MODELING OF MODERN TECHNOLOGICAL FEATURES OF THERMODYNAMIC ANALYSIS OF GAS CLEANING SYSTEMS

Abstract. Thermodynamic analysis has been a cornerstone for optimizing gas cleaning systems by evaluating their efficiency, energy consumption, and environmental impact. However, with advancements in technology, incorporating modern features into these analyses offers significant benefits. [1].

Gas cleaning systems play a crucial role in environmental protection and industrial processes by removing harmful pollutants from exhaust gases. This abstract presents a comprehensive overview of modern technological features in the thermodynamic analysis of gas cleaning systems. The modeling approaches discussed encompass various aspects including heat and mass transfer phenomena, chemical reactions kinetics, fluid dynamics, and computational techniques [2].
The abstract highlights recent advancements in modeling techniques such as Computational Fluid Dynamics (CFD), Finite Element Analysis (FEA), and Multi-Physics Simulation, which enable engineers to simulate complex interactions within gas cleaning systems with unprecedented accuracy and efficiency. These models facilitate the optimization of system design, operation, and performance prediction, leading to improved efficiency, reduced emissions, and cost-effectiveness. [3]

Furthermore, the abstract addresses the integration of artificial intelligence and machine learning algorithms into thermodynamic models, enabling real-time optimization and adaptive control of gas cleaning systems. Such approaches enhance system resilience, responsiveness, and adaptability to dynamic operating conditions.

Moreover, the abstract discusses the importance of considering the integration of renewable energy sources and advanced materials in the design and optimization of gas cleaning systems. Renewable energy integration facilitates sustainable operation, while advanced materials offer enhanced durability, corrosion resistance, and catalytic properties, thereby improving overall system performance and longevity.

In conclusion, this abstract provides insights into the cutting-edge technological advancements and methodologies in the thermodynamic analysis of gas cleaning systems, emphasizing their significance in achieving environmental sustainability, operational efficiency, and economic viability in diverse industrial applications.

**Keywords:** nozzle installation, coke gas cleaning, gas quality, particulate matter removal, computational modeling, gas-solid interactions, cleaning efficiency, optimization, thermodynamic.
МОДЕЛЮВАННЯ СУЧАСНИХ ТЕХНОЛОГІЧНИХ ОСОБЛИВОСТЕЙ ТЕРМОДИНАМІЧНОГО АНАЛІЗУ СИСТЕМ ОЧИСТКИ ГАЗУ

Анотація. Термодинамічний аналіз відігрівав визначальну роль у оптимізації систем очищення газів, оцінюючи їх ефективність, споживання енергії та вплив на навколишнє середовище. Однак з вдосконаленням технологій включення сучасних функцій у ці аналізи має значні переваги. Системи очищення газів відіграють важливу роль у захисті навколишнього середовища та промислових процесах, виділяючи шкідливі забруднення з вихлопних газів. Цей анотаційний матеріал надає всеобчісний огляд сучасних технологічних функцій у термодинамічному аналізі систем очищення газів. Обговорюються моделі підходи, що охоплюють різні аспекти, включаючи явища тепло- та масообміну, кінетику хімічних реакцій, гідродинаміку та обчислювальні техніки. У анотації висвітлюються останні досягнення в області моделювання, такі як обчислювальна гідродинаміка (CFD), метод скінчених елементів (FEA) та багатофізичне моделювання, що дозволяють інженерам моделювати складні взаємодії в системах очищення газів з неперервенною точністю та ефективністю. Ці моделі сприяють оптимізації конструкцій систем, їх експлуатації та прогнозу результатів, що призводить до покращення ефективності, зменшення викладів та економічності. Крім того, у анотації йдеться про інтеграцію штучного інтелекту та алгоритмів машинного навчання в термодинамічні моделі, що дозволяє оптимізувати системи в реальному часі та застосовувати адаптивне управління системами очищення газів. Такі підходи покращують стійкість, реакційність та адаптивність систем до динамічних умов експлуатації. Крім того, в анотації обговорюється важливість розгляду інтеграції відновлюваних джерел енергії та високорівневих матеріалів у проектуванні та оптимізації систем очищення газів. Інтеграція відновлюваних джерел енергії сприяє сталому функціонуванню, а високорівневі матеріали забезпечують підвищену довговічність, стійкість до корозії та каталітичні властивості, що покращує загальну ефективність систем та їх тривалість. Висновок цього анотаційного матеріалу надає висновки про передові технологічні досягнення і методології в термодинамічному аналізі систем очищення газів, підкреслюючи їх значення для досягнення екологічної сталості, ефективності у виробництві та економічної доцільності в різних промислових сферах.

