

Part C

1. Solving for C(r,t) when there is no reaction (V=0):

As expected, the gradient goes from a rectangle at t=0 to sloping curves to eventually a straight line, at long times/steady state.





This occurs somewhere in the vicinity of about 4000 seconds.

1. Solving for C(r,t) when V=0.05:





When reaction occurs, the gradient (ACC) is basically a result of the reactant flow in and the reactant consumption rate (IN-RXN=ACC). When these are equal (IN=RXN), the system is at steady state (ACC=0). This results in a non-linear steady state gradient for this situation. This seems to occur in the somewhere in the range of 3000 seconds.

D. Looking at the reaction situation (C-2), at early times, the model predicts that the reactant concentration inside the reactor volume near the center is actually less than the concentration at the inside flow stream boundary (see part C-2 and below). Since we assume that diffusion is controlling the movement of reactant, this means the reactant would have to flow against the concentration gradient to exit the reactor in the inside flow stream. This certainly would not occur/does not make sense.



This is due to the reaction occurring in this region before any external diffusive flow reaches this inner reactor volume. The model actually predicts the concentration inside the reactor drops to nearly 1.2 mol/cm3 near the inside flow stream before starting to increase as external diffusive flow becomes significant. In reality, it would be likely that reactant diffusion from the inside flow stream into the reactor would occur during this time. However, the model does not account for this. To be more accurate, there would have to be something like a moving zero flux region within the reactor, i.e. a change in the model assumptions/boundary conditions.