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Greybox modeling of the diesel combustion by use of the scalar dissipation rate

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Abstract

This paper deals with greybox modeling of a diesel combustion process for the purpose of model-based combustion control. For this, a real-time capable model with a high prediction quality and a high interpolation and extrapolation capability is required. An existing neural network model of the process will be introduced. The model inputs are the quantity of injected fuel, start of injection and the intake manifold fraction of recirculated exhaust gas. The variables to be predicted are the position of the combustion phasing, the indicated mean effective pressure and the maximum cylinder pressure gradient, which correlates with the combustion noise of the engine. To enhance the existing model, an analytic description of the scalar dissipation rate is used as a new input into the neural network. The aim here is to decrease the model error, improve the model robustness and reduce the complexity of the neural network. The scalar dissipation rate describes the diffusivity in mixture fraction space and represents a combustion characteristic quantity. For a couple of engine operating points, the scalar dissipation rate is calculated by 3D CFD simulations. Afterwards, the calculation results are utilized to find an analytic description. To use this new model information a restructuring of the neural network is necessary. The modeling results will be shown and compared to the existing blackbox model.

Keywords: *Greybox modeling, scalar dissipation rate, LOLIMOT, diesel combustion model*

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1. INTRODUCTION

The reduction of fuel consumption is subject of debate for a long time. In the nearer past, the reduction of pollutant emissions like soot, nitrogen oxide (NOx) and unburned hydrocarbons is increasingly focused to fulfill the high requirements of the Euro emissions norms. This implies a higher demand on engine control functions and also the underlying process models. On the one hand it is possible to fulfill the future emission requirements with expensive additional equipment for exhaust gas aftertreatment. But on the other hand it is more efficient to influence the source of pollutant emissions - the combustion process. To obtain the mentioned aim, the "Sonderforschungsbereich 686" (SFB686) at RWTH Aachen University deals with the model-based control of homogenized low-temperature combustion both in Otto and in Diesel process. An early fuel injection and thereby a higher grade of homogenization of the air-fuel-mixture within the cylinder leads to lower local temperatures during combustion and to lower pollutant emissions. Because of the fact that the homogenized low-temperature combustion is an unstable process it is crucial to control this process.

In the SFB686, model-based control strategies are developed, which require accurate process knowledge to predict the behavior of the engine. This knowledge is integrated into the control structure by real-time capable models. This paper is situated within the diesel part of the SFB686 and thereby within the modern combustion method of premixed-charge compression ignition (PCCI). The paper is concerned with creating models that can operate in real time on an engine control unit (ECU).

2. Greybox modeling using scalar dissipation rate

The existing PCCI control strategy consists of a cascaded control loop and was presented in [1]. In the outer loop, a model-based optimal controller of the combustion was implemented. Within the con-

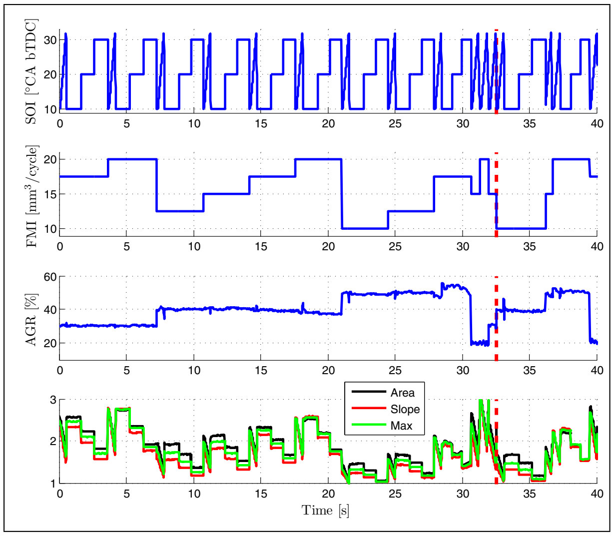

Figure 1. Calculated and scaled characteristic numbers using dissipation rate depending on training and validation data

troller, a real-time capable blackbox model is used. The model outputs or variables to be predicted by the optimal controller are the position of the combustion phasing (CA50), the indicated mean effective pressure (IMEP) and the maximum cylinder pressure gradient (DPMAX), which correlates with the combustion noise of the engine. The injected fuel mass (FMI), start of injection (SOI) and the intake manifold fraction of exhaust gas recirculation (EGR) are the model inputs.

