Chemistry3D: Robotic Interaction Toolkit for Chemistry Experiments

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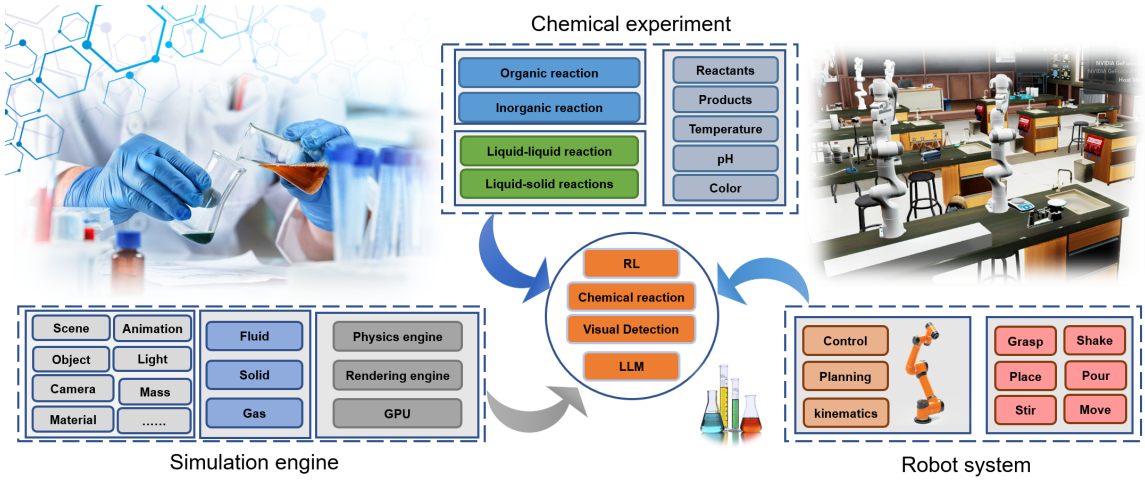

Fig. 1: Illustration of the Chemistry3D. Chemistry3D integrates a robot system, chemical experiment, and simulation engine, providing interfaces for robot manipulation, visual inspection, and fluid flow control and enabling reaction visualization.

***Abstract*— The advent of simulation engines has revolutionized learning and operational efficiency for robots, offering cost-effective and swift pipelines. However, the lack of a universal simulation platform tailored for chemical scenarios impedes progress in robotic manipulation and visualization of reaction processes. Addressing this void, we present Chemistry3D, an innovative toolkit that integrates extensive chemical and robotic knowledge. Chemistry3D not only enables robots to perform chemical experiments but also provides real-time visualization of temperature, color, and pH changes during reactions. Built on the NVIDIA Omniverse platform, Chemistry3D offers interfaces for robot operation, visual inspection, and liquid flow control, facilitating the simulation of special objects such as liquids and transparent entities. Leveraging this toolkit, we have devised RL tasks, object detection, and robot operation scenarios. Additionally, to discern disparities between the rendering engine and the real world, we conducted transparent object detection experiments using Sim2Real, validating the toolkit's exceptional simulation performance. The source code is available at https://github.com/huangyan28/Chemistry3D, and a related tutorial can be found at https://www.omni-chemistry.com.**

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I. INTRODUCTION

Chemistry is a constantly evolving and experimental discipline [17]. The birth of a new substance or material often requires thousands of experiments, making chemical experimentation demanding for researchers. The repetitive nature of this work not only imposes immense labor intensity on researchers and chemical engineers (Some chemical engineers often work up to 50 hours a week in the US, says the Bureau of Labor Statistics [18]) but also poses threats to their physical health due to exposure to harmful chemicals. In today's rapidly advancing era of embodied intelligence technology, proposing a 3D simulator that includes robot operations and chemical reaction processes is imperative, which not only improves the efficiency of experiments and reduces the cost of experiments but also liberates human beings from heavy scientific experimental tasks.

