Modelling Contaminant Transport
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The Code

For this task all code was written in MATLAB and is attached with this submission. There are two .m files, they are `ANALYTIC_ADVECTDIFF.m`, `runner_fvm.m` , `FVM_test.m`, and `FVM_Func.m` Simply run the full script `runner_fvm` to reproduce all plots and results from this report.

The Analysis

Question 2a

To numerically solve this PDE the finite volume method (FVM) was used with 4 main schemes being utilized. The FVM could numerically integrate w.r.t time either using the Backwards Euler (BE) method or the Crank Nicolson (CN) method. The advective component of the flux vector $\mathbf{J}$ was approximated using either an averaging technique (AV) or with the method of upwinding (UW) which gives preferential weighting to the nodes that the advetive component is flowing towards. This resulted in 4 total trials being run for each alteration to either the physical model parameters or the boundary condition implementation (BE-AV), (BE-UW), (CN-AV), and (CN-UW).

Model Parameters

The FVM solver as well as the physical model both had some parameters that were not changed between the 4 different implementations, these were:

- N = 300 - which was the number of node points in the FV mesh
- L = 1.5 - which was the right boundary ie x = L
- $\lambda = 0.05$ - which was the decay rate of the contaminant
- D = 0.002 - which is the diffusion constant of the physical model
- $c_0 = 1$ - which is the concentration amount released at the factory at x = 0
- u = 0.4 - which is the advective term, in the physical model it is the velocity of the river
- dt = 2×10^{-4} which is the time step length for the numerical integration (chosen to ensure monotonicity)

Error Method

For the analysis of the numerical error of all the solution schemes presented in this report the infinity norm of the difference (residual) between the exact and analytic solution was taken for each time-point at which a solution was displayed.

Monotonicity

Since we are using a numerical method to model a physical process, it is important to ensure that our numerical solution does not behave in an unphysical way, in this case we want to ensure monotonicity of our solution. The BE method will be unconditionally monotone with no advection despite our choices for grid spacing and time stepping, however this is not the case for the CN method. To ensure monotonicity in our CN schemes we must first ensure the following inequality holds

$$\delta t < \frac{2\Delta x_P}{D}\left(\frac{1}{\delta x_W} + \frac{1}{\delta x_E}\right)^{-1}$$

Taking the values used that would maximise our RHS (ie not the end nodes for δ_E or δ_W) we get

$$\delta t < \frac{2 * 0.005}{0.002}\left(\frac{1}{0.005} + \frac{1}{0.005}\right)^{-1}$$

$$\delta t < 0.0125$$

Since we have $\delta t = 2 \times 10^{-4}$ we know we satisfy this condition for monotonicity, however because we are working with an advection problem we must also check that the Peclet number is below 2 for both BE and CN (which will be identical in this case) and for both our averaging and upwinding schemes, noting for the σ method we will have our Peclet number in the form of,

$$\begin{aligned}
\text{Peclet} &= \frac{\sigma |u| \delta x_E}{D} \\
&= 0 && \text{(If } \sigma = 0\text{, hence why UW always is monotone)} \\
&= \frac{|u| \delta x_E}{D} && \text{(If } \sigma = 1 \text{ ie Averaging)} \\
&= \frac{0.4 * 0.005}{0.002} && \text{(For my values with max } \delta x_i \text{ chosen)} \\
&= 1
\end{aligned}$$

So since the Peclet number is less than 2 I know all the solutions will be monotone.

Analysis and Conclusions

Figure 6 shows both the numerical and exact solutions for the flow of the concentration of the contaminant in the river, shows at various times (in days). Figure 1 displays the associated errors between the numerical and exact solution at each of the chosen time points with the left plot being the one for the Dirichlet bounds. Each of the 4 subplots on Figure 6 represents a different FVM scheme, and from the figures it is clear that modelling the advection term with an averaging method produces more accurate results that from using upwinding.

These solutions were ran from times of 0-4 days, and it is noteworthy to point out the sharp spike in error seen in Figure 1 for all of the 4 schemes. This si due to the analytic solution showing a contaminant concerntration greater than zero at the RH boundary however the Dirichlet boundary conditions set in this model form our FVM solutions to all be 0 when $x = L$. It is possible that a poor choice for L was made, since even with the scaled distance a finite value for L had to be chose that would plausibly satisfy the condition

$$\lim_{x\to\infty} c(x,t) = 0$$

Further analysis was done by performing 4 more trials, with the same combination of schemes, however this time modelled with Neumann boundary conditions.

