Knowledge and Skills Acquisition via a “Parallel” Problem Solving Approach

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INTRODUCTION: To be competitive in today’s workforce, students in STEM undergraduate programs are expected to develop problem-solving skills. Often, this occurs through guidance and practice in the form of assignments, labs, experiential learning opportunities, teamwork, and other means. The concept of a T-shaped engineer [1] represents an engineer with deep content knowledge and awareness of engineering systems as well as multidisciplinary skills (e.g., problem-solving skills, entrepreneurship, etc.), and such skills are further emphasized by the National Academy of Engineering when communicating attributes that the engineer working in the year 2020 would ideally possess [2]. A challenge lies in how to effectively and efficiently ensure that students develop not only technical content knowledge but also multidisciplinary skills.

METHODS: *A new pedagogical approach is being explored in the Department of Chemical Engineering at Tennessee Technological University in which teams are challenged to solve a given engineering problem (see example problem statement below) using each of four approaches: 1) thought exercises, 2) analytical solution methodologies, 3) experimentation, and 4) computational/ simulation-based approaches with emphasis in using COMSOL® [3].*

Problem Statement: A porous shell containing a drug molecule is delivered into a compartment in the body at time zero (see Figure 1). Drug is released from the shell through the shell’s porous wall and into the compartment which is assumed to be well-mixed. Estimate the concentration of the drug in both the shell and in the well-mixed compartment using a thought exercise, an analytical solution methodology, experimentation, and via simulations.

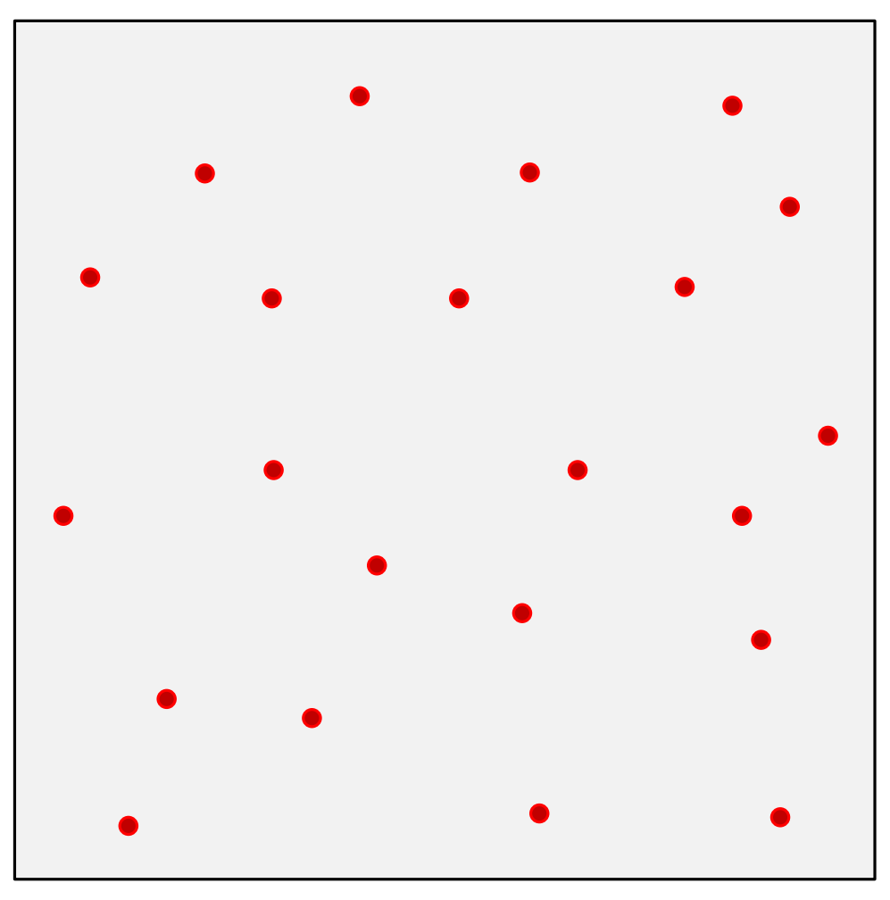

Figure 1. Representation of the drug-loaded shells (beads) in a compartment in the body.