Chemical experiments contain many chemical manipulation and visual detection tasks, which are dangerous if the robot is trained directly in a real environment. Although considerable research has been conducted into robot simulation systems [19]–[23], a dedicated chemical 3D simulation system for robots has yet to be proposed. Current research on chemical robots mainly focuses on algorithmic aspects, such as organic synthesis methods [24]–[26] and reinforcement learning(RL) [13], [27]–[30] to improve yield. This is because chemistry and robotics are interdisciplinary fields, and designing a chemical 3D simulation system tailored for robots requires addressing numerous challenges, including but not limited to: **(1) Immature rendering engines for liquids and transparent objects:** Chemical experiments

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TABLE I: Comparison of Chemistry3D with Other Researches and Toolkits

	Chemistry3D (ours)	Molecular Collision [1]	CFD [2]	ORD [3]	ORDerly [4]	ChemSpider [5]	Chemaxon [6]	RXN for Chemistry [7]	ChemReaX [8]	Robot Air Hockey [9]	Panda MuJoCo Gym [10]	Unity-based Simulator [11]	CABD [12]	ChemGymRL [13]	ML-based architecture [14]	ChemOS [15]	ARChemist [16]
Manipulation Information																	
Perception Information	✓	✗	✗	✓	✓	✗	✗	✗	✗	✓	✓	✓	✓	✗	✗	✗	✗
Transparent Object Detection	✓	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓	✗	✗	✗	✗
Contact Information	✓	✗	✗	✗	✗	✗	✗	✗	✗	✓	✓	✗	✗	✗	✗	✗	✗
Reinforcement Learning	✓	✗	✗	✗	✗	✗	✓	✓	✓	✓	✓	✗	✓	✓	✓	✗	✗
Embodied Intelligence	✓	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
Task Subdivision	✓	✗	✗	✓	✓	✗	✓	✓	✗	✗	✓	✗	✗	✗	✗	✓	✓
Chemical Information																	
Intermediate States	✓	✗	✓	✗	✗	✗	✗	✗	✓	✗	✗	✗	✗	✓	✗	✗	✗
Color Information	✓	✗	✗	✓	✓	✓	✓	✗	✗	✗	✗	✓	✗	✓	✗	✓	✗
Spectrum Information	✓	✗	✗	✗	✗	✓	✓	✗	✗	✗	✗	✗	✗	✓	✗	✗	✗
Information Collection	✓	✗	✗	✗	✓	✓	✓	✗	✗	✗	✗	✗	✗	✗	✓	✓	✗
Thermodynamic Property	✓	✗	✗	✓	✓	✓	✗	✓	✓	✗	✗	✗	✗	✗	✗	✗	✗
pH Value	✓	✗	✗	✗	✗	✗	✓	✗	✗	✗	✗	✗	✗	✗	✗	✓	✗
Temperature	✓	✗	✓	✓	✓	✗	✗	✗	✓	✗	✗	✗	✗	✓	✗	✗	✗
Fluid Simulation	✓	✗	✓	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
Database	✓	✗	✗	✓	✓	✓	✓	✓	✓	✗	✗	✗	✗	✗	✗	✓	✗
Organic Reaction	✓	✗	✗	✓	✓	✗	✓	✓	✗	✗	✗	✗	✗	✓	✓	✓	✓
Inorganic Reaction	✓	✓	✓	✗	✗	✗	✓	✗	✓	✗	✗	✗	✗	✓	✓	✓	✓

involve many liquids and transparent objects, and achieving efficient and realistic rendering engines is difficult [31]. **(2) Vast chemical reaction databases:** Chemistry is a complex discipline covering various reaction types such as organic, inorganic, liquid, solid, and gas; thus, implementing chemical simulation requires extensive database support [32]. **(3) Complex calculation methods and parameters:** Real chemical reactions involve multiple parameters such as heat, temperature, pH, color, etc.; visualizing these parameters requires a deep understanding of chemistry and complex calculation methods [33]. Therefore, to realize a chemical 3D simulation system tailored for robots, it is necessary to span multiple disciplines, such as chemistry, computer graphics, and robotics, and address the various technical challenges mentioned above.

The advancements in 3D rendering technology and the development of large language models (LLM) have presented us with new opportunities. Omniverse [34], introduced by NVIDIA, is an open virtual collaboration and simulation platform encompassing a wide array of 3D modeling tools, renderers, animation tools, and physics engines. It enables robots to create more realistic and interactive virtual environments [35]. Therefore, leveraging NVIDIA's Omniverse simulator, we propose a high-performance simulating toolkit for chemical experiments named Chemistry3D, as shown in Fig.1. This toolkit allows robots to conduct organic, inorganic, and various other experiments within simulated environments. Furthermore, to enhance the versatility of the simulator, we have opened convenient data interfaces, enabling operators to add unknown chemical reactions to the database effortlessly.

