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Investigation of performance characteristics using Stochastic Reactor Model in a biodiesel pilot-fueled natural gas engine

Biyodizel pilot yakıtlı doğalgaz motorunda performans karakteristiklerinin Stokastik Reaktör Model kullanılarak incelenmesi

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ABSTRACT

In this study, the effects of different biodiesel pilot fuel injection pressures on performance characteristics of a natural gas engine were investigated using 'Kinetics & SRM Engine Suite' software which is based on stochastic reactor model (SRM). This advanced software uses chemical kinetic mechanisms of fuels to simulate combustion process of the engine. 'Methyl decanoate/methyl-9-decenoate/n-heptane' reduced chemical kinetic mechanism including 71 species and 217 reactions were defined as a biodiesel surrogate fuel chemical kinetic mechanism to represent biodiesel fuel in this study. Theoretical model set by the way of software tools was validated by experimental data. Then, simulation was run in three different stochastic particle numbers (50, 100, and 150) to investigate engine performance characteristics of a biodiesel pilot-fueled natural gas engine. It is observed that as pilot fuel injection pressure increases, engine torque and brake power enhance, but brake specific fuel consumption decreases. Furthermore, various stochastic particle numbers used in the simulation did not dramatically affect data of engine performance characteristics simulated.

Keywords: Dual fuel engine, Natural gas, Biodiesel pilot fuel, Stochastic Reactor Model, Engine Performance.

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ÖZET

Bu çalışmada, bir doğalgaz motorunda farklı biyodizel pilot yakıt püskürtme basınçlarının performans karakteristiklerine etkileri stokastik reactor modele (SRM) dayanan 'Kinetics & SRM Engine Suite' yazılımı kullanılarak incelenmiştir. Motorun yanma işleminin benzetimini yapmak için bu gelişmiş yazılım yakıtların kimyasal kinetik mekanizmalarını kullanır. Bu çalışmada, biyodizel yakıtı yansıtmak için 71 bileşen ve 217 reaksiyon içeren 'Metil dekanoat/metil-9 dekenoat/n-heptan' kimyasal kinetik mekanizması biyodizelin yerini tutan yakıt kimyasal kinetik mekanizması olarak tanımlanmıştır. Yazılım araçları vasıtasıyla ayarlanan teorik model deneysel veri aracılığıyla doğrulanmıştır. Sonrasında, biyodizel pilot yakıtlı doğalgaz motorunun motor performans karakteristiklerini incelemek için benzetim işlemi üç farklı stokastik parçacık sayısında (50, 100 ve 150) gerçekleştirilmiştir. Pilot yakıt püskürtme basıncının artmasıyla motor döndürme momenti ve efektif gücün arttığı fakat özgül yakıt tüketiminin azaldığı gözlemlenmiştir. Buna ek olarak, simülasyonda kullanılan çeşitli stokastik parçacık sayılarının benzetimi yapılmış motor performans karakteristik verilerini önemli ölçüde etkilemediği saptanmıştır.

Anahtar sözcükler: Çift yakıtlı motor, Doğalgaz, Biyodizel pilot yakıt, Stokastik Reaktör Model, Motor Performansı

1. INTRODUCTION

Internal combustion engine (ICE) researchers have primarily focused to develop reformer engines (HCCI, PCCI and RCCI) being innovative, eco-friendly and having high fuel economy because of increasing environmental concerns and status of fossil fuels depletion (Namasivayam *et al.*, 2010; Papagiannakis *et al*., 2010). There have been numerous experimental and simulation studies to investigate reformer type of engines (Bissoli *et al.*, 2016; Wang *et al.*, 2016; Li *et al.*, 2016; Park and Yoon, 2016). Primary data have been obtained by the way of experimental studies in research activities. However, experimental studies are of some challenges and restrictions. Simulation-based approaches are briefly an important alternative used by ICE researchers. A Computational Fluid Dynamics (CFD) based engine simulation approaches are widely used in engine research activities. One Dimensional (1D) CFD and Three Dimensional (3D) CFD are called as first and second generation simulation methods (Dizy *et al.*, 2016). However, 3D CFD approach is highly time-consuming during engine simulation due to above expressions (Anetor, 2013; Pasternak *et al.*, 2014; Pasternak *et al.*, 2016). Consequently, Zero Dimensional (0D) 'Kinetics & SRM Engine Suite' Software has been developed to meet this challenge. Aforementioned software is based on Probability Density Function (PDF) methods and called as a third generation simulation method at the same time (Dizy *et al.*, 2016; Maurya and Akhil, 2017). 0D means that position of the stochastic particles have no information. 'Kinetics & SRM Engine Suite' software has been validated by experimental data related to low temperature combustion, direct injection compression ignition and direct injection spark ignition modes for twelve years and are proved oneself (Dizy

