Second Round Review General Response

I would like to again thank the reviewers for their detailed assessment of this paper.

Reviewer 2

1. Minor note: Eq. 6 looks like you forgot to insert a line break in your equation array. (This is apparent in your LaTeX changelog.)

    Solution: Thank you for catching this. The line has been broken.

2. Line 219: Looks like there's an extra 1 in the mass subscript? (m_{1i})

    Solution: Thank you for catching this. The 1 has been removed.

3. Line 391: Forgot to close parentheses

    Solution: Thank you for catching this. The closing parenthesis has been added.

4. Line 397: Perhaps indicate *figures* 9 through 13.

    Solution: Thank you for catching this. The word "Figures" has been added.

5. Lines 462-463: I think it would be more accurate to say, "These isotopes have effectively no solubility limit" rather than saying they are "infinitely soluble."

    Solution: Thank you for catching this. This has been edited exactly as suggested.

6. URL for reference 6 points to the presentation, but the paper URL (which the page number corresponds to) is: `https://inis.iaea.org/search/search.aspx?orig_q=RN:44052619`

    Solution: Thank you for catching this. This has been edited exactly as suggested.

Reviewer 3

7. I know it takes a lot of work to revise a paper. The revisions were very thorough, and this is a good paper. I am pleased to recommend this paper to be published.

Solution: Thank you.

Reviewer 4

8. It would have been helpful to include a real-life application of the method, which might also have helped improve the methods you used. This is an excellent paper however

Solution: Thank you. I hope to present a real-life application of this method, beyond the simplified homogeneous clay-like medium presented here, in a future paper.

Previous review comments and their responses are retained below for reference.

First Round Review : General Comments

I'd like to extend my immense thanks to the reviewers, whom I think have improved this manuscript dramatically with their insightful comments. Please see below for discussion of each.

Differences between the submitted version and this revision can be found at the following url: `https://goo.gl/qRQuXn`. To see line changes, click on the "files changed" tab.

Reviewer 1

9. I enjoyed reviewing this manuscript, but I found it difficult to understand. The manuscript seemed to lack specific goals and conclusions. It was very abstract and long. This reviewer wondered if the addition of examples would have made the manuscript more useful. The title used the word "rapid," but this property was not developed in the text. Was this a review paper? Some of the figures in the current manuscript were illegible. I hope that the following comments can improve the manuscript.

Solution: Thank you for your particularly detailed comments. I have edited the manuscript once through for brevity. Specific goals (to demonstrate the capabilities of the Cyder software in comparison to GoldSim) and conclusions (appropriate validity for medium-fidelity fuel cycle simulations) were added to the introduction. Figures and figure captions were reviewed and many were enlarged for better legibility. All will be provided to the journal office in high resolution.

10. This abstract seemed to lack a clear statement of the goals of the paper, the methods used, results, and conclusions.

Solution: Thank you for this comment. I have re-written the abstract to include concrete details of the purpose, models, results, and conclusions.

11. Page 2 : Somewhere in this paragraph, we needed a statement about the goals and objectives of this study.

Solution: Goals and objectives have been added. Specifically, to describe the design, development, and mathematical models within Cyder and to verify the models in Cyder against a higher fidelity DOE tool, the Clay GDSM.

12. Line 35. Was this section still part of the introduction?

Solution: It's not intended to be. This section begins the first task of this paper, which is to describe the models implemented as part of the work. This is the software-paper equivalent of the methods section.

13. Figure 1. Was z depth?

Solution: Yes, I have now added this fact to the caption.

14. Page 4 : Line 62. What were the outer and inner components?

Solution: The example intended to be general, but I see that this is a confusing approach. I have made this more explicit. The example now specifically refers to the waste form and waste package as the inner and outer components.

15. Figure 2. All abbreviations in figures need to be defined in the figure caption.

> **Solution:** Great catch. Done for Figs 2, 3, and 4.

16. Page 5: What did “10[kg]” mean?

> **Solution:** 10kg was the example source term (mass of radionuclides in the waste form).

17. Line 82 plus. An example would have been helpful.

> **Solution:** This and all other subsections of section 2.1 reference the overarching example explained in its parent section. This example will be carried through the whole timestepping section. I have added text to communicate this better to the reader.

