Бургаски държавен университет
„Проф. д-р Асен Златаров"
8010 Бургас, бул. „Проф. Якимов" №1
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REPORT

of dissertation for the acquisition of educational and scientific degree **"DOCTOR"**

Author of the dissertation: Eng. Svetlin Petrov Vasilev, "Tersa" Ltd

Topic of the dissertation: Modification of Petroleum Fluid Properties and Processes in Oil Refining

Scientific area: 5. Technical Sciences

Professional area: 5.10 Chemical Technologies

Scientific specialty: Technology of natural and synthetic fuels

The report was written by: Assoc. Prof. Dr. Vesislava Borislavova Toteva, University of Chemical Technology and Metallurgy

Eng. Svetlin Vassilev was born in 1976 in Burgas. He graduated from the Burgas English High School and earned a Master of Engineering degree from the University "Prof. Dr. Assen Zlatarov" in Burgas. In the same year, he began working at "Lukoil Neftohim Burgas" AD, where he held various positions until 2006. He currently carries out industrial design, research and consulting activities in the chemical, petrochemical, oil-refining and energy industries at "Tersa" Ltd.

The candidate fully satisfies the minimum requirements specified in the "Regulations on the terms and conditions for acquiring scientific degrees and occupying academic positions at Burgas State University "Prof. Dr. Asen Zlatarov".

In the reference for the candidate's publications are presented:

Under Indicator 7 – Articles and reports published in scientific journals, refereed and indexed in world-renowned databases with scientific information (Scopus; Web of Science): 13 publications are presented;
Under Indicator 8 - Articles and reports published in non-refereed journals with scientific peer-review or published in edited collective volumes: 3 publications are submitted;
Total points from group G: **82.7 with 30 required;**
There are 60 citations (no self-citations).

In Abstract of the dissertation, 6 publications are presented as publications on the topic of the dissertation, which correspond to 23.08 points. The PhD student had to submit both reports under Indicator 8 (No. 1 and 2), which are also on the topic of the dissertation and correspond to 13.32 points.

The dissertation on the topic: "MODELING THE PROPERTIES OF OIL FLUIDS AND PROCESSES IN OIL REFINING" is presented on 284 standard pages, includes 83 figures, 51 tables and a bibliography from 647 literature sources.

The dissertation is relevant because it combines several important scientific, technological and economic areas:

Petroleum fluids are complex multicomponent systems whose behaviour depends on composition, temperature, pressure and phase equilibrium. Modelling allows for more accurate prediction of their properties without the need for many expensive experiments.

- Oil refining requires optimization of technological processes (distillation, cracking, hydrotreating, reforming, etc.). Through mathematical models and simulations, yields, energy efficiency and quality of the resulting products can be improved.

- Modern refineries work with an increasingly diverse range of raw materials, including heavy oil fractions, mixtures from different oil sources and alternative hydrocarbon feedstocks. This increases the need for reliable models to evaluate their processing behaviour.

The dissertation is also of high economic importance, since even a small improvement in the control of technological processes can lead to significant energy savings, higher yield of valuable products and reduction of production costs.

Environmental requirements are becoming more stringent, especially in terms of sulphur content, emissions and fuel quality. Modelling supports the development of cleaner and more efficient technologies. Digitalization and the use of specialized software in the chemical and oil refining industries make modelling a key tool for analysis, design, management and control of processes.

The dissertation aims to make a critical analysis of the emerging differences between the latest advances in the characterization of petroleum fractions (including methods for converting distillation curves and determining molecular weight and critical properties); the methods implemented in the widespread process simulators used for engineering calculations and simulation of technological processes, and the constantly evolving methods for molecular reconstruction of oil and oil fractions. The peer-reviewed paper aims to review the existing correlations for modelling key properties of oil and oil fractions and models for molecular reconstruction of petroleum fluids available in the open literature and used in commercial software, and to evaluate them against modern analytical techniques and tools for evaluating influencing factors, such as nonlinear regression analysis, intercriteria analysis and the use of artificial neural networks (ANN). This analysis is expected to serve as a basis for the future development of integrated and more accurate tools for

engineering practice, capable of significantly improving the efficiency and economic feasibility of modern oil refining installations.