Question 2b

The results of these set of trials are shown in Figures 7 and 1, with the same plot layout being used as above for the solution plot, and this time the right subplot being the error for the Neumann bounds. The most immediate observation is the difference between the error plots in Figure 1. The total error with the Neumann boundaries is much lower than with the Dirichlet, most importantly there is no spike as time goes up and the exact value at $x = L$ is not zero. That is because our Neumann boundary conditions at $x = L$ do not force the FVM solution to drop to zero,only for the derivative to be zero, which is why we can see the more physical appearance of the smoothing of the curve. Again, it must be stated that for smaller values of time, and for a much larger value of L, the two boundary conditions would result in much more similar plots.

Question 2c

From the results discussed above, it seems that using Neumann boundary conditions best approximate the far field solution from the initial model. This is due to the much improved accuracy as time increases, as the unnatural "forcing" of the FVM solutions to reach zero at a finite point L will lead to increased error as time increases. The method of Averaging is the clear choice to handle the advective component of the model as it reduces the errors in both the BE and CN implementations when compared to upwinding. Possibly if the speed of our advective component was greater then upwinding may begin to be a more favoured process. While both BE and CN methods of integration are comparably accurate in regards to our error metric, CN is a second order method, and in the **Monotonicity** section, it was shown that the value needed to be chosen for δt to ensure monotonicity is not unreasonably small for our chosen grid size. Therefore the method of CN-AV would be the reccomended FVM solution method.

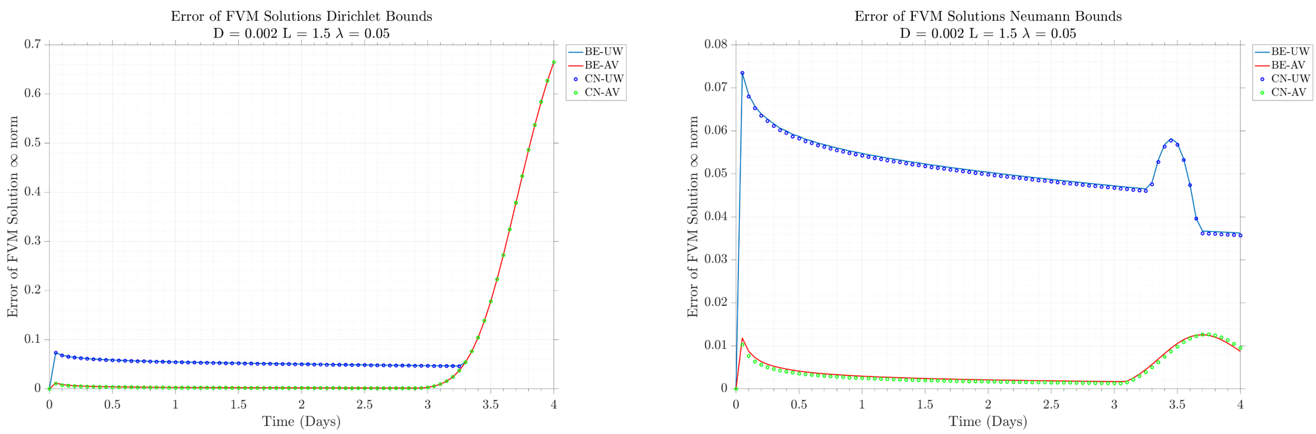

FIGURE 1. Error plots for all 4 solution schemes. Left plot displays the error when implementing Dirichlet boundary conditions on the $x = L$ boundary, with the right plot showing the errors associated with the Neumann boundary conditions.

(i) If no action is taken, how long until a lethal concentration of contaminant is absorbed by the bird colony?

By numerically integrating our FVM solution through time at our point $x = 1$ it was found that the concentration levels would reach their critical dose at approximately 3.4 days. Figure 2 is a visual depiction of how the concentration, and cumulative concentration will continue to rise as time increases if no action is taken.