18. Page 6 : Equation 4. Why 10?

> **Solution:** 10 kg was the example source term (mass of radionuclides in the waste form).

19. Page 7 Lines 115 to 128. An example would have been helpful. This manuscript was abstract, and not easy to read.

> **Solution:** This and all other subsections of section 2.1 reference the overarching example explained in its parent section. This example will be carried through the whole timestepping section. I have added text to communicate this better to the reader.

20. Line 130. This statement needs a reference.

> **Solution:** This is a very good point. Barrier materials do not degrade appreciably over short time scales, so I have rephrased this completely to recognize the general stability of most materials in a repository environment over long time scales.

21. Figure 5. Again, we need to define all figures symbols and abbreviations in the figure caption.

> **Solution:** Great catch. I have added the missing definition for V_T.

22. Page 9 Figure 6 caption. Why is only Vdf available for transport?

> **Solution:** Great question. This particular model is naive. It assumes the portion of the component that remains solid has a negligible solubility. This model is appropriate for very durable components, such as borosillicate glass. For this model (but not for all four) the dissolution of the component material is handled in the degradation rate parameter rather than in a matrix solubility parameter. A better model would include a parameter for matrix solubility as well. I believe this should be a future feature in the package. At the moment, users interested in this higher fidelity can choose the 1D PPM model instead.

23. Equation 12. What did "degraded volume" mean?

> **Solution:** This is the volume that reflects the degradation state of the component. The volume is the degradation rate times the initial volume. I have called out V_d in the text to clarify this.

24. Page 10 Equation 15. What was the "degraded solid volume?"

> **Solution:** This is the volume that has been degraded, but has not dissolved into the mobile fluid. I have added text to clarify V_{is}, V_{ds}, V_{if}, and V_{df}.

25. Page 11 Line 173. "Into" or "onto?"

> **Solution:** Great catch. I did mean onto. Fixed.

26. No line number. The "solid concentration?" What did that mean?

> **Solution:** This is the concentration of the contaminant present in the solid component matrix volume. This has been further clarified in the text.

27. Line 177. What type of degradation?

> **Solution:** I have added text to explain that the model is agnostic to the mechanism of degradation, as it is simulated based only on the rate. Release based on this degradation is congruent.

28. No line number. What did "sorbate is in the degradable solids" mean?

> **Solution:** I meant sorbed material. Since 'sorbate' was unclear, I have replace the use of sorbate with 'sorbed material' instead. Thank you.

29. Page 14 Line 210 should begin with "Because." Since is a time such as "Since this morning, I've been reading this manuscript."

> **Solution:** I chuckled. Thanks for that. I have fixed this, and noted the lesson for the future.

30. Page 22 Line 330. Were these experiments done for the current study? How much of the current manuscript is new material, and how much was already published in reference 21?

> **Solution:** Excellent question. You were not the only reviewer to find this unclear. All simulations were indeed, done specifically for this work and by this author. Indeed the Clay GDSM results (figures 14, 16, 18, and 19) were discussed in reference 21 (notably, this was just a 4-page ANS summary and not an archival journal article). I have now clarified this distinction in the captions of figures 14, 16, 18, and 19. Those simulations were used as reference, as a higher fidelity verification for the simulations discussed in the section. The simulations discussed in this section, conducted with Cyder, are the focus of all other figures and discussion.

31. Line 342. "Were conducted" Why is this statement in the results section?

> **Solution:** I'm not sure I understand the concern here. I tend to follow a style guide in which the work presented in the paper is discussed in the past tense, particularly in the results section. I think that the reviewer's comment stems from this past tense being confusing. I have clarified that sentence to state, instead, "In the present work, many numerical experiments successfully verified the capabilities of the Cyder software library". I hope this form of the sentence is more clear.

32. Line 344. What was a “global parameter”?

Solution: I just meant universal parameters, throughout the simulation. So, I have changed this text to say “simulation parameters”.

33. Line 348. What did “accepting 1 waste stream” mean?

Solution: I have changed this text to say “No more than one waste stream object is stored per waste form.” I hope that is more clear. I just mean that, in the object oriented sense, the waste form object (e.g. a certain size and shape of borosilicate glass) is associated with one waste stream object (the isotope vector of waste material, such as 1kg of Tc99 or 2kg of Cs137, or some combination of many masses of isotopes.).

