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MATTERIX: toward a digital twin for robotics-assisted chemistry laboratory automation

In the format provided by the authors and unedited

Supplementary Section 1 Assets Description

Supplementary Section 1.1 Materials

MATTERIX supports solids and fluids using position-based-dynamics (PBD) particle simulation.

Supplementary Section 1.2 Glassware

MATTERIX has different glassware available and readily-used in our environments. These include beakers, graduated cylinders, reagent bottles, funnels, test tubes and vials.

Supplementary Section 1.2.1 Laboratory Tools

Digital Pipette: This can be integrated with a robot arm to facilitate the processing of pipetting fluids through its digital interface.

Spatulas: Human scientists weigh samples (materials) using a spatula and balance. The spatula used in our environment has been demonstrated to autonomously weigh different solid materials in our previous works[59].

Supplementary Section 1.3 Laboratory Instruments

Hot plate, stirrer, and balance: A key instrument is a hot plate, balance, and stirrer, where for this setup we used the IKA RCT Digital hot plate and stirrer, which has been used in our previous works for solubility screening and crystallisation[60,61].

Syringe pump: Syringe pumps are commonly used for precise and reliable liquid handling. In our work, we have used the Tecan Cavro pumps.

Supplementary Section 1.4 Automation Platforms

Opentrons: OT-2 is an open-source bench-top liquid handler.

Supplementary Section 1.4.1 Robots

KUKA KMR iiwa: is a mobile manipulator with a 7 DoF arm that has been used in different material discovery experiments including the mobile robotic chemist for photocatalysis[6] and the multi-robot system for solid-state chemistry[7].

Franka Emika Panda: The Franka Emika Panda arm robot, equipped with either a Franka Emika Panda Hand or a Robotiq 2F-85 gripper was used as the main manipulator in the environment since it has already been demonstrated as a robotic chemist across different workflows[5,62]. To facilitate grasping objects from the side in tabletop scenarios and enhance constrained motion planning in some of the environments, we positioned the Robotiq 2F-85 end-effector parallel to the ground on the robot's last link. This configuration was attained either through a fixed linkage or by incorporating a Dynamixel XM540-W150 servo motor as an additional degree of freedom.

Supplementary Section 2 Chemistry Lab Simulated Environments

The videos of all the environment are provided on the project website at:
https://accelerationconsortium.github.io/Matterix/.

Beaker Placement in Fumehood with Franka Emika Panda 8 DoF robot arm and Robotiq gripper: The Franka Emika Panda 8 DoF robot arm, equipped with a Robotiq gripper, is precisely manoeuvring a beaker within the confines of a fumehood. The robot is executing a controlled placement of the beaker, demonstrating its ability to handle laboratory equipment in a potentially hazardous environment. An example reaching task using the cuRobo motion planner with collision avoidance is demonstrated as well.

Beaker Placement in OT2 with Franka Emika Panda 8 DoF robot arm and Robotiq gripper: The Franka Emika Panda robot with its Robotiq gripper is executing a precise placement of a beaker within the OT2 liquid handling platform's workspace.

Funnel Pick and Place with Franka Emika Panda 8 DoF robot arm and Robotiq gripper: The Franka Emika Panda with its Robotiq gripper, is performing a pick-and-place operation with a funnel. This involves grasping the funnel, transporting it, and accurately positioning it in a new location.

KUKA KMR IIWA Pick and Place Beaker: The mobile KUKA KMR IIWA robot is autonomously transporting a beaker between different locations in a representative lab.

Liquid Dispensing Station: The robot arm (Franka Emika Panda) sets up the OT-2 workstation by placing the dispensing rack, tips rack, and reservoir well in the tray. Following this, the OT-2 head connects the pipettes and begins the fluid dispensing process.

Franka Emika Panda (8DoF with Robotiq gripper) Pick and Place Beaker on Scale: The robot arm is accurately placing a beaker onto the scale, for weighing its contents.

Franka Emika Panda (8DoF with Robotiq gripper) Pour Fluid: The robot is precisely pouring a liquid from one container to another.

Franka Emika Panda Pick and Place Vial Rack: The robot arm is transporting the racks of vials between different locations.

