An Agent-Based Approach to the Convection-Dispersion-Reaction Model

Sebastian Bernasek
Graduate Student
Chemical and Biological Engineering
Northwestern University

1. INTRODUCTION

At the highest level, chemical reactors are straightforward: molecules enter, react to form new molecules, then exit. Reactors are, however, complex systems operating at the confluence of numerous phenomena originating at the molecular scale. Every reaction engineering course begins with several chapters on reaction kinetics – the mechanisms governing the rate at which individual molecules react to form new molecules. The overall rate of production, however, also depends upon fluid mechanics and bulk diffusion, the two processes that determine the residence time of reactants within the reactor. As reactor designs traverse a vast operating space, modeling complexity rapidly increases and these three competing phenomena become increasingly difficult to distinguish and interpret. This project strives to connect these phenomena to macroscopic reactor performance through the development and validation of an agent-based reactor model. Furthermore, the model is designed to serve as an instructional tool for chemical engineering students regarding the complex interplay of bulk flow, mixing, and reaction within dynamic reactors.

2. MOTIVATION

2.1 Theoretical Background on Dispersion Models

The *convection-dispersion-reaction model* combines *reaction* kinetics with both convective transport and a diffusive *dispersion* term. Reaction mechanisms assume many forms, but at their most elementary level they require the collision and/or correct orientation of reactant molecules. *Convection* is the transport of material due to bulk inertial flow. Dispersion is a macroscopic phenomenon encompassing non-idealities within a reactor that promote mixing, namely viscous effects and bulk diffusion. Its proposed mechanism is only defined at the macro-scale, where downhill concentration gradients drive dispersive flux in a manner directly analogous to molecular diffusion.

Within these *convection-dispersion-reaction* systems, the extent to which a reaction proceeds depends on the relative influence of each phenomenon [1]:

$$\frac{1}{N_{Pe}}\frac{\partial^2 C_A}{\partial z^2} - \frac{\partial C_A}{\partial z} - N_{Da}{C_A}^n = \frac{\partial C_A}{\partial t}$$
$$Dispersion + Convection + Reaction = Production \tag{1}$$

where C_A is the dimensionless concentration of a reactant species, n is the reaction order, z is a dimensionless length coordinate, t is dimensionless time, and N_{Pe} and N_{Da} are the dimensionless Peclet and Damkohler numbers. The two numbers relate the characteristic time scales associated with the three phenomena of interest:

$$N_{Pe} = \frac{convection\,rate}{dispersion\,rate} = \frac{D}{uL}$$
$$N_{Da} = \frac{reaction\,rate}{convection\,rate} = k{C_{A0}}^{n-1}\tau \tag{2}$$

where D is the dispersion coefficient, u is the linear flow velocity, L is the reactor length, k is the rate constant, C_{A0} is the inlet concentration, and $\tau = \frac{L}{u}$ is the space-time. The length coordinate, time coordinate, and concentrations in Equation 1 are non-dimensionalized by the reactor length, space-time, and inlet concentration, respectively. While available, numerical solutions to this model have inspired large volumes of work due to their mathematical complexity [2,3,4,5]. In a number of limiting cases the model converges to the idealized models familiar to all chemical engineers, namely [6]:

- $N_{Pe} \rightarrow \infty$: Ideal Plug Flow (uniform cross-section perpendicular to flow)
- $N_{Pe} \rightarrow 0$: Ideal Mixed Flow (uniform concentration throughout reactor)
- $N_{Da} \rightarrow \infty$: Complete consumption of reactant
- $N_{Da} \rightarrow 0$: No Reactant is consumed

These limiting cases are easy to independently model and understand, but real reactors operate somewhere between them. The solution space of Equation 1 is characterized by the Peclet and Damkohler numbers. For values of $N_{Pe} > 100$ the residence times of molecules are Gaussian distributed with variance inversely proportional to the Peclet number [7]. The distribution converges to the Dirac delta function as $N_{Pe} \rightarrow \infty$ [8]. As $N_{Pe} \rightarrow 0$ the residence time distribution (RTD) decays exponentially. These limiting RTDs are readily derived from the Ideal PFR and Ideal CSTR models, and provide a standard against which dispersion models may be visually and statistically validated [9].

2.2 Modeling Objective

Through the use of simple agent-level rules to reproduce dispersion models, the primary goal of this work is to paint a more intuitive portrait of convection-dispersion-reaction systems. The model operates at the macro-scale, but employs a number of micro-scale mechanisms to demonstrate the origin of emergent macroscopic behavior. In particular, molecular collisions and random-walk diffusion are proposed to yield the elementary rate laws and dispersive mixing characteristic of real systems. Despite its elementary foundations, the model should also be equipped to design and simulate real reactors. It is unlikely that an agent-based model could ever displace the numerical approach due to computational cost, but it could serve as a first-pass before significant resources are invested in complete model development.