34. Line 351. What did “a far field component” mean?

Solution: I added a parenthetical to be explicit. It now says “a far field component (i.e. the host rock)”.

35. Line 358. A solubility limitation was set? Does this mean that CYDER does not use actual solubility values?

Solution: The user must provide the solubility values. While this provides the user with complete control, it may be inconvenient for some users. Future extensions to Cyder will include a default database, ideally through the PyNE toolkit. I have added text to this effect.

36. Figure 9. We need to define all symbols and abbreviations used in a figure.

Solution: Good catch. Done.

37. Figures 10, 11, 12, and 13 are illegible. They are too small. Label all axes.

Solution: The sizes of each has been increased twofold. Axes are all labelled.

38. Page 24 Line 389 hints some of the material in the current manuscript has already been published in reference 21.

> **Solution:** Reference 21 was an ANS conference summary which presents results of the GoldSim-based Clay GDSM model from DOE. The present work uses that previous work as a benchmark for comparison. That is, in the present work, results from Cyder are compared to those Clay GDSM model results from the reference. Key plots are reproduced here. To make this distinction more clear, I have added citations to all plot captions which I produced as a part of the previous work.

39. Line 399. What is a "sharp turnover?"

> **Solution:** I just meant the elbow in the figure. I have now changed this to be more explicit about the meaning. It now says " Specifically, in Figure 15, marked transition to the solubility-limited regime is seen where the solubility limit exceeds the point at which it limits movement.

40. Figure 14 is illegible.

> **Solution:** I have increased the size of Figure 14. It will be provided separately to the journal in high resolution.

41. Page 26 Line 419. Kd has units.

> **Solution:** That is very much true. However, these results are referring to a multiplication factor applied to K_d. I have called this the K_d factor. While K_d varies by isotope, the factor was applied to all isotope K_d values.

42. Figure 16 is illegible.

> **Solution:** I have increased the size of Figure 16. It will be provided separately to the journal in high resolution.

43. Lines 432, 434, and 436. Try to use the words "high" and "low" for vertical references rather than to qualify concentrations or properties.

Solution: Great advice. I have changed the text to use fast, slow, and large instead.

44. Figures 18 and 19 are illegible.

Solution: I have increased the size of Figures 18 and 19. They will be provided separately to the journal in high resolution.

45. Line 336. Are these conclusions?

Solution: Thank you for pointing this out. You are quite right that the Results and Discussion Section is no replacement for concise conclusions. I have renamed the final subsection (previously called significance). It is now a section of its own entitled "Conclusions." I have not changed the text of that section, however.

46. Line 447. "Rapid" relative to what? Compared to what?

Solution: This is a good point. I neglected to describe (beyond the motivation in the beginning) the speed up provided by Cyder (over GDSM). I have now added a remark on their comparison in the results section and have made the magnitude of the speed up more clear there. (Cyder performs simulations in minutes where the higher fidelity GDSM requires hours.)

47. Page 29 Lines 456 to 472. The "conclusions" only seemed to promote the use of CYDER. There were no specific conclusions. What was new in this study?

Solution: Point taken. I have reworked the conclusion to focus on the facts. The design and development of Cyder itself is the primary effort being described in this paper, so a summary of Cyder's capabilities remains in the conclusion. However, I have framed this discussion to also emphasize the success of the Cyder verification effort that was the related focus of this work.

Reviewer 2

48. This article describes the implementation of a medium-fidelity contaminant transport model applicable to the Cyclus nuclear fuel cycle simulator. Overall this fills an important gap in fuel cycle simulation tools for back-end nuclear fuel cycle assessment.

Overall this article is well-written and well-organized, with careful attention given to methodological details used within the model. One minor issue I have though is that given the specialized nature of the discussion (i.e., hydrology and contaminant transport), there are a number of areas where I feel the clarity of the manuscript could be improved by simply being more explicit with nomenclature used. For example, in line 181, where is the relationship between m_ds and m_T outlined? Similarly, what does "d" (used in Eq. 30) denote - bulk density? Even with some background in the subject matter (which I cannot presume all readers to have) I found this difficult to follow without further explanation of nomenclature.