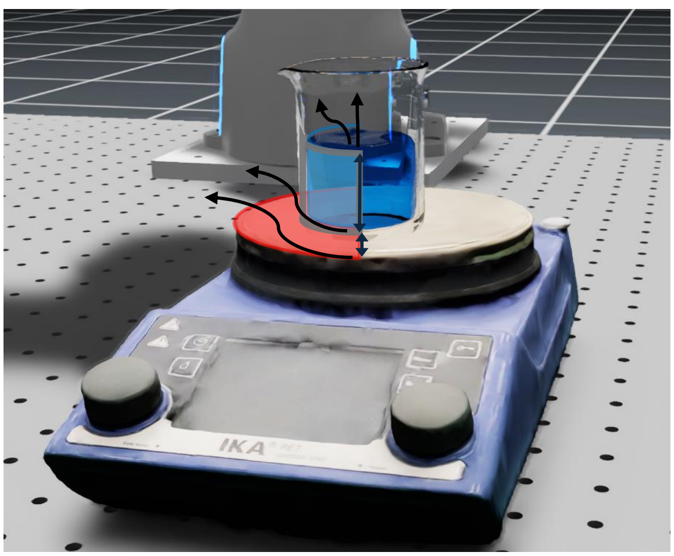
Franka Emika Panda (8DoF with Robotiq gripper)/Franka Emika Panda Vial Insertion: The robot arm is picking up a vial and inserting it in the rack.

Franka Emika Panda Wellplate Insertion in OT2: The robot arm is picking up the wellplate and inserting it in the rack locations on the OT2.

Detailed instructions and tutorials for running MATTERIX are available on the project website and repository. We encourage readers to review them.

Supplementary Section 3 Heat Transfer Semantics EngineExample

Thermal analysis is crucial in laboratory systems to ensure experimental accuracy and optimize energy efficiency. Here, we develop a thermal model for a solution-beaker-heater system as an example, applying an energy balance approach to predict temperature variations in different components over time. This approach is generic and could be applied to different laboratory components.



Supplementary Figure Supplementary Figure 1 : Heat transfer between the heater, beaker, and solution. The IKA RET control device heats the beaker through conduction, which then transfers heat to the solution. Heat exchange is bidirectional, flowing from hotter to cooler objects until equilibrium is reached. Curved arrows indicate heat dissipation to the ambient air.

System Overview The system consists of three interconnected thermal components:

- **IKA Heater**: A solid heating element providing heat input.
- **Beaker**: A glass container facilitating heat transfer between the heater and the liquid.
- **Solution**: A liquid medium subjected to thermal interactions with the beaker and ambient air.

Heat transfer in the system occurs primarily through conduction and convection.

Heat Transfer Mechanisms A uniform temperature distribution within each component is assumed in MATTERIX. Each component exchanges heat through different pathways, as shown in Supplementary Figure 1. Different pathways are described below:

- IKA Heater
  - Conductive heat transfer to the Beaker: $\dot{q}_{hb}$
  - Convective heat loss to the surrounding Air: $\dot{q}_{ha}$
  - Internal heat generation: $\dot{q}_{\text{gen}}$
- Beaker
  - Conductive heat transfer from the IKA Heater: $\dot{q}_{hb}$
  - Conductive heat transfer to the Solution: $\dot{q}_{bs}$
  - Convective heat loss to the Air: $\dot{q}_{ba}$
- Solution
  - Conductive heat transfer from the Beaker: $\dot{q}_{bs}$
  - Convective heat loss to the Air: $\dot{q}_{sa}$

Energy Balance Equations Applying the first law of thermodynamics, we obtain the governing equations:

IKA Heater

$$m_h C_h \frac{dT_h}{dt} = \dot{q}_{\text{gen}} - \dot{q}_{hb} - \dot{q}_{ha} \tag{7}$$

where:

$$\dot{q}_{hb} = \frac{k_b A_b}{d_b}(T_h - T_b) \tag{8}$$

$$\dot{q}_{ha} = h_h A_h (T_h - T_a) \tag{9}$$

The term $\dot{q}_{\text{gen}}$ represents the heat generated internally within the IKA heater due to electrical power input. Generally, the heater can be assumed to behave as a purely resistive element, the heat generation follows Joule's Law ($V^2/R = RI^2$, where V is voltage, I is current, and R is the resistance). However, in our case, we are mainly facing a temperature-controlled heating, where the heater adjusts its heat generation to maintain a target temperature. Therefore, instead assuming a constant electrical power supply, $\dot{q}_{\text{gen}}$ depend on the heater temperature using a proportional control system, where the heater generates heat depending on the difference between its current temperature, (T_h), and the target temperature, (T_{target}):

$$\dot{q}_{\text{gen}} = K_{gen}(T_{target} - T_h) \tag{10}$$

Equation 7 describes the energy balance for the heater, where the generated heat ($\dot{q}_{\text{gen}}$) is partially transferred to the beaker via conduction ($\dot{q}_{hb}$) and lost to the ambient through convection ($\dot{q}_{ha}$).

