"NEAR WALL" COMBUSTION MODEL OF SPARK IGNITION ENGINE

by

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Original scientific paper
https://doi.org/10.2298/TSCI2106189W

This paper has illustrated a "near wall" combustion model for a spark ignition engine that was included in a two-zone thermodynamic model. The model has calculated cylinder pressure and temperature, composition, as well as heat transfer of fresh and combustion gas. The CO submodel used a simplified chemical equation to calculate the dynamics of CO during the expansion phase. Subsequently, the HC submodel is introduced, and the post-flame oxidation of unburned hydrocarbon was affected by the reaction/diffusion phenomenon. After burning 90% of the fuel, the hydrocarbon reaction dominates at a very late stage of combustion. This modeling method can more directly describe the "near wall" flame reaction and its contribution to the total heat release rate.

Key words*: engine, "near wall" combustion model, CO submodel, hydrocarbon submodel*

Introduction

With the rapid development of the economy, cars have entered thousands of households and become the most commonly used means of transportation. At the same time, the growing demand for car purchases has greatly contributed to the rapid development of the automotive industry. The development of fuel vehicles to this day has already faced the dual pressures of *environmental pollution* and *energy crisis* [1]. It has turned out to be an increasingly prominent issue for China's energy and environmental research center to develop clean alternative fuel for vehicles so as to realize high-efficiency and low-polluting combustion in engines, controlling harmful emissions from automobile engines. However, this requires alternative fuels to possess both high combustion performance and low emission requirements. Fuel consumption reduction, low pollutant emission and adequate output performance features in modern SI engine designs.

In this paper, the "near wall" combustion model of a SI engine delved into, which is included in a two-zone thermodynamic model. The model has calculated cylinder pressure and temperature, composition, as well as heat transfer of fresh and combustion gas. The CO submodel used a simplified chemical equation to calculate the dynamics of CO during the

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expansion phase. This model can predict the CO change process accurately. Subsequently, the HC submodel is introduced, and the post-flame oxidation of unburned HC was affected by the reaction and diffusion phenomena. It represented the time required for the mixture to reach auto-ignition conditions, and after burning 90% of the fuel, the HC reaction dominates at a very late stage of combustion. This modeling method can more describe the "near wall" flame response directly and its contribution to the total heat release rate, but maintains faster speed and simplicity in both computation time and modeling theory.

"Near wall" combustion model of the ignition engine

Brief description

The design of SI internal combustion engines has evolved into a very difficult task because the new engines must fulfill stringent pollutant emission standards with low fuel consumption and sufficient output power. In order to satisfy the aforementioned design requirements, several technical configurations such as variable valve timing and lift (in/out) and variable compression ratio are adopted. The effects of these technical improvements are evaluated by a common engine test bench or numerical simulation.

In most models, the flame front of a SI engine is modeled as a laminar one front that fluctuates due to aerodynamic turbulence, but does not account for the occurring of "near wall" combustion when the flame approaches and reaches the combustion chamber wall. The current research on the combustion model of SI engines is the large eddy simulation (LES). Another important aspect of SI combustion is the post-flame oxidation of CO and HC when the flame front reaches the vicinity of the combustion chamber wall [2, 3]. In the combustion model of SI engines in recent years, the decrease in the rate of heat release at the end of combustion is entirely attributed to a special phenomenon, resulted from the interaction between the flame and the wall is the cause of the decrease [4-6]. In this work, in the context of 0-D physical modeling, the following method employs a simpler physical description to reproduce the complex dynamics of the post-flame reaction. The CO concentration level is controlled by chemical kinetics and exceeds its equilibrium value under exhaust pressure and temperature conditions as a result of the decrease in combustion gas temperature during expansion and exhaust stroke. This causes the CO oxidation reaction to *freeze* and the effect of CO kinetics on the rate of heat release are primarily an effect on the fuel rich mixture. Involving a combination of various phenomena, the formation of the spark ignition engine HC is extremely complicated. Nevertheless, the formation mechanism of HC is related to the flame quenching of the cylinder wall closely. The unburned HC and air mixture do not react at the flame front. It will maintain mixing with a large amount of combustion gas. After mixing, the temperature rises and oxidation occurs. In the SI engine combustion model in recent years, the decrease in the rate of heat release at the end of combustion is entirely due to a special phenomenon, and the interaction between the flame and the wall is the cause of the decrease [7].

