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MATHEMATICAL MODELING OF THE COMBUSTION PROCESS OF A TRI-FUEL MIXTURE IN A DIESEL ENGINE

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The article is dedicated to the analysis and mathematical modeling of the combustion process of three-fuel mixtures consisting of conventional diesel fuel, biodiesel (for example, based on rapeseed oil or waste), and bioethanol in diesel internal combustion engines. In the context of global environmental challenges, such as reducing harmful emissions and depleting fossil fuel resources, the authors examine the potential of these mixtures to improve engine efficiency and reduce dependence on imported oil. In particular, optimal component proportions are discussed, for example, 70% diesel fuel, 20-25% biodiesel, and 5-10% bioethanol, which allow achieving a balance between performance, economy, and environmental friendliness. Studies show that such mixtures can reduce soot emissions by 15-20%, nitrogen oxides by 25-30%, and carbon dioxide by 10-15%, depending on engine operating modes and specific physical properties of the fuel.

The work provides an overview of key experimental and theoretical studies conducted from 2008 to 2024. In particular, data from Romanian scientists at the Transilvania University of Cluj-Napoca are analyzed, who studied the physical characteristics of mixtures, such as density (0.841-0.852 kg/dm³), viscosity (2.756 mm²/s for the B25M70E5 mixture), and surface tension (up to 0.03465 N/m), as well as their impact on fuel atomization in injectors. Experiments using high-speed cameras confirmed that biodiesel additives increase the spray angle (up to 0.055 rad), while bioethanol accelerates evaporation due to its lower boiling point. In addition, the article references models from the journal Processes (2022), where a combined kinetic mechanism with 430 reactions was developed for simulating oxidation and emission formation, demonstrating a decrease in cylinder pressure by 4.31% and temperature by 1.23% with increasing ethanol content.

The mathematical apparatus of modeling is based on conservation equations for mass, momentum, energy, and species, taking into account turbulence (k-ε and k-ζ-f models), atomization (KIVA 3V), evaporation, and chemical reactions. Adapted thermodynamic models are described, such as the Wiebe function for the heat release curve ($x = 1 - exp(C \varphi^{m+1})$), with division into ignition and diffusion combustion phases, as well as gas dynamics equations for predicting parameters such as BSFC (with an error of about 1.12%). Simulations in AVL-Fire software and CFD tools confirm an increase in heat release rate due to prolonged ignition delay, but also highlight risks, such as deteriorated mixing at low loads.

The modeling results demonstrate practical value: for BE10-BE20 mixtures, BSFC increases by 18.64%, but BTE by 2.09%, with significant reductions in NOx emissions (by 29.32%), CO (by 39.57%), and soot (by 15.95%). The authors emphasize that three-fuel mixtures are suitable for implementation in agricultural machinery and transport without significant engine modifications, but recommend additional tests for material durability due to the possible impact of bioethanol on elastomers. Overall, the article contributes to the development of sustainable energy technologies, offering tools for optimizing fuel systems and reducing environmental impact.

Key words: *hree-fuel mixtures, biodiesel, bioethanol, diesel engine, mathematical modeling, CFD, emissions, combustion efficiency.*

Eq. 4. Fig. 3. Ref. 10.

1. Problem formulation

The modern development of road transport and energy is closely related to environmental challenges such as global warming, air pollution by harmful emissions and the rapid depletion of fossil fuel reserves. Diesel engines, which are widely used in freight transport, agricultural machinery and generators, are a significant source

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of nitrogen oxides (NOx), soot, carbon dioxide (CO_2) and other pollutants. According to numerous studies, traditional diesel fuel contributes to the growth of greenhouse gases, which forces the search for alternative solutions to reduce dependence on oil and improve environmental performance.

One promising direction is the transition to biofuels, in particular biodiesel (produced from vegetable oils or waste) and bioethanol. Biodiesel has a higher cetane number and contains oxygen, which contributes to more complete combustion, but its high viscosity and density worsen fuel atomization, lead to incomplete mixing and increased emissions at certain modes. Bioethanol, on the contrary, reduces the viscosity of the mixture, accelerates evaporation and lengthens the ignition delay, which can reduce soot and NOx , but reduces the energy value of the fuel and complicates the stability of the mixture.