Beaker

$$m_b C_b \frac{dT_b}{dt} = \dot{q}_{hb} - \dot{q}_{bs} - \dot{q}_{ba} \tag{11}$$

where:

$$\dot{q}_{bs} = \frac{k_b A_b}{d_b}(T_b - T_s) \tag{12}$$

$$\dot{q}_{ba} = h_b A_b (T_b - T_a) \tag{13}$$

Solution

$$m_s C_s \frac{dT_s}{dt} = \dot{q}_{bs} - \dot{q}_{sa} \tag{14}$$

where:

$$\dot{q}_{sa} = h_s A_s (T_s - T_a) \tag{15}$$

Parameter Definitions

- m (kg): Mass of the component
- C $(J/kg \cdot K)$: Specific heat capacity
- T (K): Temperature
- T_h (K): Heater temperature
- T_b (K): Beaker temperature
- T_a (K): Ambient temperature
- k $(W/m \cdot K)$: Thermal conductivity
- A (m^2): Heat transfer area
- d (m): Thickness of conductive medium
- h $(W/m^2 \cdot K)$: Convective heat transfer coefficient
- $\dot{q}$ (W): Heat transfer rate
- V (V): Voltage applied across the heater
- R (Ω): Electrical resistance of the heater
- I (A): Current flowing through the heater
- K_{gen} (W/K): Proportional control gain, which determines how aggressively the heater responds to temperature differences
- T_{target} (K): Target temperature of the IKA heater

Uniform Temperature Distribution Assumption The model employed in this work assumes a uniform temperature distribution within each component, meaning that no internal temperature gradients exist. This assumption is valid when the Biot number (Bi) is sufficiently small, indicating that internal conductive resistance is much lower than surface convective resistance[63]. The Biot number is defined as:

$$\text{Bi} = \frac{hL_c}{k} \tag{16}$$

where, h is the convective heat transfer coefficient of the surrounding fluid $(W/m^2 \cdot K)$, k is the thermal conductivity of the material $(W/m \cdot K)$, and L_c is the characteristic length (m), given by:

$$L_c = \frac{\mathcal{V}}{A} \tag{17}$$

where, $\mathcal{V}$ and A represent the volume and surface area of the object, respectively.

Although the Biot number in this study may exceed the typical threshold (0.1) depending on the object carried by the robotic system, assuming a uniform temperature distribution remains a practical simplification. This approach allows for an efficient thermal analysis that can be integrated into the MATTERIX to predict the temperature variations effectively.

In addition, it is worth mentioning that to determine whether heat transfer inside the solution is dominated by convection or conduction, we can use the Rayleigh number (Ra)[63,64]. The Rayleigh number helps predict whether buoyancy-driven fluid motion (natural convection) occurs. It is defined as follow:

$$Ra = Gr \cdot Pr \tag{18}$$

where:

- Gr is the Grashof number, representing the ratio of buoyancy to viscous forces.
- Pr is the Prandtl number, representing the ratio of momentum diffusivity to thermal diffusivity.

The Grashof number is given by:

$$Gr = \frac{g\beta(T_{\text{hot}} - T_{\text{cold}})L^3}{\nu^2}$$

where:

- g = gravitational acceleration (9.81 m/s²),
- β = thermal expansion coefficient of the liquid $(1/K)$,
- $T_{\text{hot}} - T_{\text{cold}}$ = temperature difference in the liquid,
- L = characteristic length (for example, height of the liquid column),
- ν = kinematic viscosity of the liquid (m^2/s).

The Prandtl number is given by:

$$Pr = \frac{\nu}{\alpha}$$

where:

- α = thermal diffusivity (m^2/s),
- ν = kinematic viscosity (m^2/s).