> **Solution:** Thank you for your kind words. In response to this comment, as well as other similar comments by yourself and other reviewers, I have added additional notes in the text to call out definitions of subscripts such as ds (degraded solid) and T (total). Relationships were previously described in equations (m_{ds} in Eq. 22), but I failed to give english descriptions of these. I have now added english definitions of such volume and mass subscripts to make this more clear. Thanks!

49. Similarly, in Figures 9-13, what does F_d refer to? I assume from context that S_{ref} refers to the solubility limit imposed for the nuclide, but again - please make your nomenclature more explicit.

> **Solution:** This is a great catch. I never defined F_d (fractional degradation rate). You are correct about S_{ref} I have now added a definition of both F_d and S_{ref} to all figure captions where they are used.

50. Likewise, given that the purpose of this study is a qualitative comparison of the behaviors of the Cyder generic repository model to a prior DOE-developed model (the Clay GDSM), it might be helpful to identify which figures originate from the latter. For example, are Figures 14, 18, and 19 from the Clay GDSM? If so, please indicate this explicitly in the captions.

> **Solution:** Correct. This has been fixed with citations in the captions. I think all reviewers made this comment!

51. With respect to Equations 5 and 6, if m_{ij} denotes the mass flux, then shouldn't Equation 6 specify m_{ij} as a time-integrated quantity, given that $m_j(t_n)$ is a mass quantity and m_{ij} is a mass flux?

Solution: Good catch. Fixed.

52. In equation 28, c_p should be a capital C.

Solution: Correct! Fixed.

53. Line 240 ("The correspon") appears to be a typo.

Solution: Thanks! Fixed.

54. In section 3.2.2 (lines 407-408), it would be helpful to define the relationship of the retardation factor R_f to K_d. i.e., $R_i = 1 + \rho_b * K_d/\theta$, where ρ_b is the bulk density and theta is the porosity. Similarly, this is made most clear to the reader if you then illustrate the effect of the retardation factor in terms of the effective contaminant velocity, i.e. $v_{eff} = v/R$, where v is the average linear velocity.

Solution: This is an excellent point and I have added the relationship between R_f and K_d in the text as recommended.

55. I find the comparison of Figure 20 to Figures 18 & 19 somewhat confusing; the latter two use a log-log scale, yet Figure 20 is on a linear scale. Is all we are supposed to see a saturation behavior from degradation rate? I still think this comparison would be better expressed as a log-log comparison.

Solution: I agree that the comparison would be clearer if they were both log-log. Unfortunately I did not have time to reproduce these graphs (I only had two days with your detailed comments). However, I hope to be able to make this change before publication if I am given that opportunity.

56. In both the introduction and the conclusions, you indicate that Cyder is compatible with Cyclus (specifically version 0.3). What is the status of its compatibility with the most recent Cyclus v1.5 release? Are there plans to maintain compatibility if it is not presently compatible?

Solution: Quite correct! This work was conducted with Cyclus v.0.3. Current work is ongoing to bring Cyder up to date with the most recent version of Cyclus. This work will serve as fodder for integration testing in that transition, ensuring that the same results are achieved with the new version of Cyder. I have added text to the paper indicating this.

57. Finally, with respect to citations: Is there a more complete, locatable citation for [1] and [5]? Citation [6] is incomplete: the full citation is:

    Boucher, L., Alvarez Velarde, F., Gonzalez, E., Dixon, B.W., Edwards, G., Dick, G., & Ono, K. (2012). International comparison for transition scenario codes involving COSI, DESAE, EVOLCODE, FAMILY and VISION. Proceedings of the Eleventh Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation, (p. 406). Nuclear Energy Agency of the OECD (NEA)

    ISBN: 978-92-64-99174-3 URL: `https://inis.iaea.org/search/search.aspx?orig_q=RN:44052619`

Solution: All fixed. URLs added, bibliography entry for Boucher et al. fleshed out.

58. Is citation [8] a thesis? Please make this more explicit and indicate any kind of URL or other locator device, if possible. Also, should citation [10] point to http://fuelcycle.org? Finally, citation [19] clearly appears to be in error; please check your BibTeX database for this one.