Three-fuel (ternary) blends based on diesel, biodiesel and bioethanol allow combining the advantages of the components: achieving a reduction in soot emissions by 15-30%, NOx by 20-40% and improving engine efficiency without significant modifications. However, the implementation of such blends faces a number of problems. The physicochemical properties (density, viscosity, surface tension, boiling point) are significantly different from pure diesel, which affects the processes of injection, droplet atomization, evaporation, mixing with air and combustion itself. For example, bioethanol additives can lead to phase separation of the mixture, corrosion of fuel system elements or deterioration of cold start.

Experimental studies of such mixtures require significant resources, time and expensive equipment, and the results depend on specific conditions (load, temperature, injection pressure). In addition, accurate prediction of combustion processes is complicated by nonlinear interactions: turbulence, chemical reactions (hundreds of species and thousands of reactions) and emission formation. Existing models for binary mixtures (diesel-biodiesel or diesel-ethanol) are often not accurate enough for ternary mixtures, especially when the temperature or proportions of the components change. As noted in the 2024 study, mathematical models for predicting the density of ternary mixtures at variable temperatures are still limited and less accurate.

Thus, the current problem is the development of adequate mathematical models of the combustion process of three-fuel mixtures in a diesel engine, which would take into account the influence of fuel composition on thermodynamic, hydrodynamic and kinetic processes. Such models will allow optimizing the proportions of components, predicting efficiency, emissions and engine durability, contributing to the implementation of sustainable biofuels in practice.

2. Analysis of recent research and publications

Many works are devoted to experiments and modeling of two- or three-component fuels. For example, in a 2008 Romanian study, scientists from the Transylvania University in Cluj-Napoca studied the replacement of diesel with biodiesel-diesel-bioethanol blends. They prepared ten variants of the blends, such as B 25 M 70 E 5 (25% biodiesel, 70% diesel, 5% bioethanol), and measured the physical properties: density 0.841-0.852 kg/dm³, kinematic viscosity 2.756 mm²/s for B 25 M 70 E 5 (compared to 2.485 mm²/s for pure diesel), surface tension up to 0.03465 N/m. These data are important for modeling, as they affect fuel atomization. Benchtop injector experiments showed that blends with higher biodiesel content had a larger spray angle (0.055 rad), and bioethanol accelerated evaporation. Theoretical calculations were validated using photographs of fuel spurts, with an accuracy of 90%.

Another study, published in 2022 in the journal Processes, focuses on a high-speed diesel engine with ethanol additives to biodiesel (from 5% to 20%). The authors developed a combined kinetic mechanism with 430 reactions and 122 species, combining the biodiesel mechanism (methyl decanoate, methyl-9-decanoate, n -heptane) with the ethanol one. This allowed them to simulate oxidation and emission formation. Results: with increasing ethanol, the cylinder pressure drops by 4.31%, the temperature by 1.23%, but the heat release rate increases due to the extended ignition delay.

2013 IntechOpen book describes the simulation of biofuels using CFD (computational fluid dynamics). The authors propose thermodynamic models, such as the Wiebe model for the heat release curve: $x = 1 - \exp(C \varphi \{ m +1\})$, where φ is the relative duration, m is the combustion index (0-0.7 for diesel). For biofuels, a model with two curves was adapted: for ignition and diffusion combustion, taking into account the oxygen content, which intensifies diffusion. This is relevant for three-fuel mixtures, because biodiesel and ethanol change the diameter of the droplets (increases by 1.5-2 times) and the mixing process.

Another model from 2024 in the journal Combustion Engines proposes an integration of the gas dynamics equations with k-ε turbulence for biodiesel. Continuity equation: $\partial\rho/\partial t + \nabla \cdot(\rho u) = 0$; energy: $\partial(\rho e)/\partial t + \nabla \cdot(\rho u e) = -p \nabla \cdot u +$ other terms. The model was tested on blends up to 45% biodiesel, with a BSFC error of about 1.12%.