RESULTS:

Via a Thought Exercise

I understand that a concentration gradient is associated with transport of a molecular species from an area with a relatively high concentration to another area with a relatively lower concentration. I know that differences in partitioning will affect the net driving force for this transport. Further, I know that the species could encounter resistance in transport through the boundary layers on either side of the bead wall and through the pores of the wall itself. The effect of the boundary layers might be more significant inside (rather than outside) the bead where mixing does not readily occur. Ultimately, I would expect that the drug would be transported out of the bead and into the space around the bead. Thus, the concentration of the drug in the bead would be expected to decrease with time while the concentration of the drug in the target domain would be expected to increase with time.

Via Experimentation

An experiment was conducted in which 22 beads were prepared by dropping 1 mL of a 10 mg/mL solution of Na+-alginate that contained red food coloring dye into a trough containing 14 ml of $CaCl_2$. The beads were allowed to cross-link for 5 minutes and then were transferred to a flask containing 100 ml of water which was placed on a magnetic stirrer and stirred (Figure 2). Samples were collected at t=0 and also at other times, and background subtracted absorbance at 504 nm was determined. The volume removed was then immediately returned to the flask to minimize any changes in volume. Normalized concentrations were plotted as shown in Figure 3.

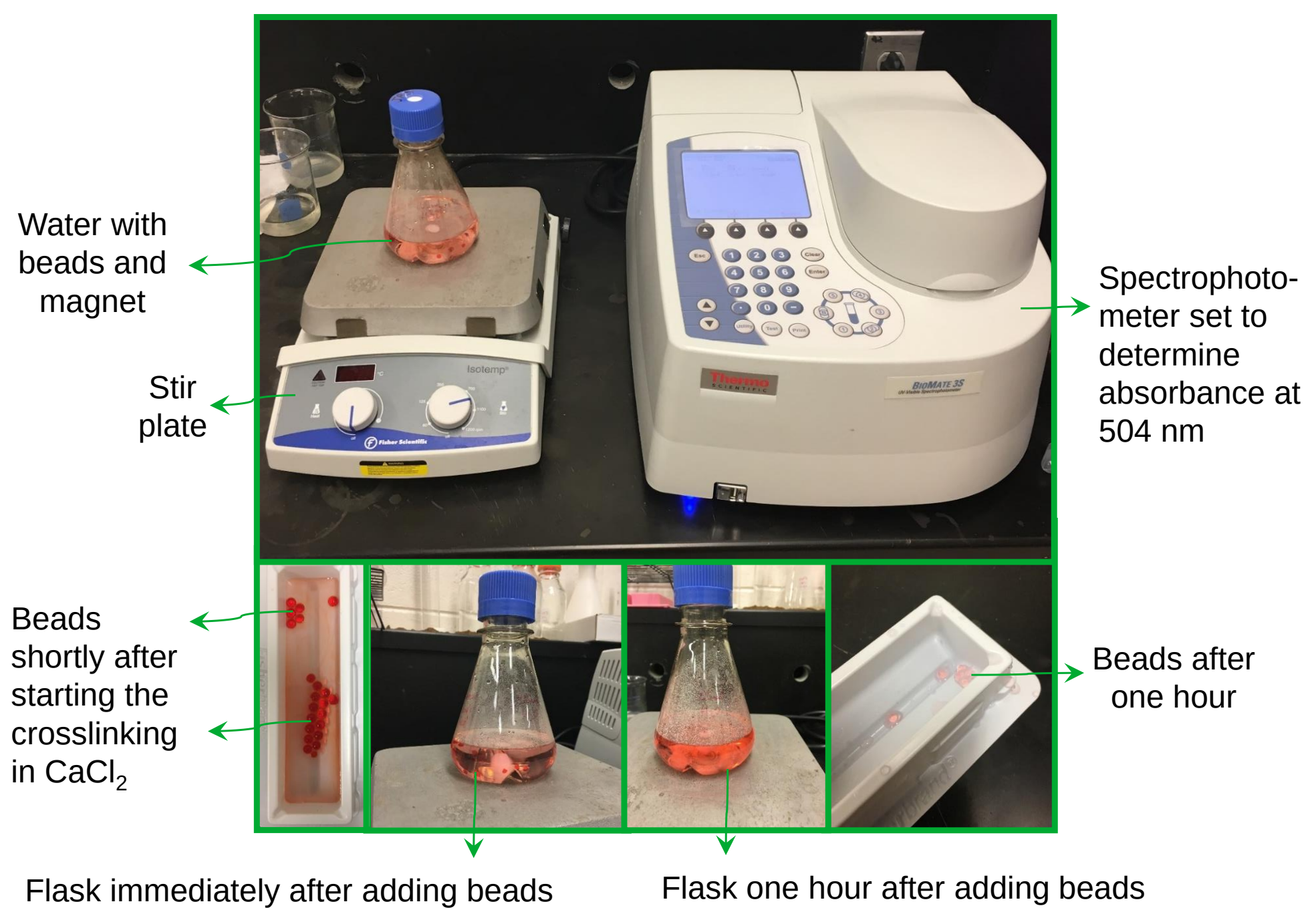

Figure 2. Depictions of experimental setup and instrumentation .

Via an Analytical Solution

It was assumed that the shells (beads) can be represented by a single, oblong bead with the same surface area and volume as multiple beads. It was further assumed that both the bead and water compartments are well-mixed. Performing a species mass balance for both compartments (see equations to the right) and solving the two equations analytically subject to appropriate initial conditions yielded expressions for concentration versus time which were plotted after estimating values for the parameters (see Figures 4 and 5).

Macroscopic Species Mass Balance Equation for Bead Compartment

$$V_{Beads}\frac{dC_{A,Bead}}{dt} = -PS\left(C_{A,Beads} - \Phi_{ABW}C_{A,Water}\right)$$

Initial Condition: $C_{A,Beads}(t=0) = C_{A0}$

Macroscopic Species Mass Balance Equation for Water Compartment

$$V_{Water}\frac{dC_{A,Water}}{dt} = PS\left(C_{A,Beads} - \Phi_{ABW}C_{A,Water}\right)$$