The agent-based approach readily lends itself to visualization and user-interaction. A successful agent-based dispersion model would be an invaluable educational tool, particularly at the undergraduate level where systems of partial differential equations are mathematically intractable. By enabling students to manipulate parameters in an environment with immediate visual feedback, the barrier to understanding these systems could be dramatically lowered. In particular, the ease of code development in NetLogo lends itself to further extensions of the model by students themselves.

2.3 Literature Review

The convection-dispersion-reaction model presented here comprises a subset of a broader class of convection-diffusion-reaction problems. These models enjoy wide use throughout the scientific community, in fields ranging from environmental to biomedical engineering. Tzatchov *et al* used Equation 1 to model the dynamic concentration of chlorine and fluoride in water distribution networks, employing a numerical Green's function technique to solve the system of equations describing the series of water channels [10]. Cameron *et al* solved an analogous form of Equation 1 to model the absorption of pesticides and nutrients within soil [11]. Their reaction term includes a rate expression reminiscent of the Langmuir-Hinshelwood kinetics used to describe heterogeneous catalytic reactions. Squires *et al* use the model to characterize various regimes of micro-sensor binding kinetics, as the ability of microarrays to monitor changes in DNA or protein activity are strongly dependent on the interplay between convection, diffusion, and adsorptive-reaction near the microarray surface [12]. Additional modeling applications include natural-convection driven polymerase chain-reaction, aquatic species population dynamics, and radioactive wastewater disposal [13,14,15]. The breadth of applications of the model suggests that an interpretable agent-based representation may prove valuable beyond the chemical engineering community. As a modeling tool, the agent-based approach may be particularly amenable to fields with inherently higher noise and consequently lower demand for accuracy than chemical reactor design, such as atmospheric or ocean science.

Despite its adoption by many hard, soft, and social sciences communities, a dearth of relevant literature suggests that agent-based modeling has not gained significant traction as a reactor modeling platform. At the smaller scale, the NetLogo Models Library contains several models connecting molecular interactions to emergent macroscopic kinetics and equilibrium states [16, 17, 18, 19]. At the larger scale, agent based models have been employed for optimization of batch reactor scheduling [20]. There are, however, two notable reactor models. Pannala *et al* studied the dynamics of fluidized bed reactors by using thousands of agents to represent rapidly colliding solute-filled bubbles [21]. The approach successfully reproduces an emergent oscillatory “slugging” phenomenon characteristic of real systems. The second exception is an agent-based model of an anaerobic sludge bioreactor published by Pereda and Zamarreño [22]. Their model, written in NetLogo, describes a stirred batch reactor in which bacterial growth is driven by uptake of substrate from wastewater. They validate their model against conventional Monod kinetics in a procedure similar to the validation method employed in this paper. While their model succeeds in reproducing Monod growth kinetics, its domain is constrained to a batch system in which perfect mixing is achieved. This corresponds to the $N_{Pe} \rightarrow 0$ limit introduced in the Background section, and is of little use in analyzing continuous flow systems. Real anaerobic sludge bioreactors do not typically operate near this limit, presenting a case in which a convection-dispersion-reaction model would be of particular utility. To the author’s knowledge, this is the first agent-based approach to modeling a reactor under the convection-dispersion-reaction model framework.

3. METHODS

Both models were developed in NetLogo. In modeling any flow system, the observer may assume either a mobile or stationary frame of reference. In fluid mechanics, these are commonly known as the Lagrangian and Eulerian viewpoints. The former describes the dynamic behavior of individual fluid elements, while the latter describes the behavior observed at a particular point in space. In the present work, separate agent-based models have been developed for each frame of reference. The Lagrangian frame of reference serves as the primary model because its mobile viewpoint is more conducive to monitoring the residence time distributions generated by dispersive mixing. The Eulerian model serves here as a validation tool, but has significant potential utility and is further discussed in the Complementary Model section.

3.1 Primary Model: Stochastic Reactions and Dispersion

All chemical species are represented by mobile turtles in the primary model. While the turtles act as discrete particles, each turtle does not represent an individual molecule. Molecules exist on a length scale $\sim 10^{10}$ times smaller than reactors, and implementing their mechanistic physical behavior (i.e. Brownian motion due to molecular bombardment) would be computationally infeasible in a model that also exhibits macroscopic behavior on the length scale of the reactor, such as convection and dispersive mixing. Instead, each turtle represents a quantum of molecules. Reactants are blue, products are red, and inert species are yellow. Molecular scale mechanisms are applied to these quanta, resulting in emergent behavior at the length scale of the reactor.