3. The purpose of the article

The purpose of this article is a systematic analysis of modern approaches to mathematical modeling of the combustion process of three-fuel mixtures (diesel fuel - biodiesel - bioethanol) in diesel internal combustion engines with an emphasis on achieving a balance between engine efficiency, economic performance and environmental characteristics. In particular, the task is to summarize the results of key

4. Results and discussion

Mathematical modeling of the combustion process in diesel engines, especially when it comes to alternative fuel blends, is a complex task that requires taking into account many physical and chemical phenomena. In the case of three-fuel blends consisting of diesel fuel, biodiesel (e.g. based on fatty acid methyl esters from vegetable oils or waste) and bioethanol, the models have to adapt to the changed properties of the fuel, such as density, viscosity, oxygen content, boiling point and cetane number. These properties directly affect the processes of injection, droplet atomization, evaporation, mixing with air, ignition and combustion itself. The basis of any model are the fundamental equations of conservation of mass, momentum, energy and components (species), which are solved within the framework of computational fluid dynamics (CFD) or quasi-dimensional approaches. Such models allow the prediction of engine parameters such as cylinder pressure, temperature, heat release rate, specific fuel consumption (BSFC), thermal efficiency (BTE), and emission levels, without the need for expensive experiments at each stage.

In practice, for three-fuel mixtures, quasi-dimensional models that simplify the cylinder geometry to zones (for example, a model with two zones: a combustion zone and a fresh charge zone) or full-fledged three-dimensional CFD models in software packages such as AVL-Fire, ANSYS Fluent, CONVERGE or KIVA are often used. Quasi-dimensional models are usually faster to calculate and are suitable for initial optimization, while CFD provides detailed analysis of the spatial distribution of flows, turbulence and reactions.

Let's take a closer look at the key components of the simulation. The mass conservation equation in CFD form looks like:

$$\partial\rho/\partial t + \nabla\cdot(\rho u) = 0, \quad (1)$$

where ρ is the density, t is the time, and u is the velocity vector.

For impulse:

$$\partial(\rho u)/\partial t + \nabla\cdot(\rho u\, u) = -\nabla p + \nabla\cdot\tau + \rho g + Sm, \quad (2)$$

where p is the pressure, τ is the stress tensor, g is the gravitational acceleration, Sm is the source terms from energy dissipation or reactions:

$$\partial(\rho E)/\partial t + \nabla\cdot(u(\rho E + p)) = \nabla\cdot(k\nabla T - \sum hj\, Jj + \tau\cdot u) + Sh, \quad (3)$$

with E as total energy, k - thermal conductivity, T - temperature, hj - enthalpy of species j, Jj - diffusion flux, Sh – source from combustion.

For components (types):

$$\partial(\rho Yi)/\partial t + \nabla\cdot(\rho u\, Yi) = \nabla\cdot(\rho\, Di\, \nabla Yi) + \omega i, \quad (4)$$

where *Yi* is the mass fraction of species i, *Di* is the diffusion coefficient, *ωi* is the rate of formation/destruction in reactions.

In models for ethanol-biodiesel blends, such as AVL-Fire, these equations are adapted for multiphase flows. Mass equation:

$$\partial\rho/\partial t + \partial(\rho u\_x)/\partial x + \partial(\rho uy)/\partial y + \partial(\rho uz)/\partial z = 0. \quad (5)$$

For momentum in the *x*-direction:

$$\partial(\rho ux)/\partial t + \nabla\cdot(\rho ux\, u) = \nabla\cdot(\mu\,\nabla ux) - \partial p/\partial x + Smx, \quad (6)$$

with similar ones for *y* and *z*.

Energy:

$$\partial(\rho T)/\partial t + \nabla\cdot(\rho u\, T) = \nabla\cdot((k/cp)\,\nabla T) + Sh/cp, \quad (7)$$

where *cp* is the heat capacity. Components:

$$\partial(\rho Ym)/\partial t + \nabla\cdot(\rho u\, Ym) = \nabla\cdot(Dm\,\nabla(\rho Ym)) + Sm. \quad (8)$$

