}{dt}$$

and

$$\frac{\partial z}{\partial y} = c_2 \frac{\partial}{\partial y} \operatorname{erf}\left(\frac{y}{\delta(t)}\right) = c_2 \frac{2}{\sqrt{\pi}} \exp\left(-\frac{y^2}{\delta^2(t)}\right) \frac{\partial}{\partial t}\left(\frac{y}{\delta(t)}\right) =$$

$$= \frac{2c_2}{\sqrt{\pi}} e^{-y^2/\delta^2} \frac{1}{\delta(t)}$$

$$\frac{\partial^2 z}{\partial y^2} = \frac{2c_2}{\delta(t)\sqrt{\pi}} e^{-y^2/\delta^2} \frac{-2y}{\delta^2(t)}.$$

To summarize:

$$\frac{\partial z}{\partial t} = \left[\frac{2c_2}{\sqrt{\pi}} e^{-y^2/\delta^2}\right] \frac{-y}{\delta^2(t)} \frac{d\delta}{dt}$$

$$\frac{\partial z}{\partial y} = \left[\frac{2c_2}{\sqrt{\pi}} e^{-y^2/\delta^2}\right] \frac{1}{\delta(t)}$$

$$\frac{\partial^2 z}{\partial y^2} = \left[\frac{2c_2}{\sqrt{\pi}} e^{-y^2/\delta^2}\right] \frac{-2y}{\delta^3(t)}.$$

Substituting to the PDE we obtain:

$$\frac{\partial z}{\partial t} - ay\frac{\partial z}{\partial y} - D\frac{\partial^2 z}{\partial y^2} = 0 \Leftrightarrow$$

$$-\frac{y}{\delta^2(t)} \frac{d\delta}{dt} - \frac{ay}{\delta(t)} + D\frac{2y}{\delta^3(t)} = 0 \Leftrightarrow$$

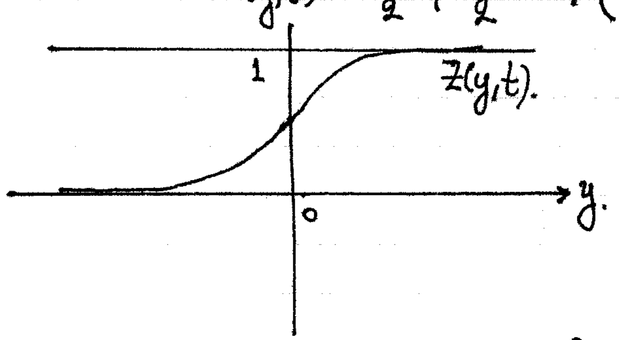
$$\frac{1}{\delta^2}\frac{d\delta}{dt} = \frac{2D}{\delta^3} - \frac{a}{\delta} \Leftrightarrow 2\delta\frac{d\delta}{dt} = 4D - 2a\delta^2 \Leftrightarrow$$

$$\Leftrightarrow \frac{d\delta^2}{dt} = 4D - 2a\delta^2.$$

Note that this works even when a is time depedent.

For the case $z_{st} = 0.5$

$$z(y,t) = \frac{1}{2} + \frac{1}{2}\operatorname{erf}\left(\frac{y}{\delta(t)}\right).$$



Solving for y/δ: $2z = 1 + \operatorname{erf}(y/\delta) \Leftrightarrow \operatorname{erf}(y/\delta) = 1 - 2z \Leftrightarrow y/\delta = \operatorname{erf}^{-1}(1-2$

$$\Leftrightarrow y/\delta = \operatorname{inverf}(1-2z).$$

Solving for y/δ: $2z = 1 + \mathrm{erf}(y/\delta) \Leftrightarrow \mathrm{erf}(y/\delta) = 2z - 1 \Leftrightarrow$
$\Leftrightarrow y/\delta = \mathrm{inverf}(2z-1)$

$$N(y,t) = D(\nabla z \cdot \nabla z) = D\left(\frac{\partial z}{\partial y}\right)^2 = D\left[\frac{1}{2}\frac{\partial}{\partial y}\mathrm{erf}\left(\frac{y}{\delta(t)}\right)\right]^2 =$$
$$= D\left[\frac{1}{2}\frac{2}{\sqrt{\pi}}\exp\left(-\frac{y^2}{\delta^2(t)}\right)\frac{1}{\delta(t)}\right]^2 =$$
$$= D\left(\frac{1}{\delta(t)\sqrt{\pi}}\right)^2 \exp(-2y^2/\delta^2) =$$
$$= N_o(t)\exp(-2\,\mathrm{inverf}^2(2z-1)) = \tilde{N}(z,t) \Rightarrow$$
$$\Rightarrow \boxed{\langle N|z\rangle_t = N_o(t)\exp[-2\,\mathrm{inverf}^2(2z-1)].}$$