The model consists of a single reactor oriented as shown in Figure 1. The feed stream of pure reactant enters through the left boundary, flows through the reactor, and exits through the right boundary. To setup, the patches lining the entrance to the reactor are asked to feed the reactor by sprouting reactants with a residence time of zero. Alternatively, the entire reactor may be filled with reactants to start. At each tick, all of the quanta undergo convection, dispersion, and reaction. Any quanta transported beyond the reactor exit are catalogued as effluent and asked to die. The residence times of the quanta are incremented before the reactor is fed more reactant.

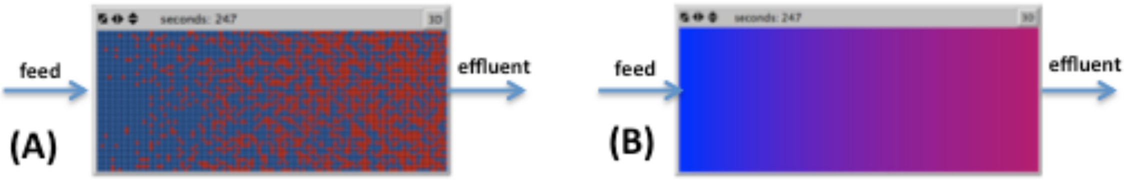

Figure 1: Visualization of flow reactors for the (A) primary turtle-based stochastic model and (B) complementary patch-based deterministic model. Feed enters the reactor at the left boundary, and effluent leaves at the right boundary. Reactants are colored blue while products are colored red.

The mechanisms selected for the three phenomena are central to the model's function. Convection is the transport of material due to bulk flow. In this model, a user-specified uniform flow velocity sets the individual velocity of each quantum. Each quantum is assumed to conserve its momentum, with no viscous momentum transfer between quanta. This assumption is consistent with the dispersion model in which viscous effects are captured by the dispersive mixing term. Most reactors also operate in a highly turbulent flow regime where a radially uniform flow profile holds. At each tick, the quanta move directly downstream by a distance equal to their flow velocity.

Dispersion encompasses the viscous and diffusive effects that lead to mixing within a reactor. The phenomenon is only defined at the macroscopic scale, where dispersive material fluxes flow down local concentration gradients. This behavior is, however, identical to molecular diffusion – the random walk process by which mass is transported from high to low regions of concentration. Consequently, dispersion is implemented with a 1-D random walk. At each tick, the quanta randomly step forward or backward by a distance set by their user-specified diffusivity.

The stochastic nature of chemical reactions at the molecular scale is preserved in the model. At each tick, the probability of a reaction occurring is determined by one of three reactions mechanisms made available to the user. The first mode, labeled concentration-independent, allows the user to specify a fixed reaction probability. In practice, reactions may or may not require collisions to proceed but will require a particular orientation. The concentration-independent mechanism corresponds to a scenario in which only molecular orientation matters. Orientation is effectively random, leading to a constant probability of reaction for this mechanism. A second concentration-dependent mode allows the user to specify a fixed reaction probability, as well as a collision-radius. Here, the likelihood of correct orientation is multiplied by the number of other reactants found within the collision radius. This mechanism corresponds to a reaction that requires collisions in order to exceed an activation barrier. The probability of correct orientation remains constant, but the particles' chances of undergoing a collision increase linearly with the local availability of other reactants. Notably, these are molecular mechanisms applied to much larger scale quanta within the model. Validation is required to determine whether these mechanisms produce realistic behavior overall.

Most of the results exhibit substantial noise due to the stochastic nature of the model. To combat this, all performance metrics are collected as a moving-average over a user-specified sampling window. The sliding window helps reduce sensitivity to noise, but decreases the response time of the system. Small (~5 s) window sizes should be used when dynamic behavior is of interest.

As discussed in the Complementary Model section, a more deterministic model operating in the Eulerian frame of reference was developed in parallel with the present stochastic turtle-model. This second model allows explicit definition of deterministic rate equations. The two models are designed to work in parallel, with Import/Export buttons enabling exchange of operating parameters and concentration profiles between the two. By importing the stochastic model's parameters and results into the deterministic model, the rate expression can be tuned to minimize the distance between reactor profiles. This scheme allows for a one-to-one mapping of the stochastic reaction mechanisms to explicit rate laws.