Similar equations are used in ANSYS Fluent for binary mixtures, where the eddy-dissipation model is used for combustion: the reaction rate is limited by turbulent mixing, with the equation for a typical biodiesel reaction:

$$C17H34O2 + 24.5O2 \rightarrow 17CO2 + 17H2O. \quad (9)$$

Turbulence is a critical factor, as the flows in a diesel engine are chaotic. Often, k-ε models (turbulence kinetic energy k and dissipation rate ε) or its variants, such as RNG k-ε in CONVERGE, are used:

$$\partial(\rho k)/\partial t + \nabla\cdot(\rho u\, k) = \nabla\cdot((\mu + \mu\_t/\sigma k)\,\nabla k) + Pk - \rho\varepsilon + Sk, \quad (10)$$

and similarly for ε with constants C1ε, C2ε. In AVL-Fire, a four-equation k-ζ-f model is used for three-fuel mixtures:

$$v\_t = C\mu\ \zeta\ k\text{^}2 / \varepsilon, \quad (11)$$

where ζ is the velocity scale, f is the elliptic relaxation function. This improves the prediction near the walls.

For injection and spraying in biodiesel-diesel-ethanol mixtures, KIVA 3V is used, which models the Lagrangian-Eulerian approach: fuel droplets as discrete particles, gas as a continuum. The injection velocity depends on the pressure: ~11.34 m/s at 300 bar, with a Sauter mean diameter (SMD) of ~0.056 cm. At 1200 bar, the SMD decreases to 0.041 cm due to better decomposition. Bioethanol accelerates evaporation due to its lower boiling point (78°C vs. 150-350°C for diesel). In the KH-RT model (Kelvin-Helmholtz-Rayleigh-Taylor), the decomposition time is τ = 3.7 Cy rw / (Λ Ω), where rw is the droplet radius, Λ is the wavelength, and Ω is the frequency. In CONVERGE for biodiesel blends, the Frossling evaporation model: the evaporation rate is proportional to the difference in partial pressures.

The heat release model for biofuels is often based on the Wiebe function:

$$x = 1 - exp(-a\ (\varphi/\varphi z)^{m+1}), \quad (12)$$

where x is the fraction of the burned fuel, φ is the crankshaft rotation angle, a, m are the parameters. For a diesel engine, it is divided into two phases: ignition (dx/dφ)I = A (1 - x) (φ/φI)^{mI}, diffusion (dx/dφ)II = C (1 - x) ξv^{mII}, where ξv is the efficiency of air use, depending on the excess air and turbulence. The parameters are adapted: for biofuels m_I = 0-0.7, with Ku = γ KuT for evaporation, where γ is a coefficient of properties.

Chemical reactions are modeled by detailed mechanisms: the rate of the species:

$$\omega k = \sum \mu k\ (v'' - v')\ Aj\ T^{aj}\ exp(-Ej / RT) \prod [Xi]^{Mi}, \quad (13)$$

where μk is the stoichiometry, Aj is the pre-exponential factor, Ej is the activation energy, R is the gas constant, T is the temperature, Xi is the concentration. For biodiesel, the mechanisms include 122 species and 430 reactions, combining n-heptane, methyl decanoate and ethanol. Emissions: NOx according to the extended Zeldovich:

$$O2 \rightleftharpoons 2O,\ N2 + O \rightleftharpoons NO + N,\ N + O2 \rightleftharpoons NO + O,\ N + OH \rightleftharpoons NO + H, \quad (14)$$

with rates dependent on T. Soot: Sps = Snuc + Sgrowth - Sox, where Snuc is nucleation, Sgrowth is growth, Sox is oxidation (Hiroyasu model). In simulations with 20% ethanol, soot drops by 15.95%, NOx by 29.32%.

These models are validated by experiments: BSFC error ~1.12%, pressure ~5%. They help optimize mixtures to reduce emissions and improve efficiency.