What about $\delta(t)$ and $N_o(t)$?
Let's solve:
$$\frac{d\delta^2}{dt} = 4D - 2a(t)\delta^2. \Leftrightarrow \frac{d\delta^2}{dt} + 2a(t)\delta^2 = 4D.$$
Homogeneous solution:
$$\frac{d\delta_o^2}{dt} = -2a(t)\delta_o^2 \Leftrightarrow \frac{1}{\delta_o^2}\frac{d\delta_o^2}{dt} = -2a(t) \Leftrightarrow$$
$$\Leftrightarrow \ln\delta_o^2 = -2\int a(t)dt \Leftrightarrow \delta_o^2 = \delta_o^2(0)\exp\left[-2\int_0^t a(t)\,dt\right]$$
Particular solution: $\delta_p(t) = 4Dt$ therefore:
$$\delta^2(t) = \delta_o^2\exp\left[-2\int_0^t a(t)\,dt\right] + 4Dt \Leftrightarrow \delta(t) \sim 2\sqrt{Dt}$$
and $N_o(t) \sim \dfrac{a}{t} \sim$ indepedent of D.

Investigation of depedence of CMC on boundary conditions.

We want to investigate the behaviour of the product CMC equation and its dependence on $N(z,t)$ and boundary condition.

The equation:

$$\frac{\partial Q_P}{\partial t} = \tilde{N}(z,t)\frac{\partial^2 Q_P}{\partial z^2} + \frac{A}{z_{st}}(z - z_{st}Q_P)[(1-z)-(1-z_{st})Q_P].$$

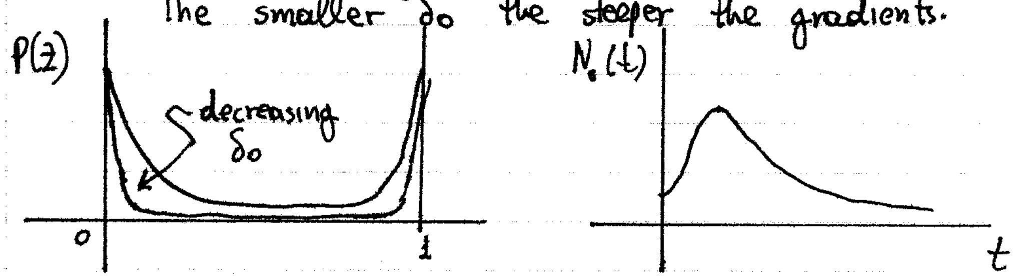
We can model $\tilde{N}(z,t)$ with counterflow:

$$\tilde{N}(z,t) = \exp[-2\,\mathrm{inverf}^2(2z-1)]\,N_0(t).$$

where $N_0(t) = \dfrac{D}{\pi(\delta_0 e^{-2at} + 4Dt)}$

The modeling parameters are δ_0 and a and their interpretation is the following:

δ_0 = the steepness of the ∇z gradient in the 1 regions to the 0 region in the initial condition. The smaller δ_0 the steeper the gradients.



a = increases as the velocity field becomes more turbulent. i.e. increases as the Reynolds number increases.

For the counterflow problem the characteristic scales are:

$u = al$, l = something and $v = D$

therefore the Reynolds number is:

$$Re = \frac{ul}{v} = \frac{al^2}{v}$$

- The meaning of a.

Note that a controls the peak of $N_0(t)$.

$$\frac{\partial N_0(t)}{\partial t} = \frac{D}{\pi}\frac{\partial}{\partial t}\left(\frac{1}{\delta_0 e^{-2at}+4Dt}\right) = \frac{D}{\pi}\,\frac{-(4D-2a\delta_0 e^{-2at})}{(\delta_0 e^{-2at}+4Dt)^2} = 0$$

$$\Leftrightarrow 2a\delta_0 e^{-2at_0} = 4D \Leftrightarrow e^{-2at_0} = \frac{2D}{a\delta_0} \Leftrightarrow$$

$$\Leftrightarrow -2at_0 = \ln\frac{2D}{a\delta_0} \Leftrightarrow \boxed{t_0 = \frac{1}{2a}\ln\frac{a\delta_0}{2D}}$$

The peak value is:

$$4D = 2a\delta_0 e^{-2at} \Rightarrow N_{max} = \frac{D}{\pi(\delta_0 e^{-2at_0}+4Dt_0)} =$$

$$= \frac{D}{\pi\left(\frac{4D}{2a}+4Dt_0\right)} = \frac{1}{\pi\left(\frac{2}{a}+4t_0\right)} =$$

$$= \left[\pi\left(\frac{2}{a}+\frac{1}{2a}\ln\frac{a\delta_0}{2D}\right)\right]^{-1} = \frac{a}{\pi}\left(2+\frac{1}{2}\ln\frac{a\delta_0}{2D}\right)^{-1}$$

$$= \frac{2a}{\pi\left(4+\ln\frac{a\delta_0}{2D}\right)}$$

therefore: $$\boxed{N_{max} = \frac{2a}{\pi\left(4+\ln\frac{a\delta_0}{2D}\right)}}$$