3.2 Complementary Model: Deterministic Reactions and Dispersion

A second model was developed from a static frame of reference in which properties are assigned to a point in space rather than individual molecular quanta. In this model a patch represents a point in the reactor. Each patch has properties corresponding to the concentration of all chemical species, and reaction kinetics are specified in the deterministic elementary $r_i = kC_i^n$ form. In this model, convection is modeled by asking each patch to inherit new properties from its upstream neighbor while passing its old properties to its downstream neighbor. Dispersion is modeled through NetLogo's built-in diffusion mechanism.

This approach is more closely representative of the conventional *convection-dispersion-reaction model*, as it creates a near-continuous space rather than discretizing the system into discrete particles representative of ~10^{20} molecules. Kinetics are specified in conventional elementary form, enabling direct input of rate parameters for a real system.

4. RESULTS AND ANALYSIS

Analyses were initially performed in NetLogo then repeated in Matlab 2014a in order to make use of its extensive library of plotting features.

4.1 Model Verification

In order to verify that the model's implementation functions as intended, each of the three main phenomena must be scrutinized. Convection describes the bulk transport of fluid, and is most easily verified during startup. Beginning with an empty reactor, in the limit of no dispersion the fluid front should move toward the reactor exit with uniform velocity. The time to reach the exit should exactly equal the space-time, τ. Dispersion is implemented as a 1-D random walk taken by each quantum of molecules. During startup, this should result in some particles jumping ahead and some jumping behind the fluid front. The noise near the leading front should also increase as the front moves down the length of the reactor, as the particles are allowed more time to undergo their random walk. For the reaction mechanisms, the rate should increase with increasing probability of correct orientation, or reaction probability. At steady state, higher rates should yield higher product concentrations in less time. All three of these phenomena are shown visually in Figure **2**, verifying that the core features of the model are implemented as intended.

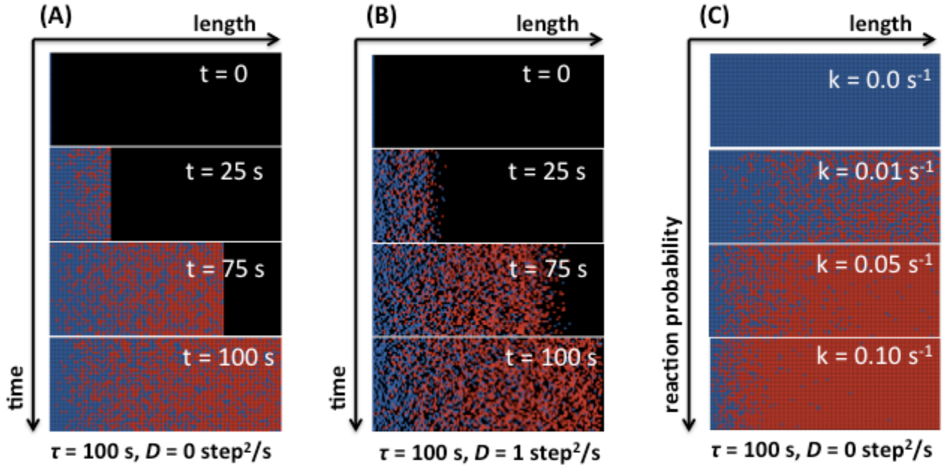

Figure 2: Verification of the (A) convection, (B) dispersion, and (B) reaction mechanisms. Convection moves the fluid front through the reactor during startup, random-walk dispersion introduces noise on the leading edge of the fluid front, and increasing reaction probability (later shown to be *k*) increases product concentration.

4.2 Model Validation: Testing the Limits of the Dispersion Model

A functioning dispersion model must span the range of behavior between the limiting cases discussed in Section **2.1**. To validate the agent-based model, concentration profiles obtained in or near these limits are compared with the analytical solutions in Table **1**. The concentration profiles obtained by both models in these limiting regions are shown in Figure **3**. By visual inspection, all of the profiles conform to those predicted by the analytical solutions of Equation 1. While the N_{Pe}→0 limit produces the expected uniform steady-state concentration profile, the concentrations are lower that those obtained under ideal plug flow conditions. Some reaction engineering insight suggests that this should not happen. Upon closer inspection of the model, this discrepancy occurs because the reactor is bounded on a length scale of similar magnitude to the random-walk step size, allowing reactants to "diffuse out of the reactor," depleting the steady state concentration. This is a limitation of operating with discretized molecular quanta, and suggests that the relationship between the specified reaction probability and steady-state concentration loses accuracy in the low Peclet regime. Despite this drawback of the random walk dispersion mechanism, the successfully quantitatively reproduces the other three limits and qualitative reproduces all of the limits.