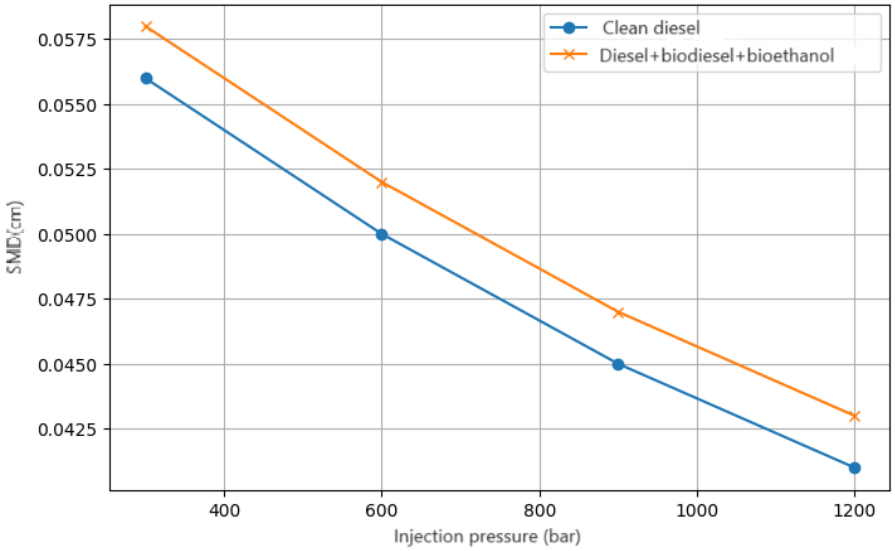

Fig. 1. Dependence of the average droplet diameter on the injection pressure

The abscissa axis shows the injection pressure in bars (from 300 to 1200 bar), and the ordinate axis shows the SMD value in centimeters. Two curves are presented: one for pure diesel fuel (marked with circles), which starts at approximately 0.056 cm at 300 bar and gradually decreases to 0.041 cm at 1200 bar; the second for the three-fuel mixture of diesel-biodiesel-bioethanol (marked with crosses), where the SMD values are slightly higher throughout the range, from 0.058 cm to 0.043 cm. The curves are nonlinear: the largest decrease in diameter occurs when moving from low to medium pressures, and then the rate slows down. This is

explained by the physical processes of atomization: higher pressure increases the fuel exit velocity from the nozzle, enhances the aerodynamic breakup of droplets according to the Kelvin-Helmholtz and Rayleigh-Taylor mechanisms, which leads to a finer spray. Bioethanol additives slightly increase the SMD due to lower viscosity and surface tension, but generally improve evaporation. The smaller droplet diameter contributes to better mixing with air, more complete combustion and reduced soot emissions.

