1. Introduction

The current research on compression ignition combustion engines is primarily oriented towards the use of alternative renewable fuels, reduction of toxic air emissions and the development of new engine diagnostic methods \[5, 6, 15\]. One of the increasingly often-addressed problems in engine research is the possibility of dual-fueling engines with the main fuel charge fed as a gaseous fuel.

An increased interest in dual-fuel compression ignition engines in recent years has contributed to the development of both experimental and model testing on this fueling method. One of the first valuable models simulating the combustion process in the full cycle of a dual-fuel engine was proposed by Raine in 1990 \[24\]. The operation of this model was limited only to the computation of the system's efficiency parameters.

Mansour et al. \[14\] proposed a simple, zero-dimensional model of combustion in a CNG-fueled engine with a pilot diesel fuel charge. Heat exchange with the chamber walls in this model was limited to convection and a number of other simplifying assumptions were adopted. The authors used a Wiebe function to describe energy release during diesel fuel and natural gas combustion in the first program.

Keywords: dual-fuel engine, engine combustion process, mathematical model, computer simulation, heat exchange.

The problem of using alternative fueling sources for combustion engines has been growing in importance recently. This is connected not only with the dwindling oil resources, but also with the growing concern for the natural environment and the fight against global warming. This paper proposes the concept for a zero-dimensional model of a multi-fuel engine, enabling the determination of thermodynamic system parameters based on the basic geometric and material object data (complete model). The basic problems in the creation of this model and the modeling of the accompanying subprocesses have been outlined and the methodology of the numerical solution of the obtained mathematical description has been proposed. The basic characteristics of the developed model are: the application of an original model of liquid fraction injection based on normal distribution, a new Assanis correlation for computing the diesel fuel self-ignition delay period in the presence of gas, first-order chemical reaction kinetic equations for describing the course of combustion for combustible components of the gas/air mixture, the implementation of a self-consistency procedure in modeling heat exchange and the effect of exhaust recirculation, the inclusion of both a single liquid fuel injection and the possibility of performing computations for a divided charge.

Keywords: dual-fuel engine, engine combustion process, mathematical model, computer simulation, heat exchange.

W ostatnim czasie problem wykorzystania alternatywnych źródeł zasilania silników spalinowych zyskuje szczególnie na znaczeniu. Związane jest to nie tylko z krawężnymi się zasobami ropy naftowej, ale również z coraz większą troską o środowisko naturalne oraz walkę z globalnym ociepleniem. W niniejszej pracy zaproponowano koncepcję zero-wymiarowego modelu silnika wielopaliwowego, umożliwiającego, wyznaczenie parametrów termodynamicznych układu w oparciu o podstawowe dane geometryczne i materiałowe obiektu (model kompletny). Nakreślono podstawowe problemy w zagadnieniu tworzenia takiego modelu i modelowania podprocesów towarzyszących oraz zaproponowano metodykę numerycznego rozwiązania uzyskanego opisu matematycznego. Podstawowe wyróżniki opracowanego modelu to: zastosowanie autorskiego modelu procesu wtrysku frakcji ciekłej opartego na rozkładzie normalnym, nowej korelacji Assanisa do obliczenia okresu zwłoki samozapłonu oleju napędowego w obecności gazu, jednostopniowych równań kinetyki reakcji chemicznej do opisu przechwatu spalania składników palnych mieszanych gaz-powietrze, implementacja procedury samouzgodnienia w modelowaniu procesu wymiany ciepła i wpływ recyrkulacji spalin, uwzględnienie zarówno pojedynczego wtrysku paliwa ciekłego jak i możliwość prowadzenia obliczeń dla dawki dzielonej.

Słowa kluczowe: silnik dwupaliwowy, proces spalania w silniku, model matematyczny, symulacja komputerowa, wymiana ciepła.

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(*) Tekst artykułu w polskiej wersji językowej dostępny w elektronicznym wydaniu kwartalnika na stronie www.ein.org.pl
step. The calculated pressure and temperature values were used as the input data for detailed kinetic computations, for which the commercial CHEMKIN package was used. The integration of complex combustion mechanisms with processes occurring in the dual-fuel engine, with the adopted simplifications, seems justified only in detailed research on exhaust toxicity, for which this model was used. In the assessment of efficiency and the power attained by the engine, the adopted simplifications in the description of individual subprocesses do not justify the need to apply very accurate combustion models, which require the use of dedicated computational environments.