Initial Condition: $C_{A,Water}(t=0) = 0$

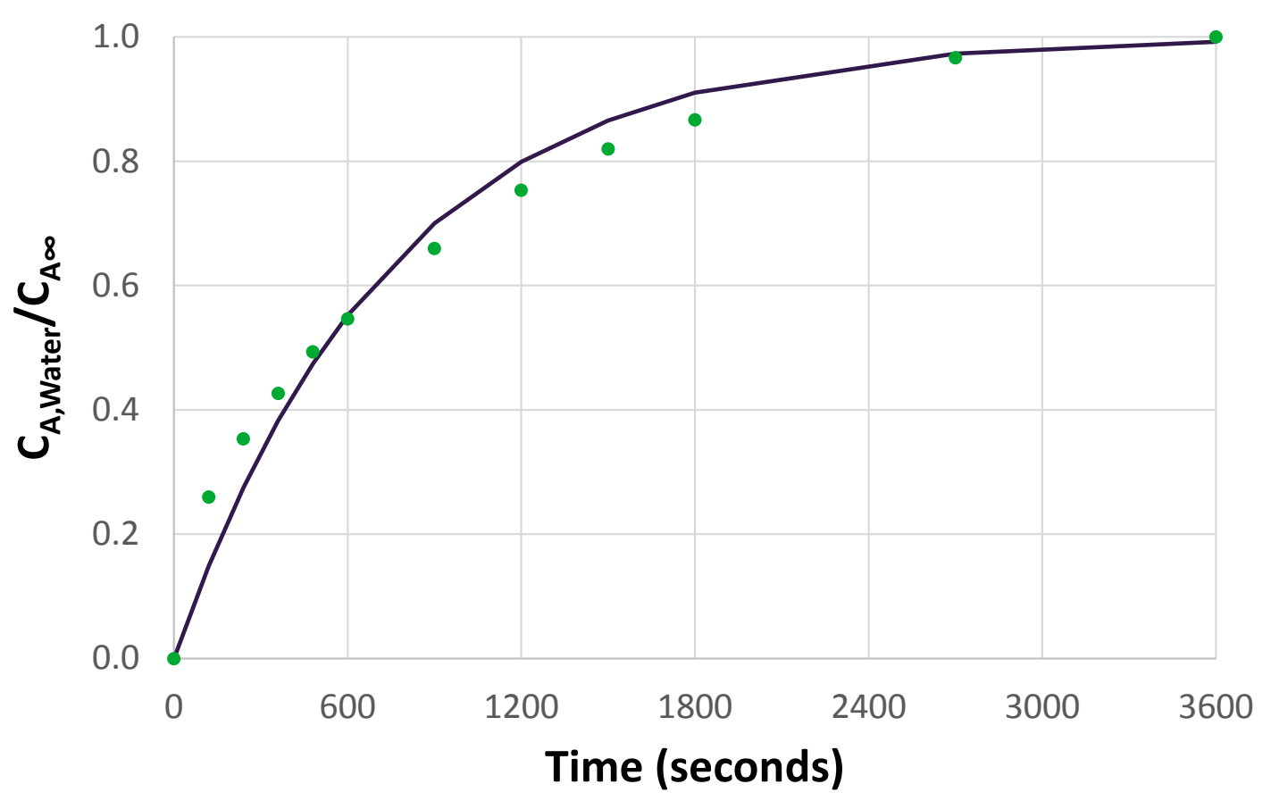

Figure 3. Normalized experimental data and the resulting best fit curve.

Analytical Solutions for Concentrations in Bead and Water Compartments

$$C_{A,Beads}(t) = C_{A0}\left(\frac{\Phi_{ABW}}{\Phi_{ABW} + \frac{V_{Water}}{V_{Beads}}} + \frac{1}{\frac{V_{Water}}{V_{Beads}}\Phi_{ABW} + 1}\right)\left[e^{-\left(\frac{PS\left(V_{Beads}\Phi_{ABW}+V_{Water}\right)}{V_{Beads}V_{Water}}\right)t}\right]$$

$$C_{A,Water}(t) = \underbrace{\frac{C_{A0}V_{Beads}}{V_{Beads}\Phi_{ABW} + V_{Water}}}_{C_{A\infty}}\left[1 - e^{-\left(\frac{PS\left(V_{Beads}\Phi_{ABW}+V_{Water}\right)}{V_{Beads}V_{Water}}\right)t}\right]$$

The concentration versus time equation for the water compartment (bottom equation above) was fit to the experimental data by varying PS (see Figure 3). The concentration versus time curves for the two compartments were then plotted using these equations based on PS estimated from the literature (see Figures 4 and 5).