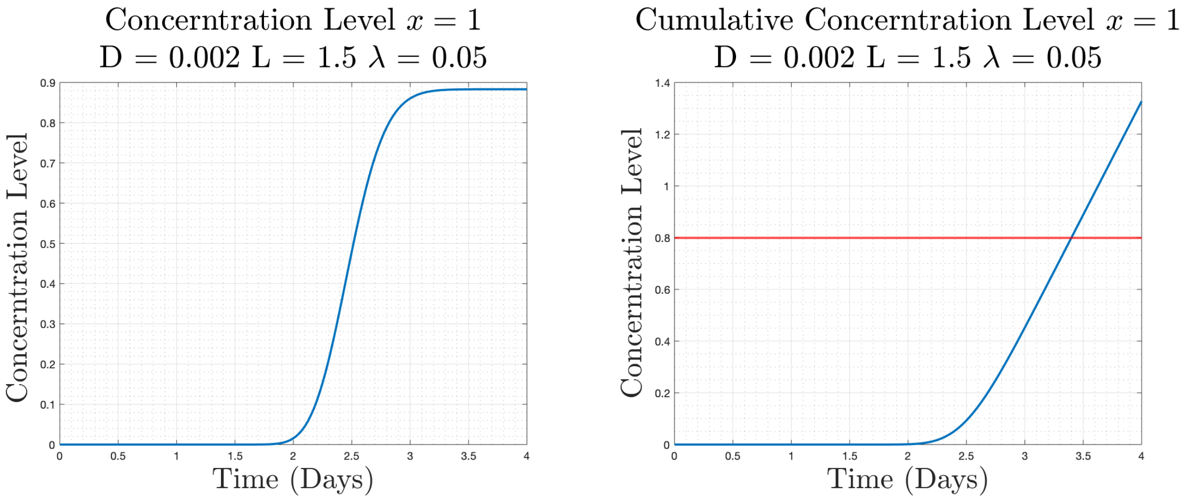

FIGURE 2. Contaminant concentration levels at Bird colony ($x = 1$) with $\lambda = 0.05$. Left plot shows the time specific concentration level, while the right plot shows the cumulative sum of the concentration (or Integral) over increasing time.

(ii) Determine if this proposed approach will be effective at limiting the amount of contaminant absorbed by the bird colony. Would this approach limit the absorbed quantity of contaminate to be less than a lethal dose?

To answer this question an FVM solution was computed with the CN-AV model using Neumann boundary conditions. It was found with this new approach the bird colony would still absorb a fatal concentration after approximately 3.8 days. Figure 3 displays two plots, on the left if a plot comparing the time-stepped solutions between the old approach and the new approach. This plot shows the new method of slowly reducing the contaminant leak does reduce the concentration levels in the spacial area, and its effect increases over time. The plot on the right is similar to the section (i) plot showing the cumulative concentration build up at the $x = 1$ area showing the critical concentration is still easily reached before any notable "levelling off" is attained.

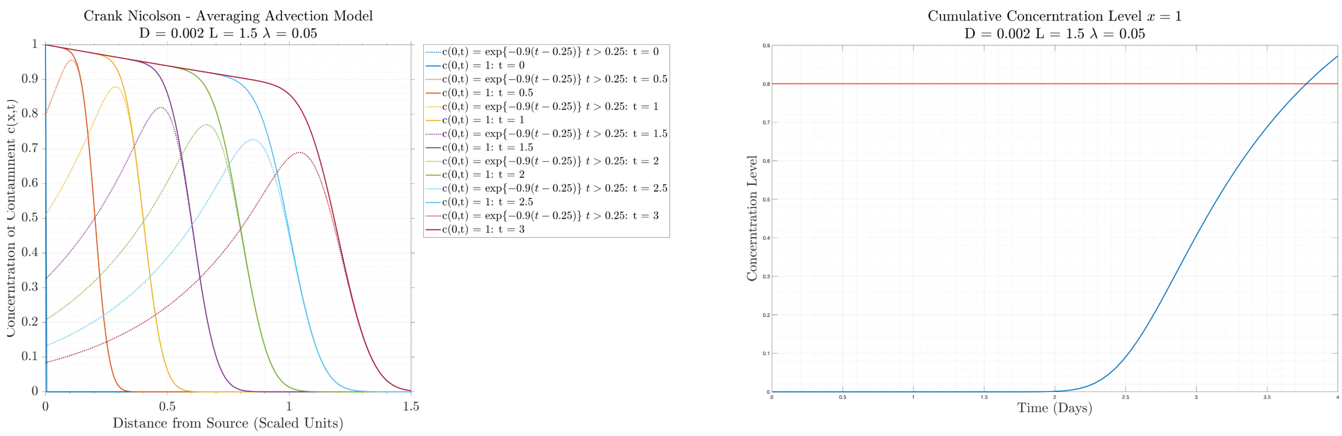

FIGURE 3. $\lambda = 0.05$ results for the factory spill. The left plot shows a comparison between the FVM solution with a constant leak of $c_0 = 1$ in the solid lines, with the time dependant c_0 plotted in the dotted lines showing the reduces concentration levels. The right plot shows the cumulative contaminant concentration at the bird colony showing that the critical concerntration is reached after roughly 3.8 days.

