Final Phase of Reactive Hazards Evaluation & Analysis Compilation Tool (RHEACT) at Purdue

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Purdue Process Safety and Assurance Center (P2SAC) Spring 2024 Conference
Day 1: Tutorials and select Purdue presentations on process safety and assurance
May 6th, 2024
West Lafayette, IN

Overview and History of P2SAC/CISTAR Safety Project

PROBLEM

Prevalence of lab safety incidents & Need for convenient tool for preliminary hazard evaluation

SOLUTION & APPROACH

LAB SAFETY INITIATIVE

Assess safety practices in academic & industrial labs

Develop tools and compile best practices for safety evaluation

IMPACT

Reduction of the occurrence and severity of safety incidents and losses

CSB Laboratory Incident Data (Jan. 2001 - Jul. 2018) www.csb.gov/csb-releases-laboratory-incident-data-jan-2001---jul-2018/

Kaufman, J. A. Memorial Wall - Killed in Lab Accident; Laboratory Safety Institute www.labsafety.org/memorial-wall
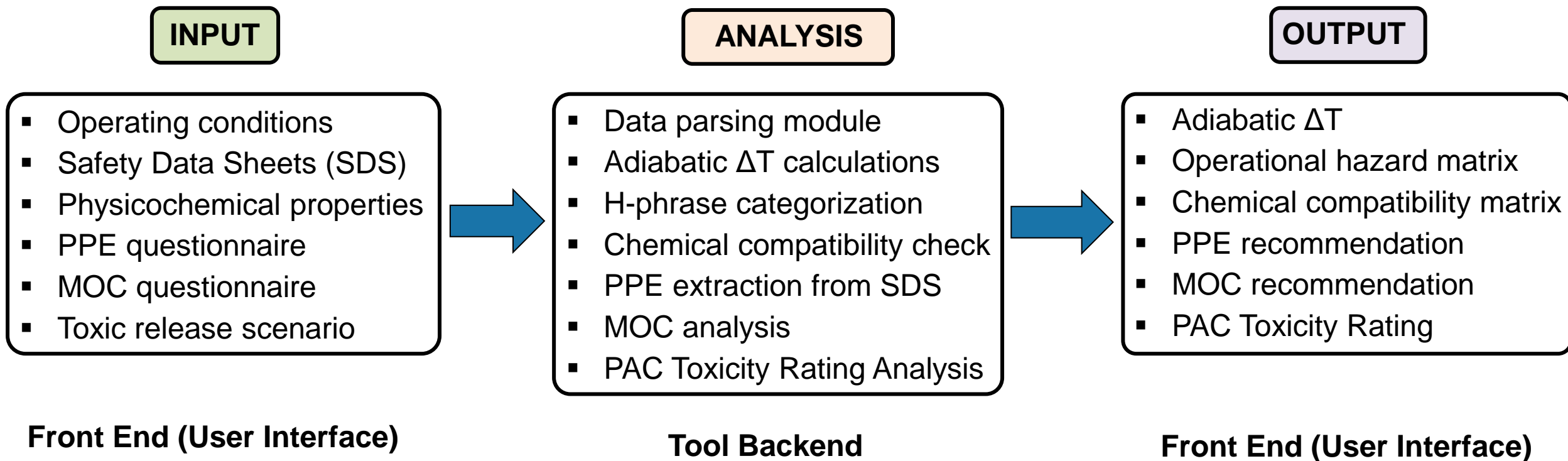
- **Summer 2018:** Project conceived following Professional Masters Project with Corteva

- **Fall 2018:** NSF-funded Lab Safety Project initiated

- **Spring 2021:** RHEACT Alpha version (1.0) developed
  - SDS parsing, Adiabatic ΔT estimation, Hazard statement summary, Chemical compatibility analysis

- **Spring 2022:** RHEACT Beta version (2.0) developed; safety survey and compiled safety best practices published
  - Redesigned user Interface, Personal Protective Equipment (PPE) Guide

- **Spring 2023:** RHEACT Beta version (3.0) developed
  - Added Heat of Reaction Calculator, Management of Change (MOC) Guide, Protective Action Criteria (PAC) toxic vapor release rating

- **Fall 2023:** RHEACT Beta version (3.0) continued development and improvements

- **Spring 2024:** External testing of RHEACT Beta version (3.0) and project completion at Purdue

Summary of RHEACT Features

RHEACT Beta Version (3.0), May 2024

Safety Data Sheets (SDS) Parsing[1]

Adiabatic ΔT Calculations[1]

Theoretical Heat of Reaction Estimation[2]