The contributions of this paper are as follows: **(1) Novel 3D scene for chemical experiments:** We introduce a pioneering scene specifically designed for chemical experiments, featuring a wide range of chemical containers and robots. **(2) Establishment of a comprehensive chemical dataset:** We have curated a dataset of over 1,000 inorganic and 100,000 organic reactions, providing intermediate products and real-time feedback on changes in temperature, color, and pH. **(3) Performance validation through various experiments:** Our simulation supports diverse robotic experiments, including RL-based object grasping training, chemical experiment operations guided by LLM, and visual Sim2Real experiments.

II. Related Work

In the realm of chemical experiment simulations, previous toolkits and researches have generally neglected the testing of robotic manipulation. Our work addresses this gap by focusing on robotic operations within chemical experiments. We conducted a comparative analysis of Chemistry3D and other tools across the fields of robotics and chemistry, as summarized in Table I. Unlike existing researches or toolkits that primarily concentrate on chemical reaction generation, our approach emphasizes robotic manipulation, including RL for robots and the development of embodied intelligence through integration with LLM.

A. Chemical Experiment Simulators

Traditionally, chemical reaction simulators focus on molecular-level processes. For example, Interactive Chemistry [1] models molecular collisions, while Computational Fluid Dynamics (CFD) [2] methods simulate gas reactions. Organic chemistry tools like ORD [3] and ORDerly [4] provide structured databases for reaction characterization, and ChemSpider [5] serves as a search tool for chemical substances. In inorganic chemistry, platforms like ChemAxon [6] and RXN for Chemistry [7], [36] are used for predicting reactions and optimizing synthesis pathways. ChemReaX [8] offers basic simulations with data on thermochemistry and reaction intermediates. However, these simulators are designed primarily for theoretical chemical research. Enabling robots to autonomously perform required chemical experiments remains an unsolved challenge.

B. Integrating Robotics in Chemical Experiment Simulations

Few simulators effectively integrate chemical experiments with robotics. Existing works focusing on robotic operations typically target specific tasks. For example, Robot Air Hockey [9] is designed for Sim2Real applications in playing air hockey, while Panda MuJoCo Gym [10] benchmarks reinforcement learning (RL) tasks such as pushing, sliding, and object manipulation. Additionally, a Unity-based Simulator [11] creates game-like scenarios for experimental manipulation, primarily for educational purposes. In terms of

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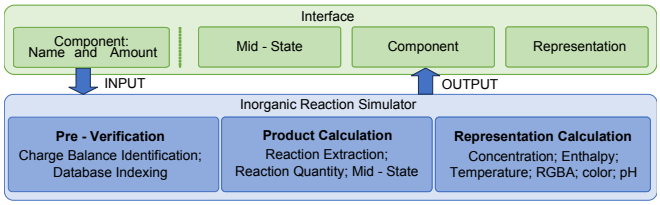

Fig. 2: The framework of the inorganic reaction simulator. It processes the input reactants as a pipeline and outputs the product information on component, representation, and mid-state.

perception tasks, CABD [12] offers benchmark datasets for image recognition of chemical apparatus, and ChemGymRL [13] provides detailed information on intermediates of chemical reactions specifically for RL purposes. For system architecture design, various pipelines have been developed to enable autonomous laboratory operations using machine learning (ML) [14] and natural language processing (NLP) [15]. Furthermore, ARChemist [16] has introduced modular managers for processing chemical recipes and interacting with robots, highlighting the emerging integration of robotics in the domain of chemical experiments.

III. Chemistry3D

Chemistry3D focuses on three main aspects: chemistry simulation, virtual chemical laboratory environments, and robotic manipulation. Chemistry3D begins by offering accurate and detailed models for simulating chemical reactions, ensuring reliable results for both organic and inorganic processes. These simulations are embedded within virtual laboratory environments that closely replicate real-world chemical experiments. Compared to previous chemistry toolkits [13], Chemistry3D uniquely supports realistic scene simulations and allows for physical interactions between robots and objects. Additionally, Chemistry3D integrates robotic manipulation, enabling robots to autonomously perform and optimize chemical reactions, thereby seamlessly combining robotic automation with experimental workflows.