Solution: Yes, 8 was a thesis, 10 now points to fuelcycle.org (an alias of cyclus.github.com), and the URL for 19 has been updated to avoid library proxy servers.

Reviewer 3

59. Revisions are more moderate than minor, but should not be overly difficult to complete. Please see the attachment. One of the main concerns was that since this a software journal, some of the math that is well known to researchers in fate and transport might not be known to readers of this journal. This is discussed more in the review.

Solution: Thank you for your very detailed comments. Your main concern is well taken. Other reviewers (above) made specific requests regarding this balance between software and method. In addressing those, I believe the paper has become much more accessible to all readers. Examples have been made more explicit, I have made attempts to reduced the wordiness and abstraction of the paper somewhat. I hope these changes have made the mathematical discussion more accessible to a broad audience. *Please note that I did not have access to your attachment for quite a while (for some reason, it was only available to the editor in evise). After phone calls and emails, it was sent to me, but only two days before the revision submission deadline. I hope you will forgive that I was rushed somewhat when responding to your comments. I very much appreciate the detail with which you reviewed this paper.*

60. Overall, this is a great paper, well structured in discussing the CYDER library, then the various means of calculating radionuclide transport behavior, then the underlying mathematical models, and finally the results and discussion. At the beginning the paper would benefit from clarifying what is meant by "technologically coupled." Placing this paper in the context a greater discussion of why nuclear waste disposal decisions rely on the full nuclear fuel cycle in the abstract and introduction would make the paper stronger. It would help to provide what a "medium-fidelity" time step is in terms of hydrologic modeling of a nuclear waste repository. Because there is a significant amount of mathematical formulations in this paper, describing the physical conditions is of high importance. Please review the figures and consider adding more descriptive content. More comments on the figures is discussed below.

Solution: Thank you. Regarding technological coupling, I have added a sentence in the introduction explaining that fuel cycles and spent fuel repositories are coupled by SNF volume, isotopic composition, mass, disposition, activity and other variables. These variables depend on the fuel cycle choices made upstream and impact repository capacity, loading strategy, and performance. Regarding the time step for medium fidelity, I should note here first that the reference to fidelity is not specifically with regard to time, but also with spatial and physical simplifications, depending on the model (among the four) chosen for each component. In the timestepping section, I have added a note about the default time step size (1 month) and its appropriateness for this level of fidelity on disposal timescales. However, the user is welcome to use arbitrarily small or large timesteps. Regarding figures and content, I have made changes according to your comments below.

61. The vertical depth is mentioned first on page 2 line 42, but not again until page 16, equation (43), and then page 18, line 263. Typically, for modeling radionuclide transport in the repository, flow would be considered in both the +x and +z directions as indicated in Figure 1. (Some models also consider matrix diffusion in the +z direction). It is not

stated in the paper why only the flow in the z direction is considered for this model. For a repository located at a 500 m depth, for example, why would the flow in the z direction be significant? There are reasonable assumptions that can be made, but this is why is it so important to describe precisely the physical conditions that this model describes in order to justify this.

Solution: I have added text on page 18 to explain that model is simply making a 1-D transport assumption for simplicity. The vertical direction was chosen because it is the most conservative choice, among directions, since it is the shortest path to the biosphere (and therefore, perhaps, humans). As you note, flow is not significant in any direction for geologic media under consideration for repository sites internationally. The far field is an excellent barrier to release and of course repositories are accordingly quite good at containment.

62. In Figures 9-13, what information exactly is being plotted on the graphs should be clearly stated. Section 3.1 generally describes the simulations, but not what is shown on each figure. The captions should be descriptive, even if this means there are only one or two figures per page.

Solution: Thank you for this comment. I have added more detail to these captions to better define all symbols that appear to make more clear the meaning of the plots.

63. Page 2 line 7-18: Explaining why dynamic waste disposal calculations are valuable, as opposed to the static outputs from other tools, would make the paper stronger.

Solution: This has been done (see previous comment in response to your initial mention of this issue.)

64. Page 2 line 21: Provide an example of what kind of time step 'medium fidelity models' includes

Solution: This has been done (see previous comment in response to your previous mention of this issue.)