Table 1: Reactant concentration profiles in the limiting cases of Equation 1

Limit	**Steady State Conc. Profile**	**Description**
$N_{Pe} \rightarrow \infty$	$\int_{1}^{C_A} \frac{dC_A}{C_A^n} = -N_{Da} z$	Ideal Plug Flow (order dependent decay)
$N_{Pe} \rightarrow 0$	$C_A^n + \frac{1}{N_{Da}} C_A = 1$	Ideal Continuous Stirred Tank (uniform profile)
$N_{Da} \rightarrow \infty$	$C_A = 0$	Complete Conversion
$N_{Da} \rightarrow 0$	$C_A = 1$	No Conversion

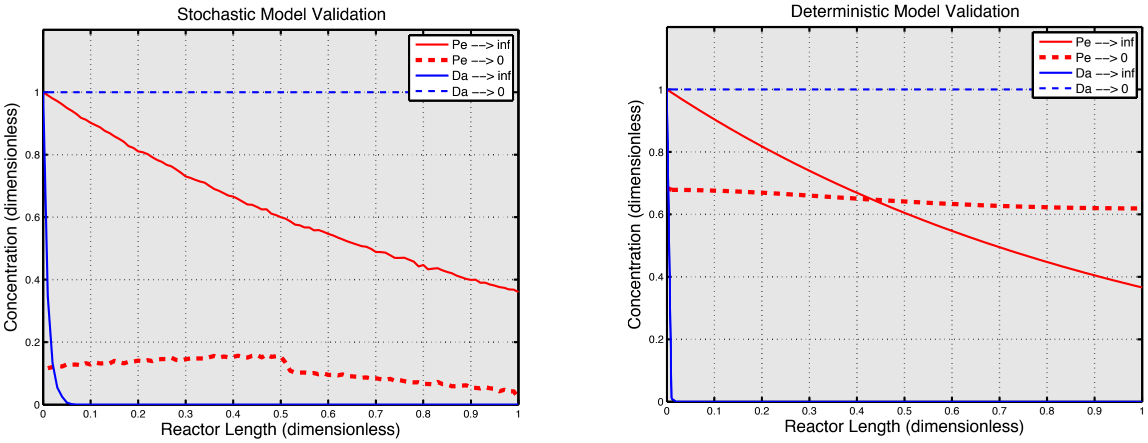

Figure 3: Validation of the (A) stochastic and (B) deterministic models' capacities to reproduce each of the limiting operating regimes. Each of these profiles correspond to one of the analytical solutions in Table **1**. The one discrepancy between the two models is in the ideal CSTR limit ($N_{Pe} \rightarrow 0$, dashed red line). The lower uniform concentration in the stochastic model is explained by a depletion of reactant as the random walk step size approaches the length scale of the reactor.

4.3 Dispersion Effects

Dispersion promotes longitudinal mixing within reactors. As discussed in Section 2.1, in convection-dominated regimes ($N_{Pe} > 100$) the residence time distribution is Gaussian, with dimensionless variance inversely proportional to the Peclet number. As dispersion increases further, the residence times converge to an exponential distribution. The agent-based model was used to generate probability density functions for the dimensionless residence time (residence time divided by space-time) across a range of dispersion coefficients. The distributions are shown in Figure 4A, where the transition from Gaussian to exponential behavior emerges. The variance of each distribution is used to calculate the statistical Peclet numbers in Figure 4B. These values are presented alongside the actual Peclet numbers calculated according to Equation 2. The two sets of Peclet numbers appear to diverge near $N_{Pe} = 10$, suggesting that this is a transition point where the Gaussian solution breaks down and the variance ceases to be inversely proportional to the dispersion coefficient. This observation is consistent with Figure 4A, where the N_{Pe} ~ 12 case shows the first signs of tending toward an exponential distribution.