Abd Alla [2] presented a model of pure methane combustion in a dual-fuel engine, calling it quasi-two zone. Leaving the nomenclature aside, the main distinguishing feature of this model was the application of detailed reaction kinetics for the description of gaseous phase combustion. A scheme of 178 elementary reactions, in which 41 chemical species participated, was used in this model, a Wiebe function was used to describe liquid phase combustion. The model description included the compression phase through combustion until the outlet valve opening. A detailed submodel of exhaust component formation was added to the basic thermochemical model. The basic advantage of this approach was the creation of connections between the progress of combustion and in-time and in-space changes in the burned zone of the engine. This model showed quite good agreement with the experiment and a high predictive capacity over a wide range of engine operating conditions.

Stelmasiak [25] proposed a relatively simple and complete approach to the problem of modeling dual-fuel systems. The zero-dimensional model assumed the separate combustion of two phases – liquid and gaseous. It is assumed in this model that the start of combustion is the same for both fuels and is determined by the ignition delay period. The combustion end angles for diesel fuel and CNG were different and set by the modeler. The heat release rate and the concentrations of the homogeneous gas/DI/air mixture components were imposed by a Wiebe function, separately for gas and diesel fuel. The empirical formula of Prakash [23] was used to predict diesel fuel ignition lag, taking into account the presence of natural gas in the cylinder.

Papagiannakis et al. used a gradually-improved model of a dual-fuel engine burning natural gas and diesel fuel in a number of their papers [9, 10, 11, 17, 18]. The authors used the fundamental laws of conservation of mass, energy and momentum for combustion process simulation. They proposed a two-zone description of the load in the cylinder, space with division into the unburned load zone and the burned zone. The fuel combustion front was described as a cone surface propagating from the point of injection. The propagation occurs in the direction normal to each cone surface with the speed defined by the jet propagation function. A scheme of 178 elementary reactions, in which 43 chemical species participated, was used in this model, a Wiebe function was used to describe liquid phase combustion. The model contains gaseous fuel mixed with air, into which liquid fuel is injected near TDC. Extremely different mechanisms dominate in the combustion of these two fractions, both of a physical (mass and energy transport processes) and chemical nature, resulting from the kinetics of fuel reaction with oxygen. All processes must therefore be analyzed, taking into account not only their effect on the gaseous and liquid fuel combustion rate, but also in regard to the proportions of individual-fuels.

Wang [26] proposed a similar model for CNG and hydrogen mixtures based on a CFD code and chemical reaction kinetics.

2. Assumptions of the model of combustion in a dual-fuel CI engine

In dual-fuel engines, a full description of the combustion process is much more difficult compared to single fuel engines. The cylinder contains gaseous fuel mixed with air, into which liquid fuel is injected near TDC. Extremely different mechanisms dominate in the combustion of these two fractions, both of a physical (mass and energy transport processes) and chemical nature, resulting from the kinetics of fuel reaction with oxygen. All processes must therefore be analyzed, taking into account not only their effect on the gaseous and liquid fuel combustion rate, but also in regard to the proportions of individual-fuels.

On the other hand, the liquid and gaseous phases are combusted at the same time, in the same space and the presence of one fraction affects the combustion of the other. The mechanisms of this influence are not yet well-known.

The examination of all these elements allowed the model assumptions to be formulated, bearing in mind both the accuracy of its results and the complexity level, affecting the autonomy (the amount of necessary experimental data) and the computational speed. The model is still innovative. Complete models are still lacking which, including all processes occurring in the cylinder, are able to predict with sufficient accuracy changes in thermodynamic working medium parameters, using only the basic object data available from its technical documentation. Among the available models, an even lower number has undergone full experimental verification, which limits their reliability. Moreover, there is a lack of research results on the effect of gas composition on the course of combustion in a dual-fuel engine. A properly constructed and verified model can significantly contribute to the filling of these deficiencies.
ignition, which initiates the gas mixture ignition. The two fuels are combusted separately and the emitted heat is the sum of heat released in the combustion of both fuels. The course of diesel fuel combustion is described by empirical equations for the ignition delay period and process rate – as represented by a Wiebe function. This is a simplified approach, but justified for dual-fuel engines because of the small pilot charge size.

