Modeling of packed-bed reactor for the water-gas shift reaction

Group Project: chemical reaction engineering S1 2025

1 Introduction

Hydrogen is rapidly emerging as a key player in the global shift toward clean energy.

The primary production route is through methane reforming, which includes three main processes: steam reforming, autothermal reforming, and partial oxidation. Steam reforming is endothermic (requires heat), while partial oxidation is exothermic (releases heat). These reactions generate hydrogen along with carbon monoxide (CO), which must be removed for applications such as fuel cells, where CO levels must be below 10 ppm due to its poisoning effect on the electrocatalyst.

The water-gas shift (WGS) reaction is a key step in hydrogen production processes, particularly for lowering carbon monoxide (CO) concentrations in reformate streams to levels suitable for fuel cell applications. Due to its exothermic nature and equilibrium-limited conversion, the WGS reaction is typically conducted in two stages: a high-temperature (HT) stage using Fe-based catalysts and a low-temperature (LT) stage using Cu-based catalysts. Among low-temperature catalysts, commercial $CuO/ZnO/Al_2O_3$ formulations have demonstrated superior performance in terms of CO conversion and operational stability.

To effectively utilize this catalyst in practical systems, there is a growing need for accurate modeling of packed-bed reactors used for the WGS reaction. These reactors are increasingly considered for compact, small-scale hydrogen generation units that can integrate with membrane reactors for producing high-purity H_2. Existing studies have provided kinetic parameters for the $CuO/ZnO/Al_2O_3$ catalyst based on Langmuir-Hinshelwood and Redox models, validated through experimental data over a range of temperatures (150–300 °C). Accurate reactor modeling is essential for designing and optimizing such systems, especially when targeting high CO conversion and integration with downstream purification units.

2 Problem description

In this project, your team has been assigned the task of developing a reaction engineering model for a fixed-bed packed-bed reactor (PBR) employing a $CuO/ZnO/Al_2O_3$ catalyst for the low-temperature WGS reaction. The model will use previously reported kinetic expressions to simulate reactor behavior and will be validated against available experimental data. In addition, the study will perform systematic parametric analyses to investigate the effects of key process variables—including temperature, pressure, and feed gas composition—on reactor performance. The goal is to develop a predictive model that captures the core reaction behavior and supports the design and operation of WGS reactors in hydrogen production systems.

The base references for this project are (Manrique et al. (2012), Zhou et al. (2023))

2.1 Reaction Engineering Aspects of the Water-Gas Shift Reaction

Prepare a comprehensive review (4-5 pages) on the reaction engineering fundamentals of the Water-Gas Shift (WGS) reaction. Cover key areas such as the industrial relevance of the WGS reaction, its role in hydrogen production, the catalytic systems used (including high-temperature iron-based and low-temperature copper-based catalysts), and mechanistic insights such as Langmuir-Hinshelwood and Redox pathways. Discuss reactor configurations (e.g., adiabatic vs. isothermal packed beds, membrane reactors), typical operating conditions, and challenges such as CO poisoning in downstream fuel cells. Highlight recent advances in catalyst development and reactor miniaturization for small-scale H_2 generation. Use the provided reference (Manrique et al. (2012), Zhou et al. (2023)) as a starting point to support discussions on kinetic models and the rationale behind the choice of catalyst and reactor type for this study.

2.2 Modeling of a Packed-Bed Reactor for the WGS Reaction

Develop a one-dimensional isothermal reaction engineering model of a packed-bed reactor (PBR) for the low-temperature WGS reaction using the $CuO/ZnO/Al_2O_3$ catalyst. Incorporate kinetic expressions as reported by Mendes et al. (2010) applying the Langmuir-Hinshelwood model at temperatures below 215 °C and a Redox mechanism above that threshold. Use the modeling approach described by Manrique et al. (2012) to formulate mass balance equations assuming ideal packed bed reactor. Simulate species concentration profiles and CO conversion using appropriate computational tool (such as python or similar tools). Validate model predictions with experimental data from literature. State all assumptions clearly, justify them with literature, and tabulate physical and kinetic parameters used.

2.3 Parametric Analysis of Process Variables

Conduct a detailed parametric study to evaluate the influence of key process variables such as temperature, pressure, feed composition (CO and H_2O content), and flow rate on reactor performance. Use conditions and data from Manrique et al. (2012). Use your engineering judgment, literature sources, etc. for any missing data. Use the validated reactor model to simulate changes in CO conversion and hydrogen yield under different operating scenarios. Analyze trends in the results with reference to thermodynamic limitations and kinetic control. Compare trends with those reported in Manrique et al. (2012), including how conversion responds to increased space time or pressure. Conclude this section with a discussion on optimal operating conditions for maximizing hydrogen production. Include brief notes on implications for reactor control and safety (e.g., sensitivity to temperature changes and implications for catalyst stability).

The project is deliberately set to be open-ended. You are expected to do some self-directed study of material outside of what has been covered in the unit.

