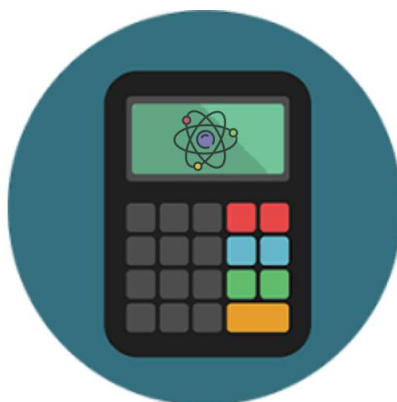


Chemical Calculator

User Manual



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User Manual

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Manish K Gupta.
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Credits & Team

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Software Logo: Khushali Shah, Nishtha Chaudhary, Ritika Lakdawala

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General Information

1. Introduction

Chemical Computing refers to computing with real molecules as well as to programming electronic devices using principles taken from chemistry. All information processing systems found in living organisms are based on chemical processes. So harnessing the power of chemistry for computing might lead to a new unifying paradigm coping with the rapidly increasing complexity and autonomy of computational systems. Chemical calculator is our attempt to exploit this power of computing with chemical reactions. We implemented four basic operations, i.e. addition, subtraction, multiplication and division. Our calculator provides the table which contains the sequence of reactions to carry out the operation given by the user. Along with that it also contains details of how the number of reactants and products varies after each chemical reaction. The sequence of reactions can also be downloaded as an XML file which can be used for further simulations.

2. Product Scope

Our web-application provides the user with:

- Display the answer for the provided operations like a normal calculator.
- Provides the table which contains the step-by-step procedure of how the answer is calculated using chemical computation.
- Option for downloading the XML file of reactions.

3. Product Perspective

The main aim of the product is to implement the operations by making use of the chemical reactions and make this process user friendly by providing a calculator UI.

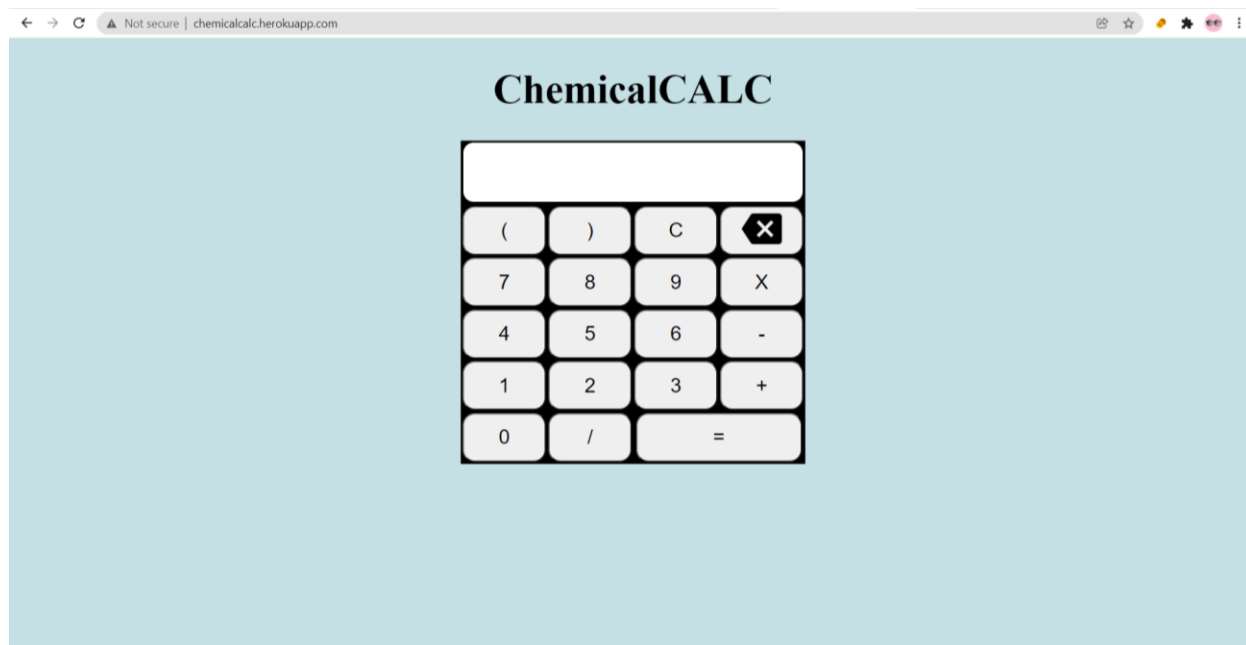
4. System Summary

Browsers: Google Chrome, Mozilla Firefox, Safari, Microsoft Edge, Opera and Brave