et al., 2016; Maurya and Akhil, 2017; Bhave *et al.*, 2004; Bjekborn *et al.*, 2012; Lundgren *et al.*, 2013; Pehlivan *et al.*, 2016).

One of the developed engine types is dual fuel engine to supply better combustion. In these engines, two different fuels (gas+liquid) are concurrently conceded in combustion chamber. The dual fuel engines can be served both current liquid fuels (diesel and biodiesel) and gaseous fuels (natural gas, biogas, producer gas, hydrogen) (URL-1, 2016; URL-2, 2016; Supee *et al.*, 2014; Bora and Saha, 2015; Korakianitis *et al.*, 2010; Carlucci *et al.*, 2013). Diesel fuel has generally used as a pilot fuel in the dual fuel engines, but recently biodiesel has been widely utilized because of high cetane number compared to diesel fuel. Natural gas as a main fuel has generally used in the dual fuel engines in that it has lower C/H ratio and higher auto-ignition temperature compared to other hydrocarbon fuels. In available literature, biodiesel pilot fueled natural gas engines are investigated with experimental studies to display the effect of pilot injection parameters (pilot injection pressure, pilot injection timing, pilot injected mass etc.) on engine performance, exhaust emissions and combustion characteristics (Ryu, 2013a; Ryu, 2013b; Gharehghani *et al.*, 2015). However, it has not found any stochastic reactor model (SRM) based theoretical study related to these type of dual fuel engines.

Therefore, SRM was set to investigate the effects of different pilot injection pressures and three different stochastic particle numbers on brake power, engine torque, brake specific fuel consumption of a biodiesel pilot fueled natural gas engine in this study.

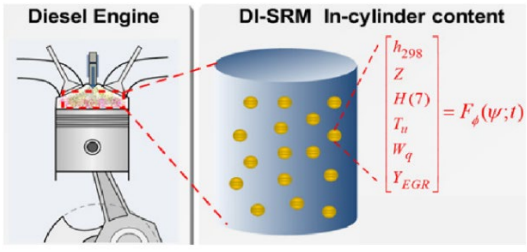
2. SRM ALGORITHM

2.1. Model Depiction

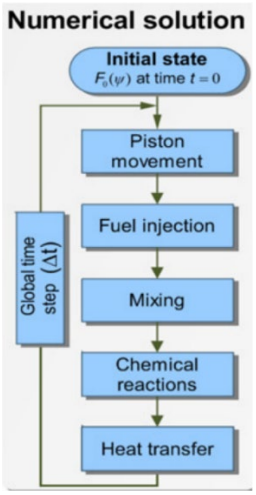
SRM is a spatially zero-dimensional model based on the opinion which real fluid particles and homogeneity inside the cylinder is switched the unreal stochastic particles and statistically homogeneity (Ahmedi *et al.*, 2014; Maurya and Akhil, 2016; Franken *et al.*, 2019). Each unreal particle has mass, chemical composition, and temperature. In addition, these particles also possess the capability of mixing with other particles next to exchange heat with cylinder walls.

Cylinder substances depend on pressure and volume changes, chemical reactions, heat transfer, mixing and fuel injection. These are independent from the space. All parameters of interest are estimated from these processes. These are subdivided as global and local parameters and obtained by solving the SRM equations using Monte Carlo particle method (Pope, 1985).

Global parameters have invariant value in the combustion chamber and include total mass, volume, mean density and pressure in the SRM model. They are assumed to remain stable spatially in the combustion chamber. If engine geometry (volume), density and equation of state (pressure) are known, global parameters can be predicted (Maurya and Akhil, 2016; CMCL, 2013; Wang *et al.*, 2016; Tunér, 2008; Tunér *et al.*, 2008). Local parameters modified in the combustion chamber are mass fractions and temperatures for each species. They can be assumed as random variables which can modify in the combustion chamber and identify the substances of the gas mixture in the cylinder. These variables are clarified using the mass density function (MDF) (CMCL, 2013). The representation of particles for diesel engines and SRM numerical solution scheme are respectively shown in Fig. 1(a) and Fig. 1(b).