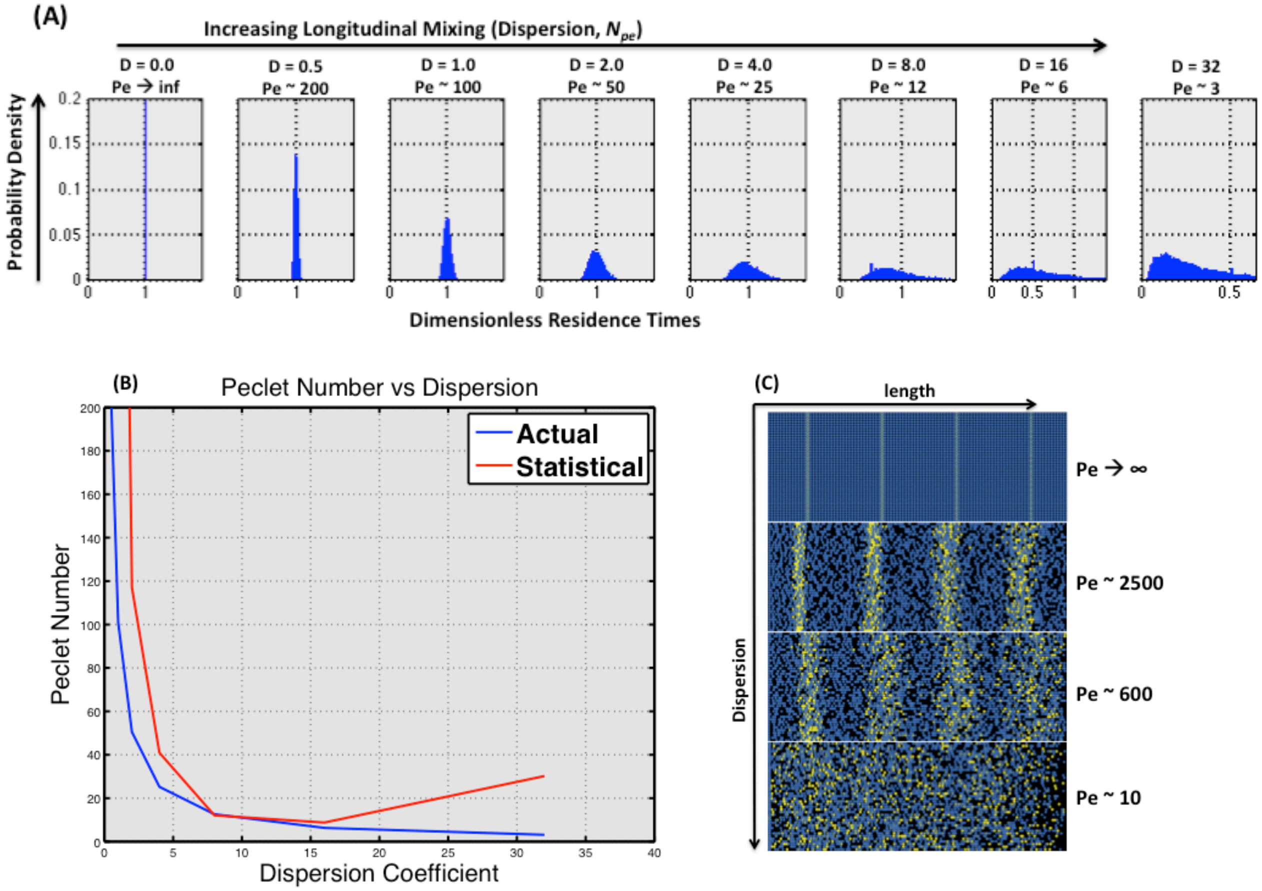

Figure 4: Influent of dispersion on residence time distributions within the reactor. (A) Probability density functions for the dimensionless residence time across a range of dispersion coefficients. (B) Comparison of Peclet numbers calculated either statistically or using Equation 2. The inverse relationship between sample variance and dispersion coefficient appears to fail near N_{Pe} ~ 10, which corresponds to a distinct transition away from Gaussian behavior. (C) Visualization of dispersive spreading within the reactor.

For undergraduates, it is not always clear what happens within the reactor that leads to these distributions. By pulsing a detectable inert tracer into the reactor feed, the characteristic spreading that is driven by axial dispersion can be visualized. This is how residence time distributions are obtained in practice, and a series of experiments are shown for varying dispersion coefficients in Figure 4C.

4.4 Reaction Mechanisms and Rate Laws

The stochastic model allows for two distinct reaction mechanisms, while the deterministic model allows the user to specify an elementary rate law. The import/export features enable direct comparison of the resultant concentration profiles, and allow for mapping the stochastic model's stochastic reaction mechanisms to deterministic rate expressions. Upon synchronizing the models, it is immediately evident that the reaction probability in the "Concentration Independent" mechanism is identical to the rate constant in a first order rate law. This revelation is demonstrated in Figure 5A, and suggests that the rate of a first order reactions is purely dependent on molecules having the correct orientation. Having taken several reaction engineering and kinetics courses at both the undergraduate and graduate levels, I find it quite surprising that I have never seen first order rate laws presented in this way.

A similar procedure was applied to the concentration dependent mechanism in the stochastic model, but no obvious connection was revealed. The concentration profile produced by the concentration dependent mechanism exhibits a rapid drop in concentration near the reactor entrance that quickly levels off to near-zero rate. This makes sense, as reactants rapidly deplete their local availability of other reactants to react with. First and second order analytical solutions were fit to the data by varying N_{Da}, but a perfect fit could not be achieved. As seen in Figure 5B, the second order rate law provides a better fit. This makes sense, as second order elementary reactions require collision of two reacting molecules.