(iii) The DERM is considering introducing legislation that would require the industry to alter the composition of their chemicals to reduce the impact of any future contaminant spill. The effect of this alteration would be that the contaminant decays rate λ would need to be increased. Given the current technology, the decay rate would be changed to $\lambda = 0.3$. Investigate the effect that such a change would have had on the present contaminant spill.

To determine the affect of this, an FVM trial was run over a much larger span of time with a fixed contaminant level of 1 at the factory site ($c_0 = 1$). The results and error are plotted in Figure 4 and it can be seen that the concentration levels in the river are much lower for all time solutions when compared to the $\lambda = 0.05$ trials. The time it would take to reach a critical dose if no action is taken at the factory site (ie $c0 = 1\ \forall t$) will also be reduced, the right plot in Figure 4 shows both the cumulative values of concentration level at $x = 1$ in the river. In this case it took approximately 4.2 days for the concentration level to reach the critical value of 0.8. By comparing this with Figure 2 we can see the Concentration levels in the left plots flatten off at a lot lower values when $\lambda = 0.3$ roughy reducing from 0.9 to 0.5.

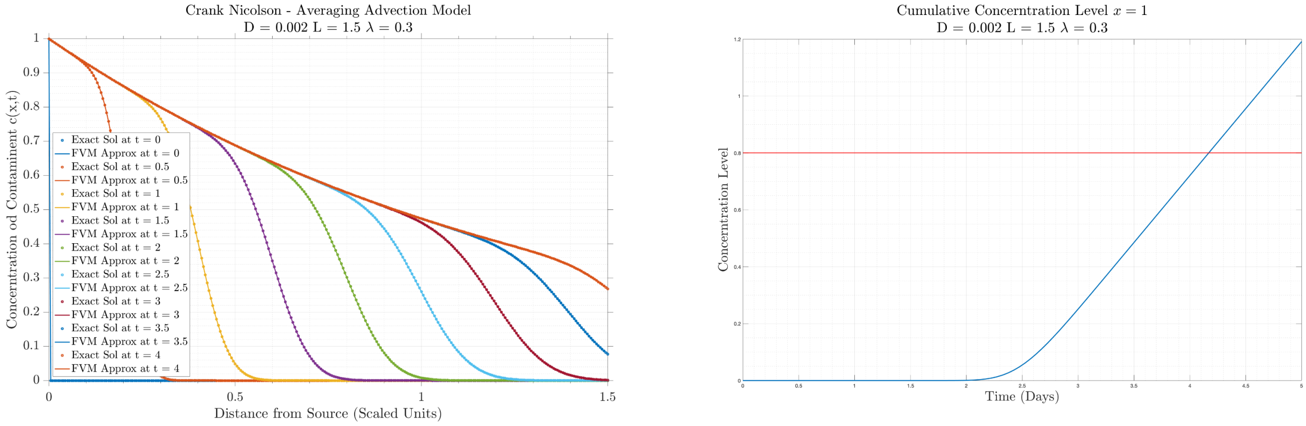

FIGURE 4. FVM solution using the Crank Nicolson and Averaging aproach to modelling the PDE. Left plot shows the concentration levels over the spacial range of the grid at various time points. The right plot shows the cumulative concentration at $x = 1$ as time increases.

An FVM trial was also run with the new λ for the time dependent $x = L$ boundary condition. Figure 5 shows the results of this trial, where it was found that this would be satisfactory action tp save the bird colony as the concentration level flattens out (then eventually starts decreasing) at approximated 0.65, which is well below the critical concentration level of 0.8.

