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Kinetic modeling, thermodynamic studies and simulation of reactions with and without boiling using temperature-time information

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THE HEAD OF SCHOOL

SCHOOL OF CHEMICAL AND METURLUGICAL ENGINEERING

UNIVERSITY OF THE WITWATERSRANG

JOHANNESBURG

SOUTH AFRICA

12-10-2015

Dear Sir,

CORRECTIONS OF PhD THESIS FOR FINAL SUBMISSION BY NANA YAW ASIEDU-STUDENT REFERENCE NUMBER-0702585V

Please find the corrections made on my PhD thesis for your approval to enable me make the final submission of my PhD thesis to the Faculty of Engineering and Built Engineering. The corrections made on the thesis has also been checked and approved by my Supervisors Prof. David Glasser and Prof. Diane Hilderbrandt.

The following are the corrections made based on the examiners specific comments:

EXAMINER-1

GENERAL COMMENTS-CORRECTIONS AND REACTIONS:

(a) **Examiners comment**: There is variations in format of the chapters

Correction: The format of the chapter titles has been corrected as suggested by the examiner.

(b) **Examiners comment**: CD ROM missing from thesis and it is misleading

Correction: The experimental data contained on CD has been attached to the thesis.

(c) **Examiners comment:** Content page; Chapters 4,5 and 6 are bold texted and the item 6.1 page

number not aligned with others on the right hand.

Correction: The contents pages, chapters 4,5 and 6 has been corrected by unbolding the text. The content page item 6.1, the page number has been aligned properly.

(d) **Examiners comment:** The title of list of tables page reads 'LIST TABLE'.Page item 5.7 is

missing a page number.

Correction: The title of the table of content has been corrected to read 'LIST OF TABLES'.

The item 5.7 has been provided with a page number.

(e) **Examiners comment:** The thesis has a page summarizing appendices A to H3 but there are no

appendices included in the thesis.

Correction: Because of the size of the experimental data collected appendixes A- H3 are contained in the attached CD to the thesis.

(f) **Examiners comment:** Scales for all graphs differ and care must be taken to standardize the graphs.

Correction: Throughout the thesis the graphs axes differ from graph to graph. This is because the software used captured the processes different reaction times and different initial and final temperature. The scales are automatically generated by the software and plots the data points capturd. One has no control of the scale. Changing the scales manually may distort the natural profile of the process.

(g) **Examiners comment:** There many assumptions in this work. It important to know the effect

in terms of error these assumptions have on the overall results.

Correction: The main assumption made in this work was that the heat of reaction is independent of temperature since the temperature range of the study is small.

(h) **Examiners comment:** Overall thesis is unnecessary long.

Corrections: The thesis has been reduced by reducing some of the graphs sizes.

(i) **Examiners comment:** Very little discussion is provided regarding kinetic and the thermo-dyamic information obtained.

Correction: Discussions on all the graphs have been done and kinetic thermodynamic information were determined based on the theoretical development made in the thesis.

SPECIFIC COMMENTS BY CHAPTERS

CHAPTER-1:

Examiners comment: The style of references in this chapter if different from that in latter chapters

This must be fixed to make the entire thesis consistent.

Corrections: The style of the references in this chapter has been changed and it is now consistent with references in chapters 2 and 3 in the thesis.

CHAPTER-2:

SPECIFIC COMMENTS:

(a) **Examiners comment:** Page 4 third word in section 2.1: 'review' should read 'reviews'.

Correction: Page 4 section 2.1; the word 'review' has been changed to 'reviews' in the thesis.

(b) **Examiners comment:** Page 4 third last line in section 2.1: '…...and its eas of application' is badly worded.

Correction: Page 4 section 2.1; the third last word wording has been changed to '..and it is easy to apply the techniques..'.

(c) **Examiners comment:** Page 10: the symbols r_A, V, N_A have units?

Correction: Page 10; the symbols; r_A,V, and N_A has been assign their appropriate units.

(d) **Examiners comments:** Page 11 third line : 'coeefficient' should read 'coefficient'

Correction: Page 11; third line the word 'coeeficient' has been corrected to 'coefficient'.

(e) **Examiners comment:** Page 12 eq(2.8): What C_P in this equation referring to? It is not explained in the text.

Correction: Page 12; Eqn (2.8), the C_p has been explained to be the specific heat capacity of the mixture in the thesis.

(f) **Examiners comment:** Page 12 eq(2.13), the variable f_i has not been defined.

Correction: Page 12; Eqn (2.13), the variable f_i has been defined as function with respect to ith order in the list of symbols page 23.

(g) **Examiners comment:** Page 15 after eq(2.28): What does 'A_i in i ' mean?

Correction: Page 15; Eqn (2.28), A_i has been explained to mean 'moles of species I present in the mixture in the list of symbols in page 23.

(h) **Examiners comment:** Page 16 eq(2.32): What does the '…….' represent?

Correction: Page 16: Eqn (2.23), has been corrected in the text.

(h) **Examiners comment:** The references in this chapter are missing paper titles.

Corrections: All the reference in this chapter has been cited properly and the style is consistent to that of chapter 1.

CHAPTER THREE

GENERAL COMMENTS-REACTIONS

This is a chapter that describes all experimental works, results and discussions of all profiles. It was stated clearly how the profiles was going to be used in latter chapters. All profiles were measured and the data can be seen in the appendices A-H3 in the CD attached.

SPECIFIC COMMENTS:

(a) **Examiners comment:** Page 61: the graph shows an initial drop before rising. Could the author comment on why this behavior occurs?

Correction: Page 61; the behavior of the drop in the initial temperature has been explained in the discussions of this chapter. This behavior is as a result of heat of mixing. The value of this heat of mixing is negligible compared to the heat of the reaction and was not considered in the analysis.

(b) **Examiners comment:** The text under section 3.1 appears to be all in the same style as the heading which makes it look like one long heading. This must be checked.

Correction: The text under section 3.1 has been checked. It describes what is inside the chapter.

CHAPTER FOUR:

This chapter is an article that has been published by the American Chemical Society (ACS) Journal of Industrial and Engineering Chemistry Research: Ind. Eng. Chem. Res. 2013, 52, 7630-7639. This chapter appears exactly as the published paper in the above stated Journal.

CHAPTER FIVE:

This chapter is an article that was published by International Institute for Science, Technology and Education (IISTE) Journal of Chemical and Process Engineering Research, vol. 10, 2013, 51-94. This chapter thus appears in the same way as published in the Journal.

CHAPTER SIX:

This chapter is also an article published in the Journal of Chemical Engineering and Process Technology: J. Chem. Eng. Process Technol. 2013. 4.8. This chapter is in the same format as published in the Journal.

EXAMINER-2

Please find my corrections to the suggestions made by the second examiner of my thesis:

1. **Examiners comment:** Thesis need English editing and I advise to do same.

Correction: English editing has been done and all spelling mistakes corrected.

2. **Examiners comment:** All the figures font should be corrected in-line.

Correction: All figures font sizes has been checked and corrected.

3. **Examiners comment:** Chapter 7 title should be corrected to 'Overall conclusions and Prospects'

Corrections: The title of chapter 7 has been changed to 'Overall conclusions and Prospects'.

EXAMINER-3

Please find my corrections to the suggestions made by the third examiner of my thesis:

The examiners comment was mainly on chapter 6. This chapter is an article published in a Journal of Chemical Engineering and Process Technology: J.Chem. Eng. Process Technol.2013.4.8. This chapter is the same as the published paper.

Thank you very much, Sir.

Yours sincerely

Nana Yaw Asiedu

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