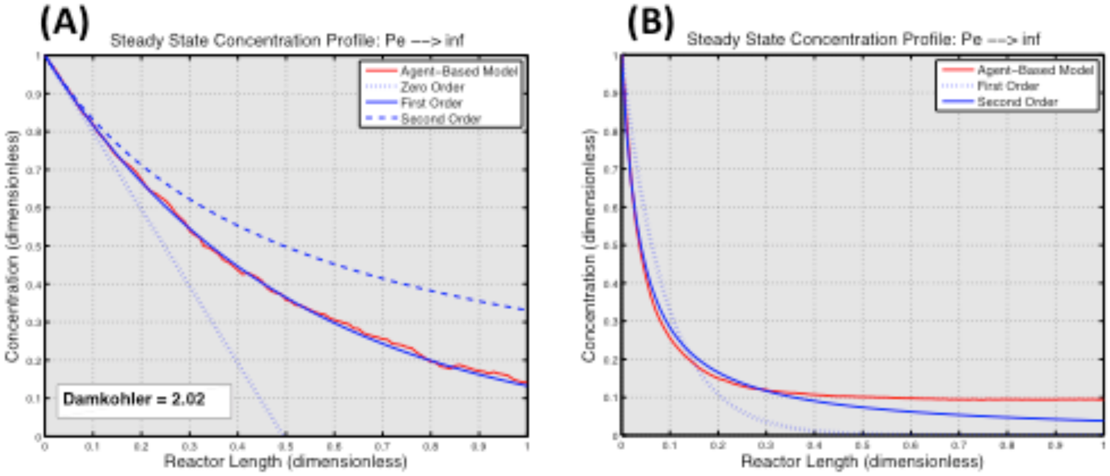

Figure 5: Comparison of reaction mechanisms with elementary rate laws. In the $N_{Pe} \rightarrow \infty$ limit, the zero, first, and second order profiles of the deterministic model are analytical solutions to the corresponding equation in Table 1. The mechanisms used were (A) concentration independent and (B) concentration dependent. In (A), all contours are based on the same reaction probability or rate constant, *k*. The perfect match between the concentration independent mechanism and the first order solution is preserved across all tested values of *k*. In (B), both the first and second order analytical models are fit to the stochastic data, but a perfect fit could not be achieved.

5. CONCLUSIONS

In light of the model validation, agent-based modeling appears to be an appropriate method of modeling chemical reactors in certain cases. This approach might be favored over numerical solutions to Equation 1 in the preliminary design stage where rigorous models are unnecessary. Agent-based reactor models might also be well suited to complex bioreactors, where growth and metabolic kinetics are not always explicitly defined. The merit of this approach requires further investigation of how computational costs scale with increasing model complexity.

During validation the concentration-independent mechanism was mapped to a first order rate law. This reaction mechanisms, while based on molecular-scale phenomenon, was applied to molecular quanta representing tens of millions of molecules. This result suggests that the mechanisms themselves are scalable, and interactions between individual molecules need not be applied to individual molecules in order to produce the emergent macroscopic rate laws observed in real systems. The mapping between microscopic mechanisms and macroscopic rate laws also suggests that the leading rate constant in elementary rate expression is just the probability of correct orientation. This is not how the rate constant is taught in conventional kinetics courses, and contributes a novel perspective on the meaning of kinetic rate constants.

The primary goal of the present model is to create a platform on which undergraduate students can develop their intuition regarding convection, dispersion, and reaction in flow reactors. A version of the turtle-based model has been demonstrated to one of the reaction engineering course instructors at Northwestern, and she has expressed interest in incorporating the model into the course curriculum next year. In this regard, the project has been a success.

6. FUTURE WORK

Both models leave ample room for extension. In both cases, the reaction mechanisms could be made increasingly complex in order to reflect real system chemistries. For instance, the inclusion of a reversible pathway would extend the system domain to include equilibrium-limited reactions where the tradeoffs between chemical and kinetics and thermodynamics are relevant. Going further, the models could be designed to import a stoichiometric matrix coding for an entire reaction network. These would be relatively simple extensions to implement, but were omitted from the current work in order to avoid obfuscating the purpose of this model.