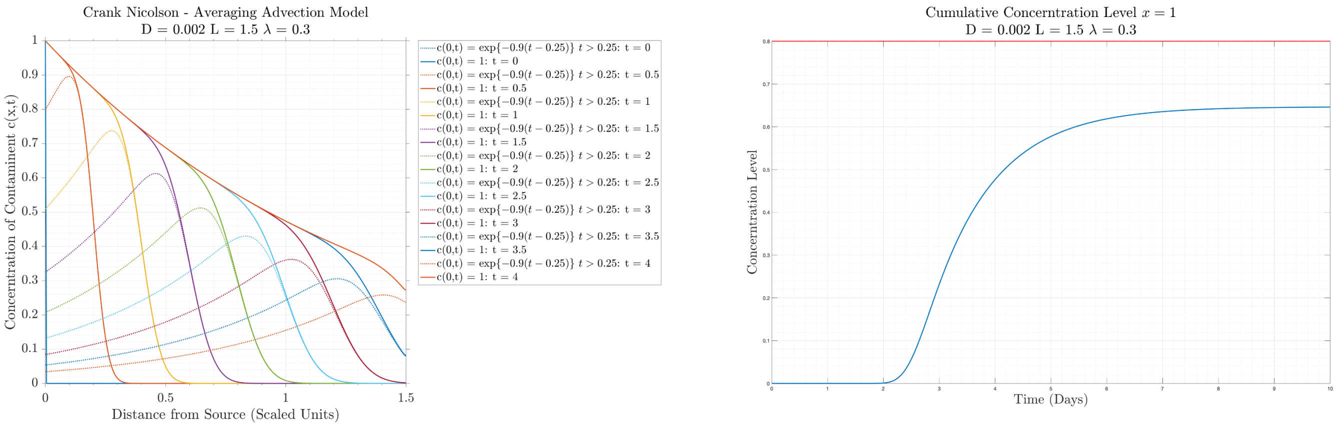

FIGURE 5. $\lambda = 0.3$ results for the factory spill. The left plot shows a comparison between the FVM solution with the new λ with a constant leak of $c_0 = 1$ in the solid lines, with the time dependant c_0 plotted in the dotted lines showing the reduces concentration levels. The right plot shows the cumulative contaminant concentration at the bird colony over a large timescale $t \to 10$ displaying the concentration levels plateau at roughly 0.65

Conclusions and Summary

The contaminant problem has been successfully modelled and for the given model parameters, it was recommended that the FVM utalizing a Crank Nicolson time integration, and an Averaging method for the advective forces should be used. If the company does nothing about the leak it was found that after approximately 3.4 days the bird colony will die. If the company implements the gradual shutdown approach, the spread will be slowed, but not significantly enough to reduce the critical concentration at the bird colony to below 0.8 and the birds are predicted to still perish after approximately 3.8 days.

The proposed changed to chemical composition of the contaminant increasing λ to 0.3 will have significant impacts, firstly if nothing was done to reduce the leak at the factory site it would take 4.2 days for a critical concentration to build up at the bird colony. More significant, if the company is using the new compound and implements their gradual shutdown of the leak, the concentration levels at the bird colony will flatten off at around 0.65 meaning that while they may get a little sick and be a little worse for weather, they should survive the leak.