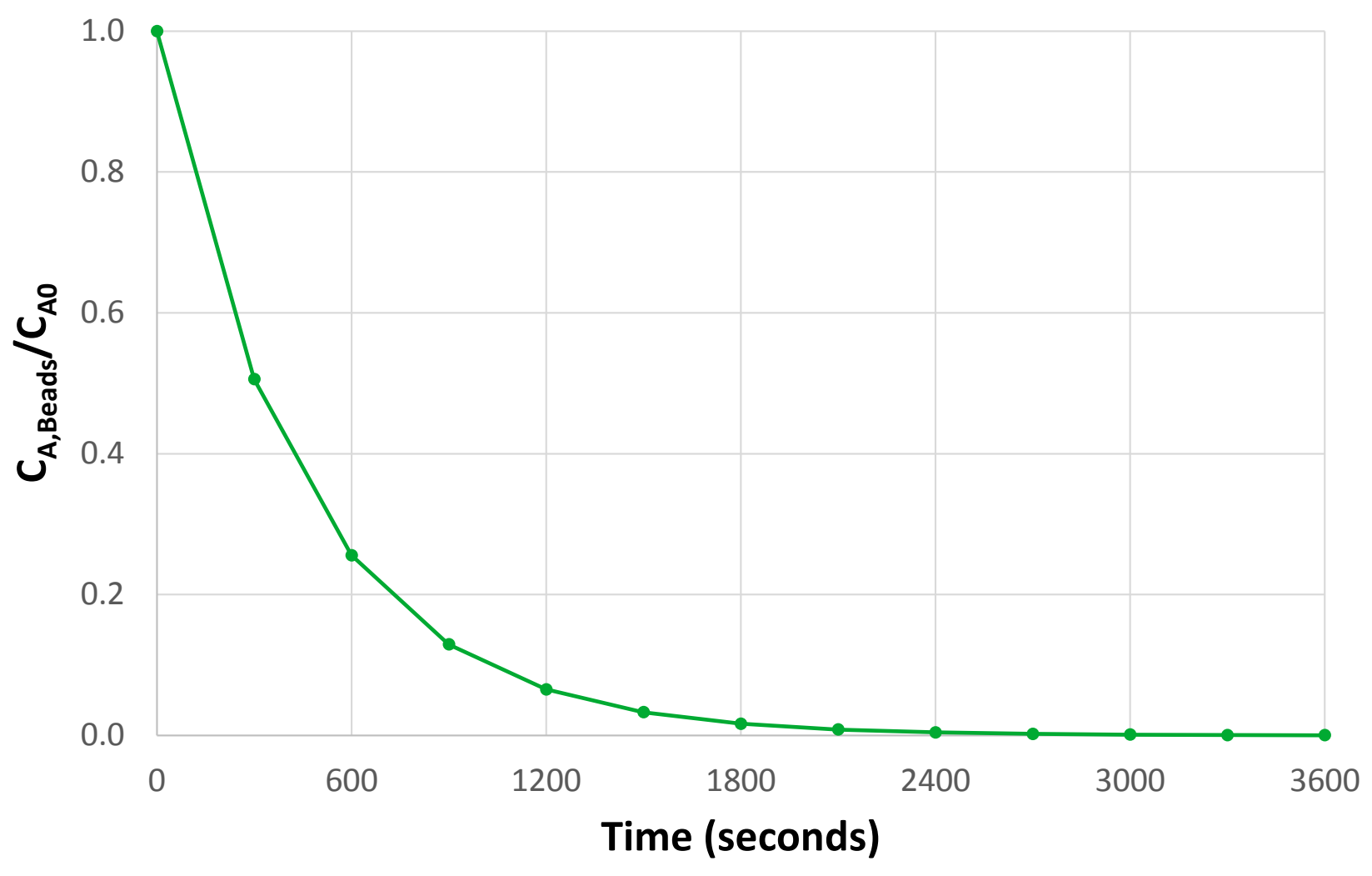

Figure 4. Normalized concentration versus time curve for the bead compartment.