The scope of the dispersion model explicitly excludes viscous effects, as they are encapsulated by the dispersion term of Equation 1. Viscous effects could be implemented if they were of interest in a convection-diffusion-reaction model, perhaps due to operation in a laminar flow regime or entirely different geometry. This would be particularly amenable to the turtle-based model, as each turtle could be assigned a momentum property. Turtles might transmit their momentum via viscous diffusion to adjacent turtles, with some form of no-slip condition implemented near the walls. Because viscous effects break radial symmetry, molecular diffusion would require at least a 2-D implementation.

REFERENCES

[1] Fogler, H. S. (1999). Elements of chemical reaction engineering.

[2] Kersner, R. (2004). *Travelling waves in nonlinear diffusion-convection reaction*(Vol. 60). Springer Science & Business Media.

[3] John, V., & Schmeyer, E. (2008). Finite element methods for time-dependent convection–diffusion–reaction equations with small diffusion. *Computer Methods in Applied Mechanics and Engineering*, *198*(3), 475-494.

[4] Douglas, J. and Russell, T. F. (1982) Numerical Methods for Convection-Dominated Diffusion Problems Based on Combining the Method of Characteristics with Finite Element or Finite Difference Procedures. *SIAM Journal on Numerical Analysis, 19*(5), 871-885.

[5] Li, M., & Christofides, P. D. (2008). Optimal control of diffusion-convection-reaction processes using reduced-order models. *Computers & chemical engineering*, *32*(9), 2123-2135.

[6] Levenspiel, O., & Smith, W. K. (1995). Notes on the diffusion-type model for the longitudinal mixing of fluids in flow. *Chemical Engineering Science*, *50*(24), 3891-3896.

[7] Michelsen, M. L., & Østergaard, K. (1970). The use of residence time distribution data for estimation of parameters in the axial dispersion model.*Chemical Engineering Science*, *25*(4), 583-592.

[8] Danckwerts, P. V. (1953). Continuous flow systems: distribution of residence times. *Chemical Engineering Science*, 2(1), 1-13.

[9] Levenspiel, O. (1999). Chemical reaction engineering. *Industrial & engineering chemistry research*, *38*(11).

[10] Tzatchkov, V. G., Aldama, A. A., & Arreguin, F. I. (2002). Advection-dispersion-reaction modeling in water distribution networks. *Journal of Water Resources Planning and Management*, *128*(5), 334-342.

[11] Cameron, D. R., and A. Klute. "Convective-dispersive solute transport with a combined equilibrium and kinetic adsorption model." *Water Resources Research* 13.1 (1977): 183-188.

[12] Squires, T. M., Messinger, R. J., & Manalis, S. R. (2008). Making it stick: convection, reaction and diffusion in surface-based biosensors. *Nature biotechnology*, 26(4), 417-426.

[13] Yariv, E., Ben-Dov, G., & Dorfman, K. D. (2005). Polymerase chain reaction in natural convection systems: A convection-diffusion-reaction model. *Europhysics Letters*, 71(6), 1008.

[14] Sibert, J. R., Hampton, J., Fournier, D. A., & Bills, P. J. (1999). An advection–diffusion–reaction model for the estimation of fish movement parameters from tagging data, with application to skipjack tuna (Katsuwonus pelamis). *Canadian Journal of Fisheries and Aquatic Sciences*, *56*(6), 925-938.

[15] Geiser, J. (2007). Discretization methods with embedded analytical solutions for convection–diffusion dispersion–reaction equations and applications. *Journal of Engineering Mathematics*, 57(1), 79-98.

[16] Wilensky, U. (1998). NetLogo Chemical Equilibrium model. http://ccl.northwestern.edu/netlogo/models/ChemicalEquilibrium. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL.

[17] Wilensky, U. (1998). NetLogo Simple Kinetics 1 model. http://ccl.northwestern.edu/netlogo/models/SimpleKinetics1. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL.

[18] Stieff, M. and Wilensky, U. (2001). NetLogo Enzyme Kinetics model. http://ccl.northwestern.edu/netlogo/models/EnzymeKinetics. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL.

[19] Wilensky, U. (1999). NetLogo. http://ccl.northwestern.edu/netlogo/. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL.

[20] Chu, Y., You, F., & Wassick, J. M. (2014). Hybrid method integrating agent-based modeling and heuristic tree search for scheduling of complex batch processes. *Computers & Chemical Engineering*, 60, 277-296.

[21] Pannala, S., Daw, C. S., & Halow, J. S. (2004). Dynamic interacting bubble simulation (DIBS): An agent-based bubble model for reacting fluidized beds. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, *14*(2), 487-498.

[22] Pereda, M., & Zamarreño, J. M. (2011, June). Agent-based modeling of an activated sludge process in a batch reactor. In *2011 19th Mediterranean Conference on Control & Automation (MED)*, 1128-1133.