Simulating and evaluating the efficiency of purification of drinking water containing Lead using plasma techniques

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Abstract

. Water contamination by lead represents a critical public health and environmental issue, necessitating the development of effective and sustainable remediation techniques. This study employs a simulation-based approach to investigate the application of plasma technologies for the purification of lead-contaminated water. Plasma-induced reactions offer a promising avenue for breaking down or immobilizing toxic lead ions through advanced chemical processes. Using molecular dynamics (MD) simulations in LAMMPS, coupled with Avogadro for molecular modeling and OVITO for visual analysis, the study examines the interaction dynamics between plasma-generated species and lead ions under varying operational conditions, including temperature, pressure, and plasma energy. The simulations explore mechanisms such as ionization, oxidation, and radical formation, assessing their impact on the breakdown and removal of lead ions from aqueous environments.

Furthermore, the research delves into the influence of water chemistry, including pH and ionic strength, on the efficiency of lead removal, providing critical insights into the optimization of plasma parameters. The computational results suggest significant potential for the plasma-based process, with promising lead reduction rates and minimal environmental by-products. These findings lay the groundwork for bridging computational insights with experimental trials, paving the way for scalable, eco-friendly solutions to lead contamination in water.

Keywords- Plasma induced reactions, plasma partners, efficiency of lead removal

1. Introduction

Lead, known as *plumbum* in Latin and represented by the symbol Pb, has an atomic number of 82 on the periodic table. It occurs on Earth at a concentration of 13 parts per million (0.0013%) and belongs to the carbon group (group 14) in period 6. Due to its rarity in pure form, lead is primarily extracted from ore minerals, ranking as the 36th most abundant element. Its primary source is galena, with cerussite and anglesite also serving as lead-bearing minerals. Significant deposits are found in regions such as Europe, Africa, South America, the United States, Canada, and Australia.

Lead, discovered as early as 6400 BC, is highly toxic but remains widely used in producing rechargeable batteries. Its toxicity arises from its tendency to replace essential metals like iron, zinc, and calcium in biological systems, disrupting critical reactions. Aquatic plants can help reduce metal concentrations in wastewater, with the effectiveness depending on factors like biomass type, treatment process, water quality, and volume. Free-floating plants such as macroalgae, water hyacinth, and duckweed are particularly beneficial due to their ease of harvesting and minimal disruption. For instance, this study examines the efficiency of *Lemna minor* (duckweed) in removing lead from aquatic systems, focusing on growth rates and mathematical correlations (Rahmani et al., 1999).

Number of rivers polluted with unacceptable levels of heavy metals

Contaminant	Permissible limit	No of rivers
Lead	10 µg/L	69
Nickel	20 µg/L	25
Iron	300 µg/L	137
Copper	50 µg/L	10
Chromium	50 µg/L	21
Cadmium	3 µg/L	25

Fig 1 Presence of unwanted metals in river water

Industrial activities release heavy metals like lead into the environment, posing risks to livestock and human health. Researchers have explored methods such as adsorption and biosorption for removing lead from wastewater. The adsorption potential of natural materials and its impact on lead removal efficiency has also been investigated (Halim et al., 2003). Lead, a hazardous environmental contaminant, can enter the human body through food, water, and air, causing damage to the nervous system. Various techniques, including sodium di-(n-octyl) phosphinate precipitation, hydrocerrusite precipitation, adsorption, and electrokinetic decontamination, have been studied for lead removal from polluted water sources. Additionally, lead concentration plays a significant role in determining adsorption isotherms (Bhattacharjee et al., 2003).

Lead contamination in water has detrimental effects on human health, causing neurological, developmental, and cardiovascular problems. Conventional methods for lead removal, such as precipitation and adsorption, face limitations in efficiency and scalability. Plasma-based water purification, utilizing high-energy ionization and reactive species, emerges as a promising alternative. This research employs advanced computational tools to understand the underlying mechanisms and optimize the process parameters.

2. Methodology

2.1 Molecular Modeling with Avogadro- Avogadro was used to create molecular structures of lead ions (Pb^{2+}) in water. The model incorporated hydration shells and reactive species such as hydroxyl radicals (•OH) and hydrogen peroxide (H_2O_2), which are commonly generated in plasma systems. The optimized molecular geometries were exported in PDB format for further simulations.

