ME2 Computing- Coursework summary

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A) What physics are you trying to model and analyse? (Describe clearly, in words, what physical phenomenon you wish to analyse)

- Transport equation for dye ("red 40" specifically) concentration (in %) in a uniform water velocity profile
- Diffusion and convection terms due to velocity profile
- Dye source in the middle (always at 100% concentration), 4 outlets on each side.
- Uniform velocity everywhere, varies over time according to different sinusoidal functions for u_x and u_y.

B) What PDE are you trying to solve, associated with the Physics described in A? (write the PDE)

$\frac{\partial}{\partial t}(\rho\phi) + \operatorname{div}(\rho\vec{u}\phi) = \operatorname{div}\left(\Gamma\overrightarrow{\operatorname{grad}}(\phi)\right) + S$, Where phi ($\phi$) is the dye concentration (%), the density term (ρ) is the volumetric mass per % concentration and Γ is the diffusion coefficient.

C) Boundary value and/or initial values for my specific problem: (be CONSISTENT with what you wrote in A)

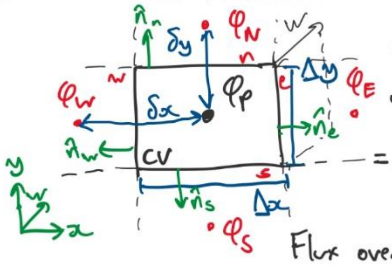
Each boundary acts as an outflow (as the dye source is in the centre) and so we assume that any dye concentration beyond the boundary is "downstream" and so there will be negligible diffusion back into the control volume (against the fluid velocity) so we set the coefficient corresponding to the boundary (a_E if the boundary is to the easy) to zero.

D) What numerical method are you going to deploy and why? (Describe, in words, which method you intend to apply and why you have chosen it as opposed to other alternatives)

We have used a Finite Volume Method in a uniform mesh to solve this problem. This method comes from chapter 5 of "Numerical Heat Transfer and Fluid Flow" (Patankar, 1980). The key steps are to integrate the equation over a cell as a control volume and over the time step. For the diffusion term, $\operatorname{div}\left(\Gamma\overrightarrow{\operatorname{grad}}(\phi)\right)$, a linear piecewise approach between cell centroids was used to find the gradient of dye concentration at each boundary and for the convection term, $\operatorname{div}(\rho\vec{u}\phi)$, the upwind scheme was used to find the value of concentration at the boundary. When integrating through time, an implicit scheme was selected due to being the most physically accurate (chapter 4) and unconditionally stable.

E) I am going to discretise my PDE as the following

Convection & Diffusion Terms $\Rightarrow$ $\boxed{\text{Discretising by integrating over CV}}$



$$\int_{CV} \operatorname{div}(\rho\vec{u}\varphi)\,dV - \int_{CV} \operatorname{div}(\Gamma\,\overrightarrow{\operatorname{grad}}(\varphi))\,dV$$

(divergence theorem)

$$= \oint_{CS} (\rho\vec{u}\varphi)\cdot\hat{n}\,dA - \oint_{CS} (\Gamma\,\overrightarrow{\operatorname{grad}}(\varphi))\cdot\hat{n}\,dA$$

Flux over "e" $= (\rho u_x \underbrace{\Delta y W}_{\text{"A"}})\varphi_e - \Gamma \underbrace{\Delta y W}_{\text{"A"}} \left.\frac{d\varphi}{dx}\right|_e$

Diffusion: $\left.\frac{\partial\varphi}{\partial x}\right|_e \approx \frac{\varphi_E - \varphi_P}{(\delta x)}$ $\Rightarrow$ Linear piecewise scheme for diffusion

Convection: $\varphi_e = \begin{cases} \varphi_P & \text{if } u_x > 0 \\ \varphi_E & \text{if } u_x < 0 \end{cases}$ $\Rightarrow$ upwind scheme for convection