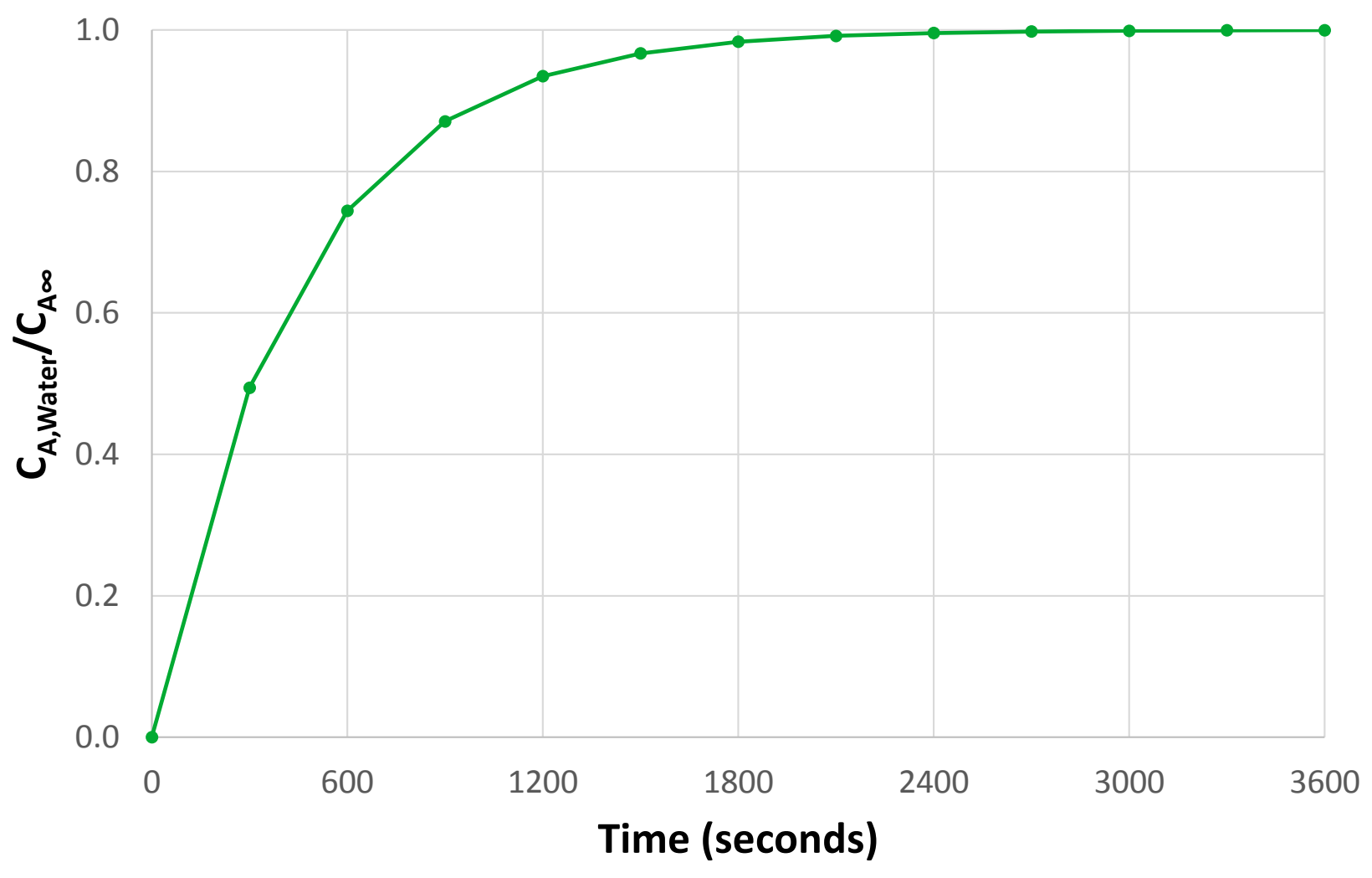

Figure 5. Normalized concentration versus time curve for the water compartment.

Via Simulation

The simulation domain was designed to illustrate the conditions of the Problem Statement with the conditions used in both the experimentation and the analytical solution (see Figure 6).