FVM Method Comparison Figures

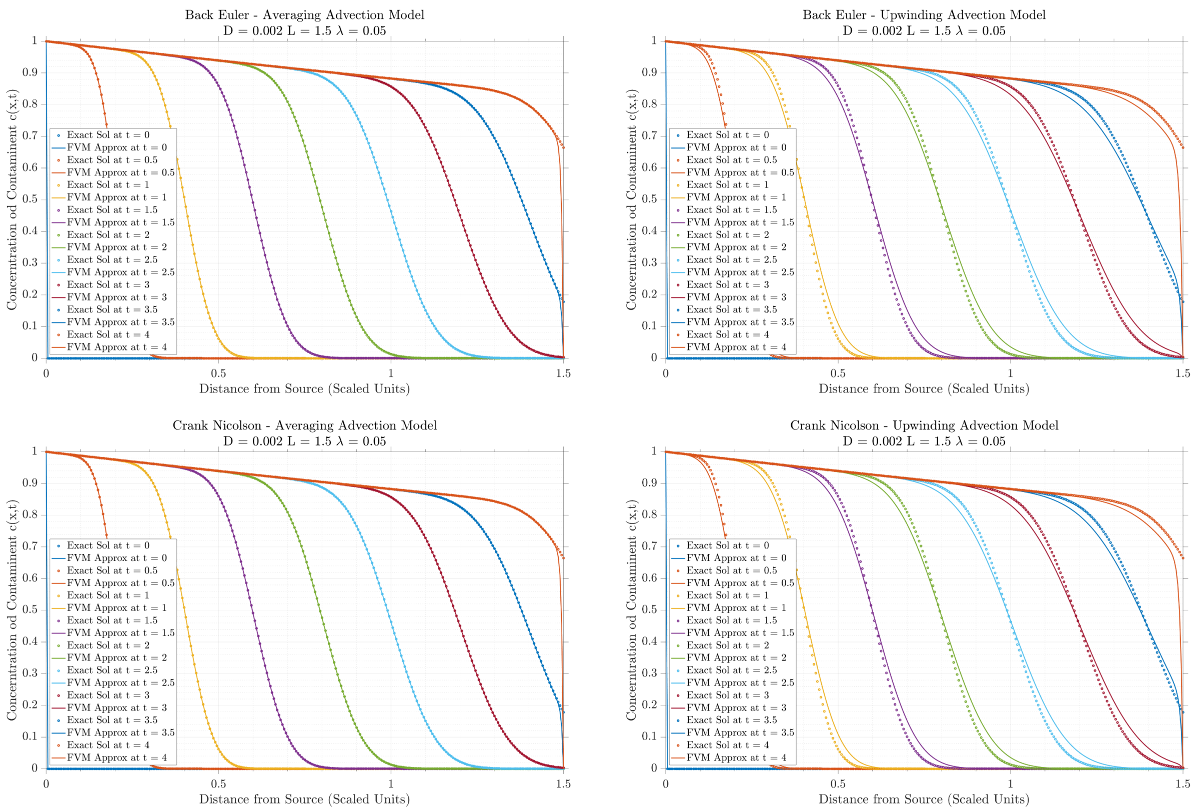

FIGURE 6. 4 different FVM solution methods for Dirichlet boundary conditions compared against analytic solutions over various times since leak.

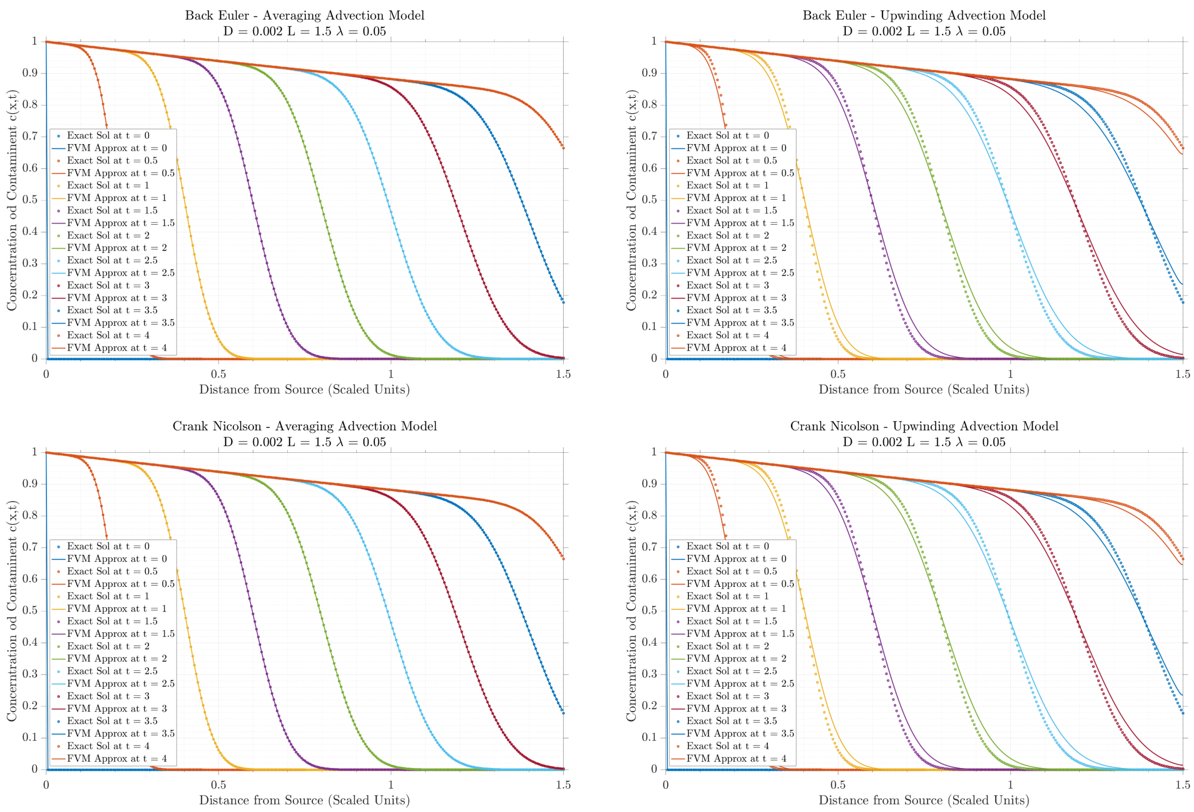

FIGURE 7. 4 different FVM solution methods for Neumann boundary conditions compared against analytic solutions over various times since leak.