3 Report

Prepare a report consisting of the following:

1. Literature review on reaction engineering aspects of the Water-Gas Shift (WGS) reaction.

   Present a comprehensive note (5–6 pages) on the WGS reaction including catalysis, reaction mechanisms, temperature regimes, reactor types, and recent advances.

2. Packed-bed reactor modeling and simulation.

   Develop a reaction engineering model for a WGS packed-bed reactor, simulate performance, and validate with available experimental data.

3. Parametric studies and analysis.

   Study the effect of key variables like temperature, pressure, and feed composition on CO conversion and H_2 production.

4. Critical review.

   Provide a reflective analysis of your modeling work: What was reliable? What assumptions were made? How can the model be improved?

3.1 Marking

Description	Marks
Short note	20
Reaction engineering aspects of WGS	
Modeling and Simulation	60
- Reactor model development and validation	*40*
- Parametric analysis	*20*
Critical Review	10
Report Presentation	10
Total	100

See detailed rubric in Section 5 for marking key.

3.2 Report format

The following guidelines are presented to ensure uniformity, clarity, and professionalism in your report submission.

3.2.1 Cover page

The cover page should have following information

Project Title:
Modeling and Simulation of a Packed-Bed Reactor for the Water-Gas Shift Reaction

Submitted by:
Student Names and IDs:
- Student 1 (ID:)
- Student 2 (ID:)
- Student 3 (ID:)
- Student 4 (ID:)

Date of Submission:
[DD Month YYYY]

Peer Contribution

Team Member	Overall Contribution (%)
Member 1	
Member 2	
Member 3	
Member 4	

3.2.2 General requirements

1. Maximum Length:
   - **30 pages** total (excluding references, appendices, and nomenclature).
   - Pages exceeding this limit will carry a 10% penalty.
2. Font & Text Formatting:
   - Font: Standard professional font either sans or sans serif
   - Font Size: Main text:11 pt minimum; Captions, footnotes, references: 9–10 pt minimum
   - Line Spacing: 1.15 minimum
   - Text Alignment: Justified
   - Paragraph Spacing: 6 pt after each paragraph
   - Section Headings: Use numbered sections (e.g., 3.2 Catalyst types and activity)
   - Subheadings: Use consistent formatting
3. Page Layout:
   - Paper Size: A4
   - Margins: minimum 2 cm on all sides
   - Header/Footer: May be used for page numbers and project title
   - Page Numbers: Bottom-center or bottom-right, starting after the cover page

3.2.3 Figures, tables, and equations

- Figures/Tables:
  - Must be numbered (e.g., *Figure 3.2*, *Table 5.1*)
  - Caption placed below figures, above tables
  - Cite in text (e.g., "as shown in Figure 3.2")
- Equations:
  - Center aligned
  - Numbered on the right (e.g., (1), (2))
  - Use consistent symbols and define them in the nomenclature section

3.2.4 References

- Citation Style: APA6 or Chicago (consistent throughout)
- All references must be cited in-text
- Include journal articles, books, and relevant technical standards
- Suggested minimum: 10 quality references

3.2.5 Technical writing

- Avoid informal language
- Use passive or formal voice (e.g., "The reactor was modeled using...")
- Define all acronyms upon first use
- Be concise and clear – avoid redundant explanations
- Avoid large blocks of text – use figures, tables, bullet points where suitable

3.3 Report structure

The following structure is recommended for your report:

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Cover page
1.0 Executive Summary
2.0 Introduction to the Water-Gas Shift Reaction
3.0 Reaction Engineering Aspects
    3.1 Reaction mechanism and thermodynamics
    3.2 Catalyst types and activity
    3.3 Operating regimes (HT/LT WGS)
4.0 Reactor Model Development
    4.1 Reactor configuration and assumptions
    4.2 Kinetic model
    4.3 Governing equations
    4.4 Numerical methods and solution approach
5.0 Model Validation
    5.1 Comparison with experimental data
6.0 Parametric Studies
    6.1 Effect of temperature
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    6.2 Effect of pressure
    6.3 Effect of feed composition
7.0 Critical Review
8.0 Conclusions and Recommendations
9.0 References
10.0 Appendices
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Appendices should include supporting material that is too detailed for the main body but still essential for completeness, transparency, or reproducibility. Here's what you can include in the appendices for your WGS reactor modeling project:

- Detailed calculations
  - Step-by-step derivations not shown in the main report
- Kinetic parameters and data tables
- Complete list of values used (e.g., from Mendes et al., 2010a)
- Experimental conditions, catalyst properties, etc.
- Python code
  - Scripts used for simulation or solving ODEs
  - Only include key parts if the full code is long
- Format guidelines
  - Use section numbers (e.g., Appendix A, Appendix B)
  - Reference them in the main text (e.g., "see Appendix B for full kinetic parameters")
  - Ensure readability and proper formatting even for raw data or code

3.4 Submission Checklist

☐ Cover page includes project title, student names, group number, and date

☐ All required sections are included

☐ Page limit not exceeded

☐ References formatted and cited properly

☐ Figures and tables clearly labeled

☐ Equation numbering is consistent

☐ Proofread for grammar and clarity

4 Submission

Bentley Students:

The project is conducted in a group of four. You are free to choose your group. Please notify the instructors of your groups as soon as you form them. If you cannot find a group, please get in touch with your instructor at the earliest.