Due to the fact that the EGR is a variable, which cannot be manipulated directly, the combustion controller requires a certain EGR from the underlying air path controller as input. The air path controller adjusts the EGR by changing the EGR-valve position and the valve position of the variable-geometry turbocharger (VGT). A linear model-based predictive control (MPC), using a model of the air path, calculates the optimal position of both valves. It is evident that in this cascaded control loop the controller models play an important role. This paper is focused on model identification and on model improvement.

2.1. Nonlinear modeling of the combustion process

To build a model of diesel combustion based on system identification, measurement data for model training are required. Therefore, an automotive 1.9 l four-cylinder diesel engine with a common rail injection system is used. The injection pressure of the common rail system is constant at 700 bar and a single injection strategy is applied for all experiments in this paper. To calculate the values of IMEP, CA50 and DPMAX in each cycle the engine testbed is equipped with hardware for thermodynamic real-time analysis (FI2RE by IAV GmbH).

In [2] it was shown that the dynamic behavior over the combustion cycles is almost linear. Therefore, the focus can be set on the static, highly nonlinear behavior of the PCCI combustion which consequently leads to stationary and quasi-stationary (very slow input variation using ramps) measurements of the combustion on engine testbed. Different operating points are measured varying the combustion inputs SOI (10 to 32 °CA bTDC), FMI (10 to 20 mm^3/cycle) and EGR (30 to 50 %). Figure 1 shows the used measurement data for model training (on the left side of the red, dashed line) and for model validation (on the right side of the red, dashed line). A neural network is trained using the training dataset of this measurement data.

The upper part of Fig. 2 represents the network structure of the existing blackbox model. The selected type of the network is named local linear model tree (LOLIMOT) with a Gaussian activation function. The standard deviation σ of this activation function is defined as $\sigma = 0.33 \cdot \Delta_{ij}$ with the width Δ_{ij} of a neuron i along input direction j. For more information about the LOLIMOT network and training algorithm see [3]. An example how to identify a blackbox air path model for uses on engine control units (ECU) applying the LOLIMOT algorithm is shown in [7]. In this paper, for each model output (CA50, IMEP, DPMAX) exists one separate network with 20 neurons and SOI, FMI, EGR as model inputs.

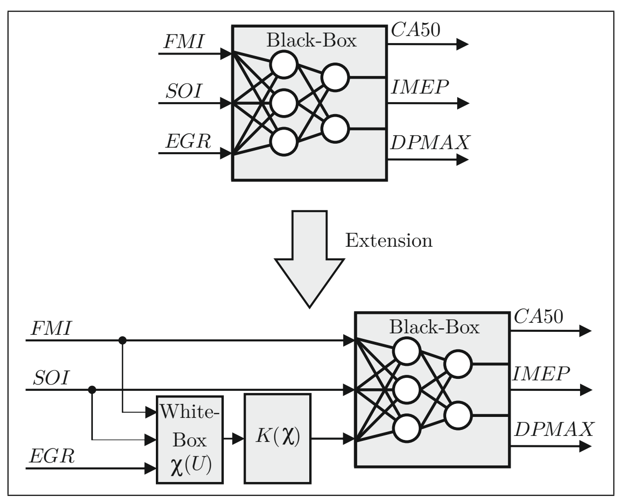

Figure 2. Basic idea to extend the existing blackbox combustion model (picture above) to a greybox model (picture below)

2.2. Analytic description of the scalar dissipation rate

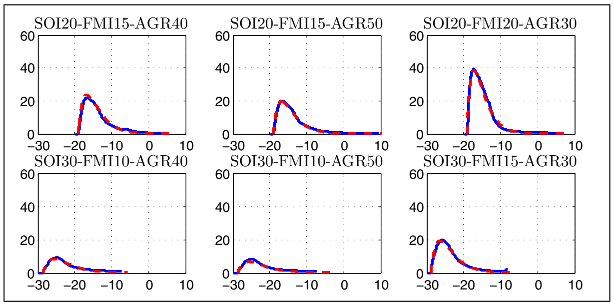

Figure 3. Comparison between calculated data of the dissipation rate in [s^{-1}] (solid line) and the corresponding model data (dashed line) over crank angle [°CA]

In the following, the existing LOLIMOT model is extended by a physical motivated approach. In this work, the main idea behind greybox modeling is to consider combustion characteristics based on, for example, chemical reactions, species mass fraction or temperature stratification during engine cycles. The aim of this approach is decreasing the model error, improving the model robustness, reducing the complexity of the neural network and increasing the interpolation and extrapolation capability. In this paper, the existing data driven model is complemented by an analytic description of the scalar dissipation rate.