A. Chemistry Simulation

Inorganic Reactions: The simulation of inorganic reactions is designed based on a database encompassing both reaction and chemical substance information. The database includes data on 69 different chemical substances, each characterized by its color, enthalpy values, and physical state. Additionally, it contains information on 65 fundamental reactions, specifying the reactants, products, and their stoichiometric ratios.

The simulator accepts input as a dictionary, with reactant names as keys and numbers of mole as values. The simulator is capable of performing iterative reactions, which allows for generating over 1000 possible reactions through various combinations.

For the output, the component interface outputs a dictionary of the same format, detailing the remaining reactants and reaction products. Furthermore, the representation interface provides a comprehensive output dictionary, including data on the color of the reaction mixture, enthalpy changes, pH levels, temperature changes, and the physical state of the resultant substances.

Precisely, the core framework of the inorganic reaction simulator is shown in Fig. 2. The detailed procedure within this simulator is discussed as follows.

- **Database Indexing:** Initially, the simulator verifies whether the input reactants satisfy charge conservation [37]. Following that, the simulator determines the impending reaction by sequentially matching in the database, i.e., whether the reactants of the retrieved reaction is included in the current reagents.
- **Reaction Extraction:** The simulator then divides current reagents into two parts. The reacting part is extracted from the current reagents according to the reactants in the retrieved reaction, and the spectating part is the remaining reagents which is not involved in this reaction. In this way, the simulator ensures that only the necessary reactions are considered in this reaction cycle, thereby streamlining the reaction prediction process.
- **Reaction Quantity Calculation:** After reaction extraction, the simulator identifies which ion is completely consumed first to calculates the reaction quantity, N. This dimensionless quantity shows how many moles of the "reaction equation" are involved in the process, thereby determines the amount of reaction. Using this number, the simulator subtracts the amount of each reactant used and adds the generated products from the current reagents, yielding the final composition of substances.
- **Mid-State Calculation** The computation of intermediate states uses a differential iteration method as (1). $n(t)$, $n(t+\Delta t)$ is the amount of substance at the current and next time step, Δt is the time increment differential. rate is the reaction rate, and ν is the stoichiometric coefficient of the substance in the reaction. The unit for each variable is indicated in the project website https://www.omnichemistry.com.

$$n(t+\Delta t) = n(t) + \text{rate} \cdot \Delta t \cdot \nu \tag{1}$$

The reaction rate [38], [39] is calculated as (2). k, $c(\text{A})$, m_a represents the rate constant,concentrations of reactants A, reaction order of A.

$$\text{rate} = k \cdot c(\text{A})^{m_a} \cdot c(\text{B})^{m_b} \tag{2}$$

The iteration starts when the reaction begins. This process continues until the reaction rate falls below a certain threshold, at which point the reaction is considered complete. During this process, the composition of current reagent at each time step is recorded and then compiled into a list, which represents the intermediate state data of the reaction.

- **Concentration Calculation:** The simulation proceeds by adding the total volume V of the mixture, then calculating the concentration c as (3) , where n is the amount of substance of a particular solute. This calculation forms the basis for subsequent concentration-dependent computations.

$$c = \frac{n}{V} \tag{3}$$

- **Enthalpy Change Calculation:** The simulator then computes the heat absorption Q based on reaction quantity as (4), where N is the reaction quantity, ΔH is enthalpy change per equation recorded in the database. For multiple reactions, Hess's Law is used to sum the enthalpy changes of individual steps to obtain the net enthalpy change.

$$Q = N \cdot \Delta H \tag{4}$$

- **Temperature Change Calculation:** Utilizing the specific heat capacity C of the solvent, the simulator calculates the temperature change ΔT resulting from the reaction. The change is determined by (5), where ρ is the density and V is the volume of the solution. Temperature changes is important in analyzing reaction rates and equilibria.

$$\Delta T = \frac{Q}{C \cdot \rho \cdot V} \tag{5}$$

- **RGBA Color Calculation:** The simulator calculates the RGBA color change in a reaction mixture by evaluating several factors. First, it determines the transparency a of the solution using an exponential model based on the concentrations of reactants and products [40], [41], with RGB values remaining constant. As (6), c is the concentration of the solute and K is a constant dependent on the identity of reactants and products.