The interpretation of the Rayleigh number is as follow:

- If $Ra \gg 10^4$ (high Ra) $\Rightarrow$ Convection dominates (buoyancy-driven fluid motion).
- If $Ra \ll 10^4$ (low Ra) $\Rightarrow$ Conduction dominates (the liquid remains mostly still).
- If $Ra \approx 10^4$ $\Rightarrow$ Transition region where both conduction and convection occur.

This work establishes an energy balance framework for multi-object systems, providing heat transfer equations for analysis and simulation integrated with chemistry and object manipulation. Future work may involve online identification of heat transfer constants using IoT sensors to align simulations with real-world results.

Supplementary Section 4 Physics and Semantics Engine Algorithm

Supplementary Algorithm 1 describes the integration of the Physics and Semantics engines. At each simulation step, we first pass the current physical states $\boldsymbol{x}_t$ and actions $\boldsymbol{a}_t$ to the physics engine to compute the next physics state. Next, we iterate over all the semantics processes and events to estimate the next semantic states $\boldsymbol{s}_{t+1}$ and $\boldsymbol{l}_{t+1}$. Additionally, events can influence the behaviours of both the physics and semantics.

Algorithm Supplementary Algorithm 1 PHYSICS&SEMANTICSENGINE()

Input: $\boldsymbol{x}_0, \boldsymbol{s}_0, \boldsymbol{l}_0, \boldsymbol{a}_t$
Output: $\boldsymbol{x}_{t+1}, \boldsymbol{s}_{t+1}, \boldsymbol{l}_{t+1}$
for all $t \in \mathcal{T}$ **do**
  $\boldsymbol{x}_{t+1} \leftarrow \boldsymbol{F}_t(\boldsymbol{x}_t, \boldsymbol{a}_t)$ ▷ physics engine
  $\boldsymbol{s}_{t+1} \leftarrow \boldsymbol{P}_t(\boldsymbol{x}_{t+1}, \boldsymbol{s}_t, \boldsymbol{l}_t, \boldsymbol{a}_t)$ ▷ semantic processes
  $\boldsymbol{l}_{t+1}, \boldsymbol{F}_{t+1}, \boldsymbol{P}_{t+1} \leftarrow \boldsymbol{E}(\boldsymbol{x}_{t+1}, \boldsymbol{s}_{t+1}, \boldsymbol{l}_t, \boldsymbol{a}_t)$ ▷ semantic events

Supplementary Section 5 Chemistry Experiment Workflows

Supplementary Figure 2 illustrates the hierarchical state machine used to run multi-scale chemistry simulations. Supplementary Figure 2.A shows the state machine that executes the organic chemistry experiment presented in Figure 5.A, controlling both the heater and the robot. Supplementary Figure 2.B shows the state machine for the two-step reduction-oxidation chemistry experiment presented in Figure 5.B. The robot begins by pouring the solution from the first beaker into the third, followed by the solution from the second beaker, mixing all three solutions in the third beaker. In both workflows, the robot's motion is calculated using inverse kinematics.

Supplementary Figure 3 presents the results of the organic chemistry experiment conducted with the IKA plate heater set to a target temperature of 40°C. As shown in the figure, the solution temperature remains close to 35°C, resulting in a relatively slow rate for the organic reaction.