(a)



(b)

Figure 1. Stochastic particles representation in Diesel-SRM model (Franken et al., 2018).

2.2. Solution Algorithm

SRM is rooted in statistical homogeneity supposed to be the same along engine cylinder of the PDF. Nevertheless, MDF has been employed rather than the PDF as the in-cylinder density changes throughout an engine cylinder. The MDF is obtained mass density multiply by PDF and given by Equation (1).

$$\mathcal{F}(\psi;t)=\rho(\psi)f(\psi;t) \tag{1}$$

In Equation (1); ρ, $\mathcal{F}$ and ψ is respectively to express the mass density, MDF and a parameter represented properties such as mass, temperature, pressure. The variation of the MDF on the time is described by the following PDF transport equation (CMCL, 2013).

$$\frac{\partial}{\partial t}\mathcal{F}(\psi;\mathrm{t})=\underbrace{-\sum_{j=1}^{N_S+1}\frac{\partial}{\partial\psi_j}\left[G_j(\psi)\mathcal{F}(\psi;\mathrm{t})\right]}_{\text{chemical reaction}}+\underbrace{\sum_{j=1}^{N_S+1}\frac{\partial}{\partial\psi_j}\left[A_j(\psi)\mathcal{F}(\psi;\mathrm{t})\right]}_{\text{turbulent mixing}}$$
$$\underbrace{-\frac{1}{V}\frac{dV}{dt}\mathcal{F}(\psi;\mathrm{t})}_{\text{piston movement}}\underbrace{-\frac{\partial}{\partial\psi_{N_S+1}}\left[U(\psi_{N_S+1})\mathcal{F}(\psi;\mathrm{t})\right]}_{\text{convective heat transfer}}+\underbrace{\frac{\mathcal{F}_C(\psi;\mathrm{t})}{\tau_{crev}}-\frac{\mathcal{F}(\psi;\mathrm{t})}{\tau_{cyl}}}_{\text{crevice flow}}+\underbrace{\frac{\mathcal{F}_f(\psi;\mathrm{t})}{\tau_f}}_{\text{fuel injection}} \tag{2}$$

In Equation (2), N_S+1 random scalar variables are to verbalize. The analysis function identifying chemical kinetic mechanisms are represented by G_j. The function defining turbulent mixing process occurred into the cylinder are by $A(\psi)$. The displacement volume is denoted by V. The function $U(\psi_{N_S+1})$ specifies the amount of heat that is transferred between the cylinder charge and cylinder walls. The MDF of the gases in the crevice and the fuel are symbolized by $\mathcal{F}_C$ and $\mathcal{F}_f$. The characteristic residence times of the in-cylinder gas, crevice gas and fuel are represented by τ_{crev}, τ_{cyl} and τ_f, respectively (CMCL, 2013). The residence time states the average amount of time that a particle in a particular system (reactor, engine etc.). The initial conditions are described by Equation (3).

$$\mathcal{F}(\psi;0)=\mathcal{F}_0(\psi) \tag{3}$$

The right-hand side of Equation (2) informs the physical in-cylinder processes of chemistry, turbulent mixing, heat transfer, piston movement, crevice flow and fuel injection (CMCL, 2013). This equation is solved by a Monte Carlo stochastic particle method (Pope, 1985; CMCL, 2013; Demir *et al.*, 2015). The PDF with ensemble average is predicated by Equation (4).

$$f(\psi;t)\approx\frac{1}{N_{par}}\sum_{i=1}^{N_{par}}\delta\left(\psi-\psi^{(i)}(t)\right) \tag{4}$$

A number of stochastic particles describing the statistical representation of the PDF is represented by N_{par}. The Dirac delta function (δ) is the PDF corresponding to discontinuous distribution function as Heaviside functions. δ is derivative of the Heaviside function (Pope, 1985). Operating splitting technique, which each term can be treated separately (Ahmedi *et al.*, 2014; Pope, 1985; Strang, 1968) is operated to solve Equation (2).