$$a = 1 - 10^{-K \cdot c} \tag{6}$$

  Second, it assigns priority to different physical states: solid substances contribute to opacity; liquids are mixed based on RGBA values; gases are excluded from the color calculation. Third, a negative mixing model is applied for color mixing in solutions without solids [42]. Finally, the simulator converts UV/Vis spectrum data into RGB values to represent the visible color of substances in the simulation [43]–[45].
- **pH Calculation:**The simulator calculates the pH of the solution through several steps. First, it establishes a reference table of water's ionization constant (K_w) for temperatures between 0 and 100 degrees Celsius at standard atmospheric pressure, enabling precise interpolation at any temperature. Then, it focuses on the ionization of strong electrolytes while ignoring weak electrolytes [46]. In this way, the simulator determines the concentrations of hydrogen (H^+) and hydroxide ions (OH^-) by (7).

$$K_w = c(\mathrm{H}^+) \cdot c(\mathrm{OH}^-) \tag{7}$$

  Based on the ionization constant and these ion concentrations, the simulator accurately calculates the pH by (8), providing insight into the solution's acidity.

$$\mathrm{pH} = -\log c(\mathrm{H}^+) \tag{8}$$

Organic Reactions: The simulation of organic reactions integrates data from RXN for Chemistry [7] for reaction information and ChemSpider [5] for chemical substance information. Similar to the inorganic simulator, this simulator also has a component and representation interface as output. The system accepts reactants represented by SMILES [47] strings and outputs the corresponding products for reaction product prediction. It's also capable of predicting reaction yields by RXN for Chemistry, therefore determines the component output for the specific reaction. For the representation, the simulator employs web scraping to query substance information; given a SMILES string, it retrieves a dictionary of properties and values. For more comprehensive data, users can query additional information using the CAS number [48] of the substance.

Simulator Interface: To integrate the chemical aspects with the operational aspects seamlessly, the simulator is embedded into a container class, which features three main methods: initialization, updating, and information retrieval. The initialization method distinguishes between organic and inorganic reactions and sets the chemical components by name, amount, and volume. The updating method simulates sampling or mixing operations and can automatically conduct reactions. The output of this method represents the intermediate state of the container's contents, calculated through rate equations with an adjustable time step to suit simulation tasks in Omniverse. The information retrieval method allows access to component or representation information, enabling direct queries about concentration, color, and other properties for any container. This approach binds chemical information to simulated reagent bottles, facilitating clear demonstrations. It also aligns chemical reactions with operational actions, making the simulation intuitive. This integrated simulating method allows for accurate predictions and detailed representation calculations. It's essential for further studies in chemistry, including analysis of intermediate states and RL.

B. Chemical Environment

Chemistry3D offers an advanced and meticulously designed environment for simulating chemical experiments, as shown in Fig. 3. This environment, built upon the NVIDIA Omniverse platform, integrates a variety of features essential for both chemical and robotic research.

Rich Chemical Assets: Chemistry3D is endowed with an extensive series of chemical containers and instruments, meticulously designed to facilitate a diverse range of chemical reactions. These encompass both organic and inorganic reactions, as well as liquid-liquid and liquid-solid interactions. This vast collection of chemical assets allows for the simulation of various chemical experiments, offering

Fig. 3: Illustration of simulated chemistry environment. The chemical containers with a green background were 3D scanned from real objects. This environment is designed to support a wide range of chemical and robotic experiments, providing a highly detailed and interactive platform.

researchers and educators a versatile platform to explore different reaction dynamics.

Robotic Assets: The environment is equipped with numerous robotic arms and robotic grippers, enhancing the potential for robotic simulations. These robotic systems are capable of performing precise tasks such as grasping, shaking, pouring, stirring, placing, and moving chemical containers. This capability significantly expands the possibilities for robotic experimentation and automation within the chemical laboratory setting.

Fluid and Rigid Body Simulation: Chemistry3D excels in simulating both fluid and rigid body interactions with high fidelity. This capability is particularly beneficial for visualizing intricate chemical processes involved in both inorganic and organic experiments. For instance, the platform can realistically simulate the dissolution of solid compounds in a liquid. Additionally, it can accurately depict the merging of two liquids and the resultant color changes, providing a vivid representation of reaction progress and intermediate states.

High-Fidelity Rendering: The platform supports highly realistic rendering and light simulation, which is essential for accurately representing chemical experiments involving transparent materials. In many chemical lab settings, instruments such as glass beakers and flasks are transparent, posing challenges for vision-based tasks. Chemistry3D excels in simulating these transparent objects, providing detailed visual representations of chemical reactions, including changes in color and clarity. This enhances the effectiveness of visual inspections and analyses, which is crucial for monitoring and understanding chemical processes.