65. Page 2 line 24: Explain the difference between using Cyder as a standalone library and in collaboration with Cyclus

> **Solution:** I have explained this statement by emphasizing that it is compiled as an independent shared object library with its own application programming interface. This terminology will be appropriate for the readers of this journal.

66. Page 4 lines 59-61: "These calculations proceed from the inner-most component to the outermost component, with mass transfer calculations conducted at the boundaries." Could use a labeled diagram that describes what the inner components are versus the outer components or provide more detail in Figure 1. I cannot tell what is the "geosphere" and what are the various containment layers.

> **Solution:** You are not the only reviewer to feel this way, and I appreciate that you have pointed out how confusing this is. I have elected to add additional detail to the caption of Figure 1 to address this. It now says "In CYDER, as in a canonical drift-tunnel repository, waste form components (the innermost components) are contained by waste package components which are, in turn, emplaced in a buffer component (the backfilled emplacement tunnel into which waste packages are loaded). That buffer component contains many other waste packages, spaced evenly in a horizontal grid. The geosphere (the outermost component) occupies all space below the repository surface and outside of the buffer components (emplacement tunnels). The CYDER repository layout has a depth (Δz) and package spacing defined by the user input (Δx within the drifts and Δy between drifts."

67. Page 4 line 74: Please explain source and sink more thoroughly for non-Cyclus users, and include more description of these in Figure 2.

> **Solution:** Excellent observation. These are actually unrelated to the CYCLUS notion of the source and sink. So an explanation may be even more important for Cyclus users (for whom the term is overloaded)! Thanks for pointing this out. I have added a sentence to clarify the meaning of these two components in the example.

68. Page 5, Figure 4: The asterisk for t_n^* is not defined

> **Solution:** I have added, to the caption, more detail about this timestep updating syntax and all other symbols used in this figure.

69. Page 6, Equation 5: While is standard notation for mass flow rate, it might be helpful to clearly define it in the text

> **Solution:** This equation has been clarified with a statement in the text as well as an additional equation 6 describing the integral relationship between m and $\dot{m}$.

70. Page 7-16: Might be more clear to include a table that shows the differences between the four Radionuclide Mass Balance models; include the inputs, the built in assumptions, the strengths and the weaknesses.

> **Solution:** This is an excellent idea. I sketched a bit of this table idea to see it could be done clearly, but I'm afraid I came up short. The table quickly became unweildy, given the detail necessary to differentiate the models in their many facets. I like this suggestion, but was unable to make it work.

71. Page 8, Equation 9: m_{jk} should be defined right below Equation 9 where it is introduced first as opposed to below Equation 10.

> **Solution:** Fixed.

72. Page 9, line 148: Would readers of this journal know the Dirichlet boundary condition? Perhaps include a description of it.

> **Solution:** Good question. It is my understanding that readers of this journal are engineers who write research software for engineering. After looking at some examples among previous articles in this journal, I think this is something that the reader will understand, particularly since the form of the boundary condition is given in the figure.

73. Page 9, line 150-151: "is the average concentration throughout the degraded volume" at which point (j or k), or at the boundary between the two? The wording is a bit confusing.

> **Solution:** Good catch. I intended to refer to $C(r_j)$, the concentration at r_j, which is the boundary between j & k.

74. Page 9, Figure 6: This figure would be clearer if V_T was shown as full of the various constituent parts.

Solution: This seemed like a great idea, so I tried it (see below). However, I'm not convinced it isn't actually more confusing, so I have chosen not to make this change. If the reviewer feels strongly that the below image is more clear, I can certainly make this change, but I do feel like it may actually add to the confusion.

