

Test Report: Stoichiometry Mass-Mass Program

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1 Revision History

Date	Version	Notes
26/12/2019	1.0	First version of the document

2 Symbols, Abbreviations and Acronyms

symbol	description
T	Test
SMMP	Stoichiometry Mass-Mass Program

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This document report result from unit test cases found in Unit Verification and Validation Plan document (1).

3 Functional Requirements Evaluation

Functional requirement is evaluated using unit test cases from T1 to T17. All the details regarding functional requirements evaluation can be found in section 6. The traceability between unit test cases and functional requirement found in table 2 of section 9.

4 Nonfunctional Requirements Evaluation

Nonfunctional Requirements Evaluated in unit test cases T18 - T19. All the details regarding Nonfunctional requirements evaluation can be found in this section. The traceability between unit test cases and Nonfunctional requirement found in table 3 of section 9.

4.1 Usability

Unit test T18 measures the Usability of SMMP system. The survey measured the satisfaction level of potential user after using SMMP. How easy and understandable the system is?. It needs to be filled by any user and if satisfactory level is low then enhancement need to be taken into account.

4.2 Reliability

Unit test T19 measures the Reliability of SMMP system. 25 different unbalanced chemical reactions were tested and compared to answer of online balancer (2) as parallel testing. the aim was to get 100% of correct answers that includes right balance reaction and correct mass value. Below table shows the final result compared to the online balancer and the final percentage of correctness

The goal of Reliability had been accomplished. all tested reactions were balanced correctly as compared to the online balancer.

Unbalanced Chemical Reaction	Online Balancer Result	SMMP Result	correctness
$CH_4 + O_2 \rightarrow CO_2 + H_2O$	$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$	$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$	correct
$Fe_2O_3 + C \rightarrow Fe + CO_2$	$2Fe_2O_3 + 3C \rightarrow 4Fe + 3CO_2$	$2Fe_2O_3 + 3C \rightarrow 4Fe + 3CO_2$	correct
$N_2 + O_2 \rightarrow N_2O_5$	$2N_2 + 5O_2 \rightarrow 2N_2O_5$	$2N_2 + 5O_2 \rightarrow 2N_2O_5$	correct
$CH_4 + Cl_2 \rightarrow CCl_4 + HCl$	$CH_4 + 4Cl_2 \rightarrow CCl_4 + 4HCl$	$4CH_4 + Cl_2 \rightarrow CCl_4 + 4HCl$	correct
$N_2 + H_2 \rightarrow NH_3$	$N_2 + 3H_2 \rightarrow 2NH_3$	$N_2 + 3H_2 \rightarrow 2NH_3$	correct
$Fe + H_2O \rightarrow Fe_3O_4 + H_2$	$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$	$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$	correct
$Xe + F_2 \rightarrow XeF_6$	$Xe + 3F_2 \rightarrow XeF_6$	$Xe + 3F_2 \rightarrow XeF_6$	correct
$Hg + O_2 \rightarrow HgO$	$2Hg + O_2 \rightarrow 2HgO$	$2Hg + O_2 \rightarrow 2HgO$	correct
$CaO + C \rightarrow CaC_2 + CO$	$CaO + 3C \rightarrow CaC_2 + CO$	$CaO + 3C \rightarrow CaC_2 + CO$	correct
$S_8 + F_2 \rightarrow SF_6$	$S_8 + 24F_2 \rightarrow 8SF_6$	$S_8 + 24F_2 \rightarrow 8SF_6$	correct
$Mg + N_2 \rightarrow Mg_3N_2$	$3Mg + N_2 \rightarrow Mg_3N_2$	$3Mg + N_2 \rightarrow Mg_3N_2$	correct
$BeF_2 + Mg \rightarrow MgF_2 + Be$	balance	balance	correct
$Zn + HCl \rightarrow ZnCl_2 + H_2$	$Zn + 2HCl \rightarrow ZnCl_2 + H_2$	$Zn + 2HCl \rightarrow ZnCl_2 + H_2$	correct
$SiC + Cl_2 \rightarrow SiCl_4 + C$	$SiC + 2Cl_2 \rightarrow SiCl_4 + C$	$SiC + 2Cl_2 \rightarrow SiCl_4 + C$	correct
$MnS + HCl \rightarrow H_2S + MnCl_2$	$MnS + 2HCl \rightarrow H_2S + MnCl_2$	$MnS + 2HCl \rightarrow H_2S + MnCl_2$	correct
$UF_4 + Mg \rightarrow MgF_2 + U$	$UF_4 + 2Mg \rightarrow 2MgF_2 + U$	$UF_4 + 2Mg \rightarrow 2MgF_2 + U$	correct
$S + N_2O \rightarrow SO_2 + N_2$	$S + 2N_2O \rightarrow SO_2 + 2N_2$	$S + 2N_2O \rightarrow SO_2 + 2N_2$	correct
$SiH_4 + O_2 \rightarrow SiO_2 + H_2O$	$SiH_4 + 2O_2 \rightarrow SiO_2 + 2H_2O$	$SiH_4 + 2O_2 \rightarrow SiO_2 + 2H_2O$	correct
$TiCl_4 + Mg \rightarrow MgCl_2 + Ti$	$TiCl_4 + 2Mg \rightarrow 2MgCl_2 + Ti$	$TiCl_4 + 2Mg \rightarrow 2MgCl_2 + Ti$	correct
$Si + S_8 \rightarrow Si_2S_4$	$4Si + S_8 \rightarrow 2Si_2S_4$	$4Si + S_8 \rightarrow 2Si_2S_4$	correct
$SiO_2 + HF \rightarrow SiF_4 + H_2O$	$SiO_2 + 4HF \rightarrow SiF_4 + 2H_2O$	$SiO_2 + 4HF \rightarrow SiF_4 + 2H_2O$	correct
$P_4 + O_2 \rightarrow P_2O_5$	$P_4 + 5O_2 \rightarrow 2P_2O_5$	$P_4 + 5O_2 \rightarrow 2P_2O_5$	correct
$Sb + O_2 \rightarrow Sb_4O_6$	$4Sb + 3O_2 \rightarrow Sb_4O_6$	$4Sb + 3O_2 \rightarrow Sb_4O_6$	correct
$UO_2 + HF \rightarrow UF_4 + H_2O$	$UO_2 + 4HF \rightarrow UF_4 + 2H_2O$	$UO_2 + 4HF \rightarrow UF_4 + 2H_2O$	correct
$Al + O_2 \rightarrow Al_2O_3$	$4Al + 3O_2 \rightarrow 2Al_2O_3$	$4Al + 3O_2 \rightarrow 2Al_2O_3$	correct