Basic research on combustion processes proves that methane combustion is a very complex process and consists altogether of a system of 132 chemical reactions, whose rates are interrelated by the concentration of individual reactants. The implementation of such a complex model in a complete dual-fuel engine working cycle is unjustified due to the applied simplifications in the description of the other subprocesses (heat exchange, fuel injection etc.). A satisfactory representation of the combustion process can be obtained using even one methane combustion macromodel [20]. In the proposed model, a system of three interrelated global reactions, including the combustion of the most important combustible components used to fuel gas engines, was implemented for the description of gaseous phase combustion.

It is assumed that the developed model with the adopted assumptions will enable precise examination of the effect of gas composition on the character of combustion in a dual-fuel engine.

3. Basic equations of the developed model of fuel combustion in a dual-fuel engine

According to the discussed assumptions, the cylinder load is a homogeneous mixture of air, natural gas, diesel fuel and exhaust at each moment of time. The proportions of individual components change with the stages of the injection and combustion of combustible components. With such assumptions, starting from the energy conservation law, the basic equations of the model can be introduced in a differential form:

\[
\frac{dQ_{in}}{da} + p \frac{dV}{da} + \frac{dQ_{out}}{da} - h_{ON} \frac{dM_{ON}}{da} = p \cdot V = n(\alpha)\bar{R}T
\]

(1)

The first equation expresses the first law of thermodynamics in a differential form for an open system, where: \( dU \) – increase in the internal energy of the system, \( p, V \) – are the pressure and volume of the working medium in the cylinder, respectively, \( Q_{out} \) represents the heat exchanged with the cylinder walls, \( Q_{in} \) – heat fed to the system, \( h_{ON} \) – is diesel fuel enthalpy and \( M_{ON} \) – the mass of injected fuel. The second equation of the system represents an equation of state, where: \( \bar{R} \) is the universal gas constant, \( n \) – medium moles in the cylinder and \( T \) its temperature. All the quantities in the system (1) are functions of the crank angle.

Heat exchange with the walls was included in the developed model as the sum of three fluxes passing through the cylinder wall and head and the piston head. Because the main part of heat is removed in CI engines as a result of convection between gas in the working space and the given surface, it can be written:

\[
\frac{dQ_{out}}{da} = \frac{1}{\sigma} h_{ch}(T, p, V) \left[ A_{g} \cdot (T - T_{g}) + A_{s} \cdot (T - T_{s}) + A_{h}(\alpha) \cdot (T - T_{h}) \right]
\]

(2)

A simplified model of heat exchange in a combustion chamber wall and on the side of the coolant is included in equation (2) by expressions for the mean value of cylinder piston (\( t \)), head (\( g \)) and wall (\( s \)) temperatures:

\[
\bar{T}_{ch} = \frac{\bar{T}_{h} + \gamma_{ch} \bar{T}_{ch}}{\gamma_{ch} + 1}
\]

\[
\bar{T}_{ch} = \frac{h_{ch}}{\sqrt{\pi}} \bar{T}_{ch} \left[ \frac{1}{\sigma} \left( \frac{1}{\gamma_{ch}} + \gamma_{ch} \bar{T}_{ch} \right) \right]
\]

(3)

These temperatures were computed as the weighted mean from the mean temperature \( \bar{T} \) of the medium in the chamber with the mean heat transfer coefficient \( \gamma_{ch} \) and coolant temperature \( T_{cool} \) with the coefficient of heat transmission through the respective wall \( \gamma_{ch} \):

\[
\gamma_{ch} = \frac{1}{1} \left( \frac{\delta_{ch}}{\alpha_{ch}} \right)
\]

(4)

where: \( \gamma_{ch} \) – heat transfer coefficient of the wall material, \( \delta_{ch} \) – wall thickness.

Heat transfer occurs under a number of conditions – variable cylinder gas pressure and temperature and with locally variable rates of medium flow in the cylinder. These conditions are taken into account in the model by adopting an appropriate heat exchange coefficient \( h_{ch} \). Washin’s formula was used for this purpose, in the form modified by Hohenberg [9]:

\[
h_{ch} = 130 \left( \frac{P \cdot 10^6}{T} \right)^{0.8} \left( C_{pf} + 1.2 \right)
\]

(5)

where: \( C_{pf} \) – mean piston speed.