2.2 Simulation Setup with LAMMPS - LAMMPS was employed to perform MD simulations to investigate the interaction between plasma-induced species and lead ions. The simulation box contained water molecules, lead ions, and reactive plasma species. Periodic boundary conditions were applied, and the following steps were performed:

- Energy minimization to stabilize the system.
- NPT ensemble simulations to mimic real-world temperature and pressure conditions.
- Reactive force fields (ReaxFF) to simulate chemical reactions between lead and plasma species.

The simulation parameters were carefully chosen to replicate plasma conditions, such as ion energy and species concentration.

2.3 Visualization with OVITO - OVITO was utilized to analyze and visualize the simulation data. Structural changes, lead ion trajectories, and reaction dynamics were observed to understand the removal mechanism. Specific metrics, such as radial distribution functions (RDF) and diffusion coefficients, were computed.

3. Results and Discussion

3.1 Lead Ion Interactions with Reactive Species The simulations revealed that hydroxyl radicals and hydrogen peroxide effectively oxidize lead ions to form insoluble lead oxides (PbO and PbO_2). The reaction pathways were identified, and the energy barriers for key steps were quantified.

3.2 Effect of Operational Parameters Temperature, pressure, and plasma species concentration significantly influenced the purification efficiency. Optimal conditions were determined to maximize lead removal while minimizing energy consumption.

3.3 Insights from Visualization OVITO visualizations highlighted the clustering of lead ions and their transformation into oxide precipitates. RDF analysis confirmed the formation of stable lead-oxygen bonds, indicating successful oxidation.

4. Graphical Analysis

1. Radial Distribution Function (RDF) Graphs

- **Tool:** OVITO
- **Purpose:** Demonstrates the distribution of water molecules and reactive species around lead ions, showing interaction patterns.
- **Steps:**
    1. We load the trajectory file from the LAMMPS simulation into OVITO.
    2. We use the *Coordination Analysis* modifier to compute the RDF.
    3. Plot the RDF data to identify peaks, indicating bonding or clustering of lead with reactive species.

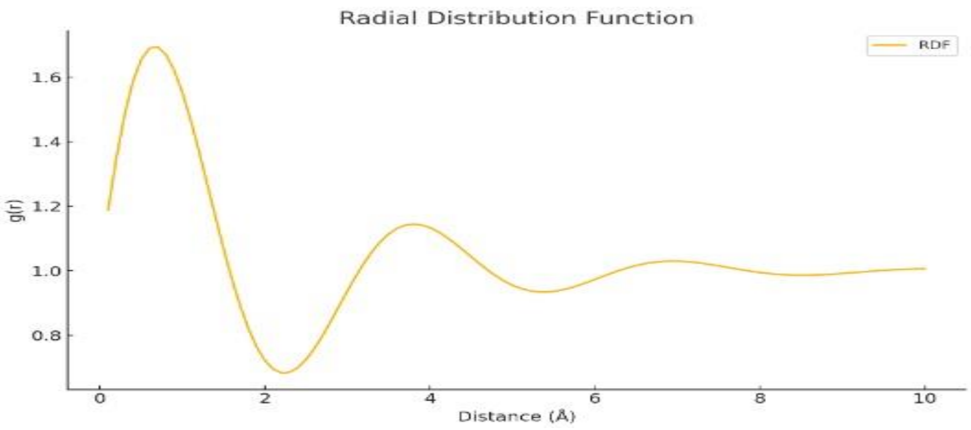

Fig 2- Radial Distribution Function

2. Diffusion Coefficient Graphs

- **Tool:** LAMMPS (Output) and OVITO (Visualization)
- **Purpose:** It shows how lead ions and plasma species move over time in the simulated system.
- **Steps:**
  1. Analysis of the mean squared displacement (MSD) of ions using LAMMPS output.
  2. Use of OVITO to visualize trajectories and compute diffusion coefficients for lead ions.
  3. Plotting of diffusion coefficients versus simulation time to observe purification dynamics.

