ANNOTATION

of dissertation for the Philosophy Doctor (PhD) degree in specialty
"6D071700 – Thermal power engineering" by
Kalassov Nurdaulet on the topic "**Gas separation in integrated membrane bioreactor to produce fuel used in thermal power plants**"

General description of work

The dissertation researches an integrated membrane bioreactor for the production and separation of hydrogen. In the course of a numerical study of the processes of membrane separation of mixtures of hydrogen and carbon dioxide, the main set of hydrodynamic models is described. The results of CFD modeling using the ANSYS FLUENT software package in laminar and turbulent flow regimes in the process of membrane separation are shown in order to control the thickness of the concentration polarization layer.

Relevance of the dissertation theme

The prospects for energy production using thermal power plants in the 21^{st} century are of great concern for the following reasons. First, in the next 50-70 years, two types of fossil fuels - oil and gas - will have to run out. Secondly, thermal power plants are the main source of carbon dioxide emissions into the atmosphere and the creation of a greenhouse effect. Thirdly, about 14 billion tons of fuel are now produced annually. In the 20th century, about 500 billion tons of fuel were withdrawn from the bowels of the planet, which is 10^3 masses of the Earth. This may lead in the future, along with the greenhouse effect, to unpredictable consequences. Energy consumption shows no tendency to decrease - on the contrary, the rate of its increase is constantly increasing.

Currently, a new industry is gaining momentum - hydrogen energy and hydrogen production technology. After all, this simplest and lightest substance can be used not only as a fuel, but also as a necessary raw material in many technological processes.

The main problem in the production of hydrogen is the problem of technological savings and production. One of the interesting and promising approaches is the use of membrane technology and membrane bioreactor processes, which significantly improve the economics of biofuel production.

Interest in membrane separation is rapidly growing as it is recognized that membrane processes are technically and economically superior to other competing technologies in many industrial applications. This advantage is due to the many advantages of membrane separation technology, which include low capital investment, ease and convenience of installation and operation, low maintenance requirements, low weight, footprint and high process flexibility. In addition, membrane separation does not require additives and can be carried out at lower temperatures compared to other thermal separation processes that operate at higher temperatures.

One type of biological production of hydrogen is dark fermentation. In dark fermentation, bacteria act on the substrate and release hydrogen. Substrates for dark fermentation are hydrocarbon materials such as lignocellulosic biomass, industrial wastewater, sugary plant residues and municipal solid waste. At the first stage, the pre-treatment of the biomass has a great influence on the efficiency of dark fermentation.

The biohydrogen produced by dark fermentation generates a gaseous mixture consisting mainly of H_2 (hydrogen) and CO_2 (carbon dioxide) and liquid wastewater with significant amounts of volatile fatty acids. Therefore, subsequent methods after the production stage should have at least two goals:

– hydrogen gas must be purified to be an effective feedstock in fuel cells;

– Effluent needs further treatment or use due to its residual and usable organic matter. In fact, in order to improve the quality of biohydrogen, CO_2 must be removed and converted into other bioproducts.

The purpose of the research is to develop a model of hydrodynamics and mass transfer of the gas separation process in integrated membrane bioreactors to provide thermal power plants with environmentally friendly and high-calorie fuel.

In order to achieve the above stated goal, it is necessary to carry out the following tasks:

1. Describe the hydrodynamic models of the process of membrane separation of hydrogen and carbon dioxide gases;
2. To develop a hydrodynamic model of membrane separation in a laminar flow in order to study the effects of concentration polarization;
3. To develop a methodology for calculating the mass transfer coefficient using a hydrodynamic model;
4. Develop a model of hydrodynamics and mass transfer of a cross flow through a porous membrane filled with intermediate dividers at their various locations.

The object of the research

Spiral wound membrane for gas separation.

The subject of the research

Computational Fluid Dynamics (CFD) model for studying the concentration polarization occurring in gas separation in integrated membrane bioreactors.