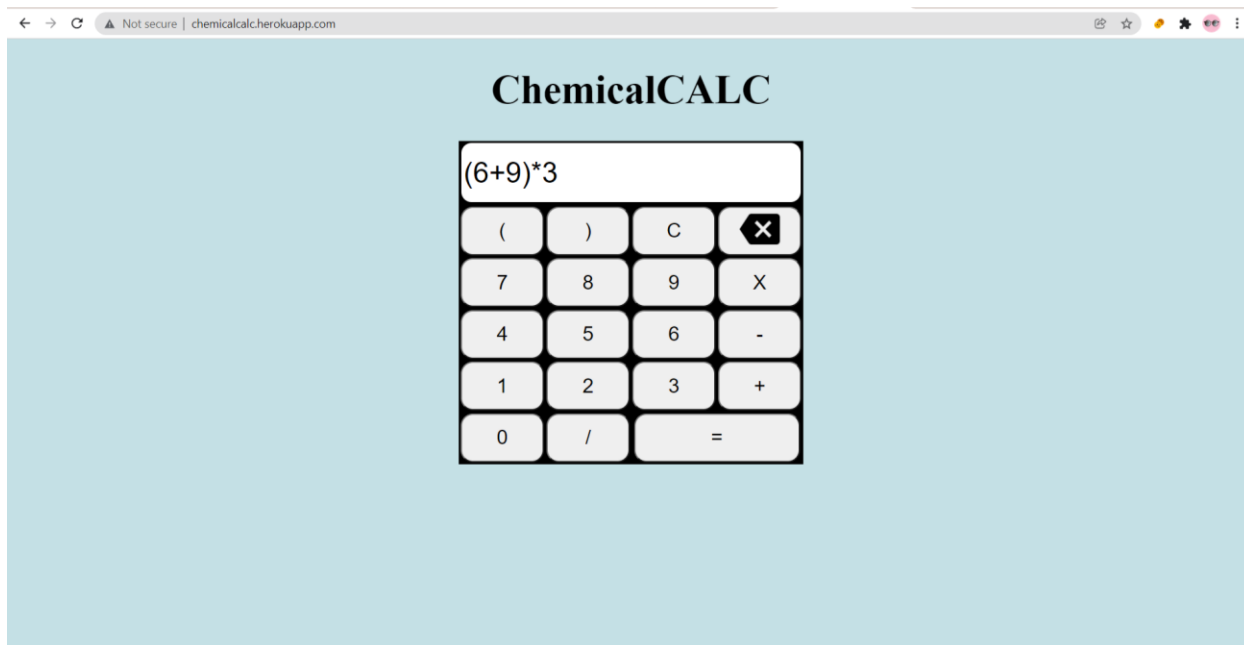
Getting Started

1. Calculator UI:

Once you open the website, the basic calculator UI is shown. It includes buttons for numbers (0-9), operations (+, -, /, *,=), brackets, clear, and delete.