Table 1: Reliability testing of SMMP as comparison to online balancer.

5 Comparison to Existing Implementation

This is stand alone system. If there is any existing systems with same functionalities and goals the developer is not aware about them and no comparison had been made.

6 Unit Testing

6.1 T1: get number of chemical reaction elements

The goal of this test is to make sure that at least one element for reactant1 , reactant2 and product1 were entered by the user. this test is to fulfill the minimum requirements of balancing reaction with two reactant and one

product. If user enter less than this requirement , an error message should be shown. pictures below illustrates all possible entries by user that matches all cases of T1 ,Table1 in (1). The tests had been passed correctly and system responded as intended.

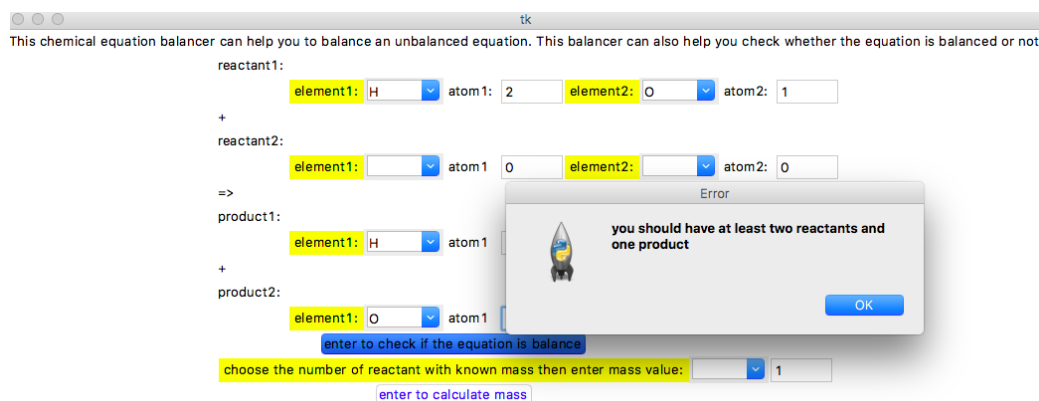


Figure 1: error message if user enter only one reactant

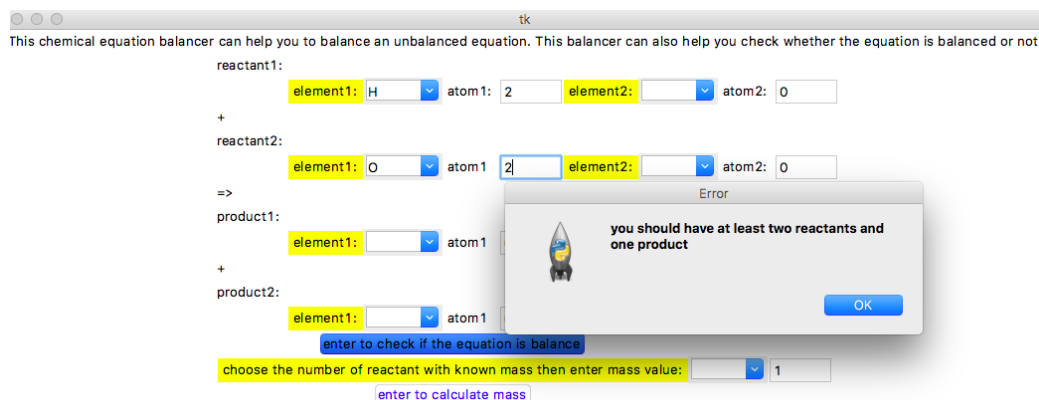


Figure 2: error message if user did not enter at least one product

tk

This chemical equation balancer can help you to balance an unbalanced equation. This balancer can also help you check whether the equation is balanced or not