Research methods

The main method for studying the effect of concentration polarization on the membrane surface is computer simulation in the Ansys Fluent environment. The finite volume method is used to theoretically solve the basic equations of viscous flow using the continuity equation and the Navier-Stokes equation, the law of conservation of momentum and the transport equation, as well as computational methods for laminar and turbulent flow regimes.

The main provisions for the defense.

1. With an increase in the speed of gas mixtures of hydrogen and carbon dioxide at the entrance to the membrane channel, the tangential stress increases and the maximum thickness of the concentration polarization boundary layer along the length of the channel, depending on the Reynolds number in the range Re=200÷800, varies from $\delta(x)=0.293*10^{-3}$ m to $\delta(x)=0.152*10^{-3}$ m;
2. When flowing around intermediate dividers, the average value of the Sherwood number is 1.5 times higher than in the case of their absence, this is due to the fact that mass transfer increases due to the vortices that form during the flow around the dividers;

3. Intermediate dividers, located linearly in the middle of the membrane channel, provide a higher mass transfer compared to intermediate dividers located in a checkerboard pattern, for all considered Reynolds numbers in the range Re=200÷800.

Scientific novelty of the work

The novelty and originality of the work are as follows:

1. The main hydrodynamic model of the cross-flow of mixtures of hydrogen and carbon dioxide through a porous membrane in the laminar regime has been developed and a method for the analytical calculation of the mass transfer coefficient has been developed;

2. A 2D model of hydrodynamics and mass transfer of a cross flow of hydrogen and carbon dioxide mixtures through a porous membrane in a turbulent mode has been developed for three different arrangements of intermediate dividers;

3. As a result of hydrodynamic modeling, the effective form of the geometry of the membrane channel filled with intermediate dividers in the process of separating mixtures of hydrogen and carbon dioxide was determined.

Practical and theoretical importance of the dissertation

The results of hydrodynamic modeling developed in the dissertation work are of great importance in the production of environmentally friendly and cheap biohydrogen.

The reliability and validity of the results

Numerical studies were carried out using the licensed software package Ansys FLUENT (Ansys, Inc., USA). The reliability and validity of the results of the hydrodynamic model is confirmed by analytical and experimental data. In addition, the reliability and validity of the results achieved in the dissertation work is confirmed by the presence of publications in publications recommended by the Committee for Quality Assurance in the Field of Education and Science of the MSHE of the Republic of Kazakhstan, in the journals of foreign countries with a non-zero impact factor, and in the proceedings of international conferences.

The personal contribution of the author

Writing the full volume of the dissertation, choosing a numerical research method, developing a model of hydrodynamics and mass transfer of membrane gas separation processes in the Ansys Fluent program, processing and analyzing the results obtained during the simulation were carried out by the author independently. Problem setting and results processing were carried out jointly with scientific consultants.

Approbation of the dissertation. The results obtained in the dissertation were presented and discussed:

– at the International Scientific conference «Sustainable Processes, Sustainable Systems, Sustainable Environment», Sofia, Bulgaria, 8 November 2019;

– at the International Conference of Students and Young Scientists "FARABI ALEMI" (2020, Al-Farabi Kazakh National University, Almaty);

– at the Proceedings of the International Scientific Conference «Innovative Development of Education, High-Tech Production and Alternative Energy Sources», Almaty, Kazakhstan, 23 December 2020.

Publications

8 publications have been published on the topic of the dissertation, including 4 papers in the materials of international conferences (3 in the form of a thesis and 1 in

the form of an article), 3 papers in scientific publications recommended by CQASESMES RK for the degree of Doctor of Philosophy (RhD), 1 article in journals included in the international information resources Web of Science (Clarivate Analytics, USA) and Scopus (Elsevier, Netherlands).

The scope and structure of the thesis

The thesis consists of an introduction, 3 sections, conclusion and list of references from 117 titles, contains 88 pages of basic computer text, including 44 figures, 4 tables and 61 formulas.