The scalar dissipation rate originates from the flamelet concept to describe a turbulent diffusion flame as an ensemble of flamelets [6], which are thin reactive-diffusive layers located within an otherwise nonreactive flow field. With the mixture fraction $Z = \frac{m_F}{m_F + m_{Ox}}$ as the independent variable, the scalar dissipation rate is defined by $\chi = 2D|\nabla Z|^2$. Here, the mixture fraction Z is a normalized fuel-air ratio with m_F and m_{Ox} indicating fuel and oxidizer mass, respectively, and D representing a species independent diffusion coefficient.

The scalar dissipation rate χ is a parameter imposed by the mixture fraction field, which can be viewed as an diffusivity in mixture fraction space. Thus, the scalar dissipation rate is an essential parameter for the description of Diesel engine combustion. The derivation of the flamelet equations for premixed and diffusion flames is outlined in [4] and the development of the representative interactive flamelet (RIF) model for Diesel engine combustion can be found in [5]. In the presented work, the scalar dissipation rate is calculated with 3D CFD (computational fluid dynamics) simulations of the diesel engine. The CFD code is the in-house RANS flow solver AC-FluX, which is coupled to the well-known RIF model to account for the chemical source term. For the determination of the scalar dissipation rate with respect to the model inputs $\chi = f(SOI, FMI, EGR, CA)$, 27 engine operating points were simulated with the initial pressure (1.08 bar), initial temperature (355 K) and the composition of EGR held constant:

- SOI = 10, 20, 30 °CA bTDC
- FMI = 10, 15, 20 mm^3/cycle
- EGR = 30, 40, 50 %

Figure 3 shows the resulting data of the scalar dissipation rate for six different engine operating points (variations of SOI, FMI, EGR). Here, for each cycle the evolution of the scalar dissipation rate as function of crank angle is calculated with the increase of the scalar dissipation rate directly connected to the start of injection. In a first step, it is necessary to identify an analytic description, which represents the correlation between χ and the input variables SOI, FMI, EGR. Therefore , an exponential approach is chosen (1):

$$\chi_{\text{analytic}} = a \cdot \left(e^{-b \cdot CA^*} - e^{-c \cdot CA^*}\right) \quad (1)$$

This approach is physically motivated by the fact of using an injection impulse to introduce fuel mass into cylinder. Furthermore, the fuel mass possesses inertia and has to be accelerated. The impulse of the fuel mass and its later distribution are directly correlated to the dissipation rate. This leads automatically to the chosen approach, using the impulse response of a second order lag, to describe the dissipation rate.

To optimize the approach (1), it is necessary to shift the beginning (first value greater than zero) of calculated dissipation rate to the origin of co-ordinates (to zero). This shifting is represented by $CA^* = CA +$ offset. a, b and c are parameters to be optimized using nonlinear optimization (in this paper the Levenberg-Marquardt algorithm is applied). Analyzing the calculated dissipation rates turned out that each parameter a, b, c depends on the input variables SOI, FMI, EGR too.

The model complexity and the reached model quality can be used as selection criterions for the number of free parameters. Functions with several numbers of free parameters were investigated. In the present work, the function with 11 parameters was selected (2) as the best trade-off between model complexity (number of parameters) and prediction capability (low model error).

$$
\begin{aligned}
a &= a_1 + a_2 \cdot SOI + a_3 \cdot FMI + a_4 \cdot EGR \\
&\quad + a_5 \cdot SOI \cdot FMI + a_6 \cdot SOI \cdot EGR \\
b &= b_1 + b_2 \cdot FMI \qquad (2) \\
c &= c_1 + c_2 \cdot FMI + c_3 \cdot SOI \cdot FMI
\end{aligned}
$$

Figure 3 shows the optimized analytic function (dashed line) compared to the calculated data of the scalar dissipation rate (solid line). An absolute error average of 0.82 s^{-1} of the analytic function relating to the simulation data is achieved. This error average is calculated over all 27 engine operating points. Compared to the maximum value of the dissipation rate ($\chi_{textmax} = 55s^{-1}$ within all simulation data), this error average is quiet small and therefore, the chosen analytic function is able to approximate the dissipation rate with only small prediction error.