Robot Operating System: Chemistry3D inherits robust support from Isaac-Sim, including integration with ROS and ROS2. This compatibility allows for a diverse range of robotic development and experimentation, enabling users to leverage advanced robotic operating systems for controlling and simulating robotic behavior within the chemical environment. This integration is crucial for developing and testing sophisticated robotic applications and workflows.

C. Robotic Manipulation

Chemistry3D aims to integrates robotic operations with the simulation of chemical experiments, leveraging Nvidia Omniverse, PhysX 5, and IsaacSim for realistic simulations of rigid bodies, fluids, soft bodies. This platform enhances realism through accurate physics simulation and light rendering effects. To advance robotic operations within Chemistry3D, we proposes tasks focused on chemical experimental manipulation, embodied intelligence manipulation, and RL tasks.

Chemistry manipulation: Chemical experimental manipulations frequently involve the desired motions of target objects, e.g., pouring. Consequently, the tasks in Chemistry3D encompass a variety of chemical experimental operations. We have selected four common chemical experimental operations including picking, placing, pouring, stirring, and shaking. In our experiments, we developed simulation tasks within Chemistry3D to demonstrate these operations.

Embodied intelligence: Embodied intelligence involves the interaction of semantic information between agents and humans, enabling robots to understand and perform desired chemical operations. This capability is vital for the automation of chemical processes. However, since LLMs cannot always accurately produce results as expected in experiments, we introduced LLM-based agents in Chemistry3D to support debugging these agents within the simulator. We designed specific chemical experiment scenarios to demonstrate that the development of embodied intelligence is possible in Chemistry3D. These scenarios showcase the potential for robots to autonomously observe the environment and complete specified tasks within the platform.

RL task: RL has become a significant algorithm in dexterous manipulation involving grasping, moving, and even stirring objects [49], [50]. We believe that the techniques developed in these works are transferable to operations involving chemical instruments. IsaacGym is a well-regarded simulation environment specifically designed to support robot learning. The Omniverse Isaac Gym Reinforcement Learning (OmniIsaacGymEnvs) for Isaac Sim repository provides RL examples compatible with IsaacSim and has become a widely adopted environment for RL research. Utilizing this repository, we implemented a reward function setup similar to the provided examples and successfully achieved the picking of chemical containers. The RL task demonstrates that Chemistry3D can support RL research in robotic manipulation.

IV. Experiments

In this section, we investigate the capabilities of chemical reaction simulation and robotic manipulation within the Chemistry3D. All experiments are conducted within a simulated chemistry environment. As shown in Fig. 4, we have carried out four experiments based on Chemistry3D, covering chemical manipulation, visual Sim2Real, embodied intelligence, and RL. Additionally, we have integrated the chemical simulator to perform both organic and inorganic experiments.

A. Chemical Experiments

In chemical experiments, we focus on inorganic and organic reactions, integrating robotic operations within Isaac-Sim to enhance the experimental process. (See the project website for more details.)

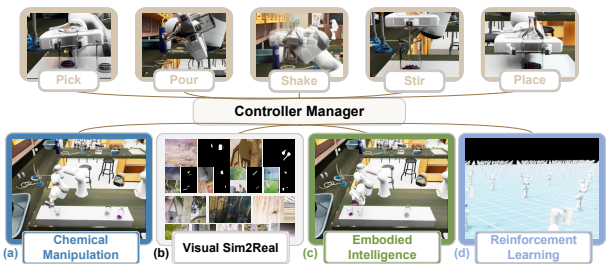

Fig. 4: Illustration of the motion and experiments in Chemistry3D.

Inorganic Experiment: We selected redox reactions due to their notable color and state changes. Experiments involved potassium permanganate ($KMnO_4$) with ferrous chloride ($FeCl_2$), and hydrochloric acid (HCl) with iron(II) oxide (FeO). The center of mass of reactants determines contact points, triggering color and state transformations. Chemistry3D outputs detailed reaction data such as temperature, enthalpy change, and pH at each time step.