Reference is made below to a 0-D SI combustion model that includes the geometry of the combustion chamber and a sub-model of the average flame surface, laminar flame velocity, turbulent fluctuations of the free flame, and the interaction of the flame with the wall [8]. In this paper, the combustion model of a 0-D SI engine is embedded in the thermodynamic and heat transfer model of a SI internal combustion engine. Furthermore, the model considered the effect of post-flame reaction on heat release, and analyzed its effectiveness under different working conditions. Finally, it compares with the experimental results and evaluates the performance of the model.

Combustion model and its submodel

Firstly, the turbulent combustion model is briefly introduced. In order to summarize the principle of the model, the overall 0-D equation of combustion quality is proposed and analyzed:

$$\dot{Q}_{\text{comb}} = \dot{Q}_{ff} + \dot{Q}_{pf} \tag{1}$$

$$\dot{Q}_{ff} = \dot{m}_{\text{fuel},ff}\Delta h_{r,\text{fuel}} \tag{2}$$

$$\dot{Q}_{pf} = \dot{m}_{\text{CO}}\Delta h_{r\text{CO}} + \dot{m}_{\text{HC}}\Delta h_{r,\text{fuel}} \tag{3}$$

The rate of heat release from combustion, $\dot{Q}_{\text{comb}}$, includes the heat release, $\dot{Q}_{ff}$, of the flame front and the heat release of the reaction after the flame, $\dot{Q}_{pf}$. The evaluation of $\dot{Q}_{ff}$ is based on a flame propagation combustion model using the fuel consumption rate, $\dot{m}_{\text{fuel},ff}$, of the flame front and the reaction, $\Delta h_{r,\text{fuel}}$ of the fuel.

The schematic diagram of the combustion model (pre-flame model and post-flame model) is shown in fig. 1, which provides the interaction between the sub-models and gives the key variables of combustion modeling within the framework of each sub-model [9].

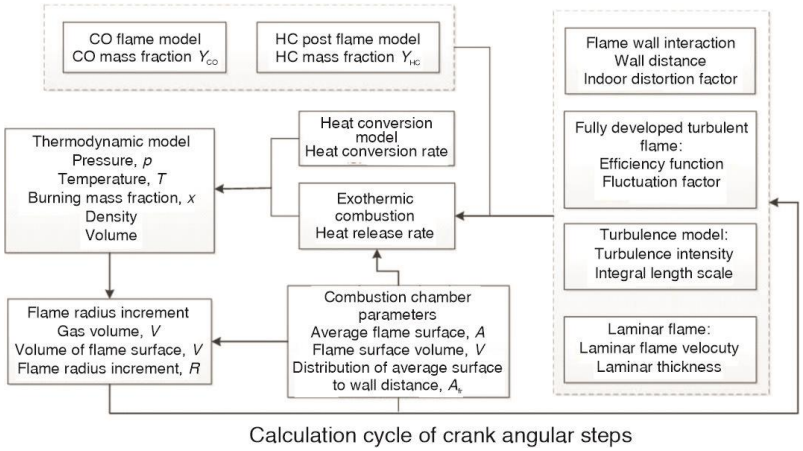

Figure 1. Schematic representation of the entire model

Thermodynamic heat transfer model (dual zone model)

Energy, mass and material conservation equations

The two-zone thermodynamic model describes mass conservation and energy conservation in the combustion chamber [10]. In order to write these equations, some simplifying assumptions must be made from the closing angle of the intake valve to the opening angle of the exhaust valve. First, the total mass, *M*, is conserved and the loss is assumed to be zero:

$$\dot{m} = \dot{m}_u + \dot{m}_b = 0 \tag{4}$$

where $\dot{m}_b$ represents the mass burning rate, which is $\dot{m}_b = \dot{m}_{b,ff}\,p + \dot{m}_{b,pf}$ determined by the flame propagation model and the flame propagation model, where $\dot{m}_{b,ff}$ is determined by the flame propagation model and $\dot{m}_{b,pf}$ corresponds to the mass of gas consumed by the reaction after CO and HC flame. The mass ratio $\dot{m}_u$ is one of the fresh gases.