The literature review of the dissertation systematizes and analyses the main directions in the modern characterization of oil, oil fractions and oil fluids. At the beginning, the methods for converting data on boiling points obtained by standard laboratory distillations to true boiling point (TBP) are considered, including the conversion of distillation curves according to ASTM D86, ASTM D1160, ASTM D2887 and ASTM D7169.

The next important thematic block is devoted to correlations for predicting the molecular weight of oil fractions. Due to the key importance of molecular weight in the design of new equipment, evaluation of existing installations and determination of the physicochemical characteristics of oil fluids, the review presents and critically compares the results of scientific papers aimed at its modelling and forecasting.

Attention is paid to the methods for predicting the critical temperature and critical pressure of oil fractions and individual hydrocarbons. The consideration of these properties allows us to assess the applicability of various empirical and semi-empirical dependencies in modelling phase behaviour, thermodynamic characteristics and technological modes. The review highlights both the practical usefulness of the existing correlations and their limitations when working with complex and heavy oil systems.

To achieve the purpose of the dissertation, after a thorough literature review, the following tasks have been formulated:

1. To conduct a study using distillation curves from physical vacuum distillation (ASTM D1160) and gas chromatographic high-temperature simulant distillation (ASTM D7169) to predict the yield of target products and to carry out an industrial experiment to validate the results obtained and determine which distillation method provides more reliable information to determine the amount of more valuable light fractions in the separation product.

2. Compare the available and most commonly used correlations for predicting the molecular weight of hydrocarbons and petroleum fluids and determine which of these correlations are most suitable for predicting molecular weight in the range of 70 to 1685 g/mol. Use the collected molecular weight data to conduct nonlinear regression and create an artificial neural network (ANN) to predict the molecular weight of petroleum fluids.

3. Compare the available and most used correlations for predicting the critical temperature and pressure of hydrocarbons and petroleum fluids and determine the accuracy of predicting these properties among a wide range of hydrocarbons. Perform an InterCriteria Analysis to assess the relationships between the different input variables, correlation analysis with available data to obtain improved correlation dependencies and apply artificial neural networks (ANN) to predict these properties.

4. To perform an analysis of the available correlations for empirical and metaheuristic modelling of the viscosity of heavy fractions dilute with low molecular weight oil fluids using experimentally obtained results from measurement of the viscosity of individual fractions and the resulting mixtures. To compare the result of the best empirical model with the predictions of the artificial neural network model.

5. To perform an analysis of the available software libraries for automated prediction of the properties of libraries of components used for molecular modelling of oil and oil fractions. To analyse the accuracy of the most used models with group components for predicting the properties of individual components in the light fractions – gasoline and diesel, compared with the available experimental data.

The methods chosen to achieve the objectives of the dissertation are well su artificial neural network

ited to the tasks set. They include experimental approaches and industrial validation, as well as comparative analysis of existing correlations, nonlinear regression, intercriterion and correlation analysis, as well as the application of artificial neural networks. Thus, the methodological approach chosen allows for a reliable assessment of the properties of oil fluids and processes in oil refining and provides a good basis for obtaining scientifically based and practically applicable results:

For each task, a toolkit is selected that corresponds to the desired property or process: experimental validation, comparative analysis of correlations, statistical modelling, nonlinear regression, intercriteria/correlation analysis and artificial neural networks.

For the extraction of target products, the use of ASTM D1160 and ASTM D7169 is appropriate because both methods provide information on the distillation behaviour of heavy oil fractions. Their comparison and subsequent industrial validation are particularly adequate, as they allow not only laboratory evaluation, but also verification of feasibility under real process conditions.