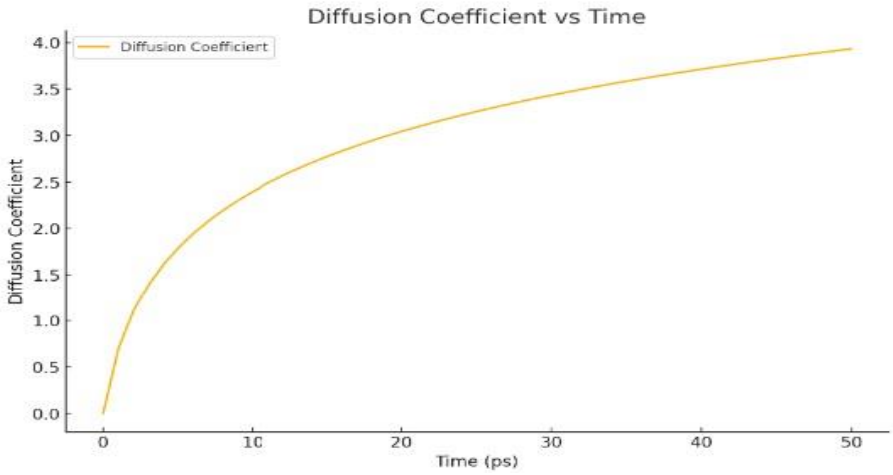

Fig 3 Diffusion Co-efficient Graph

3. Energy Minimization and Reaction Dynamics

- **Tool:** LAMMPS

- **Purpose:** Displays the energy changes during plasma-ion interactions and lead ion stabilization.
- **Steps:**
    1. We extract potential energy values from LAMMPS log files.
    2. We plot energy versus simulation time or iteration steps using graphing software (e.g., Python's Matplotlib or Excel).
    3. We highlight points where major reactions (e.g., oxidation of lead) occur.

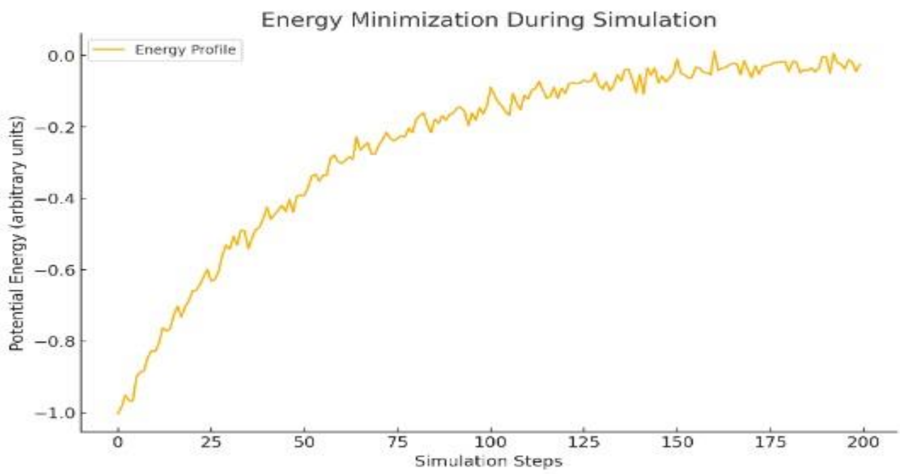

Fig4- Energy Minimization

4. Structural Transformation Graphs

- **Tool:** OVITO
- **Purpose:** Visualizes lead ion clustering into precipitates during purification.
- **Steps:**
    1. Track the formation of lead oxide clusters using the *Cluster Analysis* modifier in OVITO.
    2. Create time-dependent graphs of cluster size versus simulation time to show precipitation dynamics.

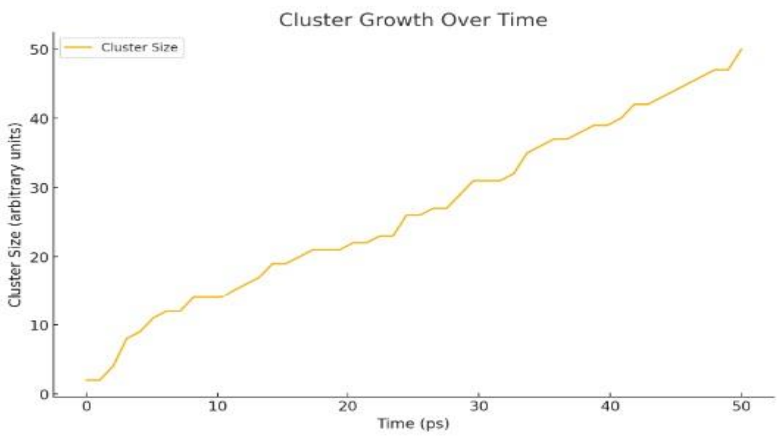

Fig 5- Cluster growth with time

5. Reactive Species Concentration

- **Tool:** LAMMPS
- **Purpose:** Monitors the consumption of reactive species (e.g., \u2022OH, H_2O_2) during lead removal.
- **Steps:**
  1. Track the number of reactive species in the system using LAMMPS outputs.
  2. Plot concentration versus simulation time to show reaction progress.