The instantaneous cylinder volume, V, is equal to that of the sum of the volumes of the combustion zone, V_b, and the unburned zone, V_u. The derivative of the volume of the two zones is equal to the derivative of the volume of the combustion chamber (given by the kinematics of the piston rod):

$$V = V_b + V_u \tag{5}$$

In addition, during compression and expansion strokes, pressure is considered to be in an infinitely fast manner throughout the cylinder. Therefore, the pressure, P, is considered to be spatially uniform and varies only with changes in the crank angle. Fresh and burning gas zones are considered to be chemically balanced. During the flame propagation, it is assumed that the fresh and burning areas are separated by an infinitely thin flame front with no heat exchange between them. The energy of eq. (4) and fresh gas entropy (S_u – fresh gas entropy and s_u – fresh gas specific entropy) conservation equations of eq. (5) and volume conservation eq. (3) complete the equations of the thermodynamic model. (h is the specific enthalpy, u – the specific internal energy, T_u – the temperature of the fresh gas, and q – the heat exchanged by the gas with the external environment, which is determined by using the wall heat transfer model):

$$\dot{Q} = m\dot{u} + p\dot{V} \tag{6}$$

$$\dot{S}_u = -\dot{m}_u s_u - \frac{\dot{Q}_u}{T_u} \tag{7}$$

All gases are considered ideal gases. The specific heat difference ($r = c_p - c_v$) is at constant pressure, c_p, and constant volume, c_v. The $\rho_{v,b}$ and $T_{v,b}$ are unburned and burned density and temperature respectively.

Heat transfer model

The thermodynamic model requires input of initial pressure and composition, combustion chamber volume and its rate of change as a function of crank angle, and a cyclic heat transfer rate model. The wall temperatures of the cylinder head, piston crown and cylinder liner are constant and equal to 453 K. The heat transfer rate ($\dot{Q} = \dot{Q}_u + \dot{Q}_b$) is commonly used:

$$\dot{Q}_u = A_{u,w} h_{c,u} \left(T_u - T_w\right) \tag{8}$$

$$\dot{Q}_b = A_{b,w} h_{c,b} \left(T_b - T_w\right) \tag{9}$$

The wetted area ($A_{u,w}$ and $A_{b,w}$) of each zone was modeled as a function of combustion mass fraction, hole and cylinder height. Convection heat transfer coefficient (HC) is composed of pressure, temperature, cylinder inner diameter and average gas velocity. The coefficients of the model were calibrated so that the cylinder pressures before ignition were equal to their respective measured values, and the sum of the net heat release and heat transfer was equal to the fuel energy for combustion.

Post flame reaction

Effect of CO on heat release rate

During SI engine combustion, chemical equilibrium usually does not occur. because of extremely short time and smaller scale of the engine cycle than the chemical scale of the main reaction. Throughout the expansion process, the combustion gas, due to the high tem-

perature, the combustion gas contains a large amount of CO and NO gas, so it participates in a variety of CO oxidation reactions during the expansion process, so that the chemical reaction cannot be balanced. If the system's chemical reactions are in equilibrium at this time, the concentration of each reaction can be ignored. Based on this, a CO concentration model controlled by kinetics was established, and the effect of CO concentration on the heat release rate are penetrated into.

In order to maintain the speed and simplicity of the global 0-D model, a simple chemical kinetic model based on partial equilibrium technology is implemented. According to Valerio *et al*. [11] , the most basic chemical equation for controlling the kinetics of CO is:

$$\mathrm{CO+OH} \xleftrightarrow[K_{b,1}]{} \mathrm{CO_2+H} \tag{10}$$

$$\mathrm{O_2+O} \xleftrightarrow{K_{f,2}} \mathrm{CO+O_2} \tag{11}$$

where K_f and K_b are forward and backward rate constants.