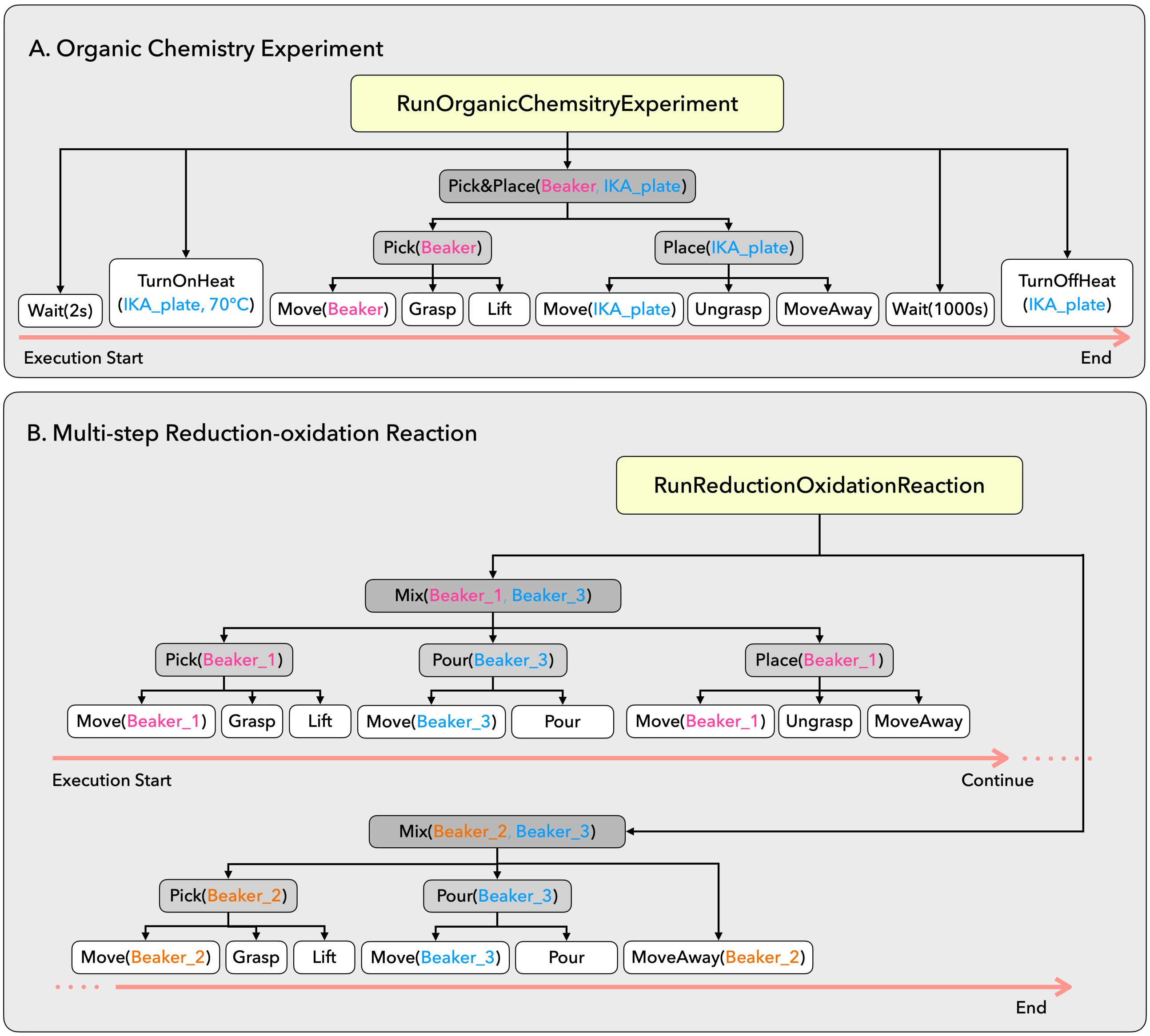
Supplementary Section 6 Deployment of Digital Twin Workflows to Real Setup

The videos of the deployment of digital twin workflows to the real setup are provided on the project website at: `https://accelerationconsortium.github.io/Matterix/`.

