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ВЕБ-ПЛАТФОРМА «CHEMGRAPH» ДЛЯ МОДЕЛИРОВАНИЯ ИНТЕГРИРОВАННЫХ ПРОЦЕССОВ ПРОИЗВОДСТВА БУТАНОЛА–ЭТАНОЛА (IBE/ABE)

Аннотация. *В статье представлена веб-платформа Chemgraph, предназначенная для моделирования интегрированных биопроцессов получения бутанола–этанола (IBE/ABE). Платформа выступает открытой альтернативой проприетарным симуляторам, опираясь на облачные вычисления, открытые термодинамические пакеты и интеграцию данных химической информатики. Описаны архитектура, модели данных, структура моделирования и результаты верификации. Chemgraph обеспечивает интерактивное проектирование, оптимизацию и образовательное применение в химической и биохимической инженерии.*

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WEB-BASED SIMULATION FRAMEWORK “CHEMGRAPH” FOR INTEGRATED BUTANOL–ETHANOL (IBE/ABE) BIOPROCESS MODELING

Abstract. *The paper presents Chemgraph — a web-based simulation platform developed as an open research tool for modeling integrated butanol–ethanol (IBE/ABE) bioprocesses. The system provides an accessible alternative to proprietary simulators through cloud computing, open-source thermodynamic packages, and cheminformatics-based data integration. Its architecture, data models, simulation workflow, and validation results are described. Chemgraph supports interactive process design, optimization, and educational use in chemical and biochemical engineering.*

1. Introduction

Modern bioprocess simulation remains dominated by proprietary environments such as Aspen HYSYS or SuperPro Designer. These tools, while powerful, are costly and closed-source, limiting their integration with cheminformatics workflows and machine learning environments. To address these challenges, Chemgraph was developed as a web-based, modular process simulator designed specifically for IBE/ABE bio-refinery systems.

The goal of this work is to demonstrate how a cloud-native, data-driven simulation framework can replicate essential functionalities of conventional process simulators while enabling broader access for research and education.

2. System Architecture and Methodology

Chemgraph consists of three main layers:

1. Front-End (User Interface):
   Implemented using modern web technologies, allowing real-time visualization of process flow diagrams, thermodynamic property data, and unit operation parameters.
2. Simulation Engine:
   Built on Python and integrated with open-source packages such as NumPy, SciPy, and CoolProp. Mass and energy balances are solved iteratively through modular blocks representing reactors, separators, and heat exchangers.
3. Data Layer and API:
   Supports cheminformatics data import (e.g., molecular properties, thermodynamic coefficients) and REST-based data exchange with external systems such as laboratory information management systems (LIMS) or AI-based optimization engines.

A schematic representation of Chemgraph's architecture is shown in Fig. 1.

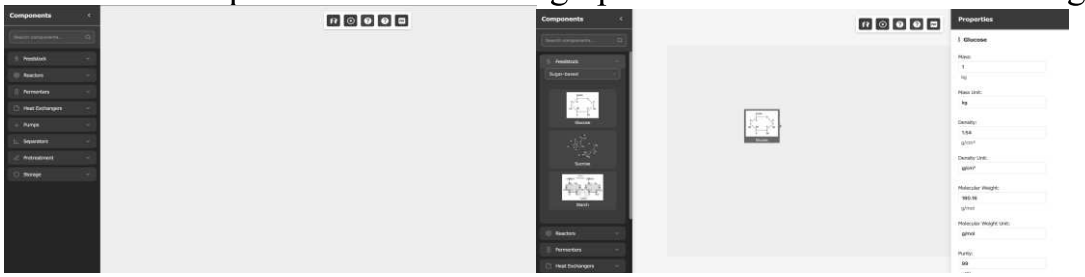

Fig. 1. Schematic structure of the Chemgraph process simulation framework.

3. Case Study: IBE/ABE Process Simulation

The system was validated on a continuous IBE/ABE fermentation and separation process, which involves multiple coupled unit operations: fermentation reactor, distillation column, liquid–liquid extractor, and dehydration unit.

Key model features:

- Component database for acetone, butanol, and ethanol mixtures.
- Thermodynamic models: NRTL and UNIQUAC (via CoolProp interface).
- Dynamic mass balance of microbial conversion.
- Separation optimization via equilibrium-based distillation algorithms.

Simulation results were benchmarked against Aspen HYSYS reference data. The average deviation for outlet stream compositions was below 4 %, confirming computational reliability for academic applications.

4. Results and Discussion

Chemgraph successfully reproduces steady-state process parameters for solvent fermentation systems and demonstrates potential for:

- Educational use — allowing students to design process flows directly in a browser.
- Collaborative research — enabling multiple users to edit and compare process scenarios online.
- Integration with AI tools — machine learning models can optimize process conditions using Chemgraph's API.

Compared to traditional simulators, Chemgraph achieves faster iteration, open data interoperability, and reduced cost for small research labs.

However, further work is required to integrate advanced thermodynamic libraries, dynamic simulation of control systems, and visualization of 3D reactor geometries.

5. Conclusions

Chemgraph demonstrates that open, web-based simulation tools can achieve accuracy comparable to commercial simulators in modeling IBE/ABE bioprocesses.

The framework supports educational and research integration, providing a foundation for collaborative digital process design. Future developments will focus on cloud deployment, hybrid modeling using experimental datasets, and integration with cheminformatics repositories.

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