Ключові слова: установка форсунок, очищення коксового газу, якість газу, видалення часток, обчислювальне моделювання, газ-тверді взаємодії, ефективність очищення, оптимізація, термодинаміка

Formulation of the problem. Gas cleaning systems are integral components of various industrial processes, aimed at reducing emissions of pollutants such as...
particulate matter, sulfur dioxide, nitrogen oxides, and volatile organic compounds. The design and optimization of these systems require a thorough understanding of thermodynamic principles and complex interactions between multiple variables. However, traditional modeling approaches often oversimplify these complexities, leading to suboptimal designs and inefficiencies in operation [4].

The problem at hand revolves around the need for advanced modeling techniques that can accurately capture the intricate thermodynamic processes occurring within gas cleaning systems. This includes:

**Multi-Physics Interactions:** Gas cleaning systems involve a combination of heat transfer, mass transfer, fluid dynamics, and chemical reactions. Traditional models often treat these phenomena independently, neglecting their interdependence. Advanced modeling must account for the coupled interactions between these processes to provide a comprehensive understanding of system behavior.

**Complex Geometries and Configurations:** Gas cleaning systems exhibit diverse geometries and configurations, such as packed beds, scrubbers, electrostatic precipitators, and catalytic converters. Conventional models may struggle to accurately represent the intricacies of these complex structures. Advanced modeling techniques should enable the simulation of realistic geometries with high fidelity to real-world conditions. [5]

**Dynamic Operating Conditions:** Industrial processes are subject to fluctuations in operating conditions, including variations in gas flow rates, temperatures, and pollutant concentrations. Traditional models often rely on steady-state assumptions, disregarding transient behavior. Advanced modeling should account for dynamic conditions to facilitate real-time optimization and adaptive control strategies.

**Integration of Advanced Materials and Technologies:** With advancements in materials science and technology, gas-cleaning systems can benefit from novel materials with improved catalytic activity, corrosion resistance, and thermal stability. Advanced modeling should incorporate the effects of these materials on system performance and explore their potential for enhancing efficiency and durability.

**Computational Efficiency and Scalability:** As gas cleaning systems become increasingly complex, computational resources required for modeling also escalate. Advanced modeling techniques should balance accuracy with computational efficiency, enabling the simulation of large-scale systems within reasonable timeframes. [6]

**Analysis of the latest research and publications.** Analyzing the latest research and publications in the field of advanced modeling for thermodynamic analysis of gas cleaning systems reveals a growing focus on several key areas:

**Multi-Physics Modeling:** Recent studies emphasize the importance of integrating multiple physical phenomena, such as fluid dynamics, heat transfer, mass
transfer, and chemical reactions, into comprehensive models. Advanced Computational Fluid Dynamics (CFD) techniques are employed to simulate the complex interactions within gas cleaning systems accurately.

**High-Fidelity Simulation:** Researchers are increasingly utilizing high-fidelity simulation techniques, such as Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS), to capture turbulent flow behavior and particle dynamics within gas cleaning devices like scrubbers, filters, and electrostatic precipitators.

**Dynamic Modeling and Control:** There is a growing interest in dynamic modeling and control strategies for gas cleaning systems to address transient operating conditions and optimize system performance in real-time. Model Predictive Control (MPC) and Adaptive Control algorithms are explored to enhance system responsiveness and efficiency.

**Machine Learning Integration:** Machine learning algorithms are being integrated into thermodynamic models to improve predictive capabilities, optimize system operation, and facilitate fault detection and diagnosis in gas cleaning systems. Reinforcement learning techniques are utilized to develop adaptive control strategies that can dynamically adjust system parameters based on changing conditions.

**Materials Science and Catalysis:** Advanced materials with tailored properties, such as high surface area, catalytic activity, and chemical stability, are investigated for their potential in enhancing gas cleaning system performance. Computational methods, including Density Functional Theory (DFT) calculations and Molecular Dynamics (MD) simulations, are employed to understand the behavior of these materials at the molecular level and optimize their integration into gas cleaning devices.

**Sustainability and Energy Efficiency:** Researchers are exploring the use of renewable energy sources and energy-efficient technologies in gas cleaning systems to reduce environmental impact and improve overall sustainability. Coupled thermo-economic modeling approaches are developed to assess the environmental and economic implications of different system configurations and operating strategies.

**Validation and Experimental Validation:** Validation of advanced thermodynamic models is essential for ensuring their accuracy and reliability. Recent studies emphasize the importance of experimental validation through field measurements and laboratory-scale tests to validate model predictions and optimize model parameters.

**Purpose of the article** – The article aims to provide a comprehensive overview of the current state-of-the-art in advanced modeling techniques for gas cleaning systems. It synthesizes recent research and publications to present a holistic understanding of the advancements in thermodynamic analysis within this field.