reactant1:
 element1: H atom1: 2 element2: atom2: 0

+

reactant2:
 element1: O atom1: 2 element2: atom2: 0

=>

product1:
 element1: H atom1: 2 element2: O atom2: 1

+

product2:
 element1: atom1: 0 element2: atom2: 0

enter to check if the equation is balance

not balance

the balance form is: 2H2 + O2=2H2O

choose the number of reactant with known mass then enter mass value: 1

enter to calculate mass

Figure 3: system works fine with two reactants one product

tk

This chemical equation balancer can help you to balance an unbalanced equation. This balancer can also help you check whether the equation is balanced or not

reactant1:
 element1: Fe atom1: 1 element2: Cl atom2: 3

+

reactant2:
 element1: Mg atom1: 1 element2: O atom2: 1

=>

product1:
 element1: Fe atom1: 2 element2: O atom2: 3

+

product2:
 element1: Mg atom1: 1 element2: Cl atom2: 2

enter to check if the equation is balance

not balance

the balance form is: 2FeCl3 + 3MgO=Fe2O3+3MgCl2

choose the number of reactant with known mass then enter mass value: 1

enter to calculate mass

Figure 4: system works fine with two reactants two product

6.2 T2: get name of chemical reaction elements

The goal of this test is to make sure that any chemical element involved in the reaction need to be in both sides, reactants and products sides. Every element enter the reaction must be also one of products. Failing to fulfill this requirement will cause an error message. pictures below illustrates all possible entries by user that will rise an error message which matches cases of

T2 ,Table2 in (1). The tests had been passed correctly and system responded as intended.

The screenshot shows a graphical user interface for a chemical equation balancer. At the top, a title bar reads 'tk'. Below it, a subtitle states: 'This chemical equation balancer can help you to balance an unbalanced equation. This balancer can also help you check whether the equation is balanced or not'. The interface is divided into sections for reactants and products. Reactant 1 is set to 'Fe' with an atom count of 1. Reactant 2 is set to 'Cl' with an atom count of 3. Product 1 is set to 'Fe' with an atom count of 2 and 'O' with an atom count of 3. Product 2 is currently empty, with element dropdowns set to blank and atom counts set to 0. A red error message is displayed: 'wrong entry! element should be in the products side as well'. Below the error message, there are two buttons: 'enter to check if the equation is balance' and 'enter to calculate mass'. At the bottom, a label says 'choose the number of reactant with known mass then enter mass value:' followed by a dropdown menu set to 1 and a text input field.

Figure 5: error message if user enter element only in reactant side

The screenshot shows the same chemical equation balancer interface. Reactant 1 is 'C' with an atom count of 1. Reactant 2 is 'O' with an atom count of 2. Product 1 is 'C' with an atom count of 1 and 'H' with an atom count of 4. Product 2 is 'O' with an atom count of 2. A red error message is displayed: 'wrong entry! element should be in the reactants side as well'. The same buttons and bottom controls as in Figure 5 are present.

Figure 6: error message if user enter element only in product side

6.3 T3: get atom value of chemical reaction elements

The goal of this test is to make sure user change the default value of atom from 0 if he chose an element and enter a number greater than 0. pictures

below illustrates all possible entries by user that cause error message which matches cases of T3 ,Table3 in (1). The tests had been passed correctly and system responded as intended.