The thermodynamic medium parameters change during liquid fuel injection into the engine’s combustion chamber. The effect of the fuel mass flux supplied to the cylinder must therefore be taken into account. In direct ignition engines, temperature change as a result of stream evaporation can be neglected, because of a low ratio of the injected fuel volume to the working medium volume. This assumption is all the more justified for dual-fuel engines with diesel fuel charges of up to fifteen percent of the main charge. Another paper by the authors [16] discusses using complex hydraulic models to describe the diesel fuel mass flux in zero-dimensional models. It was demonstrated that a simple, complete model based on normal distribution with normalization to the total fuel charge could be used in this case without an observable loss of accuracy:

\[
M_{ON}(\alpha) = \begin{cases} 0 & \alpha_{pw} > \alpha < \alpha_{kw} \\ \frac{hB_{ON}}{\sqrt{\pi}} e^{-\frac{(a-a_{max})}{\alpha_{pw} \alpha_{kw}}} & \alpha_{pw} < \alpha < \alpha_{kw} \\ 10^{-3} B_{ON} & \alpha_{pw} = \alpha = \alpha_{pw} \end{cases}
\]

(6)

In a dual-fuel engine, the air/gas mixture ignites from the energy released from the combustion of the pilot diesel fuel charge. Test results show that even for a pilot charge lower than 1% of the total energy, the ignition energy can be by around 35 J higher in a dual-fuel engine than the electric pulse energy in a spark engine [25]. It can thus be assumed that in a dual-fuel engine the start of the combustion of both fractions (liquid and gas) is the same and the problem of ignition moment determination comes down to the accurate modeling of pilot charge ignition lag. This process, however, takes place under conditions significantly different from those in a classical compression ignition engine. Increasing the concentration of combustible gases in the cylinder causes, in most cases, a longer diesel fuel self-ignition delay. In an earlier paper [22], the authors examined the possibility of us-
ing ignition delay correlations verified for traditional CI engines. The equation proposed by Assanis [3] was used in the developed model to determine self-ignition lag:

$$\tau_{id} = 2.4\varphi^{-0.2}p^{-1.02} \exp\left(\frac{E_a}{RT}\right)$$  \hspace{1cm} (7)

It was demonstrated in the paper [22] that this correlation, taking into account cylinder load composition, describes self-ignition delay in dual-fuel engines better than others.

Diesel fuel combustion was represented in the developed model with a Wiebe function [7]. This allows the effect of the course of diesel fuel combustion on gaseous fraction combustion to be tested; however, this requires prior model validation for single fueling.

The natural gas combustion model was based on first-order oxidation macroractions for the main combustible mixture components: methane (CH₄), ethane (C₂H₆) and propane (C₃H₈). This leads to a system of three global reactions of the form:

$$nC_H + \frac{s}{4}O_2 \rightarrow nCO_2 + (n + 1)H_2O$$  \hspace{1cm} (8)

for \( n = 1...3 \). The expression for the global reaction rate in this case will assume the form:

$$\frac{d[C_nH_{2n+2}]}{dt} = A_n \exp\left(-\frac{E_a}{RT}\right) [C_nH_{2n+2}]^{s/4}[O_2]^{s/4}$$  \hspace{1cm} (9)

The constant values present in equation (9), for individual gases, were collected in Table 1.

### Table 1. Values of the constants included in equation (9). Activation energy \( E_a \) (kcal/mol).

| No | Fuel | \( A \) | \( E_a \) | \( a \) | \( b \) |
|----|------|--------|--------|------|------|
| 1  | CH₄  | 8.3\times10⁶ | 30     | -0.3 | 1.3  |
| 2  | C₂H₆ | 1.1\times10¹² | 30     | 0.1  | 1.65 |
| 3  | C₃H₈ | 8.6\times10¹¹ | 30     | 0.1  | 1.65 |

The solution of each equation of the system (9) fully determines the course of heat release in the gas combustion process at any moment.

### 4. Methodology of the model’s numerical computations

The developed mathematical model was implemented in the MathWorks MATLAB environment. The basis for creating the software program was the assumption of its modular structure. Individual submodels (e.g. of heat exchange, fuel injection, ignition delay, heat release during combustion, change in medium moles etc.) were treated as separate functional m-files called by the main program built around the basic system of differential equations for state variables (1). This approach guarantees program clarity, which facilitates its verification and optimization. The modular structure ensures, moreover, project expandability, by easy exchange of individual submodels with others – more detailed – when these are available.

