Models to Predict the Removal of Emerging Micropollutants from Water by Novel Adsorbents in Fixed-Bed Column Processes

Informational Webinar Questions and Answers

August 15, 2024

Application Information

- **Will the models developed be owned by EPA entirely, open source, or be owned by the applicant?**
  Answer: Models developed with assistance funds are not owned by EPA. They are intended to be used by the public consistent with the federal grant and cooperative act and EPA Order 5700.1. EPA may use the models consistent with § 200.315, "The non-Federal entity may copyright any work that is subject to copyright and was developed, or for which ownership was acquired, under a Federal award. The Federal awarding agency reserves a royalty-free, nonexclusive and irrevocable right to reproduce, publish, or otherwise use the work for Federal purposes, and to authorize others to do so."

  Also, as stated on page 7 of the funding opportunity, "it is expected that the model development and code for these models will be made publicly available upon completion of this project." However, the full scope of uses will be subject to the provisions within § 200.315 and any additional uses expressly permitted by the rights holders or applicable law.

  For more information, you can find requirements associated with data access, information release and copyrights at the EPA Solicitation Clauses webpage: https://www.epa.gov/grants/epa-solicitation-clauses-20240614.

- **Can you clarify what two classes of adsorbents mean? Are Metal Organic Frameworks (MOFs) one class only, or can the proposal include two different MOFs?**
  Answer: Different classes of novel adsorbents means that the targeted adsorbents under each class have different design parameters and removal mechanisms. Therefore, two different MOFs are not considered as two different classes. You should pick two different classes (e.g., MOFs and covalent organic frameworks [COFs], etc.). These are just examples, and the selection is not limited to them. The important aspect is to justify the selections and how to link them to your hypothesis.

- **For approaches that require significant high-performance computing (HPC), can we use National Science Foundation-managed HPC resources without overburdening the budget? More specifically, can federally-owned HPC resources be added on top of the $1,000,000?**
  Answer: You may use federal resources for the computations that you need. Please be sure to provide written justification and/or a letter of support, if possible. Note that the budget must not exceed $1,000,000 in federal funds per award and a minimum 35% non-federal cost share/match of the total project costs is required, so the federal resources may not be included as part of the cost share as noted in section III.C. Please feel free to reach out to Ron Josephson (josephson.ron@epa.gov) for more specifics.

As stated in section III.A. of the funding opportunity: “The applicant institution may enter into an agreement with a Federal Agency to purchase or utilize unique supplies or services unavailable in the private sector to the extent authorized by law. Examples are purchase of satellite data, chemical reference standards, analyses, or use of instrumentation or other facilities not available elsewhere. A written justification for federal involvement must be included in the application. In addition, an appropriate form of assurance that documents the commitment, such as a letter of intent from the Federal Agency involved, should be included.”

- **Can machine learning be used to correlate multiple mechanistic models? Or can machine learning not be used at all?**
  Answer: Artificial intelligence or machine learning, which are essentially “black box” models, are not favorable. The models are expected to have physical meaning and should inform better design of novel adsorbents.

- **Can the outcome be a code or model that needs to be fed to proprietary software like Comsol or Aspen to design full-scale systems?**
  Answer: Yes, but a demonstration of the developed model implemented using free and open-source software would be preferred.

- **Should we focus on adsorbents and reactive adsorbents?**
  Answer: Your application should justify selecting the specific adsorbents to support the steps of building a new model. If that is the technology you are proposing to model, then it should be documented.

- **Adsorption and absorption are defined differently. Can you please clarify if the funding opportunity will focus on adsorption or absorption?**
  Answer: The application can focus on adsorption, absorption, or both, as appropriate for the sorbent. The developed model should capture the expected behavior of the novel sorbent. Proposals should describe the appropriate mechanisms and discuss associated experiments to validate the associated model. The key feature is that an appropriate mechanism can be described mechanistically to help test the associated sorbent and aid in the future design of that class of sorbents.

- **Can each class of adsorbent target be a different family of micropollutants?**
  Answer: Yes, it is even encouraged that each class is a different family of micropollutants. Be sure the justification and hypothesis for each are clearly indicated.

- **Can you clarify how you define pollutant classes? Are perfluoroalkyl sulfonic acids a different class from perfluoroalkyl carboxylic acids? Are perfluoroalkyl acids different from perfluoroalkyl ether acids? Are pesticides a class? Are triazines a class?**
  Answer: Per- and polyfluoroalkyl substances (PFAS) are a class, pesticides are another class, and submissions on other classes (that are not PFAS or pesticides) are welcome. There are no limitations on the selections as long as the justification of the selections is clear, and they can

help build meaningful models. Examples of other classes would be herbicides, personal care products or pharmaceuticals. Ultimately, it is expected that cross comparisons between these groups will be made, for example, by comparing negatively, positively, neutral, and Zwitterionic groupings.

- **If PFAS is one class, what about pesticides? Are pesticides one class or are triazines an example of a class?**
  Answer: Yes, pesticides are one class. Justification of any selection is expected to explain how this selection supports the model development and validation.

- **Would more holistic approaches involving multiple classes like non-targeted analysis (NTA) also be allowed?**
  Answer: Holistic approaches like NTA can help inform some aspects of the project but should not be used as a primary approach.

- **Is there any difference in your preference between chemical and physical adsorption processes?**
  Answer: There is no preference, as long it is defined and justified in your project.

- **Are microplastics considered a class of micropollutants in the scope?**
  Answer: No, microplastics would not be within the scope of this funding opportunity.

- **Is there a list of adsorbents that would generally be considered novel, or can any adsorbent be considered novel as long as it is well justified**
  Answer: The adsorbent should be well justified. For this funding opportunity, a novel adsorbent is defined as a modular adsorbent that has been designed and synthesized to have specific characteristics and functionalities to selectively remove a certain class or classes of contaminants in a fashion that is not defined by existing modeling programs.

Eligibility

- **Are international collaborations allowed/encouraged? Specifically with universities in other countries.**
  Answer: Collaborations with foreign universities are permitted. Research involving populations in foreign countries is allowed as long as the results of research under this funding opportunity benefit the U.S. and are applicable/transferable across the U.S. International organizations cannot be the primary applicant but can be a sub-awardee.

- **What do you define as a consultant? What can and can't they do?**
  Answer: The funding opportunity states, “Consultants are individuals with specialized skills who are paid at a daily or hourly rate.” A lead institution from academia may propose consultants in their application, but the grant recipient must follow the competitive procurement procedures

described in the RFA. Consultants are not to be listed as PIs or co-PIs. See page 32, section IV.C.5.iv.f for more information.

As stated in the funding opportunity, "Any procurement of services from individual consultants or commercial firms (including space for workshops) must comply with the competitive procurement requirements of 2 CFR Part 200.317-200.327. Please see EPA Solicitation Clauses for more details. EPA provides detailed guidance on procurement requirements in the Agency's Best Practice Guide for Procuring Services, Supplies, and Equipment Under EPA Assistance Agreements."

- **Is there any possibility for us to discuss our proposal ideas with one of the program coordinators before drafting a full proposal?**
  Answer: To be fair to all potential applicants so that everyone has the full range of information about the funding opportunity when applying, we cannot discuss specific proposals in advance of submission. However, feel free to email the project officer, Rich Callan, (callan.richard@epa.gov) for more general or technical questions.

- **Can we submit a white paper or one-pager?**
  Answer: No. You can email the project officer, Rich Callan (callan.richard@epa.gov), to ask if something is clearly outside the scope, but we will not assess the quality of your ideas for the application by reviewing a white paper or one-pager.