Let $\begin{cases} D = \frac{\Gamma A}{\delta} & \text{(conductivity)} \\ F = \rho u A & \text{(mass flowrate)} \end{cases}$ $\boxed{\text{eq. becomes:}}$ $F_x(\varphi_e - \varphi_w) - D_x(\varphi_E - \varphi_P) + D_x(\varphi_P - \varphi_W) + F_y(\varphi_n - \varphi_s) - D_y(\varphi_N - \varphi_P) + D_y(\varphi_P - \varphi_S)$

(linear form)

($[\![A, B]\!]$ = larger of A or B)

$a_P\varphi_P = \sum_n a_n\varphi_n + b$ $\Rightarrow$ $a_E = [\![-F_x, 0]\!] + D_x$

$a_P = a_E + a_W + a_N + a_S \underbrace{+ F_e - F_w + F_n - F_s}_{\text{Should = 0 if continuity maintained}}$

$a_W = [\![F_x, 0]\!] + D_x$

$a_N = [\![-F_y, 0]\!] + D_y$

$a_S = \underbrace{[\![F_y, 0]\!]}_{\text{consequence of upwind scheme}} + D_y$

Unsteady Term $\Rightarrow$ integrate over time step "Δt"

$$\boxed{\int_t^{t+\Delta t} \varphi\,dt = \varphi\Delta t}$$ where $\varphi(t) = \varphi^0$, $\varphi(t+\Delta t) = \varphi$

$\Rightarrow$ Implicit scheme: unconditionally stable

$\therefore$ all previously derived coefficients should be multiplied by Δt

For: $\underbrace{\int_{CV}\int_t^{t+\Delta t} \frac{\partial}{\partial t}(\rho\varphi)\,dt\,dV}_{\text{the unsteady term}} = \rho\overbrace{\Delta x\Delta y W}^{\text{Volume}}(\varphi - \varphi^0)$

we can divide everything by Δt now

$\Rightarrow \boxed{a_P^0 = \frac{\rho\Delta x\Delta y W}{\Delta t}}$ $\therefore$ $a_P = a_E + a_W + a_N + a_S + a_P^0$