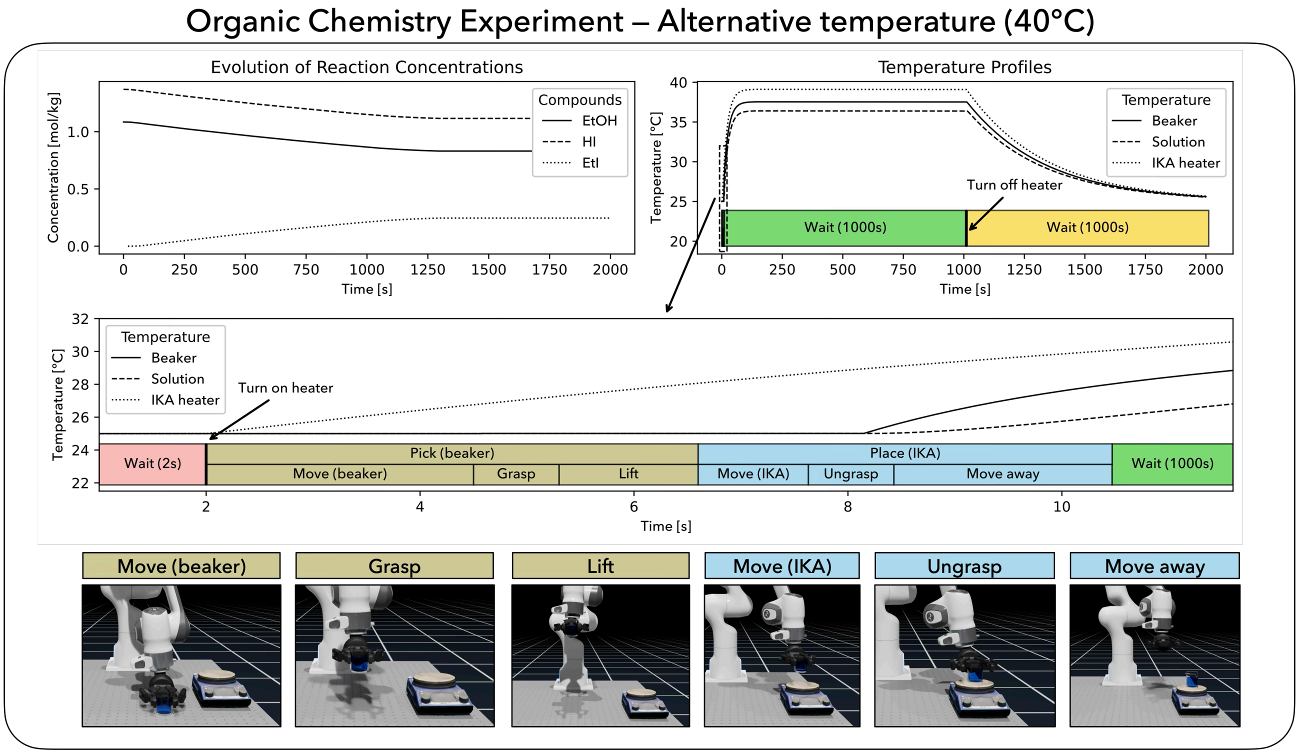
Robot Pouring Liquid from a beaker to another: The Franka Emika Panda 7 DoF robot arm, equipped with a Robotiq gripper, is transfers liquids during a pouring task (related to Figure 6.B).

Liquid Hnadling Station with Opentrons and Franka Arm: The Franka Research 3 (FR3) robot arm setups the Opentrons liquid hanlder in a real-world chemistry lab (related to Figure 6.C).

Multi-step Reduction-Oxidation Chemistry Experiment: The Franka Panda arm (FR3) robot arm equipped with a Robotiq gripper runs a two-step reduction-oxidation chemistry experiment (related to Figure 5.B).



Supplementary Figure Supplementary Figure 2 : Visualization of hierarchical state machine for different chemistry experiments. (A) demonstrates the workflow of the organic chemistry experiment as shown in Figure 5.A. (B) demonstrates the workflow of the multi-step reduction-oxidation reaction as shown in Figure 5.B.

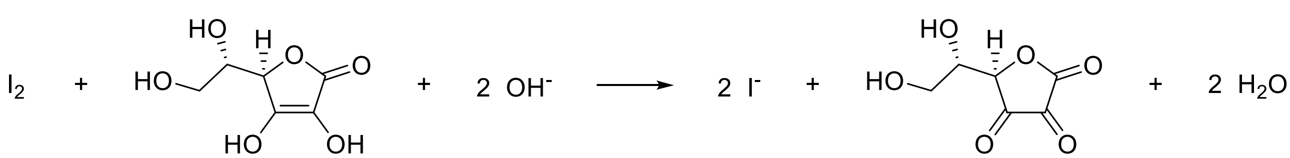


Supplementary Figure Supplementary Figure 3 : Multi-scale simulation of an organic chemistry experiment. A single-step organic chemistry experiment demonstrating the interaction of physical manipulation, heat transfer, and chemical kinetics simulation. The target temperature for the IKA plate heater is set to 40°C. Compared to Figure 5.A, the reaction proceeds at a slower rate at 40°C.

Step 1

$$2\ I^- + H_2O_2 \longrightarrow I_2 + 2\ OH^-$$

Step 2



Supplementary Figure Supplementary Figure 4 : Reaction equations of two step organic-inorganic redox-oxidation experiment. (Step 1) Oxidation of iodide to elementary iodine with hydrogen peroxide, reflected by the dark color of the iodine-starch complex. (Step 2) Reduction of iodine with ascorbic acid (Vitamin C), reflected by the diminishing of the iodine-starch dark color.