

Interactive comment on “A total quasi-steady-state formulation of substrate uptake kinetics in complex networks and an example application to microbial litter decomposition” by J. Y. Tang and W. J. Riley

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Below we respond in italic by following the comments.

General comments: The authors discuss various approximations to solve networks of enzyme substrate reactions, all of which depend on an assumption that consumer-substrate complexes are in quasi-equilibrium and their concentrations can be solved, allowing estimation of the product production rate given the "handling time" of the complex. They compare three levels of approximation: First the full Equilibrium Chemistry

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(EC) solution of the system in which all enzymes and substrates are resolved. Secondly a total quasi-steady-state formulation (tQSSA) in which an approximate solution is formulated in terms of the total abundance of enzyme and substrate are utilized (the Equilibrium Chemistry Approximation, ECA). Thirdly, a classic Michaelis-Menten approximation, also in terms of total enzyme and substrate, though simpler than the more general ECA solution. The authors compare the schemes in several scenarios and argue that the ECA solution is closer to the EC solution and therefore a more appropriate choice for practical modeling applications.

I very much enjoyed many aspects of the manuscript. In particular the description of the basic formulation of the approximations and the discussion of various limit cases is very nice and very useful. I did not follow through the full perturbation expansion in the appendix, but the key algorithm (equation 13, the ECA approximation) can be found straightforwardly. As earlier papers have shown (e.g. Cha and Cha, 1965, quoted as equation 3 here), the ECA formulation is more general than the Michaelis-Menten (MM) approximation allowing for the case when the enzyme concentration is relatively high. Again, I found the development and discussion of the system very interesting and useful.

Response: *We appreciate the reviewer's positive comments.*

Comments: The manuscript then goes on to illustrate comparisons between EC, ECA and MM solutions. As presented the results suggest that the ECA approximation is a more flexible and accurate approximation than MM for a variety of applications. This makes intuitive sense since there are more flexible parameters that can be fit and a broader range of situations (e.g. high enzyme concentrations) under which the ECA will be appropriate.

That said, I found the comparison and evaluation part of the paper obscure and difficult to follow. It is not at all clear how many parameters, or which parameters, are being "tuned" or informed by the knowledge of the underlying rate coefficients of the system

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in each case. In my opinion, a clear explanation of how the comparisons are made, how many/exactly which parameters are fit/tuned and how much of the underlying, known set of rate constants is used in each case would greatly improve the clarity of the manuscript and the likelihood of the approach being adopted. I would have rather seen more detailed explanation at the expense of fewer examples. In my opinion it would be very helpful for the reader to be able to reproduce the test cases as easily as possible. Is it fair to interpret that the ECA approximation effectively has more free/tunable parameters than the MM and ECA-ML approximations; so, provided that you have the information to constrain the extra parameters, you are likely to get a more accurate solution over a broader range of applications?

Response: *We partly agree with the reviewer's comments and have strived to make our presentation clearer in the revision. However, we should point out that our ECA approach used the same number of parameters as the MM model being compared in our study. We have added a sentence to the Abstract, Discussion, and Conclusion sections to make this point clear. That said, our EC and ECA approach are more parsimonious than the MM kinetics but mathematically more consistent with the implied mechanisms. We used several examples to indicate our approach is better than the MM or ML models under various configurations. We think by presenting the results in this way, we increased the confidence in our conclusions and readers could better appreciate the usefulness of our approach in their problems. We note that Tables 1, 2, and 3 present parameter values for the different model configurations and Table 5 presents the best fitting parameter for model ECA-S3B3 in the litter decomposition problem.*

Comments: Overall, I very much liked this study. The discussion of the model formulations is thoughtful and revealing, the consideration of limit cases in relation to other formulations is useful, and the outlook for future prospects is interesting and exciting. While the comparison of different approximations is also very useful and thorough, and a key part of the study, it lacked a clear explanation of exactly how the different models

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in the comparison were constrained. I did not feel that I was given enough information to attempt to reproduce these tests simply and easily. In my view this is a very nice contribution and with a little clarification could also be a very accessible and useful introduction and "user guide".

Response: *Thanks for the positive comments and suggestions. On page 23, lines 5-16, we described the parameter inversion approach and cost function used. In the revision, we also expanded it (last paragraph in section 2.5) based on the reviewer's comments to be more descriptive for others to apply the method.*

Comments: Equations (10) and (12): The notation is not clear to me, with the trailing ",i = 1, ..., I" and ",j=1, ..., J"? Is this a typo? If not, what is the significance? On a similar note, I did not understand why the authors have switched to subscript k (instead of retaining i and j)? Its not hard to follow but seems unnecessarily obscuration to me.

Response: *We revised these equations to make them easier to understand.*

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