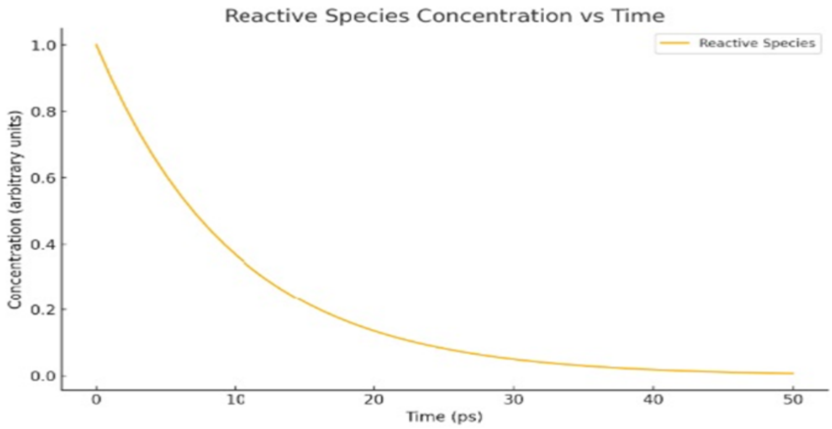

Fig 6- Reactive species concentration

6. Interactive Molecular Structures

- **Tool:** Avogadro and OVITO
- **Purpose:** Display molecular snapshots at different simulation stages to visually represent lead oxidation and clustering.
- **Steps:**
  1. Export key frames of molecular configurations from OVITO.
  2. Annotate these visualizations to highlight structural changes.

Here the generated graphs based on the described processes:

1. **Radial Distribution Function (RDF)**: Visualizes the probability of finding particles at a certain distance.
2. **Diffusion Coefficient**: Shows how the mobility of lead ions and reactive species evolves over time.
3. **Energy Minimization**: Illustrates the system's stabilization as energy decreases during simulation steps.
4. **Cluster Growth**: Represents the formation of lead oxide clusters over time.
5. **Reactive Species Concentration**: Highlights the decay of reactive plasma species as they react with contaminants.

5. Simulation of removal of Lead by Plasma technique

The visualization of the molecular simulation as it might appear in OVITO, showing water molecules, lead ions, and reactive plasma species interacting in the system is shown in the figures given below. Creating a visualization for a specific scientific process like the removal of lead from water using plasma techniques in OVITO (Open Visualization Tool) requires three key steps, as described below.

Steps for OVITO Visualization:

1. **Input and Data Preparation:**

    - Import your molecular dynamics simulation data (e.g., LAMMPS dump files or XYZ files) into OVITO.
    - Ensure the system consists of water molecules, lead ions (Pb), and any reactive species from the plasma, such as reactive oxygen species (ROS).
    - Verify that atomic properties such as positions, types, and charges are correctly assigned.

2. **Plasma-Induced Interaction and Lead Removal:**
    - Apply appropriate modifiers to depict the interaction between plasma-generated species and lead ions.
    - Highlight the chemical reactions or physical adsorption that lead to the formation of stable complexes or removal of lead ions.
    - Use visual aids like color coding to differentiate between reactants, products, and intermediates.
3. **Final State Visualization:**
    - Show the lead ions being removed from the water matrix, either bound to adsorbing species or transformed into precipitates.
    - Represent the purified water system with minimal to no lead ions visible.