2.3. Engine Performance Algorithm

The calculations for this section are the standard definitions in engine technologies (Heywood, 1988). In the event that the simulation typifies a *closed system only* (i.e. intake valve *closed* to exhaust valve opening), the open portions of the cycle are guessed to be same to the intake ($P_{int.man.}$) and exhaust manifold pressures ($P_{exh.man.}$), respectively.

2.3.1. Indicated work per cycle

The indicated work ($W_{c,in}$) is calculated by integration of pressure and volume throughout the whole cycle.

$$W_{c,in} = \oint pdV \tag{5}$$

2.3.2. Indicated power per cylinder

The indicated power per cylinder (P_i) is determined depending on the indicated work in Equation (6).

$$P_i = \frac{W_{c,in} \times n}{n_R} \tag{6}$$

where n_R is the number of crank revolutions for each power stroke per cylinder (two stroke n_R=1, four stroke n_R=2).

2.3.3. Mean effective pressure

The Mean Effective Pressure (MEP) is given by Equation (7).

$$\text{MEP} = \frac{P \times n_R}{n \times V_d} \tag{7}$$

where V_d is the displacement volume and n the engine speed.

2.3.4. Engine Torque

The MEP can be used from Equation (8) to obtain the engine torque (T).

$$T = \frac{\text{MEP} \times V_d}{n_R} \tag{8}$$

2.3.5. Brake mean effective pressure and mechanical efficiency

The IMEP and BMEP are related via frictional losses predicted by calculating the FMEP in Equation (9).

$$\text{BMEP} = \text{IMEP} - \text{FMEP} \tag{9}$$

A mechanical efficiency (in percentages), η_m can also be gained by relating indicated, P_i and brake P_b power.

$$\eta_m = 100 \times \frac{P_i}{P_b} \tag{10}$$

2.3.6. Specific fuel consumption and emissions

Specific outputs are obtained by calculating the mass flow rate and dividing by the brake P_b power.

$$\text{Specific Emissions or SFC} = \frac{\dot{m}}{P_b} \tag{11}$$

2.4. Chemical Kinetic Model

The theory of SRM Engine Suite software depends on chemical kinetic mechanism of related fuel. Improved chemical kinetic mechanisms were put to use within software. These mechanisms were initially developed as detailed chemical kinetic mechanism, but use of these mechanisms has considerably been time-consuming. Reduced chemical kinetic mechanisms of

fuels were employed using some reduction methods to solve this problem. In the wake of disposal reduced chemical kinetic mechanism, simulations in CFD or SRM Suite have considerably been fast. 'methyl decanoate/methyl-9-decenoate/n-heptane' biodiesel surrogate reduced chemical kinetic mechanism (Brakora, 2012) was used to depict biodiesel fuel in this study.

2.5. Dual Fuel Engine Specifications and Experimental Data

Experimental data was extracted from the literature (Ryu, 2013a) related to biodiesel pilot fueled dual fuel engine and used to validate the presented SRM model. Specifications of the dual fuel engine are given in Table 1.

Table 1. Specifications of test engine (Ryu, 2013a; Ryu, 2013b).

Description	Specification
Engine model	ND 130DI
Type	Single cylinder DI engine
Bore × Stroke (mm)	95 × 95
Displacement volume (cm^3)	673
Compression ratio	18
Intake valve opening	BTDC 340°
Intake valve closing	ATDC 136°
Exhaust valve opening	ATDC 136°
Exhaust valve closing	BTDC 340°
Combustion chamber	Open chamber
Maximum horse power (ps/rpm)	13/2400
Maximum engine torque (N.m/rpm)	42/2000
Cooling water temperature (°C)	70 ± 2

3. RESULTS AND DISCUSSION

In this study, the effects of five biodiesel pilot fuel injection pressures (30, 60, 90, 120 and 150 MPa) on engine performance characteristics were investigated at three different stochastic particle numbers (50, 100 and 150) by SRM model (using Kinetics & SRM Engine Suite software). Experimental data were obtained at constant engine speed (1800 rpm) and engine load (75 %) by Ryu (2013a). Values of engine performance characteristics were calculated at the same engine operation condition in the SRM model. The simulation results were presented in Fig. 2-5. The optimum biodiesel pilot injection pressure (120 MPa) value was defined via indicated mean effective pressure (IMEP). Validation of the model, shown in Fig. 2, was performed by the cylinder pressure history at optimum biodiesel pilot fuel injection pressure. It was seen that there was modest difference for maximum cylinder pressures in between the simulation and experimental data by 6.6% at optimum case (Pehlivan, 2016).