Miri Students:

Your project group will be same as your assigned lab group.

Submission instructions:

You will need to submit all the files created electronically on blackboard There should be one submission per group. Please follow the instructions given below carefully for preparing the files for submission. Failure to follow these instructions may result in us not being able to assess the files.

You will be uploading two files.

1. Report (pdf file containing the report). You need to name the file as STUDENTID_CHEN3010_project_report.pdf (or) STUDENTID_CHEN5040_project_report.pdf (Replace STUDENTID with your Student ID; Miri students replace STUDENTID with Group number). You need to make only one submission per group.

2. Create a zip file named STUDENTID_CHEN3010_project_Supporting_files.zip. The zip file should contain a) All supporting files for design, modeling, and simulation activities (excel, python, ...) presented in the PDF report file. You may upload the supporting file to a cloud storage of your preference and share a link with us.

5 Marking rubric

Marking Criteria	Unsatisfactory (Fail) [0 – 49%]	Satisfactory (Pass) [50 – 59%]	Competent (Credit) [60 – 69%]	Very Competent (Distinction) [70 – 79%]	Excellent (High Distinction) [80 – 100%]
1. Reaction Engineering Aspects of the WGS Reaction (20 marks)	No or incomplete discussion, lacking key concepts. [0 – 9.8]	Basic discussion on WGS reaction, with minimal detail. [10.0 – 11.8]	Covers mechanism, catalysts, and process conditions with some technical depth. [12.0 – 13.8]	Covers all core aspects in detail with comparisons and literature support. [14.0 – 15.8]	Thorough, well-structured, and critically informed note with detailed references and examples. [16.0 – 20.0]
2. Packed-Bed Reactor Modeling (40 marks)	No clear modeling approach or incorrect equations used. [0 – 19.6]	Basic plug-flow model with limited explanation and minimal validation. [20.0 – 23.6]	Clear model development with reasonable assumptions and comparison to some data. [24.0 – 27.6]	Detailed modeling using literature kinetics, supported with validation and analysis. [28.0 – 31.6]	Complete model, well-validated, technically sound, and thoroughly justified using reference data. [32.0 – 40.0]
3. Parametric Analysis of Process Variables (20 marks)	No analysis or disconnected from the model. [0 – 9.8]	General trends described, limited linkage to model outputs. [10.0 – 11.8]	Effect of key parameters like temperature/flow rate analyzed using model. [12.0 – 13.8]	Parametric trends explained with supporting simulations and discussion. [14.0 – 15.8]	Deep and insightful analysis with clear linkage to design and optimization decisions. [16.0 – 20.0]
4. Critical Review (10 marks)	No reflection or irrelevant content. [0 – 4.9]	Basic reflection on results and limitations. [5.0 – 5.9]	Highlights strengths and weaknesses with some suggestions. [6.0 – 6.9]	Thoughtful insights on model reliability and areas for improvement. [7.0 – 7.9]	Critical and structured review supported with benchmarking or literature comparisons. [8.0 – 10.0]

Marking Criteria	Unsatisfactory (Fail) [0 – 49%]	Satisfactory (Pass) [50 – 59%]	Competent (Credit) [60 – 69%]	Very Competent (Distinction) [70 – 79%]	Excellent (High Distinction) [80 – 100%]
5. Report Presentation (10 marks)	Poorly structured, major formatting/grammar issues. [0 – 4.9]	Basic structure and formatting, some clarity issues. [5.0 – 5.9]	Clear layout with acceptable writing and referencing. [6.0 – 6.9]	Professional formatting and writing with minimal errors. [7.0 – 7.9]	Polished, professional report, free of errors, in the tone of a graduate engineer. [8.0 – 10.0]

References

Manrique, Yaidelin A., Carlos V. Miguel, Diogo Mendes, Adelio Mendes, and Luis M. Madeira. 2012. "Modeling and Simulation of a Packed-Bed Reactor for Carrying Out the Water-Gas Shift Reaction." *International Journal of Chemical Reactor Engineering* 10 (1). https://doi.org/10.1515/1542-6580.3105.

Mendes, Diogo, Vânia Chibante, Adélio Mendes, and Luis M. Madeira. 2010. "Determination of the Low-Temperature Water–gas Shift Reaction Kinetics Using a Cu-Based Catalyst." *Industrial & Engineering Chemistry Research* 49 (22): 11269–79. https://doi.org/10.1021/ie101137b.

Zhou, Limin, Yanyan Liu, Shuling Liu, Huanhuan Zhang, Xianli Wu, Ruofan Shen, Tao Liu, et al. 2023. "For More and Purer Hydrogen-the Progress and Challenges in Water Gas Shift Reaction." *Journal of Energy Chemistry* 83 (August): 363–96. https://doi.org/10.1016/j.jechem.2023.03.055.