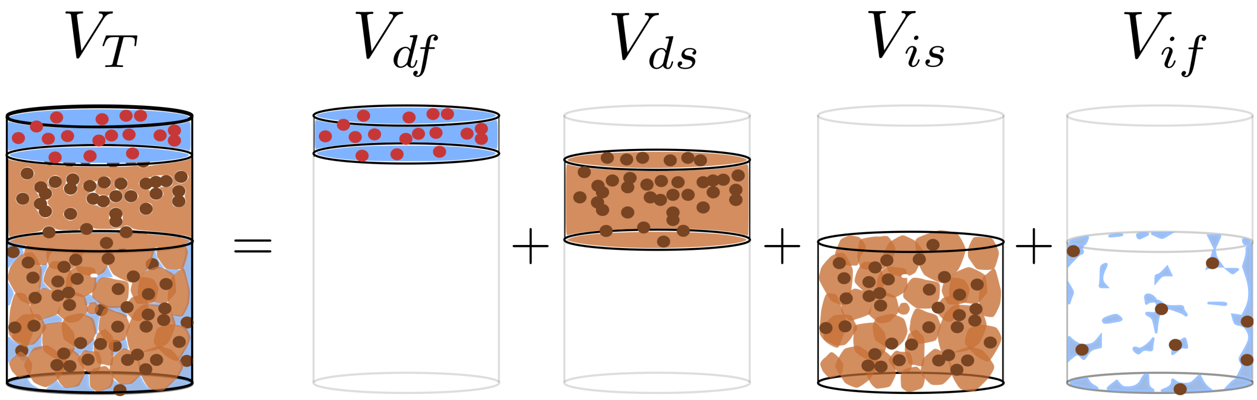

Figure 1: The degraded volume is modeled as a degraded solid volume, V_{ds}, and a degraded fluid volume, V_{df}. The intact volume is modeled as an intact solid volume, V_{is}, and an intact fluid volume V_{if}. Only contaminants in V_{df} are available for transport.

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75. Pages 9-10, equations 13-21: θ is not defined.

Solution: The porosity, θ, is defined in the paragraph immediately preceeding this set of equations.

76. Page 10, line 161: Define contaminant masses and why they are the ones available to adjacent components.

Solution: Thank you for this comment. I didn't realize how unclear this was. All masses are contaminant masses in this context. I have added a reminder of this to the beginning of the section at what was previously line 114.

77. Page 10, line 165: The use of the word 'available' is not really mathematically based. Because there are so many equations, the mass transfer of the contaminants should be precisely described.

Solution: Very true. I have replaced this with the more explicit wording, "mass m_{ij} that can be transferred to the adjacent component in the mass transfer phase."

78. Page 12, Equations 30 & 31: It is not clear how the result in 31 was obtained from 30.

Solution: Great catch. This was based on the definition of V_{df} as a function of V_T. I have added text to this effect. But, more importantly, as you noted, there was an extra d. Thanks for noticing this level of detail. I have double checked the source code and you will be pleased (as I was) to know that in the implementation, the V_{df} definiton is plugged in directly, so this typo is in the paper only and did not appear in the code itself.

79. Page 15, lines 220-27: Similar to the comment on the Dirichlet condition, both the Cauchy and Neumann conditions should be clearly defined. They are used in Figure 8 but not clearly indicated either.

Solution: I have called these out by name in equations (40) and (41). Given the engineering computation background of the readership, I suspect an elementary explanation of Cauchy and Neuman conditions would underestimate the readers. I hope that common differential equation boundary conditions of this type are well understood by engineers, particularly the computationally trained readers of this journal.

80. Page 16, Equation 43: Based on experience, D and v should be diffusion coefficient (or dispersion) and advection, respectively, although they are not defined here. Would the readers of this journal inherently understand this, however? It is typically just good form to reference all the variables in an equation, or state that D and v were defined previously in equation (x).

Solution: You are quite correct, I have moved the definitions of D and v to their first mention. I do believe that the readers of this journal are engineers and engineers are typically familiar with flow (so advection and diffusion kernels will be familiar). However you are correct that the explanation needs to be pointed out in this first mention. I have referenced the discussion of advection and dispersion (which appears in the following mass transfer section) from this section in which they first raise their heads. Thank you for this suggestion.

81. Page 16, Equation 44: The retardation factor is not physically defined. This is an important parameter in radionuclide transport studies.

> **Solution:** A definition has been added to its first mention, as a function of bulk density.

82. Page 16, line 240: This line is cut off and sentence starting 'The correspon' does not make sense.

> **Solution:** This has been fixed, see previous comments to reviewer 1.

83. Page 16, line 246-49: If there are results comparing the explicit and implicit modes of mass transfer, might be worth mentioning where they are discussed below. If there are not results, might be worth discussing the general success of the implicit mode.