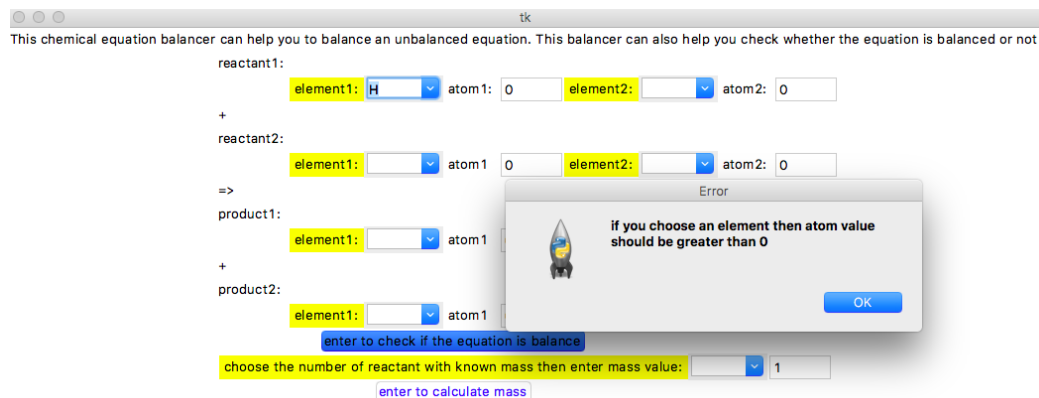


Figure 7: error message if user enter atom less than 1 if he selected an element

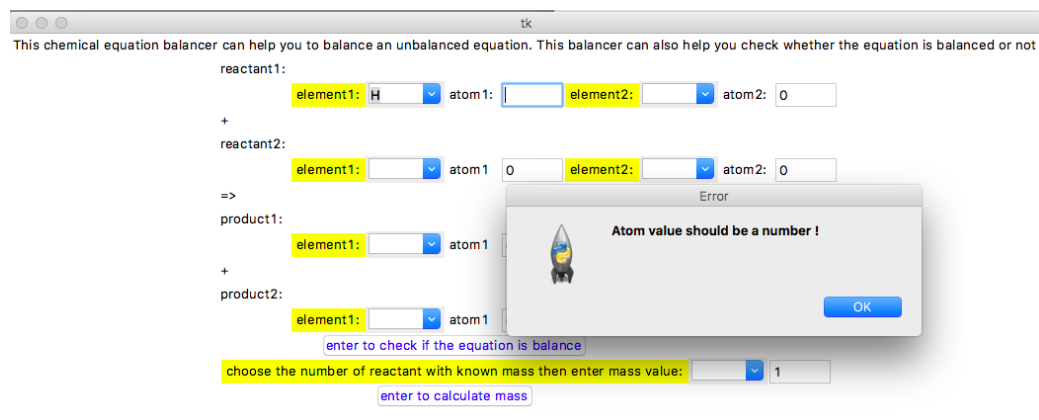


Figure 8: error message if user enter non number atom value

6.4 T4: get Mass Input

The goal of this test is to make sure user enter a positive number in mass value widget. the default mass value is 1. pictures below illustrates all possible entries by user that cause error message which matches cases of T4 ,Table4 in (1). The tests had been passed correctly and system responded as intended.

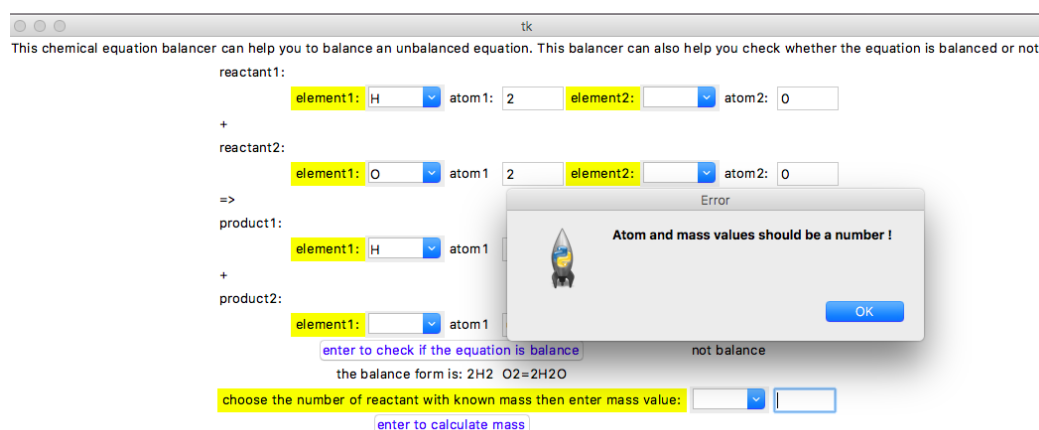


Figure 9: error message if user enter non number mass value

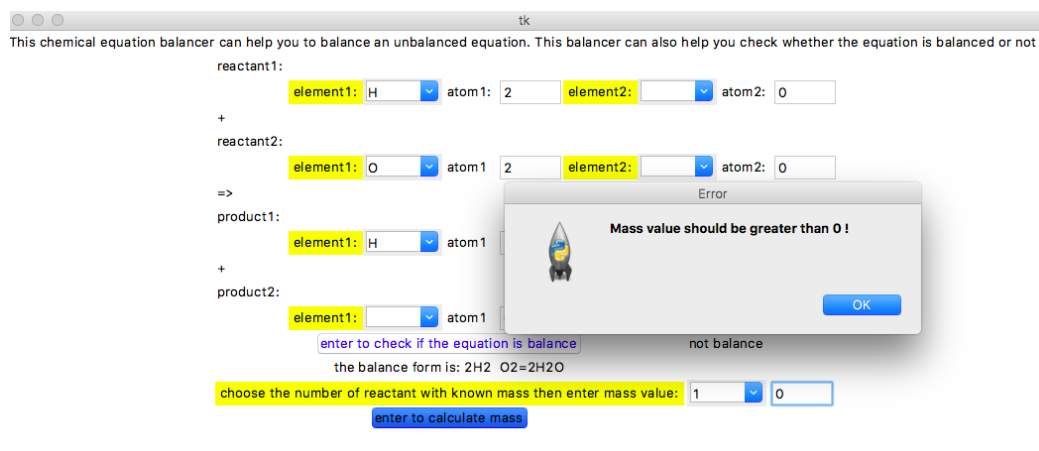


Figure 10: error message if user enter mass less than 1

6.5 T5: get reactant of known Mass

The goal of this test is to make sure user select a reactant of a known mass along with entering the mass value before enter the mass calculation button. picture below shows error message when user did not select a reactant number. The test passed correctly and system responded as intended.