Operational Hazard Analysis[1]

Chemical Compatibility Analysis[1]

Personal Protective Equipment (PPE) Guide[3]

Management of Change (MOC) guide[3]

Protective Action Criteria (PAC) for Chemical Release[4]
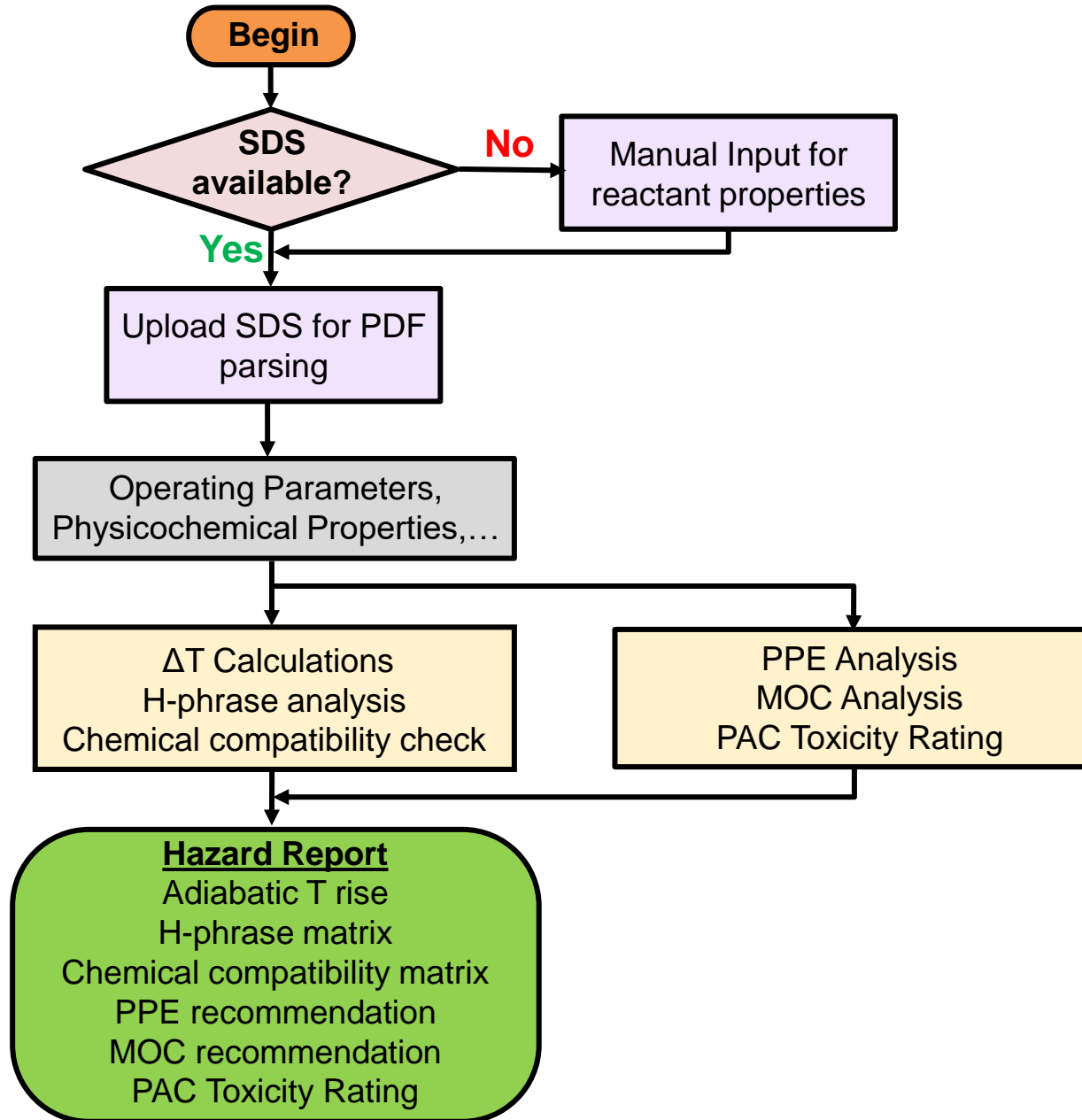
Safety Resource Links[5]

Beta version: rheact.github.io

1. Talpade, Ghanekar, Ezenwa,…,Devaraj, Ribeiro, Mentzer, Promoting a Safe Laboratory Environment Using the Reactive Hazard Evaluation and Analysis Compilation Tool. *ACS Chem. Health Saf.* **2021**