- <u>The meaning of δ_0.</u>

The initial counterflow field is given by:

$$\overset{o}{z}(y,t) = \frac{1}{2}+\frac{1}{2}\operatorname{erf}\left(\frac{y}{\delta_0}\right)$$

The slopes are given by:

$$\frac{\partial z}{\partial y} = \frac{1}{2}\frac{\partial}{\partial y}\operatorname{erf}\left(\frac{y_0}{\delta}\right) = \frac{1}{4\sqrt{\pi}}\exp\left(-\frac{y_0^2}{\delta_0^2}\right)\frac{1}{\delta_0} \Rightarrow$$

$$\Rightarrow \left.\frac{\partial z}{\partial y}\right|_{y=0} = \frac{1}{4\sqrt{\pi}\,\delta_0}$$ $\rightsquigarrow$ at $y=0$ we have maximum slope.

so $\delta_0 \sim 1/\text{slope} \sim 1/k_{max} \rightsquigarrow$
where k_{max} = max <u>integer</u> wavenumber.

- The investigation.

Define $\tilde{N}(z,t;\delta) = \begin{cases} \tilde{N}(z,t) & \text{if } z \in [\delta, 1-\delta]. \\ 0 & \text{otherwize.} \end{cases}$

Timestep CMC with $\tilde{N}(z,t) \rightsquigarrow$ treat this as an exact solution
Timestep CMC with $\tilde{N}(z,t;\delta) \rightsquigarrow$ compare max-norm error as $e(t)$ and find point in time t where the error is largest.

δ should control: maximum error e_{max}.
time where the error is largest.
These should also depend in changes in a and S_0.

e_{max} must also be checked against using $\langle N_t \rangle$.
as well as δ-truncated $\langle N \rangle$?

↳ effects on $Q_F(z,t)$, errors on $Q_F(z,t)$.
what about $\langle Y_F \rangle$?

Can $P(z,t,D)$ be known if it is known for $D=1$?

Sensitivity of counterflow CMC on behaviour of $N(z,t)$

The CMC equation we study is:

$$\frac{\partial Q_P}{\partial t} = N(z,t)\frac{\partial^2 Q_P}{\partial z^2} + \frac{A}{z_{st}}\left(z - z_{st} Q_P\right)\left[(1-z)-(1-z_{st})Q_P\right]$$

The counterflow model of $N(z,t)$ is:

$$N(z,t) = N_0(t)\exp\left[-2\,\mathrm{inverf}^2(2z-1)\right]$$

where $N_0(t)$ must be obtained by simulation runs with the corresponding $P(z,t)$.
Then the average $N_0(t)$ can be obtained from

$$\langle N\rangle_t = \int_0^1 N(z,t)\,P(z,t)\,dz = N_0(t)\int_0^1 \exp\left[-2\,\mathrm{inverf}^2(2z-1)\right]P(z,t)\,dz$$

Let $\sigma^2 = \langle z^2\rangle - \langle z\rangle^2$ be the varience of the z field.
It can be shown then that

$$\boxed{\frac{d\sigma^2}{dt} = -2\langle N\rangle_t}$$

In order for $P(z,t)$ and $N_0(t)$ to make physical sense together, they must respect the relationship above.
Moreover, $P(z,t)$ can be modeled by:

$$P(z,t) = \frac{z^{a(t)-1}(1-z)^{b(t)-1}}{B(a,b)}$$

where $a(t) = \mu\left[\frac{\mu(1-\mu)}{\sigma^2} - 1\right]$ with $\mu = \langle z\rangle$, $\sigma^2 = \langle z^2\rangle - \langle z\rangle^2$

$$b(t) = \frac{a}{\mu} - a$$

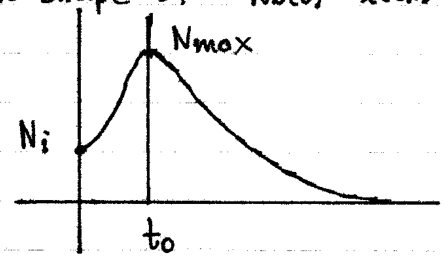
Note of course that $\frac{d\mu}{dt} = 0$ so time dependence enters only by the varience.

• Counterflow model for $N_o(t)$.