The operation of the program starts with the entry of the basic input data into the global memory, i.e. engine geometry, engine material data (necessary for heat exchange computations), engine operating parameters etc. The thermodynamic load parameters (\( V_{in}, T_{in}, p_{in} \)) at the start of compression are then computed, from which the computation of cylinder temperature and pressure during the entire cycle starts.

The computational cycle of the main program was divided into 3 main processes: compression, combustion and expansion. The system of equations (1) for compression can be reduced to a single, nonlinear first-order differential equation for cylinder medium temperature as a function of the crank angle. Developing the expression for the internal energy of the system and heat exchanged with the walls (2), we obtain in this case:

$$\sum nC_H \frac{dT}{da} + \frac{p}{V(a)} \frac{dV(a)}{da} \cdot \frac{T}{a} = \frac{1}{a} \left[ \begin{array}{c} (30 \times 10^{-3}) \frac{R^3.8}{p^{0.8}} \cdot (C_{V} + 1.40) \end{array} \right] \cdot (a) \cdot (T - T_{a}) = 0$$  \hspace{1cm} (10)

Due to the complexity level of the above equation, using the dedicated MATLAB package functions for solving differential equations was dropped in favor of a solution by the iterative method. The temperature derivative can be expressed, based on its definition, as the difference quotient limit:

$$\frac{dT}{da} = \lim_{\Delta a \to 0} \frac{T(a + \Delta a) - T(a)}{\Delta a}$$  \hspace{1cm} (11)

In the numerical solution approximation, the quantity \( \Delta a \to 0 \) can be replaced with a finite value, obtaining instead of the differential equation (10) the corresponding difference equation, in which the successive temperature values are calculated based on the values computed in the previous step. The accuracy of the computations will be higher, the lower the value of the computational step is. The parameters for the next angle \( \alpha \) + \( \Delta a \) are calculated this way starting from the values \( T_{a}, p_{a} \), corresponding to the crank angle \( \alpha \) falling on the inlet valve closure. The other quantities in the equation (10) are calculated by complementary subprograms: the moles of individual components \( n_i(a) \) and the total load moles \( n_o(a) \) from the solution of the kinetics equations (9). The volume \( V(a) \) is calculated from rod-crank system geometry etc.

The procedure continues until the angle for which liquid fuel pumping starts is reached. Starting from this point, the pilot charge injection submodel (6) is included. For the same point, the ignition angle \( \alpha_i \) is computed based on the calculated temperature and pressure values, according to the adopted model (7). The compression procedure continues until the calculated \( \alpha_i \) value is reached, starting from which combustion starts. In this loop, computations are performed analogously as for combustion including the heat flux released during combustion, with variable instantaneous values of load moles depending on the rotation angle. The combustion end angle is defined by the moment when combustible components burn out.

Expansion proceeds according to an analogous equation as for compression with the moles of individual components determined at the combustion end point. The parameters for expansion are calculated until the angle corresponding to the outlet valve opening is reached, which ends the model operation.

It should be noted that the heat exchange equation used in the model (2) requires the mean temperature and the mean heat exchange coefficient for the cylinder load over the entire cycle for the computation of cylinder wall, head and piston head temperatures (3). It is obvious that these values are not known until the instantaneous values of these parameters are calculated. In the simplest approximation, the above mean values can be set as model operation parameters, based on the modeler’s experience or the results of experimental tests on the given engine. The first solution causes high uncertainties of computation results and the second leads to considerable limitation of model autonomy. These problems were solved by running the discussed
The developed model in its present specification can be used as a research tool in two main ranges, i.e. autonomous operation and semi-autonomous operation, in the analysis of experimental changes. In the autonomous operation range, only the basic technical data of the tested engine and the parameters characterizing the working point are used as the input data. Each input parameter can be used as an independent variable, which enables the simulation of different real processes. Moreover, it is possible in the model to insert the calculation of some parameters and their introduction into the computational program as an independent variable, e.g. the ignition delay angle. With such model applicability, the effect on the course of combustion in a dual-fuel engine can be tested for such parameters as:

- engine geometry;
- injection start angle (of both a single and a dual charge);
- temperature of the medium sucked into the cylinder;
- consumption (of air, liquid fuel, gas);
- ignition delay angle;
- gaseous fuel composition;
- diesel fuel combustion time.