2. Sheng, Practical Estimation Techniques for Determination of Reaction Heat. *Org. Process Res. Dev.* **2021**

3. Bolton, Ezenwa,…, Devaraj, Ribeiro, Mentzer, A Guide for Personal Protective Equipment and Management of Change in Chemical Research Labs. *In Preparation* **2024**

4. Ezenwa, Bolton,…, Devaraj, Ribeiro, Mentzer, Protective Action Criteria Toxicity Rating: A Tool for Evaluating Toxic Vapor Release Events *In Preparation* **2024**

5. Ezenwa, Talpade, Ghanekar, Joshi, Devaraj, Ribeiro, Mentzer, Toward Improved Safety Cultures in Academic and Industrial Chemical Laboratories: An Assessment and Recommendation of Best Practices. *ACS Chem. Health Saf.* **2022**

RHEACT Overall Workflow

INPUT

- Operating conditions
- Safety Data Sheets (SDS)
- Physicochemical properties
- PPE questionnaire
- MOC questionnaire
- Toxic release scenario

ANALYSIS

- Data parsing module
- Adiabatic ΔT calculations
- H-phrase categorization
- Chemical compatibility check
- PPE extraction from SDS
- MOC analysis
- PAC Toxicity Rating Analysis

OUTPUT

- Adiabatic ΔT
- Operational hazard matrix
- Chemical compatibility matrix
- PPE recommendation
- MOC recommendation
- PAC Toxicity Rating

Front End (User Interface)

Tool Backend

Front End (User Interface)

RHEACT is a modular-designed online interactive web tool for hazard evaluation

Data workflow for RHEACT

Several case studies used to validate and demonstrate RHEACT capabilities

- University of Hawaii Incident (March 2016)

- Sodium azide mixtures in water or acid

- Aqua regia preparation and handling

- T2 Laboratories incident (December 2007)

- …

|	
Operational Hazards:	**Quick visual summary of physical and health hazards**
Chemical Compatibility:	**User alerts for chemical compatibility hazards**
Adiabatic ΔT:	**Preliminary caution for thermal runaways**
Personal Protective Equipment:	**Recommendations of required PPE based on SDS and questionnaire**
Management of Change (MOC):	**Recommendations on effective change management practices based on hazard matrix and questionnaire**
Protective Action Criteria (PAC):	**Evaluates release scenarios for adequate risk management**

RHEACT is a preliminary screening tool that alerts users about potential hazards and pushes them to perform further analysis.

Feedback from external testing by industrial partners

Bug fixes, feature testing, and general feedback was provided by industrial partners of P2SAC/CISTAR

Legend:
- Strongly Agree
- Somewhat Agree
- Somewhat Disagree
- Strongly Disagree
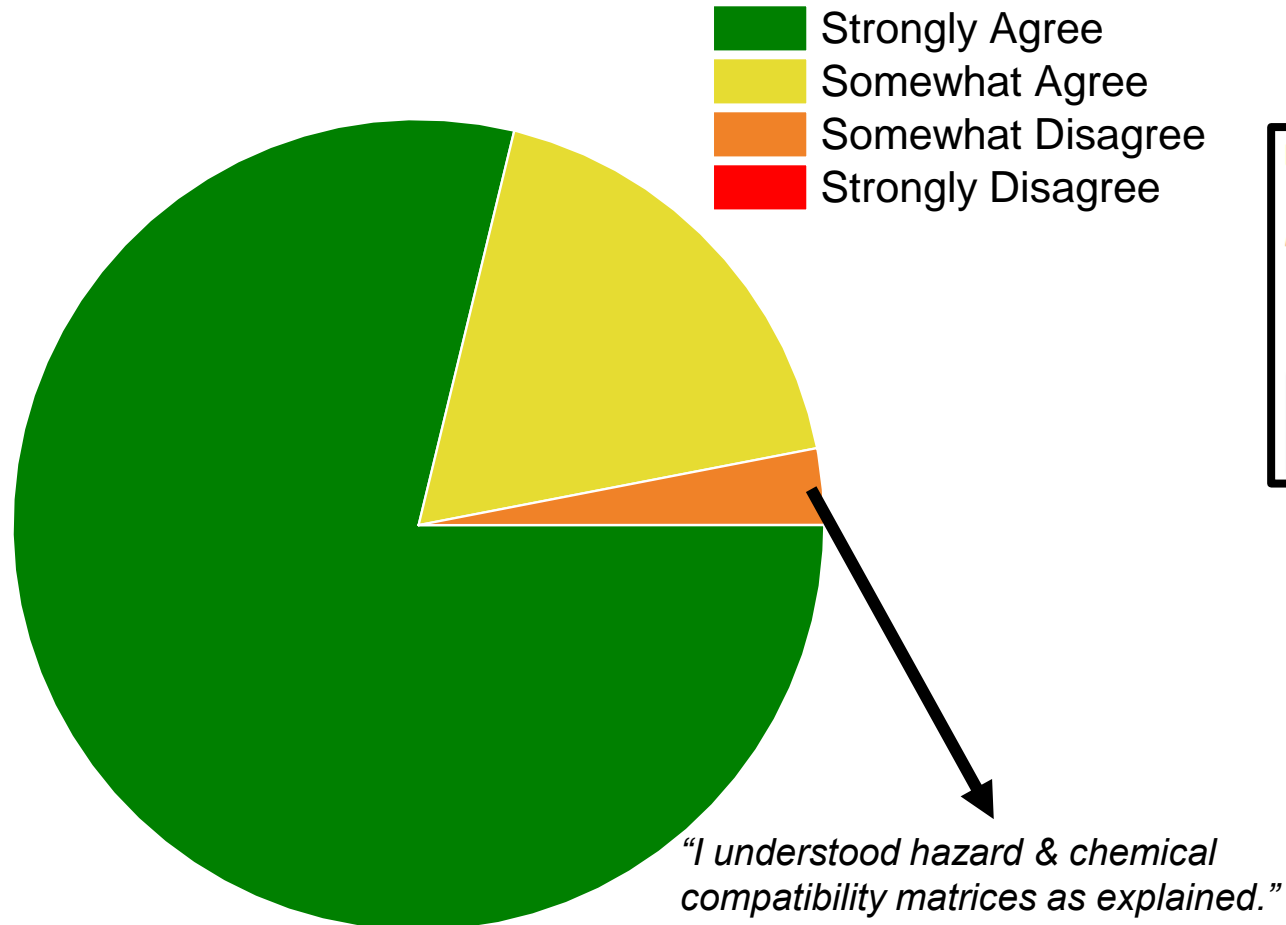
Semi-quantitative feedback obtained through survey