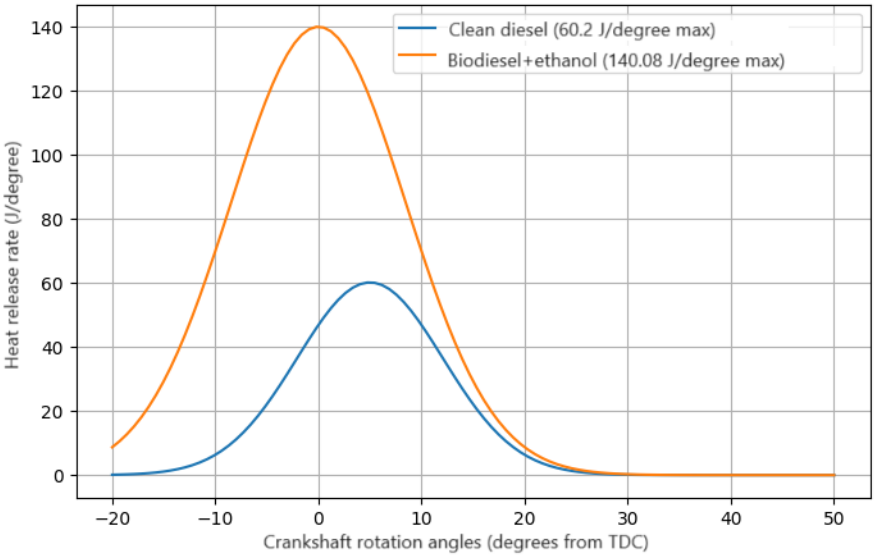

Fig. 2. Heat release curve for different fuels

Fig. 2 shows the curves of the heat release rate (HRR) as a function of the crankshaft angle (Crank Angle, CA) in degrees relative to the top dead center (TDC, 0°). Axes: abscissa – angle from -20° to +50°, ordinate – HRR in J per degree. The curve for pure diesel fuel has a lower peak – about 60 J/deg, with the maximum shifted to the right (approximately +5° after TDC), which reflects a typical diffusion combustion profile with a noticeable ignition delay. The curve for the biodiesel and ethanol mixture is much higher – the peak reaches 140 J/deg closer to TDC (about 0°), with a wider base. The shape of both curves is close to a Gaussian bell: a sharp rise after ignition, a peak and a gradual decline. The higher and earlier peak in the mixture occurs due to the extended ignition delay (due to the lower cetane number of ethanol), which accumulates more fuel for premix combustion, and the presence of oxygen in the biodiesel, which intensifies the reactions. This results in faster heat release, higher efficiency at full loads, but can increase noise and engine stress.

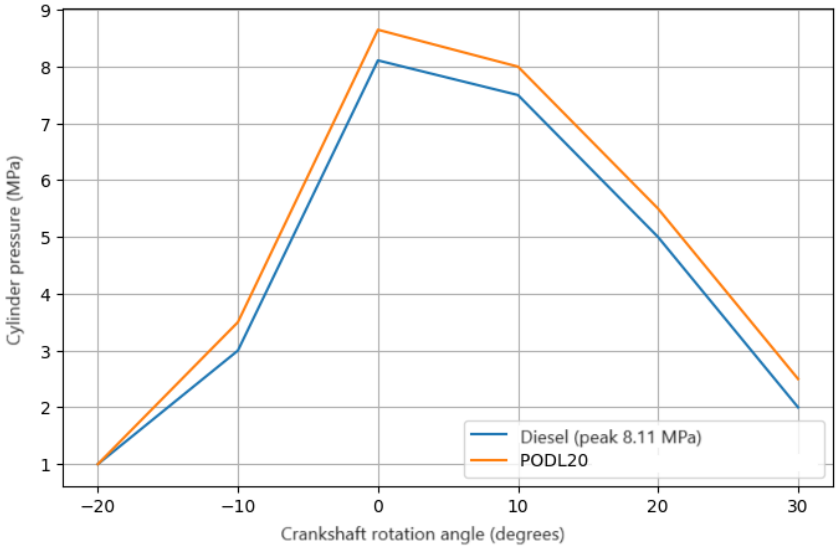

Fig. 3. Pressure versus angle for biodiesel blends

The graph shows the change in cylinder pressure depending on the crankshaft rotation angle. Axes: abscissa - angle from -20° to +30°, ordinate - pressure in MPa. The curve for diesel fuel starts at 1 MPa on compression, reaches a peak of 8.11 MPa near TDC and drops to 2 MPa on expansion. For a biodiesel mixture

(for example, PODL20 or with ethanol), the rise is steeper, the peak is higher - 8.65 MPa, and the decline is slower. Both curves have a characteristic "hump" on compression due to compression, a sharp jump after ignition and a smooth decline. The higher pressure in the mixture is explained by more intense heat release due to oxygen in biodiesel molecules and better premix combustion with ethanol, which increases thermodynamic efficiency (BTE up to +2%). However, this may reduce the maximum temperature and pressure in some modes due to the cooling effect of ethanol. Such profiles validate CFD models with energy and component equations, with a prediction error of up to 5%.

5. Conclusion

The analysis of modern approaches to mathematical modeling of the combustion process of three-fuel mixtures in diesel engines shows that the combination of traditional diesel fuel with biodiesel and bioethanol opens up real opportunities for improving the environmental and operational characteristics of internal combustion engines. Such mixtures, with proportions such as 70% diesel, 20-25% biodiesel and 5-10% bioethanol, allow achieving a noticeable reduction in emissions of harmful substances: soot by 15-20%, nitrogen oxides by 25-30%, carbon dioxide by 10-15%, and carbon monoxide by up to 40% compared to pure diesel. These effects arise due to the synergy of the components - oxygen in biodiesel molecules contributes to more complete oxidation, and bioethanol extends the ignition delay, which enhances premixed combustion and reduces soot formation.