**Presentation of the main material.** Overview of the importance of gas cleaning systems in environmental protection and industrial processes. [7]
Introduction to the thermodynamic principles governing gas cleaning processes.

Identification of limitations and challenges associated with traditional modeling approaches.

Discussion on the need for advanced modeling techniques to address these challenges.

Overview of advanced modeling techniques such as Computational Fluid Dynamics (CFD), Finite Element Analysis (FEA), and Multi-Physics Simulation.

Discussion on how these techniques enable a more comprehensive analysis of gas cleaning systems by capturing multi-physics interactions.

Exploration of how machine-learning algorithms can enhance thermodynamic analysis by providing predictive capabilities and adaptive control strategies.

Examples of how machine learning is integrated into modeling for gas cleaning systems. [8]

Discussion on the role of advanced materials in improving the efficiency and performance of gas cleaning systems.

Introduction to computational methods such as Density Functional Theory (DFT) and Molecular Dynamics (MD) for modeling materials at the molecular level.

Overview of dynamic modeling techniques for gas cleaning systems to account for transient operating conditions. [9]

Introduction to control strategies such as Model Predictive Control (MPC) and Adaptive Control for optimizing system performance in real-time.

Emphasis on the importance of sustainability and energy efficiency in gas cleaning systems.

Discussion on how advanced modeling can contribute to optimizing system design for reduced environmental impact and improved energy efficiency.

Presentation of case studies illustrating the application of advanced modeling techniques in real-world gas cleaning systems.

Examples of how these techniques have led to improved performance, reduced emissions, and cost-effectiveness [10].

Discussion on future research directions in the field of advanced modeling for gas cleaning systems.

Conclusion summarizing the key findings and emphasizing the significance of advanced modeling in addressing the challenges of environmental protection and industrial sustainability.

The scrubber operates as follows: gas enters for purification, is directed through a gas duct to the lower part of the scrubber, and ascends through the body. In the upper part of the scrubber, there are three wetting tiers consisting of centrifugal nozzles. A pressurized aqueous solution of CaCO₃ is atomized. The formed droplets of the CaCO₃ water solution fall in the direction of the contaminated gas under the force of gravity. The capture of dust particles by water droplets occurs
due to the inertial and diffusive mechanisms, hydrodynamic and electrostatic forces, and turbulent diffusion. Gas purification from sulfur dioxide (SO$_2$) occurs through absorption technology. Reaction takes place upon contact of the suspension with the gas.

\[
\text{CaCO}_3 + \text{SO}_2 + \frac{1}{2} \text{H}_2\text{O} = \text{CaSO}_3 \cdot \frac{1}{2}\text{H}_2\text{O} + \text{CO}_2
\]  

(1)

The experiment data were summarized in a single table 1

<table>
<thead>
<tr>
<th>Experiment</th>
<th>The method of laying the nozzle</th>
<th>Consistent</th>
<th>Disorderly</th>
<th>block, successively angular</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>before</td>
<td>after</td>
<td>before</td>
<td>after</td>
</tr>
<tr>
<td>CO$_2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0,322</td>
<td>0,154</td>
<td>0,320</td>
<td>0,154</td>
</tr>
<tr>
<td>2</td>
<td>0,336</td>
<td>0,158</td>
<td>0,332</td>
<td>0,158</td>
</tr>
<tr>
<td>3</td>
<td>0,318</td>
<td>0,155</td>
<td>0,316</td>
<td>0,155</td>
</tr>
</tbody>
</table>

**Conclusions.** Advanced modeling techniques such as Computational Fluid Dynamics (CFD), Finite Element Analysis (FEA), and Multi-Physics Simulation offer a more comprehensive understanding of gas cleaning systems by capturing the complex interactions between fluid dynamics, heat transfer, mass transfer, and chemical reactions.

The experiment revealed that employing a triangular nozzle with cross-shaped cutouts, combined with cooling the coke gas temperature to 15°C and adding KOH alkali at a concentration of 20%, significantly enhances the efficiency of coke gas cleaning. This configuration proved to be the most optimal for tray-type scrubbers, leading to a notable increase in purification efficiency, up to 50%.

The integration of machine learning algorithms into thermodynamic models enables enhanced predictive capabilities, adaptive control strategies, and real-time optimization of gas cleaning systems. This facilitates improved system performance, efficiency, and reliability.

**References:**


10. J. Elm An Atmospheric Cluster Database Consisting of Sulfuric Acid, Bases, Organics, and Water ACS Omega, 4 (6) (2019), pp. 10965-10974, 10.1021/acsomega.9b00860

Література:


10. J. Elm An Atmospheric Cluster Database Consisting of Sulfuric Acid, Bases, Organics, and Water ACS Omega, 4 (6) (2019), pp. 10965-10974, 10.1021/acsomega.9b00860