Please rate the following statements regarding your experience with RHEACT

Please leave any untested features blank

	1 - Strongly Agree	2 - Somewhat Agree	3 - Somewhat Disagree	4 - Strongly Disagree
The interface is easy to navigate.	○	○	○	○

"I understood hazard & chemical compatibility matrices as explained."

We asked a series of 14 questions designed to collect data on all aspects of RHEACT

- *User experience*
- *SDS parsing*
- *Adiabatic temperature rise*
- *Hazard matrix and summary*
- *PPE questionnaire*
- *MOC*
- *PAC toxicity*

Feedback from external testing by industrial partners

Bug fixes, feature testing, and general feedback was provided by industrial partners of P2SAC/CISTAR

Key takeaways from survey comments

Data input through SDS parsing loads data without errors, improves usability

Saving current projects allows for updates to be made easily (In line with MOC)

Hazard statement summaries and compatibility matrix are best used as a "high level" description of potential issues

The PPE guide, MOC report, and PAC toxicity calculator meet their designed intent towards a continued safety culture

Feedback from external testing by industrial partners

Bug fixes, feature testing, and general feedback was provided by industrial partners of P2SAC/CISTAR

Suggestions for long-term improvement

- Robust unit converter for input values

- Designated interface for mobile use

- Interpretation of ChemDraw compound entry/search

- Heat of reaction calculations for compounds with limited thermochemistry data

- Alternate or industry-specific release calculators to account for varied standards

- Ability to catalogue manually entered compounds

- Implement a dedicated feature for scale-up calculations and safety considerations

Invitation for testing and use of RHEACT

rheact.github.io

Particularly interested in:

- **Required clarifications on wording of prompts, data fields, and results**
- **"Bugs" or other issues encountered with incorrect calculations**
- **Experience with unique or specific chemical systems**
- **Ability to consult with the quick start and user guides to address questions**

We will continue to actively monitor for feedback through the end of June

Outlook of permanent implementation

- Permanent home with CISTAR for publicly-accessible, robust hosting
  - ***https://cistar.us/RHEACT***
  - Expected June 2024

> **Target users**
> Academic chemical research and teaching labs
> Small and mid-size enterprises' (SME) R&D labs

- Hosting RHEACT on Purdue CISTAR is in line with our target user base
  - Small and mid-sized industrial labs and academic labs will not be required to have their own hosting and development resources

Upcoming publications (Summer 2024)

A Guide for Personal Protective Equipment and Management of Change in Chemical Research Labs
Ezenwa, S.[‡]; Bolton, B. [‡]; et al., *In Preparation*