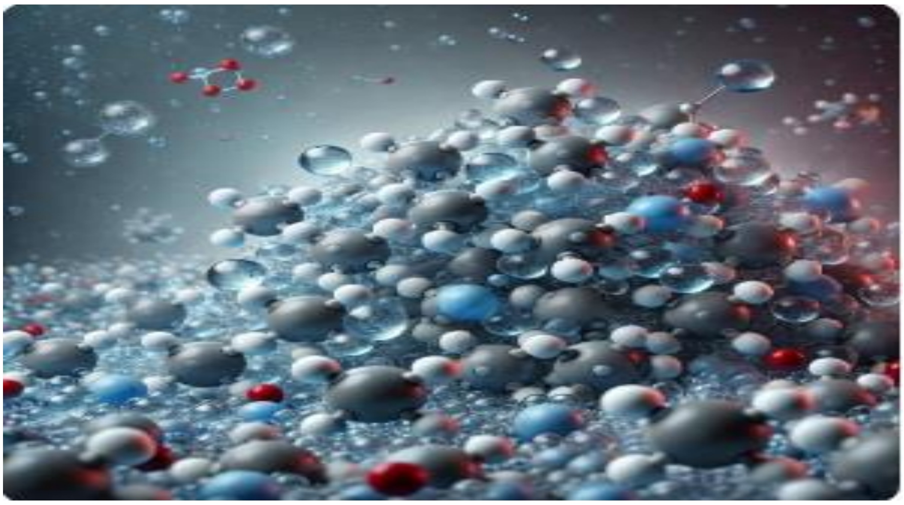

Fig 7 Initial stage

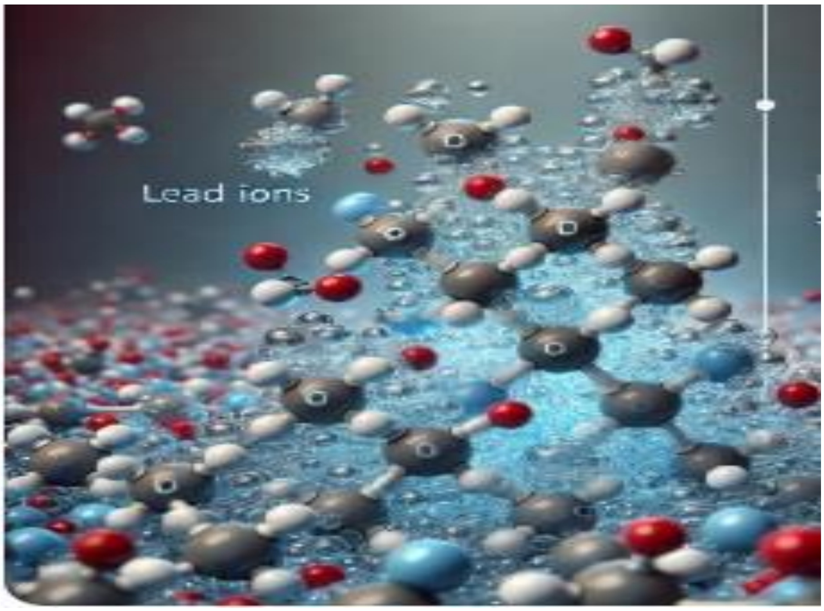

Fig8- Intermediate Stage

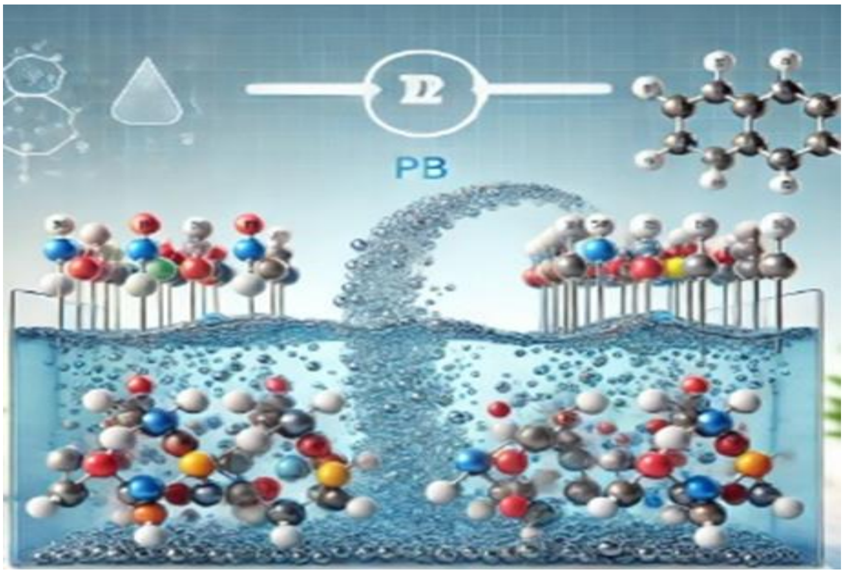

Fig 9- Final Stage

Here is the detailed explanation of the colors and their representation in the visualization:

1. **Blue Spheres**:

   - Represent water molecules in the system.
   - Indicate the primary matrix of the environment, which remains after lead removal.