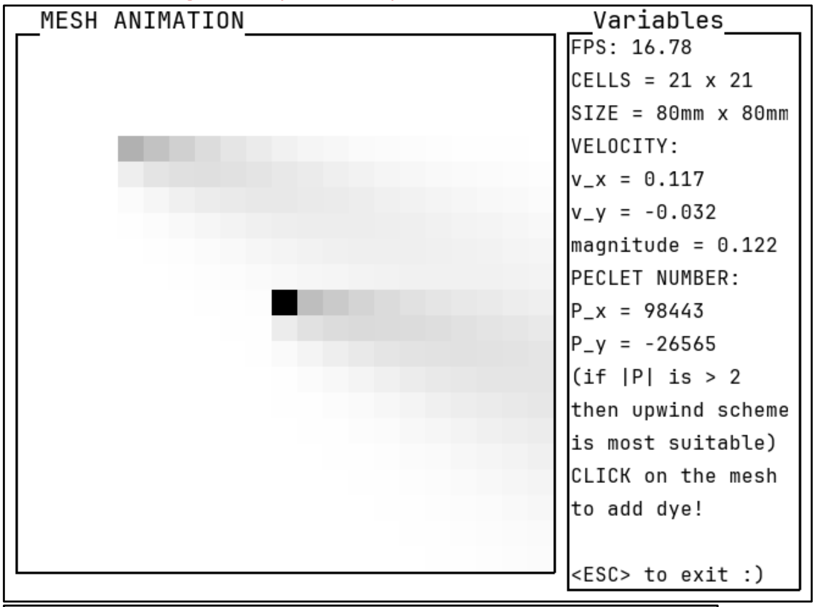
$b = a_P^0\varphi_P^0$

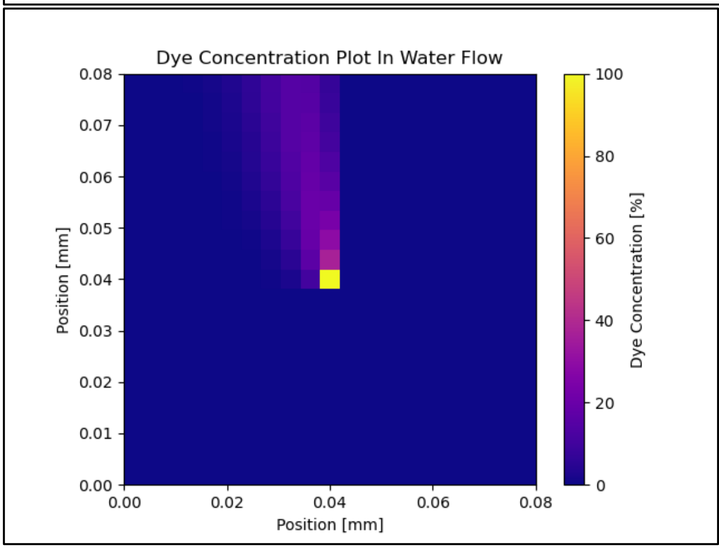
and the rest remained unchanged//

E) I am going to discretise my PDE as the following

To summarise the working above: the partial differential equation becomes a system of equations for every cell centroid in the mesh of the form $a_p\phi_p = a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S + b$. The previous derivation shows that:
$a_E = [\![-F_x, 0]\!] + D_x,\quad a_W = [\![F_x, 0]\!] + D_x,\quad a_N = [\![-F_y, 0]\!] + D_y,\quad a_S = [\![F_y, 0]\!] + D_y,\quad a_P = a_E + a_W + a_N + a_S + a_P^0$
and finally $b = a_P^0\phi_P^0$. Where the superscript "nought", eg. ϕ^0, corresponds to the value at the previous time step and the double brackets, eg. $[\![A, B]\!]$, means "the larger of A or B" and is a result of using the upwind differencing scheme. These equations are made into a system for every cell and then solved using the "numpy.linalg" library. Due to our analysis of boundaries being outlets in question C, any coefficients corresponding to boundaries are made zero.

F) Plot the numerical results comprehensively and discuss them (discuss how the results describe the physics and comment on any discrepancies or unexpected behaviours). Use multiple types of visual graphs. Present and discuss any outcomes of the grid analysis, as requested in Task 9, too.





The screenshot to the left is of the interactive pygame GUI (make sure to run `pip install pygame` before running) built to showcase the solver – black represents 100% concentration and white represents 0. The source at the top right is due to the user pressing there to add dye. The screenshot beneath is equivalent but with a matplotlib heatmap instead. A 2D heatmap representation is the most appropriate plot as our problem is literally the movement of colour in a 2D plane.

One key discussion point is that of the Peclet number which is $P = \frac{\rho u \delta}{\Gamma}$ or the ratio of convective strength over diffusive strength. At high Peclet number (at a boundary) we can prove analytically (Same textbook as discussed in section D) that:

$$\left.\frac{\partial \phi}{\partial x}\right|_{boundary} = 0$$

Therefore, no diffusion happens between cells due to overwhelming influence of convection. While at high Peclet number the upwind scheme is accurate for our convection discretisation as:

$$\phi_{boundary} = \phi_{upwind}$$

The linear piecewise approach, however, to diffusion, outlined in the derivation (part E), becomes an overestimate and so the results shown to the left show a disproportionate influence of diffusion, and so are not fully physically accurate.

G) Other remarks (limits of the model, convergence problems, possible alternative approaches, anything you find relevant and important to mention):

Following the above discussion of Peclet number, the distribution of ϕ between two nodes of ϕ_0 and ϕ_L is shown according to an analytic model in the graph to the right. One way to fix the overestimation of diffusion at high Peclet numbers (where $\frac{\partial \phi}{\partial x} = 0$) is using a so called "Hybrid" scheme that "turns off" diffusion at $|P| \gg 0$. This is too complicated to have done for this project, however.