Protective Action Criteria Toxicity Rating: A Tool for Evaluating Chemical Release Events
Ezenwa, S.[‡]; Bolton, B. [‡]; et al., *In Preparation*

Adaptation and development by industry

Target users
Academic chemical research and teaching labs
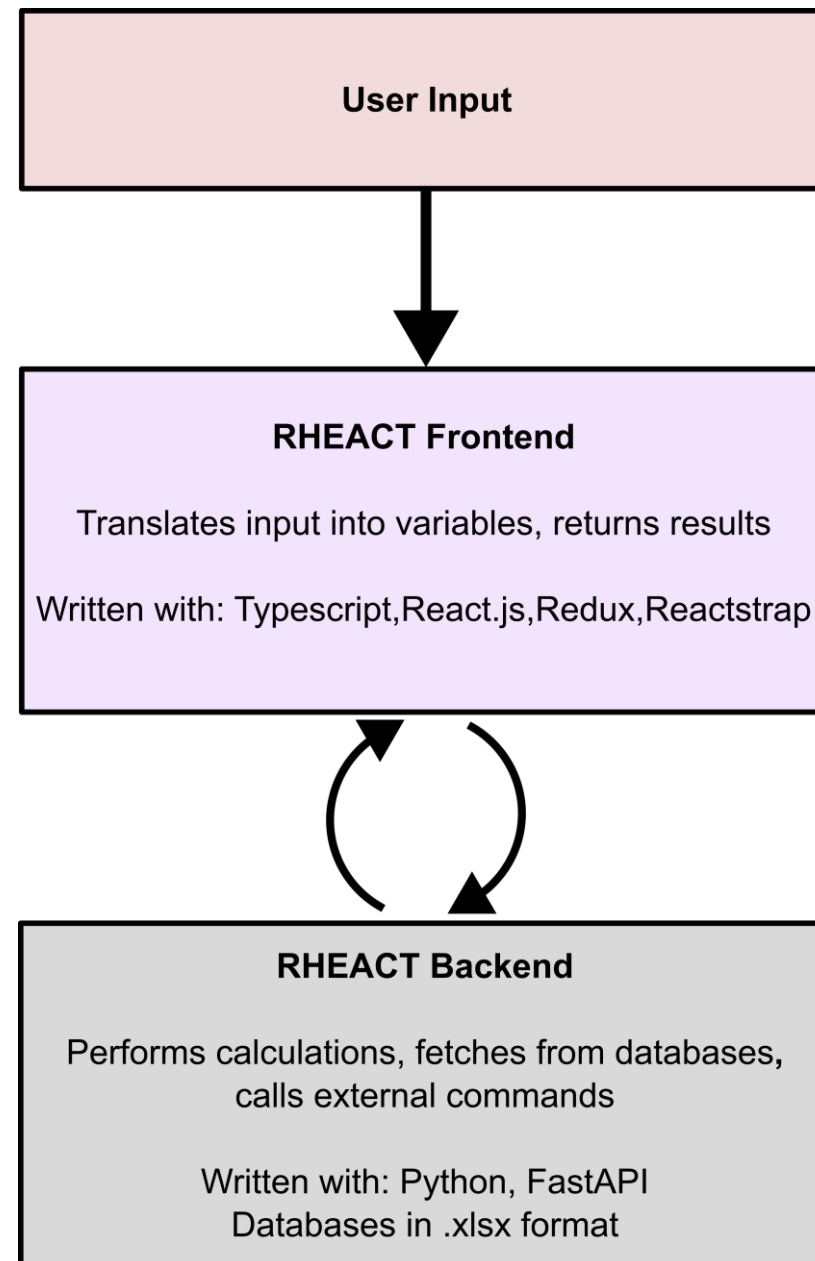Small and mid-size enterprises' (SME) R&D labs

We also recognize that larger organizations, with their own dedicated resources and use cases, may have need for various RHEACT features

We encourage organizations to adapt the RHEACT framework to deploy their own version and tailor it to their needs or integrate with existing services

The RHEACT implementation has been documented and organized such that it can be easily adapted

Code repository
https://github.com/rheact

User Input

↓

RHEACT Frontend

Translates input into variables, returns results

Written with: Typescript,React.js,Redux,Reactstrap

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RHEACT Backend

Performs calculations, fetches from databases, calls external commands

Written with: Python, FastAPI
Databases in .xlsx format

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CISTAR Industry Partners: *https://cistar.us/industry-innovation*
P2SAC Industry Partners: *https://engineering.purdue.edu/P2SAC/people/partners*

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