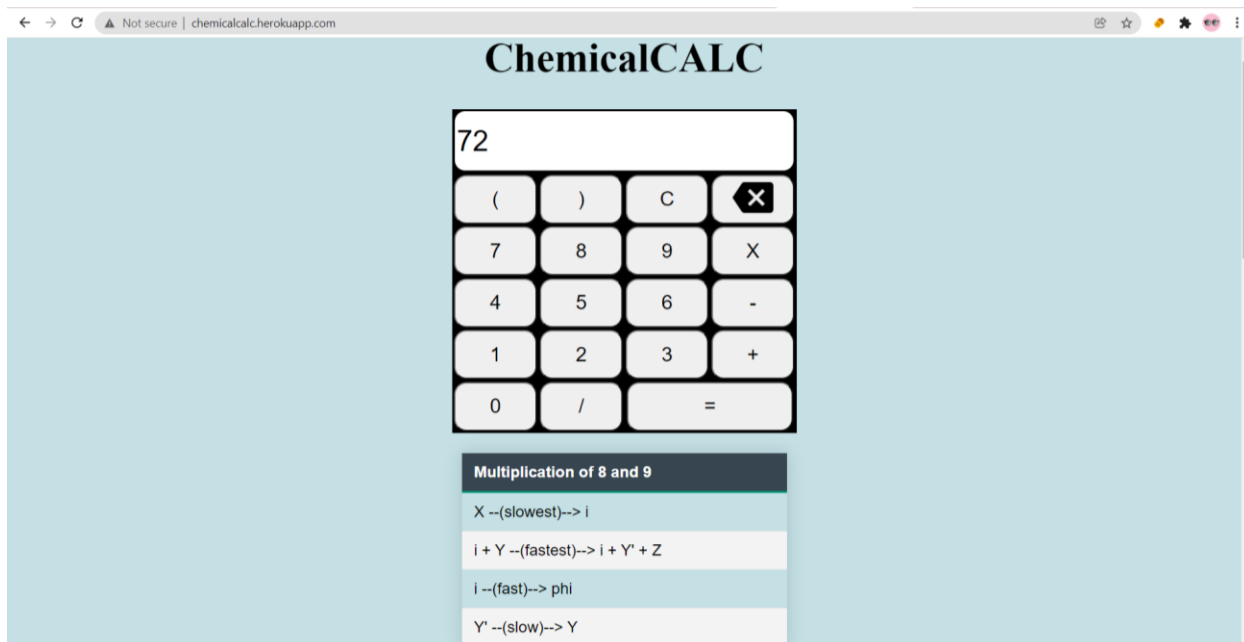


You can enter any number and operation you want to perform and it can be seen in the calculator display as shown below:



2. Reaction Table:

After pressing the '=' button, The reaction table will be displayed under the calculator UI as mentioned below:



Reaction	Number Of Iterations	X	Y	i	Y'	Z
Initial Values	0	8	9	0	0	0
X $\xrightarrow{\text{slowest}}$ i	8	7	9	1	0	0
i + Y $\xrightarrow{\text{fastest}}$ i + Y' + Z	9	7	0	1	9	9
i $\xrightarrow{\text{fast}}$ phi	1	7	0	0	9	9
Y' $\xrightarrow{\text{slow}}$ Y	9	7	9	0	0	9
X $\xrightarrow{\text{slowest}}$ i	7	6	9	1	0	9
i + Y $\xrightarrow{\text{fastest}}$ i + Y' + Z	9	6	0	1	9	18
i $\xrightarrow{\text{fast}}$ phi	1	6	0	0	9	18
Y' $\xrightarrow{\text{slow}}$ Y	9	6	9	0	0	18
X $\xrightarrow{\text{slowest}}$ i	6	5	9	1	0	18
i + Y $\xrightarrow{\text{fastest}}$ i + Y' + Z	9	5	0	1	9	27
i $\xrightarrow{\text{fast}}$ phi	1	5	0	0	9	27
Y' $\xrightarrow{\text{slow}}$ Y	9	5	9	0	0	27
X $\xrightarrow{\text{slowest}}$ i	5	4	9	1	0	27
i + Y $\xrightarrow{\text{fastest}}$ i + Y' + Z	9	4	0	1	9	36
i $\xrightarrow{\text{fast}}$ phi	1	4	0	0	9	36

Y' $\xrightarrow{\text{slow}}$ Y	9	4	9	0	0	36
X $\xrightarrow{\text{slowest}}$ i	4	3	9	1	0	36
i + Y $\xrightarrow{\text{fastest}}$ i + Y' + Z	9	3	0	1	9	45
i $\xrightarrow{\text{fast}}$ phi	1	3	0	0	9	45
Y' $\xrightarrow{\text{slow}}$ Y	9	3	9	0	0	45
X $\xrightarrow{\text{slowest}}$ i	3	2	9	1	0	45
i + Y $\xrightarrow{\text{fastest}}$ i + Y' + Z	9	2	0	1	9	54
i $\xrightarrow{\text{fast}}$ phi	1	2	0	0	9	54
Y' $\xrightarrow{\text{slow}}$ Y	9	2	9	0	0	54
X $\xrightarrow{\text{slowest}}$ i	2	1	9	1	0	54
i + Y $\xrightarrow{\text{fastest}}$ i + Y' + Z	9	1	0	1	9	63
i $\xrightarrow{\text{fast}}$ phi	1	1	0	0	9	63
Y' $\xrightarrow{\text{slow}}$ Y	9	1	9	0	0	63
X $\xrightarrow{\text{slowest}}$ i	1	0	9	1	0	63
i + Y $\xrightarrow{\text{fastest}}$ i + Y' + Z	9	0	0	1	9	72
i $\xrightarrow{\text{fast}}$ phi	1	0	0	0	9	72
Y' $\xrightarrow{\text{slow}}$ Y	9	0	9	0	0	72

3. Download XML

Once the reaction table is generated, you can download the XML file with the help of **'Download XML'** button given below the table:

i + Y --(fastest)--> i + Y1 + Z	9	0	0	1	9	72
i --(fast)--> phi	1	0	0	0	9	72
Y1 --(slow)--> Y	9	0	9	0	0	72

Download (XML)

4. References

https://www.youtube.com/watch?v=yIdA6HvUi_Q&t=1610s

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<https://www.geeksforgeeks.org/deploy-python-flask-app-on-heroku/>