Organic Experiment: Focused on the simulation of mid-state products rather than color changes, we synchronized reaction steps with IsaacSim simulation. Using the substitution reaction between bromine (Br_2) and anthracene ($C_{14}H_{10}$) as an example, mid-state products are generated upon reactant contact. This enables real-time optimization of final products and robotic manipulations.

B. Chemical Manipulation

As shown in Fig. 4(a), chemical manipulation often involves tasks such as picking and placing. Our experiments demonstrated the effective deployment of robotic picking and pouring operations in chemical processes. We designed modular operations, including picking, pouring, shaking, stirring, and placing, managed by a Controller Manager. This manager ensures the sequential and integrated execution of these operations. We successfully combined picking, pouring, and placing operations, as illustrated in our experimental results. (See the project website for more details.)

C. Visual Sim2Real

Chemical experiment containers are mostly transparent objects. Transparent objects possess intricate optical properties, and current visual tasks for transparent objects often concentrate on depth completion [51], [52], multi-modal analysis [53], and other research areas. Regardless of the approach, most studies rely heavily on large-scale simulation datasets [54], [55], making high-fidelity transparent simulations a crucial foundation for research and grasping tasks involving transparent objects. Our framework integrates Segmentation Models PyTorch [56], offering mainstream encoder-decoder architectures to facilitate network deployment in deep learning research areas such as depth completion and multi-modal analysis. We deployed various network combinations and conducted quantitative experiments on our simulation datasets. As illustrated in Table II, quantitative comparisons using Intersection over Union (IoU), Pixel Accuracy (PA), F1-Score, and F2-Score showed that the EfficientNet-DeepLabV3 combination outperformed others, achieving top scores across all metrics.

TABLE II: Performance Metrics of Different Encoder-Decoder Combinations

Encoder	Decoder	IoU	PA	F1-Score	F2-Score
TGCNN [53]	-	0.6604	0.9875	0.7851	0.7220
ResNet [57]	Unet [58]	0.7097	0.9902	0.8181	0.7813
VGG [59]	Unet++ [60]	0.6963	0.9896	0.8056	0.7494
EfficientNet [61]	DeepLabV3 [62]	0.7582	0.9917	0.8558	0.8112

Additionally, we further validated the Sim2Real ability by performing an object detection task. For this task, we selected YOLO [63] as our algorithm. The model trained within the simulation environment was evaluated for object detection in both simulated and real-world environments. The results are consistent with results in the semantic segmentation task, confirming that Chemistry3D effectively supports visual Sim2Real.(See the project website for more details.)

D. Embodied Intelligence

We integrated multiple functional agents into Chemistry3D using LLMs to understand and execute tasks. We designed an inorganic chemistry experiment scene (as shown in Fig. 4(c)), where the robot is expected to carry out the desired experimental operations through natural language input. The scene includes containers with $KMnO_4$, $FeCl_2$, and empty beakers and the robot can implicitly acquire object labels to observe the environment. Using Chemistry3D's chemical database, our agent can predict possible reactions and execute the corresponding actions. Additionally, with the controller manager described in Section IV-B, the experiment supports combining various manipulations.(See the project website for more details.)

E. Reinforcement Learning

OmniIsaacGymEnvs facilitates complex RL tasks in Chemistry3D. We demonstrated the capability of RL research by setting the RL task of picking as shown in Fig. 4(d). Using Proximal Policy Optimization (PPO) [64] as the algorithm, The experiment involved 2048 environments, 3500 epochs, and a learning rate of 5×10^{-4}, applied consistently across multiple experiments. We plotted the reward and success rate curves, showing robust outcomes. The results confirmed that robotic arms could successfully grasp chemical containers within Chemistry3D. (See the project website for more details.)

V. Conclusion

We presented a 3D robot simulation toolkit based on NVIDIA's Omniverse platform for chemical experiments. This system encompasses various chemical containers and robotic models, supporting transparent objects and fluid simulations. We have established an extensive chemical dataset that provides real-time feedback on various parameter changes during experiments. Through RL tasks, large language modeling, and Sim2Real experiments, we have demonstrated the significant potential of this system in machine learning applications. However, simulating chemical reactions balances computational complexity with model accuracy, requiring more resources for precise models. Inorganic reaction simulations are limited by database quality, which may not cover all reactions. Omniverse's current capabilities can't fully replicate gas-phase reactions. This system enhances the visualization and interactivity of chemical experiments and offers a new tool for interdisciplinary research in chemistry and robotics, promising to advance related fields.

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