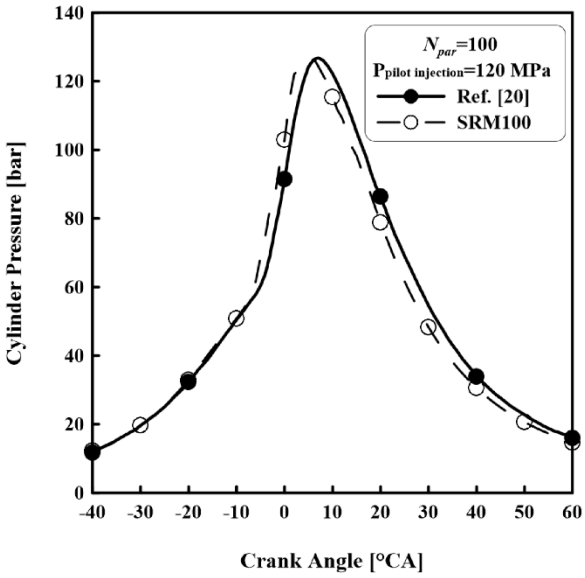


Figure 2. Model validation process for 120 MPa pilot fuel injection pressure

There have been small differences between calculated and experimental cylinder pressure data at the early stage of the combustion and the late stage of expansion process. Conceivable causes have been specified as below:

- Crevice volume (%) was roughly computed and set as an input in the simulation process.
- Initial boundary conditions (initial pressure and initial temperature) required for numerical solution was not fully known. Therefore, they

were predicted with trial and error method.

- Convenient turbulent mixing model was chosen. Its default value of the parameters (swirl ratio, tumble ratio etc.) were used in the simulation.
- Heat transfer parameters such as piston top temperature, cylinder liner temperature, etc. were approximately determined.
- Reduced chemical kinetic mechanism for biodiesel was used in terms of reducing computational time.
- The reduced chemical kinetic mechanism for biodiesel may not fully represent biodiesel fuel.

Engine performance characteristics (brake power, engine torque and brake specific fuel consumption) at three different stochastic particle numbers are given in Figs. 3-5, respectively. Due to giving better simulation results, the optimum stochastic particle number was chosen as 100. It was observed that 120 MPa pilot fuel injection pressure give the best results to brake power, engine torque and brake specific fuel consumption data for different stochastic particle numbers. Furthermore, as pilot fuel injection pressure was increased, it was observed that brake power and engine torque increased (Abd Alla *et al.*, 2000) and brake specific fuel consumption decreased.

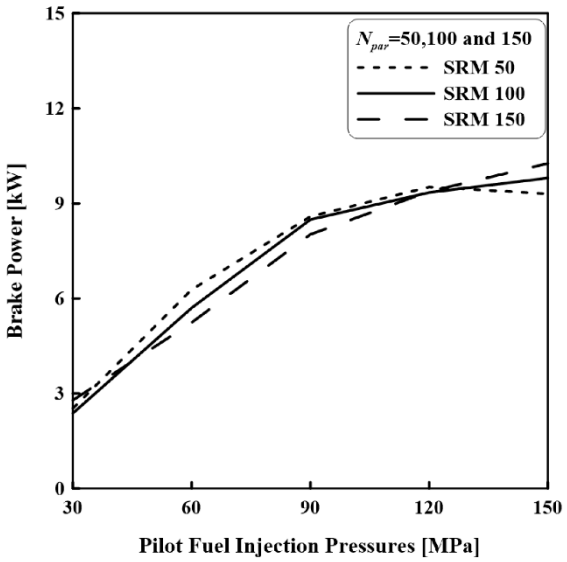


Figure 3. The variation of brake power on different pilot fuel injection pressures.