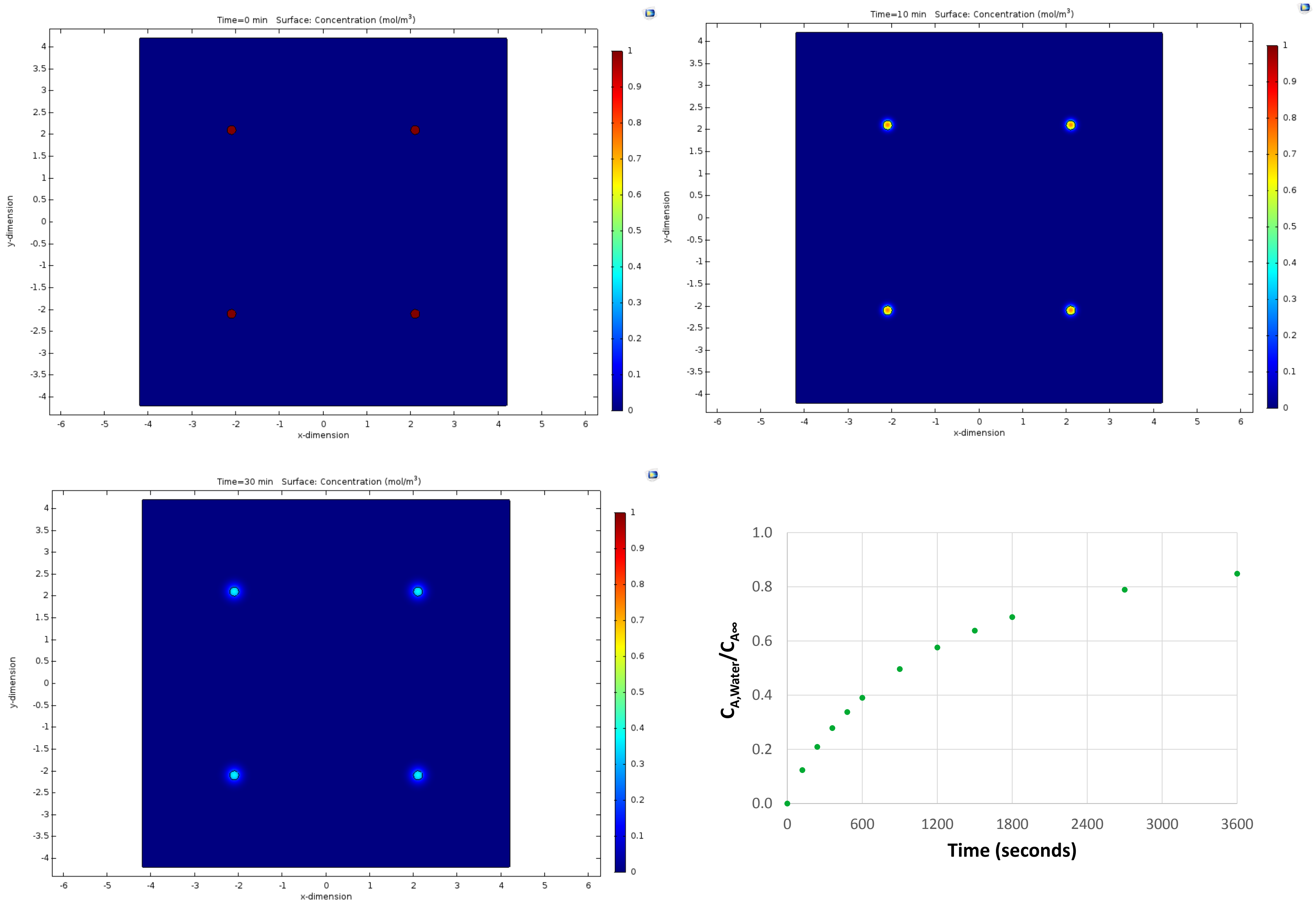

Figure 6. Representative concentration profiles from simulations with results at t = 0 (top left), 10 (top right), and 30 minutes (bottom left) as well as the normalized concentration in water versus time (bottom right).

CONCLUSIONS and OTHER COMMENTS:

Thought Exercise: Thinking about a problem is an effective strategy to develop a preliminary understanding of a solution. Sometimes this is enough. Often times, we have to do more. **Analytical Solution:** The macroscopic species mass balance approach provides us with useful information about how the average concentrations in the two compartments change with time. The value for PS was estimated using literature values for diffusivity and an assumption that the thickness of the bead wall represented 40% of the diameter of the bead and an idealized approach in which it was envisioned that the surface area through which the dye could migrate was 20% of the total surface area of the outside of the bead. In biological systems, it is generally not possible to distinguish P from S. Thus, PS as a single parameter is typically used. **Experimentation:** These experiments were based on a study by Farrell and Vernengo [4]. The use of Solver allowed us to use the analytical solution equations to fit the experimental data by adjusting PS until a best fit (based on minimization of the sum-of-squared-errors, SSE) was obtained. **Simulations:** The radius of the bead was made to be 0.105 cm with a “Thin Diffusion Layer” of 0.06 cm being added through which diffusion would occur. The bead domain was selected to be water though a porous material with selectable porosity could have been chosen instead. The lower normalized concentrations obtained via simulation when compared to the other methods is associated with either the fact that the simulation does not include stirring and/or the choice to set the radius at 0.105 cm with a thin diffusion layer on the surface of the bead. Simple changes could be made to the model, and the results then predicted via the simulation. Ultimately, all four techniques hold a lot of value in helping us with various aspects of the problem.

REFERENCES:

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3. COMSOL is a registered trademark of COMSOL AB.
4. Ferrell, S. and J. Vernengo. A Controlled Drug-Delivery Experiment Using Alginate Beds. *Chemical Engineering Education*. 46(2): 97-109, Spring 2012.

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