The previous formula gives the total formation of CO. Combining the two formulas above can be obtained:

$$\left[\dot{\mathrm{CO}}\right] = -k_{\mathrm{f},1}\left[\mathrm{CO}\right]\left[\mathrm{OH}\right] + k_{\mathrm{b},1}\left[\mathrm{CO_2}\right]\left[\mathrm{O}\right] - k_{\mathrm{b},2}\left[\mathrm{CO}\right]\left[\mathrm{O_2}\right] \tag{12}$$

Therefore, taking all factors into account, the formation rate of $\dot{\mathrm{CO}}$ can be expressed:

$$\left[\dot{\mathrm{CO}}\right] = \left(R_1 + R_2\right)\left(1 - \frac{\left[\mathrm{CO}\right]}{\left[\mathrm{CO}\right]_{\mathrm{eq}}}\right) \tag{13}$$

where R_1 and R_2 designed in the formula are:

$$R_1 = k_{f,1}e[\mathrm{CO}]_{\mathrm{eq}}[\mathrm{OH}]_{\mathrm{eq}} = k_{b,1}[\mathrm{CO_2}]_{\mathrm{eq}}[\mathrm{H}]_{\mathrm{eq}}$$

$$R_2 = k_{f,2}[\mathrm{CO_2}]_{\mathrm{eq}}[\mathrm{O}]_{\mathrm{eq}} = k_{b,2}[\mathrm{CO_2}]_{\mathrm{eq}}[\mathrm{O}]_{\mathrm{eq}}$$

The reaction rate constants $k_{f,1}$ and $k_{f,2}$ are:

$$k_{f,1}\left[\frac{\mathrm{cm}^3}{\mathrm{mol\,sec}}\right] = 6.76\cdot 10^{10}\exp\left(\frac{T_b}{1102}\right) \tag{14}$$

$$k_{f,2}\left[\frac{\mathrm{cm}^3}{\mathrm{mol\,sec}}\right] = 2.5\cdot 10^{12}\exp\left(\frac{-24055}{T_b}\right) \tag{15}$$

The two-zone thermodynamic model takes into account the energy contained in the equilibrium state because the combustion mixture contains multiple gases. However, energy storage is not included in CO dynamics, so this energy loss has been calculated in eq. (1).

Effect of HC on heat release rate

The main reasons for HC emissions from SI engines with good premixing and stoichiometry is [2]:

- When the flame approaches the wall of the combustion chamber, the flame goes out, leaving a layer of unburned HC near the wall.
- The blow-by gas leaking into the crankcase from the combustion chamber through the gap between the piston and the cylinder.
- Absorption and desorption in lubricating oil during intake and compression.

All of these mechanisms lead to high HC concentrations in adjacent walls.

Through the numerical analysis of the convection, diffusion and reaction phenomena occurring during the expansion stroke, the effects of diffusion and oxidation on heat release can be observed.

Rakopoulos *et al*. [12] gives a detailed explanation of the 1-D model and gave all assumptions and equations, including the reaction diffusion process of the post-oxidation phenomenon. In the 0-D model, the thermodynamics of the cylinder provides the temperature of the combustion gas and the temperature of the fresh gas. These two variables are consistent in their respective regions:

$$\left(\frac{\partial Y_i}{\partial t}+u\frac{\partial Y_i}{\partial x}\right)-\frac{\partial}{\partial x}\left(\rho D_i\frac{\partial Y_i}{\partial x}\right)-\dot{\omega}_i=0 \tag{16}$$

where i is the composition index, u – the flow velocity, x – the spatial dimension, D – the species diffusion coefficient, ρ – the density, and ω – the reaction rate.

The flow near the wall of the combustion chamber is highly viscous, and the diffusion phenomenon is dominant. Therefore, the convection term is negligible.

Analysis of the post-oxidation phenomenon indicates that the unburned HC-air mixture diffuses from the cold boundary to the combustion gas [13]. This diffusion process brings about the increase in the temperature of the mixture until it reaches the local thermodynamic conditions of auto-ignition.

Fuel consumption is controlled by a special chemical time, τ_{HC}, which can be defined as (Y_{HC} is the HC mass):

$$\dot{\omega}_{\mathrm{HC}}=\rho\dot{Y}_{\mathrm{HC}}^{\mathrm{ch}}=-\rho\frac{Y_{\mathrm{HC}}}{\tau_{\mathrm{HC}}} \tag{17}$$

Compared with other characteristic time scales, this one is shorter, indicating that fuel consumption is very rapid after auto-ignition. The thermodynamic conditions and physicochemical properties in the "near wall" region are considered to be uniform. The thickness δ_{HC} is only 0.2 mm. Therefore, a global species diffusion coefficient of D_{HC} is used [14]. The conservation equation of HC is given:

$$\frac{\partial\xi}{\partial t}=D_{\mathrm{HC}}\frac{\partial\xi}{\partial\chi^2} \tag{18}$$