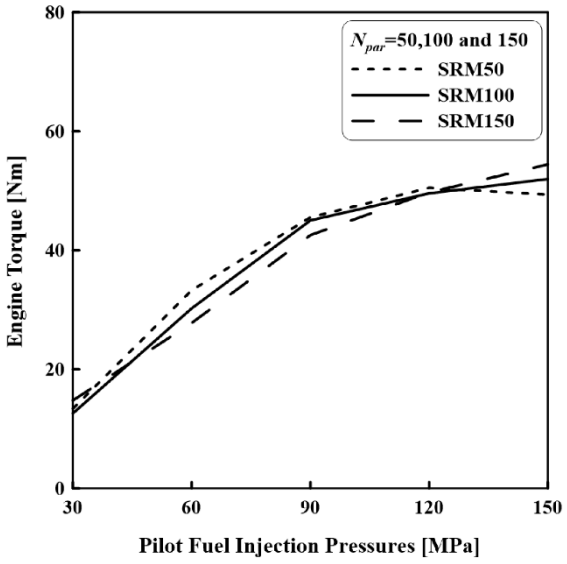


Figure 4. The variation of engine torque on different pilot fuel injection pressures.

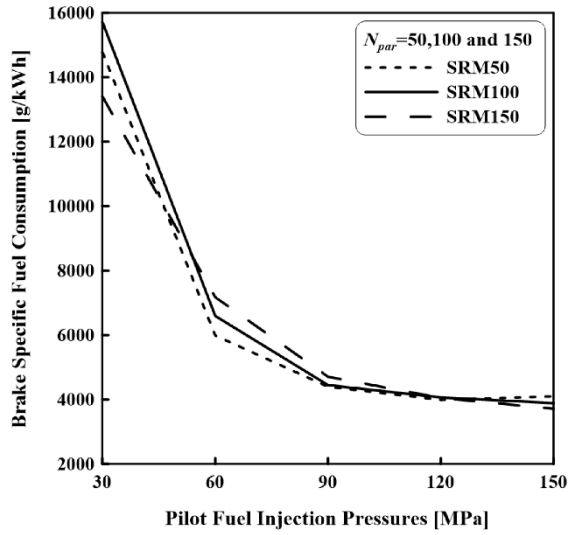


Figure 5. The variation of brake specific fuel consumption on different pilot fuel injection pressures.

4. CONCLUSIONS AND FUTURE WORK

In this study, it was investigated the variation of different biodiesel pilot fuel injection pressures on engine performance characteristics (brake power, engine torque and brake specific fuel consumption). The dual fuel engine operated natural gas and biodiesel was preliminary investigated using SRM approach with this study. It was seen that SRM Engine Suite was a good tool to predict engine performance characteristics of a biodiesel pilot fueled natural gas engine. Presented results can be improved and performed simulation process using different engine parameters such as engine speed, engine load, pilot fuel injection amounts if chemical kinetic mechanisms for each biodiesel (soy bean, canola, rapeseed methyl esters) are advanced. Presented model can be extended on dual fuel marine engines with various pilot fuels (dimethyl ether, alcohol, diesel etc.) and gas fuels (biogas, producer gas, Liquified Petroleum Gas, shale gas etc.).

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NOMENCLATURE AND UNITS

BMEP: Brake Mean Effective Pressure [bar]
CFD: Computational Fluid Dynamics
$\mathcal{F}_C$: Mass Density Function of the crevice gas
$\mathcal{F}_f$: Mass Density Function of the fuel
HCCI: Homogeneous Charge Compression Ignition
IMEP: Indicated Mean Effective Pressure [bar]
MDF($\mathcal{F}$): Mass Density Function
N_{par}: Stochastic particle numbers
N_S+1: Random scalar variable numbers
n: Engine speed [rpm]
PCCI: Premixed Charge Compression Ignition
PDF(f): Probability Density Function
P_i: Indicated Power [W]
P_b: Brake Power [W]
RCCI: Reactivity Charge Compression Ignition
SE: Specific Emissions [g/kWh]
SFC: Specific Fuel Consumption [g/kWh]
SRM: Stochastic Reactor Model
$W_{c,in}$: Indicated work [J]
0D: Zero Dimensional
1D: One Dimensional
3D: Three Dimensional
(i): Individual particle

ρ: Mass Density [kg/m^3]
ϕ: Equivalence ratio
η_m: Mechanical efficiency [%]
τ_{crev}: Characteristic residence time of the crevice gas
τ_{cyl}: Characteristic residence time of the cylinder gas
τ_f: Characteristic residence time of the fuel
ψ : Chemical and physical characteristics such as mass, pressure and temperature

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