In the semi-autonomous operation mode, the model can be successfully used for the analysis of real changes obtained during the performed experiments. For example, cylinder pressure changes do not have to be calculated by the model, they can be introduced there from an external file. In this case, the model can calculate all the other thermodynamic load parameters for the real cycle.

The proposed model, regardless of the mode of operation, based on available data without additional experimental tests on the data, enables the calculation of thermodynamic cylinder load parameters as a function of the crank angle (Fig. 3). The basic changes generated by the computational program are:

- cylinder pressure changes;
- cylinder temperature changes;
- cylinder volume changes;
- changes in the (total) heat flux removed through the surface of the cylinder, piston head, cylinder head, changes in DF, CH₄, C₂H₆, C₃H₈ combustion;

### Table 2. Range of conditions for which the model was verified and a synthetic summary of verification results

| Engine operation type | verification parameters | maximum error |
|-----------------------|-------------------------|---------------|
|                       | n | M₀ | P₀ | U₀ | instantaneous | in cycle |
| compression and expansion | 750 | 3400 | 0 | 27 | 42 | 0 | 1,1 | 5 | 6,6 |
| DF operation non-divided charge | 2300 | 3400 | 50 | 49 | 92 | 100 | 6,5 | 8 | 8,4 |
| DF operation divided charge | 1500 | 20-200 | 36-87 | 100 | 3,7 | 6 | 6,8 |
| DF+CNG operation non-divided charge | 3400 | 50-200 | 35-48 | 80 | 6,5 | 11 | 6,1 |
| DF+CNG operation divided charge | 1500 | 50 | 150 | 40 | 72 | 16 | 80 | 8 | 15 | 6,2 |
The model uses around fifteen submodels to determine these relationships, which compute a number of additional parameters in real time. The results of these partial computations can also be used in the testing procedure in inference. The most important additional parameters computed by the program include:

- excess air coefficients for the cylinder mixture ($\lambda_{ON}$, $\lambda_{CNG}$, $\lambda_A$);
- ignition delay angle (and combustion start angle);
- mean temperatures (of the load, cylinder, piston head, cylinder head);
- specific heats (for CO₂, CO, N, O₂, H₂, H₂O, CH₄, C₂H₆, C₃H₈);
- changes in the moles in the cylinder (for CO₂, O₂, H₂O, CH₄, C₂H₆, C₃H₈, DF) – under the adopted combustion model.

Different parameters and synthetic characteristics can be calculated based on the generated changes, including:

- $P/V$ characteristics;
- phase portrait of the engine;
- mean indicated pressure;
- indicated power and thermal efficiency of the engine.

6. Summary

The developed zero-dimensional simulation model of the working cycle of a dual-fuel engine fed with gaseous fuel with an initiating diesel fuel charge includes the compression, combustion and expansion phases. The main characteristics of the proposed model are:

- application of an original approach to modeling liquid fuel injection, based on normal distribution;
- application of a new Assanis correlation for describing diesel fuel self-ignition delay in the presence of gas;
- application of chemical reaction kinetics equations for describing the course of combustion for combustible components of the gas/air mixture in the zero-dimensional dual-fuel engine model;
- implementation of a self-consistency procedure in modeling heat exchange and the effect of exhaust recirculation, which allows a high degree of model completeness to be maintained;
- inclusion of both a single liquid fuel injection and the possibility of performing computations for a divided charge.

The basic advantages of this model include:

- a high degree of completeness, which permits autonomous computational program operation, using only the basic technical data of the tested engine;
- a wide spectrum of model applicability;
- relatively fast computational time, which enables model use on standard PC computers;
- a modular structure, ensuring easy modification and expandability of the model. The model can be developed by adding new submodels or changing the existing ones when more accurate correlations are available, without the need to change the main program;
- the model was subjected to thorough verification in several stages, which ensures its high reliability.

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Maciej MIKULSKI
Sławomir WIERZBICKI
Andrzej PIĘTAK
University of Warmia and Mazury in Olsztyn
Faculty of Technical Sciences
ul. Słoneczna 46A
10-710 Olsztyn, Poland

E-mails: maciej.mikulski@uwm.edu.pl, slawekw@uwm.edu.pl, apietak@uwm.edu.pl