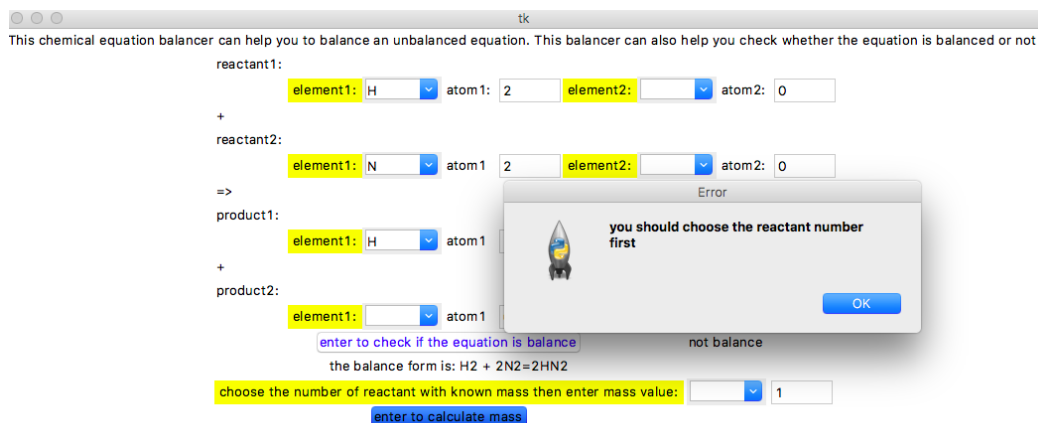


Figure 11: error message if user did not select number of reactant with known mass.

6.6 T6: Count total number of atoms for each element in each side

The goal of this test is to make sure that the system count the total of atom values each element involved in the reaction correctly in each side of reaction. add the element name along with the atom total value in dictionary structure to conclude with two dictionaries. one for reactant side and one for product side. picture below shows dictionaries for this reaction: $\text{FeCl}_3 + \text{MgO} \rightarrow \text{Fe}_2\text{O}_3 + \text{MgCl}_2$. The test passed correctly and system responded as intended.

```

Run: project x
/Users/deemaalomair/PycharmProjects/CAS741/venv/bin/python /Users/deemaalomair/PycharmProjects/CAS741/project.py
Reactant dictionary: {'Fe': 1, 'Cl': 3, 'Mg': 1, 'O': 1}
Product dictionary: {'Fe': 2, 'O': 3, 'Mg': 1, 'Cl': 2}

```

Figure 12: Reactant and Product dictionaries that count the total atoms value for each element

6.7 T7: Check Balance Test

The goal of this test is to check if the entered reaction is balance or not. Display "balance" if yes and "not balance" with new balanced form if not. Pictures below shows how system respond to balance and non balance reactions. The test passed correctly and system responded as intended.

This chemical equation balancer can help you to balance an unbalanced equation. This balancer can also help you check whether the equation is balanced or not