Among them, $\xi=Y_{HC}-Y_{HC}^{ch}$. This equation has an analytical solution to independent variables: the dimensionless variable $\xi(\hat{\chi},\hat{t})=X(\hat{\chi})T(\hat{t})$ represents the dimension of space, $\hat{\chi}=\chi/\delta_{\mathrm{HC}}$, t represents time, $\hat{t}=(t/\hat{\tau})\tau=\delta_{\mathrm{HC}}^2/D_{\mathrm{HC}}$ and so on. The $X(\hat{\chi})$ has the form:

$$X(\hat{\chi})=A\cos\left(\lambda^{1/2}\hat{\chi}\right)+B\sin\left(\lambda^{1/2}\hat{\chi}\right)$$

The value of λ corresponds to the eigenvalue of the Sturm-liouville problem, and the constants A and B are associated with the boundary conditions [15]. If the fresh gas has diffused and reached the boundary of the opposite wall of the combustion chamber, then they are completely consumed and the constants A and B can be calculated:

$$X'(\hat{\chi}=0)=0\rightarrow B\lambda^{1/2}=0\rightarrow B=0 \tag{19}$$

$$X(\hat{\chi}=1)=0\rightarrow A\cos\left(\lambda^{1/2}\right)=0\rightarrow\lambda^{1/2}=\frac{\pi}{2}(2n-1) \tag{20}$$

In this paper, the area studied is the "near wall" area, which can be regarded as a thin-walled system. In the "near wall" region, the initial conditions can be thought of as uniform, and the initial value of the HC mass fraction originates from the combustion model [16].

In order to verify the HC sub-model, an operating point with an engine speed of 2000 rpm and an average effective pressure of 8×10^5 pa was selected as the influence of the HC reaction diffusion mechanism on the heat release rate [17]. The evolution of the combustion mass fraction, fig. 2, and cylinder pressure, fig. 3, supplies the calculation results of the combustion model, as is shown in fig. 2.

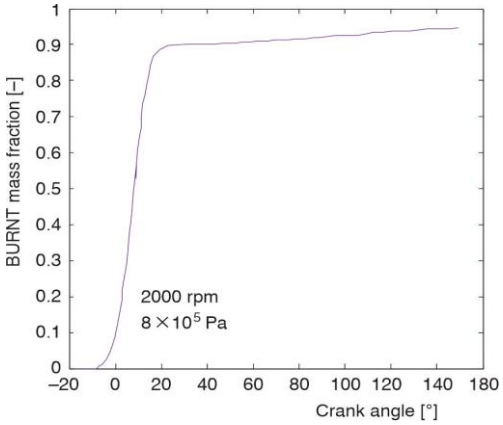

Figure 2. Calculation of combustion mass fraction, experimental combustion angle, and combustion efficiency

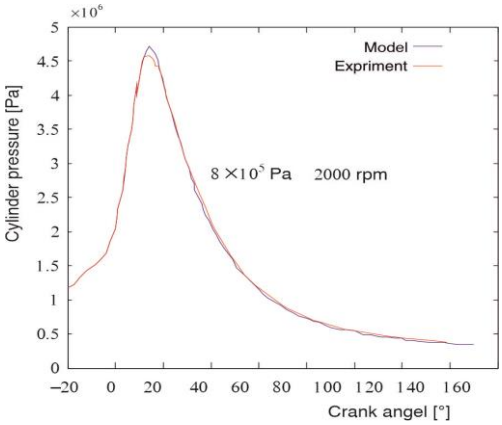

Figure 3. Measuring and simulating cylinder pressure

Conclusion

It has been verified that the CO model proposed earlier is correct because it predicts that the CO concentration will increase as the fuel-air equivalent ratio rises, and accordingly the available amount of oxygen decreases. Such being the case, the system is prone to incomplete combustion and CO generation cannot be avoided.

In this paper, the "near wall" combustion model of SI engine is studied and studied. By calculating cylinder pressure, the temperature, composition and heat transfer of fresh and combusted gas, the chemical equation of the simplified CO sub-model is used to calculate the dynamic process of CO in the expansion phase. The model can accurately predict the CO change process. The HC emission is caused by several kinds of phenomena. For a mixed, stoichiometric specific charge, the phenomena together prompt HC to squeeze into various gaps, add a certain amount of HC during the compression process, and re-enter the volume during the expansion stroke. Gas will be an improvement of flame reaction after HC.