In general, tri-fuel blends are suitable for practical use in agricultural machinery and transport without significant changes in engine design, contributing to reducing dependence on imported oil and meeting environmental standards. However, full implementation requires additional research into the durability of fuel system materials due to possible corrosion from ethanol and the stability of blends at low temperatures. Future developments should focus on more detailed kinetic mechanisms and real-world conditions with variable loads to maximize the potential of biofuels in sustainable energy.

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МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ПРОЦЕСУ ГОРІННЯ ТРЬОХПАЛИВНОЇ СУМІШІ В ДИЗЕЛЬНОМУ ДВИГУНІ

Стаття присвячена аналізу та математичному моделюванню процесу горіння трипаливних сумішей, які складаються з традиційного дизельного палива, біодизеля (наприклад, на основі ріпакової олії чи відходів) та біоетанолу, в дизельних двигунах внутрішнього згоряння. У контексті глобальних екологічних викликів, таких як зменшення викидів шкідливих речовин і вичерпання викопних ресурсів, автори розглядають потенціал цих сумішей для підвищення ефективності двигунів та зниження

залежності від імпортованої нафти. Зокрема, обговорюються оптимальні пропорції компонентів, наприклад, 70% дизельного палива, 20-25% біодизеля та 5-10% біоетанолу, які дозволяють досягти балансу між продуктивністю, економічністю та екологічністю. Дослідження показують, що такі суміші можуть скоротити викиди сажі на 15-20%, оксидів азоту на 25-30% та вуглекислого газу на 10-15%, залежно від режимів роботи двигуна та конкретних фізичних властивостей палива.

У роботі наведено огляд ключових експериментальних і теоретичних досліджень, проведених у період з 2008 по 2024 роки. Зокрема, аналізуються дані румунських вчених з Університету Трансільванії в Клуж-Напоці, які вивчали фізичні характеристики сумішей, такі як щільність (0,841-0,852 кг/дм³), в'язкість (2,756 мм²/с для суміші B25M70E5) та поверхневий натяг (до 0,03465 Н/м), а також їх вплив на розпилення палива в інжекторах. Експерименти з використанням високошвидкісних камер підтвердили, що добавки біодизеля збільшують кут розпилення (до 0,055 рад), тоді як біоетанол прискорює випаровування завдяки нижчій температурі кипіння. Крім того, стаття посилається на моделі з журналу Processes (2022 рік), де розроблено комбінований кінетичний механізм з 430 реакціями для симуляції окислення та утворення викидів, що демонструє зниження тиску в циліндрі на 4,31% та температури на 1,23% при зростанні вмісту етанолу.

Математичний апарат моделювання базується на рівняннях збереження маси, імпульсу, енергії та компонентів, з урахуванням турбулентності (моделі k-ε та k-ζ-f), розпилення (KIVA 3V), випаровування та хімічних реакцій. Описуються адаптовані термодинамічні моделі, як функція Вібе для кривої тепловиділення ($x = 1 - exp(C\ \varphi\{m+1\})$), з поділом на фази запалювання та дифузійного згоряння, а також рівняння газової динаміки для прогнозування параметрів, таких як BSFC (з помилкою близько 1,12%). Симуляції в програмному забезпеченні AVL-Fire та CFD-інструментах підтверджують зростання швидкості тепловиділення завдяки подовженій затримці запалювання, але також вказують на ризики, як погіршення змішування на низьких навантаженнях.

Результати моделювання демонструють практичну цінність: для сумішей BE10-BE20 BSFC зростає на 18,64%, але BTE – на 2,09%, з істотним зменшенням викидів NOx (на 29,32%), CO (на 39,57%) та сажі (на 15,95%). Автори підкреслюють, що трипаливні суміші придатні для впровадження в сільськогосподарській техніці та транспорті без значних модифікацій двигунів, але рекомендують додаткові тести на довговічність матеріалів через можливий вплив біоетанолу на еластомери. Загалом, стаття сприяє розвитку стійких технологій у енергетиці, пропонуючи інструменти для оптимізації паливних систем і зменшення екологічного навантаження.

Ключові слова: *трипаливні суміші, біодизель, біоетанол, дизельний двигун, математичне моделювання, CFD, викиди, ефективність згоряння.*

Ф. 14. Рис. 3. Літ. 7.

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