reactant1:
 element1: Na atom1: 1 element2: atom2: 0

+

reactant2:
 element1: Cl atom1: 1 element2: atom2: 0

=>

product1:
 element1: Na atom1: 1 element2: Cl atom2: 1

+

product2:
 element1: atom1: 0 element2: atom2: 0

enter to check if the equation is balance balance

choose the number of reactant with known mass then enter mass value: 1

enter to calculate mass

Figure 13: balance reaction

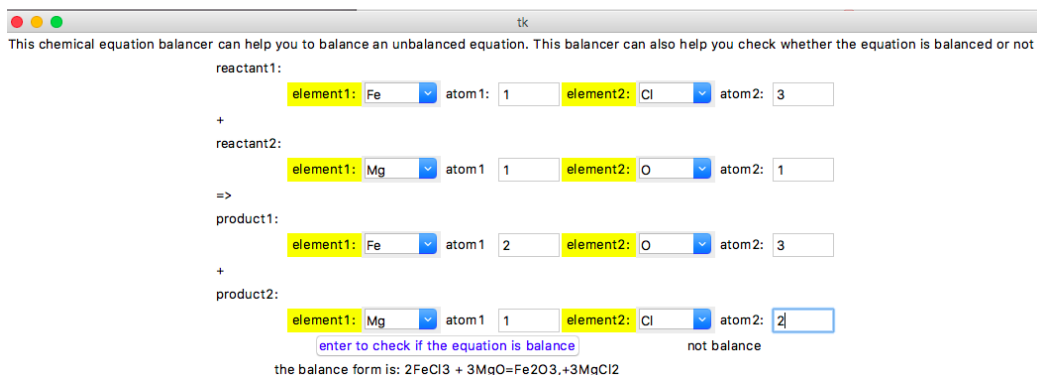


Figure 14: non balance reaction

6.8 T8: Balance Test

The goal of this test is to update the created dictionaries: Reactant,Product to make the total atom values for each element in both sides equal. The new dictionaries called : Reactant1, Product1. Picture below shows test passed correctly and system responded as intended.

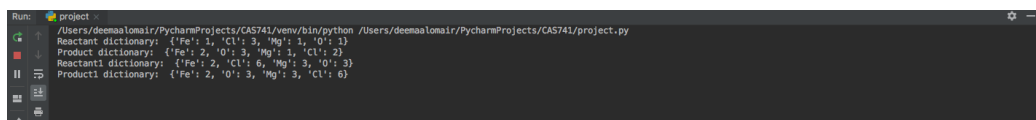


Figure 15: Reactant1 and Product1 dictionaries after balancing

6.9 T9: Coefficients Test

The goal of this test is to place appropriate coefficients in front of each reactant and product to get the balance form displayed to user . Picture below shows Coefficients values as in test case T9 in (1). test passed correctly and system responded as intended.

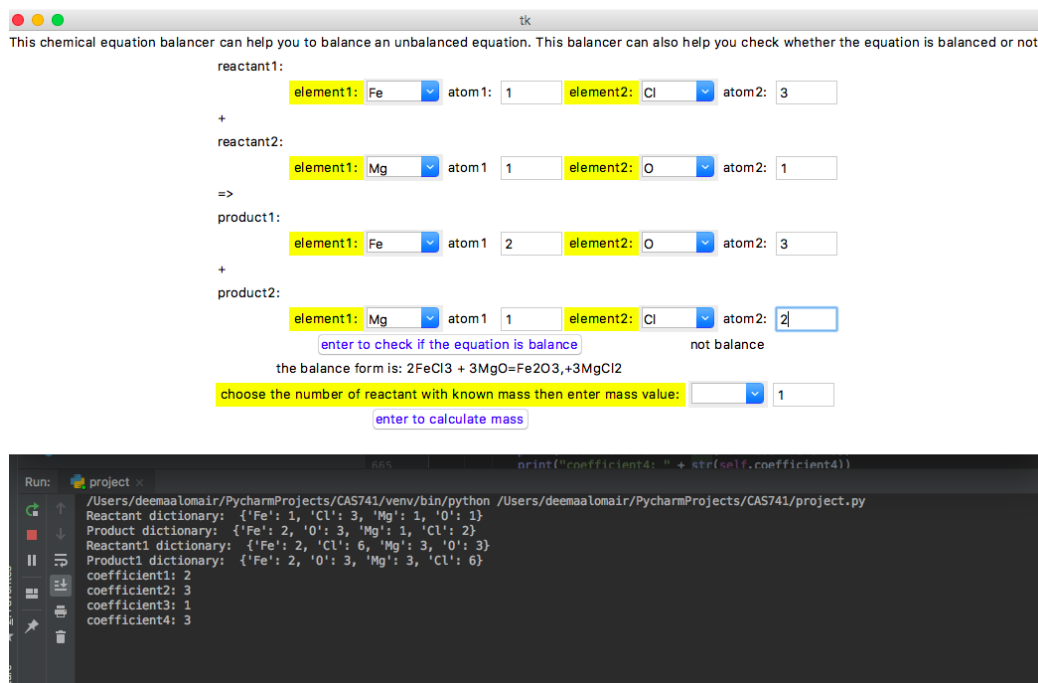


Figure 16: coefficients values

6.10 T10: atomic mass Test

The goal of this test is to get the atomic mass for each element from atomic mass library. Picture below shows atomic mass for element "Fe" and element "O". test passed correctly and system responded as intended.

```

element name: O atomic mass: 15.9994
element name: Fe atomic mass: 55.845

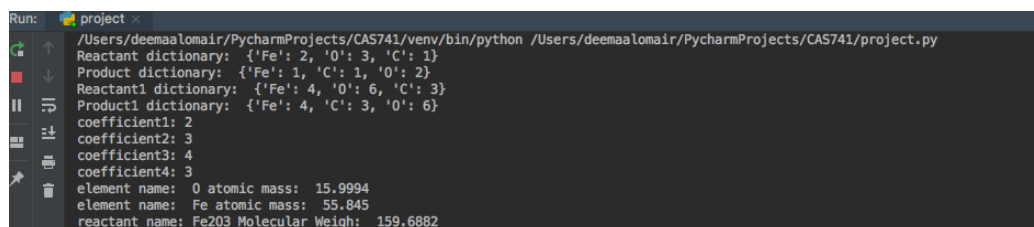
```