> **Solution:** Any difference introduced by the explicitness vs. implicitness of the modes is dwarfed by the differences between the models themselves. Nonetheless, in the results section, I have added a reference to the much longer dissertation where such additional results can be found.

84. Page 16, lines 250 & 251: Advection and dispersion have been mentioned enough to warrant a definition at its first mention in the paper. It is defined on page 17, line 253, but discussed numerous times in the paper already.

> **Solution:** This has been solved on page 16 by referencing this definition at first mention.

85. Page 16, line 251: 'equationfor' needs a space inserted.

> **Solution:** Fixed.

86. Page 20, Line 299: Equation (44) is mentioned as an afterthought as to imply that the reader should have known that (43)-(44) was what C(z,t) represents in this section. Because there is a lot of derivations, an earlier mention to this in Section 2.3 should be included.

Solution: I'm sorry to say that I don't understand this comment. Section 2.3 is after, not before, (43) - (44). If you mean section 2.2.3, then please note that each of the four subsections (2.2.1, 2.2.2, 2.2.3, and 2.2.4) seek to describe *different* models for determining C(z,t). So, in fact, equation (44) only applies to the model discussed in 2.2.4 and is not at all related to the model in 2.2.3.

87. Page 23, figure 9: Unclear what the CompID values represent, do not know what F_d represents.

Solution: These two items have now been defined in the captions of all of the figures that use them. See response to reviewer 1.

88. Page 23, figures 10-13: Unclear why the IsoID legend is present as the graphs only appear to include ^{238}U.

Solution: The graphs include all isotopes listed. It is simply the case that the vast majority of the material in the example was made of ^{238}U isotopes. So, blue is the predominent color, and all others are dwarfed at the bottom of the plot.

89. Page 24, line 372: 'accross' is spelled wrong

Solution: Fixed.

90. Page 26, Figure 16: Both ^{129}I and ^{79}Se exhibit a markedly distinct behavior than the other radionuclides and should be explained as to why. Additionally, because only K_D is shown on the graph, but in fact the analysis is focused on the retardation coefficient, the relationship between the two should be shown. Additionally, the effects of the retardation factor and K_D are dependent on the sorption isotherm that is assumed. This should be included in the discussion.

Solution: This is correct, I have pointed out that the different behavior of these nuclides is due to their near infinite solubility. Additionally, I have now added a definition of the relationship between K_d and R_f at the very beginning of the section.

91. Page 28, Figure 18, 19: The text on the graphs is really small and hard to read unless one zooms to 200%. While this isn't really that much of an issue, it might be prudent to enhance the graphs if possible, just fyi.

Solution: I have increased the size of Figures 18 and 19. These will be provided separately to the journal in high resolution.

Reviewer 4

92. Some aspects of material transport are treated somewhat superficially. The first is that the radionuclide waste material that would be transported by groundwater is essentially insoluble uranium dioxide to the surface of which fission products are bound by adsorption, which is essentially a weak chemical bond. This suspension of particles in water is treated as if it were a water solution rather than a suspension. Relatively straightforward laboratory experiments investigating the difference in transport between a true solution and a suspension might have resulted in somewhat different parameter values. Alternatively, discussion of such experiments might be found in the literature. The Hanford site provides a physical example of contaminated groundwater (from the French drains) moving through an adsorbing matrix, and might have been cited. In addition, published data of groundwater movement at the proposed repository site in Nevada might have been cited. Some tabulation of Cyder results with results from some of the cited models would be illuminating.

Solution: Thank you for these suggestions. It is true that some of the models treat transport very superficially. The software implementation aimed for speed, rather than high fidelity. I hope that future improvements can emphasize fidelity without sacrificing speed. Regarding the treatment of particle suspension as solution rather than solution, you're quite right that this is a weakness. Your suggestion for including data retrieved from Handford or Yucca Mountain would be excellent future feature improvements to this framework. The current implementation made comparisons with simulations of a homogenous medium, reducing chemistry, generic clay host rock environment. Given the renewed interest in Yucca Mountain, verification against high fidelity tuff models is very desirable. The comparisons between Cyder and the cited GDSM model were displayed as plots, rather than tables, due to the sheer size of the tables that would be needed. Importantly, the raw data for the Cyder results can be retrieved in its open source repository. Thank you so much ffor these suggestions.