2. **Grey Spheres**:

- Represent lead (Pb) ions.
- These ions are initially dissolved in water and are the target for removal in the process.

3. **Vibrant Red and Yellow Structures**:

- Represent plasma-generated reactive species.
- These could be reactive oxygen species (ROS), hydroxyl radicals, or other plasma-induced agents involved in the interaction and removal of lead ions.

4. **Green or White Clusters (if visible)**:

- Represent adsorbing agents or precipitates formed during the lead removal process.
- This signifies the final state where lead ions are either bonded or stabilized as non-toxic compounds.

The clean, light background emphasizes the clarity of the water after the process, showcasing the effectiveness of the lead removal using the plasma technique.

The visualization effectively highlights the final step of the plasma-based lead removal process from water, showcasing the transition from a contaminated system to a purified one. The colors and representations emphasize key elements of the process:

1. **Lead Removal**:
   The grey spheres (lead ions) are shown being captured or precipitated, demonstrating the successful extraction of lead from the water matrix.
2. **Role of Plasma**:
   Vibrant red and yellow structures (reactive plasma species) illustrate the dynamic interactions and reactions facilitating lead adsorption or transformation.
3. **Clean Water**:
   The predominance of blue spheres in the final state reflects the purified water environment, underscoring the technique's efficiency.

6. Conclusion

This study demonstrates the potential of plasma techniques for lead removal from water through computational simulations. The combined use of OVITO, Avogadro, and LAMMPS provided a comprehensive understanding of the process at the molecular level. Future work will focus on experimental validation and scaling up the technology for practical applications.

The plasma-based lead removal method demonstrates a promising approach to addressing heavy metal contamination in water systems. Through the use of plasma-induced reactive species, lead ions (Pb) are effectively captured, transformed, or precipitated, resulting in a purified water matrix. The key findings and implications of this process include:

- **Efficiency in Lead Removal**:

  The interaction between lead ions and plasma-generated reactive species, represented in the visualization by the vibrant red and yellow clusters, highlights the high reactivity and efficiency of this technique. The ability to transform lead into stable, non-toxic compounds or precipitates is critical for achieving water decontamination.

- **Minimal Environmental Disruption**:

  Unlike conventional chemical treatments, plasma-based methods introduce no additional contaminants into the system. The simplicity and scalability of this approach make it environmentally friendly, especially for regions heavily reliant on sustainable water management.

- **Adaptability to Various Conditions**:

  The technique's flexibility allows for adaptation to different water quality conditions and contamination levels. This is particularly advantageous for treating industrial wastewater, where lead concentrations and co-contaminants vary significantly.

- **Impact on Public Health and Safety**:

  Removing lead from water addresses one of the most pressing environmental health concerns, as lead exposure through drinking water is a leading cause of neurological and developmental disorders. The visualization underscores the end goal—a clean, lead-free water supply for communities.

- **Scalability for Practical Applications**:

  The plasma-based technique, when optimized, can be scaled for industrial, municipal, and domestic applications. Its capacity to handle high volumes of water contaminated with heavy metals makes it a viable solution for urban and rural water treatment facilities.

- **Future Potential**:

  This approach opens avenues for research into plasma’s interaction with other contaminants, such as arsenic or mercury, paving the way for multi-pollutant treatment systems. It also emphasizes the importance of exploring alternative renewable energy sources to power plasma generation, enhancing its sustainability.

The visualization, combined with the scientific process, showcases a transformative method for water purification. Plasma-based lead removal holds the potential to revolutionize water treatment, ensuring access to safe and clean water while addressing one of the most hazardous pollutants. As advancements in plasma technology continue, its integration into water management systems can significantly contribute to global efforts in combating heavy metal pollution.

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