Figure 17: atomic mass value

6.11 T11: Molecular Weight Calculation Test

The goal of this test is to get molecular weight for a reactant. Picture below shows molecular weight is printed for reactant " Fe_2O_3 " as the test case

in T10 in (1) and the result is identical. Test passed correctly and system responded as intended.



```

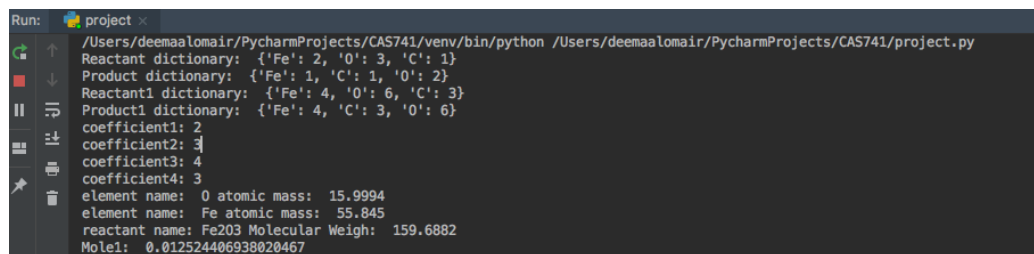
Run: project x
/Users/deemaalomair/PycharmProjects/CAS741/venv/bin/python /Users/deemaalomair/PycharmProjects/CAS741/project.py
Reactant dictionary: {'Fe': 2, 'O': 3, 'C': 1}
Product dictionary: {'Fe': 1, 'C': 1, 'O': 2}
Reactant1 dictionary: {'Fe': 4, 'O': 6, 'C': 3}
Product1 dictionary: {'Fe': 4, 'C': 3, 'O': 6}
coefficient1: 2
coefficient2: 3
coefficient3: 4
coefficient4: 3
element name: O atomic mass: 15.9994
element name: Fe atomic mass: 55.845
reactant name: Fe2O3 Molecular Weigh: 159.6882

```

Figure 18: molecular weight value

6.12 T12: Mole1 Calculation Test

The goal of this test is to get mole for reactant with known mass. we name this mole "Mole1". Picture below shows Mole1 value printed for reactant " Fe_2O_3 " as the test case in T12 in (1) and the result is identical. Test passed correctly and system responded as intended.



```

Run: project x
/Users/deemaalomair/PycharmProjects/CAS741/venv/bin/python /Users/deemaalomair/PycharmProjects/CAS741/project.py
Reactant dictionary: {'Fe': 2, 'O': 3, 'C': 1}
Product dictionary: {'Fe': 1, 'C': 1, 'O': 2}
Reactant1 dictionary: {'Fe': 4, 'O': 6, 'C': 3}
Product1 dictionary: {'Fe': 4, 'C': 3, 'O': 6}
coefficient1: 2
coefficient2: 3
coefficient3: 4
coefficient4: 3
element name: O atomic mass: 15.9994
element name: Fe atomic mass: 55.845
reactant name: Fe2O3 Molecular Weigh: 159.6882
Mole1: 0.012524406938020467

```

Figure 19: Mole1 value

6.13 T13: Mole Ratio Calculation Test

The goal of this test is to get mole ratio between given reactants. Picture below shows Mole Ratio value for coefficient of reactant2/coefficient of reactant1 printed as the test case in T13 in (1) and the result is identical. Test passed correctly and system responded as intended.

```

Run: project x
/Users/deemaalomair/PycharmProjects/CAS741/venv/bin/python /Users/deemaalomair/PycharmProjects/CAS741/project.py
Reactant dictionary: {'Fe': 2, 'O': 3, 'C': 1}
Product dictionary: {'Fe': 1, 'C': 1, 'O': 2}
Reactant1 dictionary: {'Fe': 4, 'O': 6, 'C': 3}
Product1 dictionary: {'Fe': 4, 'C': 3, 'O': 6}
coefficient1: 2
coefficient2: 3
coefficient3: 4
coefficient4: 3
element name: O atomic mass: 15.9994
element name: Fe atomic mass: 55.845
reactant name: Fe2O3 Molecular Weight: 159.6882
Mole1: 0.012524406938020467
ratio 1.5

```

Figure 20: Mole Ratio value

6.14 T14: Mole2 Calculation Test

The goal of this test is to get mole for reactant with unknown mass. we name this mole "Mole2". Picture below shows Mole2 value printed as the test case in T14 in (1) and the result is identical. Test passed correctly and system responded as intended.

```

Run: project x
/Users/deemaalomair/PycharmProjects/CAS741/venv/bin/python /Users/deemaalomair/PycharmProjects/CAS741/project.py
Reactant dictionary: {'Fe': 2, 'O': 3, 'C': 1}
Product dictionary: {'Fe': 1, 'C': 1, 'O': 2}
Reactant1 dictionary: {'Fe': 4, 'O': 6, 'C': 3}
Product1 dictionary: {'Fe': 4, 'C': 3, 'O': 6}
coefficient1: 2
coefficient2: 3
coefficient3: 4
coefficient4: 3
element name: O atomic mass: 15.9994
element name: Fe atomic mass: 55.845
reactant name: Fe2O3 Molecular Weight: 159.6882
Mole1: 0.012524406938020467
ratio 1.5
mol2: 0.008349604625346977