For the purposes of studying the CMC equation mathematically, we may use the expression for $N_o(t)$ obtained by the counterflow model:

$$\boxed{N_o(t) = \frac{D}{n\delta^2(t)}} \quad \text{where} \quad \boxed{\delta^2(t) = \delta_o^2 e^{-2at} + 4Dt}$$

The shape of $N_o(t)$ looks like this:



The characteristic values N_i, t_o, N_{max} depend on D, δ_o, a as follows:

a) N_i ~~dend~~pendence

$$N_i = N_o(0) = \frac{D}{n\delta^2(0)} = \frac{D}{n[\delta_o^2 e^0 + 0]} = \frac{D}{n\delta_o^2} \rightsquigarrow \text{not dependent on } a.$$

b) t_o dependence

Note that

$$\frac{\partial N_o}{\partial t} = \frac{D}{n}\frac{\partial}{\partial t}\left(\frac{1}{\delta^2(t)}\right) = \frac{-D}{n\delta^4(t)}\frac{\partial \delta^2(t)}{\partial t} = 0 \Leftrightarrow$$

$$\Leftrightarrow \frac{\partial \delta^2}{\partial t} = \frac{\partial}{\partial t}\left[\delta_o^2 e^{-2at} + 4Dt\right] = -2a\delta_o^2 e^{-2at} + 4D = 0 \Leftrightarrow$$

$$\Leftrightarrow e^{-2at} = \frac{4D}{2a\delta_o^2} = \frac{2D}{a\delta_o^2} \Leftrightarrow -2at = \ln\frac{2D}{a\delta_o^2} \Leftrightarrow 2at = \ln\frac{a\delta_o^2}{2D}$$

$$\Leftrightarrow t = \frac{1}{2a}\ln\frac{a\delta_o^2}{2D}$$

Therefore we find that $\boxed{t_o = \frac{1}{2a}\ln\frac{a\delta_o^2}{2D}.}$

c) At $t=t_0$, $4D = 2a\delta_0^2 e^{-2at}$ therefore:

$$N_{max} = N(t_0) = \frac{D}{\pi \delta^2(t_0)} \quad \text{where:}$$

$$\delta^2(t_0) = \delta_0^2 e^{-2at_0} + 4Dt_0 = \frac{4D}{2a} + 4Dt_0 = 4D\left(\frac{1}{2a} + t_0\right) =$$

$$= 4D\left[\frac{1}{2a} + \frac{1}{2a}\ln\frac{a\delta_0^2}{2D}\right] = \frac{2D}{a}\left[1 + \ln\frac{a\delta_0^2}{2D}\right] \Rightarrow$$

$$\Rightarrow N_{max} = \frac{D}{\pi}\,\frac{a}{2D}\left(1+\ln\frac{a\delta_0^2}{D}\right)^{-1} = \frac{D}{2\pi}\left(1+\ln\frac{a\delta_0^2}{D}\right)^{-1}.$$

To summarize:

$$\boxed{N_i = \frac{D}{\pi\delta_0^2}} \qquad \boxed{t_0 = \frac{1}{2a}\ln\frac{a\delta_0^2}{2D}} \qquad \boxed{N_{max} = \frac{D}{2\pi}\left(1+\ln\frac{a\delta_0^2}{D}\right)^{-1}}$$

- Sensitivity of the CMC equation.

Let $Q_p(z,t)$ be the solution using the counterflow based $N(z,t)$.
Let $b_1, b_2 \in [0,1]$ with $b_1 < b_2$ and let:

$$N_1(z,t;b_1,b_2) = \begin{cases} N(z,t) & \text{if } b_1 \le z \le b_2 \\ 0 & \text{otherwise} \end{cases} \quad \text{(Steve's way)}$$

$$N_2(z,t;b_1,b_2) = \begin{cases} N(z,t) & \text{, if } b_1 \le z \le b_2 \\ N(b_1,t) & \text{, if } z < b_1 \\ N(b_2,t) & \text{, if } b_2 < z \end{cases} \quad \text{(another way).}$$

$$N_3(z,t;b_1,b_2) = \begin{cases} N(z,t). & \text{, if } b_1 \le z \le b_2 \\ N(b_1,t)\,z/b_1 & \text{, if } z < b_1 \\ N(b_2,t)(1-z)/(1-b_2). & \text{, if } b_2 < z \end{cases} \quad \text{(Velbjorn's way)}$$

Solve the CMC equation with these and obtain the following solutions:

$$N_1(z,t;b_1,b_2) \longrightarrow Q_1(z,t;b_1,b_2).$$
$$N_2(z,t;b_1,b_2) \longrightarrow Q_2(z,t;b_1,b_2)$$
$$N_3(z,t;b_1,b_2) \longrightarrow Q_3(z,t;b_1,b_2).$$

and look at how much they deviate from $Q_p(z,t)$ in terms of the max-norm.