References

[1] Dimitriou, P., Tsujimura, T. A Review of Hydro as a Compression Ignition Engine Fuel, *ScienceDirect, 42* (2017), 38, pp. 24470-24486
[2] Misdariis, A., *et al*., A Methodology Based on Reduced Schemes to Compute Autoignition and Propagation in Internal Combustion Engines, *Proc. Combust. Inst., 35* (2015), 3, pp. 3001-30008
[3] Knop, V., *et al*., On the Use of a Tabulation Approach to Model Auto Ignition During Flame Propagation in SI Engines, *Appl Energy, 88* (2017), 12, pp. 4968-4979
[4] Rivas, M., *et al*., Validation and Application of a New 0-D Flame/Wall Interaction Sub Model for SI Engines, *SAE Int. J. Engines, 5* (2016), 10, pp. 718-733

[5] Bougrine, S., *et al*., Simulation of CO and NO Emissions in a SI Engine Using a 0-D Coherent Flame Model Coupled with a Tabulated Chemistry Approach, *Appl Energy, 113* (2014), Jan., pp. 1199-1215
[6] Decan, G., *et al*., Evaluation of Wall Heat Flux Calculation Methods for CFD Simulations of an Internal Combustion Engine Under Both Motored and HCCI Operation, *Applied Energy, 232* (2018), 2, pp. 451-461
[7] Fontanesi, S., *et al*., Large-Eddy Simulation Analysis of Spark Configuration Effect on Cycle-to-Cycle Variability of Combustion and Knock, *Int. J. Engine Res., 16* (2015), Mar., pp. 403-418
[8] Demesoukas, S., *et al*., Near Wall Combustion Modeling in Spark Ignition Engines. Part A: Flame-Wall Interaction, *Energy Convers Manage, 106* (2015), Dec., pp. 1426-1438
[9] Cuhla, O., *et al*., Heat Exchanger Applications in Wastewater Source Heat Pumps for Buildings: A Key Review, *Energy and Buildings, 104* (2015), Oct., pp. 215-232
[10] Demesoukas, S., *et al*., Near Wall Combustion Modeling in Spark Ignition Engines. Part B: Post-Flame Reactions, *Energy Conversion and Management, 106* (2015), Dec., pp. 1439-1449
[11] Valerio, M., *et al*., Model for Kinetic Formation of CO Emissions in Internal Combustion Engines, SAE Technical Paper, 2003-01-3138, 2003
[12] Rakopoulos, C. D., *et al*., Development and Validation of a Multi-Zone Combustion Model for Performance And Nitric Oxide Formation in Syngas Fueled Spark Ignition Engine, *Energy Convers Manage, 49* (2017), 10, pp. 2924-2938
[13] Khalique, C. M., *et al*., On Optimal System, Exact Solutions and Conservation Laws of the Modified Equal-Width Equation, *Applied Mathematics and Nonlinear Sciences, 3* (2018), 2, pp. 409-418
[14] Yang, C., *et al*., Energy Efficiency Modeling of Integrated Energy System in Coastal Areas, *Journal of Coastal Research, 103* (2020), sp1, 995
[15] Lu, H., *et al*., Evaluating the Global Potential of Aquifer Thermal Energy Storage and Determining the Potential Worldwide Hotspots Driven by Socio-Economic, Geo-Hydrologic and Climatic Conditions. *Renewable and Sustainable Energy Reviews, 112* (2019), Sept., pp. 788-796
[16] Du, X. S., *et al*., Flame-Retardant and Solid-Solid Phase Change Composites Based on Dopamine-Decorated BP Nanosheets/Polyurethane for Efficient Solar-to-Thermal Energy Storage, *Renewable Energy, 164* (2021), 5, pp. 1-10
[17] Jiang, J., *et al*., Thermal Effect of Welding on Mechanical Behavior of High-Strength Steel, Journal of Materials in Civil Engineering, 33 (2021), 8, 04021186

Paper submitted: May 11, 2021
Paper revised: July 10, 2021
Paper accepted: July 13, 2021