```

Figure 21: Mole2 value

6.15 T15: Mass Calculation Test

The goal of this test is to get the final mass result for reactant with unknown mass. Picture below shows mass value printed as the test case in T15 in (1) and the result is identical. Test passed correctly and system responded as intended.

```

Run: project x
/Users/deemaalomair/PycharmProjects/CAS741/venv/bin/python /Users/deemaalomair/PycharmProjects/CAS741/project.py
Reactant dictionary: {'Fe': 2, 'O': 3, 'C': 1}
Product dictionary: {'Fe': 1, 'C': 1, 'O': 2}
Reactant1 dictionary: {'Fe': 4, 'O': 6, 'C': 3}
Product1 dictionary: {'Fe': 4, 'C': 3, 'O': 6}
coefficient1: 2
coefficient2: 3
coefficient3: 4
coefficient4: 3
element name: O atomic mass: 15.9994
element name: Fe atomic mass: 55.845
reactant name: Fe2O3 Molecular Weigh: 159.6882
Mole1: 0.012524406938020467
ratio 1.5
mol2: 0.008349604625346977
reactant name: C10 Molecular Weigh: 12.0107
Final Mass: 0.10028459627365494

```

Figure 22: final mass value

6.16 T16, T17 : Mass and Reaction Output Test

The goal of this test is to output the final result including the mass and balance reaction to GUI. This is the main goal of the system. Picture below shows how system will print out the final result to end user. this test is for test case in T16, T17 in (1). Test passed correctly and system responded as intended.

tk

This chemical equation balancer can help you to balance an unbalanced equation. This balancer can also help you check whether the equation is balanced or not

reactant1:
 element1: Fe atom1: 2 element2: O atom2: 3

+

reactant2:
 element1: C atom1: 1 element2: O atom2: 0

=>

product1:
 element1: Fe atom1: 1 element2: O atom2: 0

+

product2:
 element1: C atom1: 1 element2: O atom2: 2

[enter to check if the equation is balance](#) not balance

the balance form is: 2Fe2O3 + 3C=4Fe,+3CO2

choose the number of reactant with known mass then enter mass value: 1 2

[enter to calculate mass](#)

{The mass value for the reactant} C = 0.10028459627365494 g

Figure 23: final system output

7 Changes Due to Testing

No changes are necessary to the first stage of implementation due to these test results.

8 Automated Testing

- coverage testing was preformed using coverage package without any error. blew picture shows coverage testing.

```
(venv) deema-2\CAS741 deemaalonair$ coverage run project.py
Reactant dictionary: {'H': 2, 'O': 2}
Product dictionary: {'H': 2, 'O': 1}
Reactant1 dictionary: {'H': 4, 'O': 2}
Product1 dictionary: {'H': 4, 'O': 2}
coefficient1: 2
coefficient2: 1
coefficient3: 2
coefficient4: 0
element name: H atomic mass: 1.00794
reactant name: H2O Molecular Weight: 2.01588
Mole1: 0.9921225469770825
ratio 0.5
mol2: 1.984245893954085
reactant name: O2O Molecular Weight: 31.9988
Final Mass: 63.49346191241541
```

Figure 24: coverage testing

9 Trace to Requirements

	T1	T2	T3	T4	T5	T6	T7	T8	T9	T10	T11	T12	T13	T14	T15	T16	T17
R1(input)	X	X	X	X	X												
R2(output)																X	X
R3(calculation)						X	X	X	X	X	X	X	X	X	X		
R4(VerifyInputOutput)	X	X	X	X	X											X	X

Table 2: Traceability Matrix Showing the Connections Between unit test cases and functional requirements

10 Trace to Modules

A complete description of modules is found in the MG (3) . A traceability of unit tests to modules can be found in Table 5 in Section 5.3 of the Unit

	T18	T19
NF1		X
NF2	X	

Table 3: Traceability Matrix Showing the Connections Between unit test cases and Nonfunctional requirements

VnV Plan (1).

11 Code Coverage Metrics

coverage test was done for the whole system and covers all functional requirements. It covers test cases from T1 to T17.

References

- [1] <https://github.com/deemaalomair1/CAS741project/blob/master/docs/VnVPlan/UnitVnVPlan/UnitVnVPlan.pdf>
- [2] <http://www.endmemo.com/chem/balancer.php>
- [3] <https://github.com/deemaalomair1/CAS741project/tree/master/docs/Design>