Regarding molecular weight, the use of nonlinear regression and INM is adequate because the relationships between composition, physical characteristics and molecular weight are often nonlinear and difficult to describe with a simple analytical formula.

For critical temperature and critical pressure, the approach is justified because these properties are difficult to measure experimentally for complex oil systems. Correlation comparison, InterCriteria Analysis, correlation analysis, and INM make it possible to simultaneously assess the accuracy of available models and develop improved dependencies.

The methods used for the viscosity of heavy fractions and mixtures are appropriate because the viscosity is highly dependent on the composition, temperature and

degree of dilution. The combination of experimentally measured data, empirical models, metaheuristic approaches and ANN allows for a reliable comparison between classical and modern forecasting methods.

Analysis of available software libraries and models with group constituents is adequate because molecular modelling of petroleum fractions requires automated prediction of properties for many components. Comparison with experimental data for gasoline and diesel fractions is a correct criterion for assessing accuracy.

The PhD student eng. Svetlin Vassilev has formulated his contributions as follows:

1. The correlations derived in this dissertation for predicting the molecular weight, critical temperature and pressure of oil fractions and individual hydrocarbons can be used in the simulation and modelling of oil fluids and oil refining processes, improving or complementing the predictions of the existing correlations used so far.

2. The studies carried out demonstrate the superiority of gas chromatographic methods of simulant distillation over physical distillation methods in performing distillation analysis of petroleum fluids. Confirmation of the equivalence of the obtained data with those of the true boiling point curve reinforces the advantage of these methods, due to the elimination of the need to convert the obtained data into a true boiling point curve.

3. The proposed correlations for the calculation of the viscosity of mixtures of heavy fractions and thinners of lighter fractions shall provide an opportunity to model the viscosity of such mixtures to improve the transport properties of heavy fractions using the optimal number of lighter fractions used as diluent. Those lighter fractions have a correspondingly higher cost, and the reduction of their input has direct economic benefits.

4. The detailed overview of the growing popularity and application approach to molecular reconstruction and the analysis of criticality in the preparation of the initial information on the properties of molecules in the libraries used for molecular reconstruction can serve to further improve the accuracy of the results obtained and the scope of application of molecular reconstruction.

The contributions of the dissertation are clearly related to the goals and objectives of the dissertation and have a significant both scientific and scientifically applied nature. The main contribution can be pointed out the development of new correlations for predicting important physicochemical properties of petroleum fluids and individual hydrocarbons, which is essential for modelling and simulation of processes in oil refining. The results related to the comparison of distillation methods, the modelling of the viscosity of mixtures of heavy and light fractions, as well as the analysis of molecular reconstruction are also of practical value.

The scientific value of the dissertation is expressed in the development and evaluation of new correlation dependencies and models for predicting molecular weight, critical temperature, critical pressure and viscosity of petroleum fluids and

individual hydrocarbons. Additional scientific significance is the comparative analysis of existing models and the application of modern approaches such as nonlinear regression, InterCriteria Analysis and artificial neural networks.

The application value consists in the possibility to use the obtained results in the simulation, design and optimization of processes in oil refining. Of particular importance are the results related to the selection of an appropriate distillation method, the modelling of the viscosity of heavy fractions when diluted with lighter components and the increase in accuracy in molecular reconstruction. This creates prerequisites for more efficient use of raw materials, cost reduction and improvement of technological solutions in practice.

A practically significant technological approach to increasing the efficiency of oil refining processes has been proven, leading to an improvement in the productivity of the refinery and the realization of a significant economic effect (increased conversion and production of diesel fraction).

Based on the above, I appreciate the dissertation very highly. It is distinguished by the relevance of the issues under consideration, an in-depth analytical approach, significant scientific and applied contributions and a clear practical orientation to solving important tasks in the field of oil refining.

My overall assessment of the dissertation of Eng. Svetlin Petrov Vassilev is POSITIVE.

The report was written by:

Date: 15.09.2026