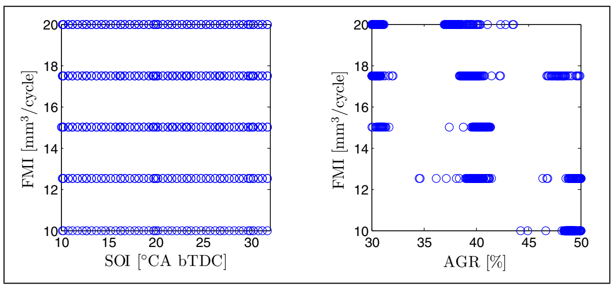

Figure 4. Distribution of the training data

2.3. Identification of characteristic numbers

Due to the fact that the real-time combustion model is calculated only one time per combustion cycle, it is not possible to integrate the analytic function of the scalar dissipation rate into the blackbox model: the analytic approach is a function of the crank angle and varies within a cycle. Thus, characteristic numbers are necessary, which adequately describe the dissipation rate of a complete cycle. Therefore the optimized analytic function is used to calculate an appropriate characteristic number, which describes the dependency on the actual operating point. Several approaches can be used:

- **Area**: Calculation of the area below the scalar dissipation rate
- **Slope**: Identification of a secant slope to determine the gradient between the first point and the maximum value of the dissipation rate within a cycle
- **Max**: Definition of the maximum value of the dissipation rate

The lower part of Figure 1 illustrates the results of the three different characteristic numbers (Area, Slope, Max) relating to the measured testbed data. Here, the values are scaled between 1 and 3 for an easier comparison. It is easy to see that the characteristic numbers are different but possess almost the same information content. Due to this fact, the maximum value of the scalar dissipation rate is selected as a new model input into the existing LOLIMOT network. It is worth mentioning that using one of the other characteristic numbers leads to almost the same results.

3. Modeling results

The new model structure of the greybox model is shown in the lower part of Figure 2. In this new model structure the variable EGR is removed as input of the neural network and is only used to calculate the scalar dissipation rate. This is realized because one aim of the greybox modeling is to reduce the network complexity. Due to this fact, an increase of the number of model inputs is not desirable. The data distribution of SOI and FMI is uniformly in the model input space and for this reason very important for the LOLIMOT training algorithm (division of the neurons in the middle). In contrast the EGR depends on the position of EGR- and VGT-valve and is less uniformly distributed in the input space (Figure 4). For this reason, the EGR is replaced by the physical input. In addition considering the EGR value only in the physical part of the greybox model does not lead to a loss of model information.

Table 1. RMSE of the blackbox and greybox model with 20 neurons related to the validation dataset

RMSE	CA50	IMEP	DPMAX
Unit	°CA bTDC	bar	bar/°CA
Blackbox	1.693	0.143	1.182
Greybox	1.276	0.132	0.909

In Table 1 the errors of the blackbox model and the greybox model according to Figure 2 are compared. Both models possess 20 neurons in their neural network. The utilized model error is the root mean squared error (RMSE). Only the validation data (on the left side of the red, dashed line in Figure 1) are considered in the RMSE as shown in Table 1. With the validation dataset, which is not used during the network training, it is possible to compare the generality of the models. In this context, generality means the interpolation and extrapolation capability of the model. In comparison with the blackbox model, the greybox model structure leads to a better model prediction for all model outputs (CA50, IMEP, DPMAX) and therewith the model generality increases. Even though the error in predicting the IMEP is small for both models, the results are improved for the greybox approach. To quantify the increase of model quality, it is possible to do it in a percentile manner: relating the RMSE to the maximum deviation of the output variables (Table 2). In this case, the greatest gain of model quality can be found in the DPMAX greybox model: the RMSE decreases for 1.7 % compared to the blackbox model.

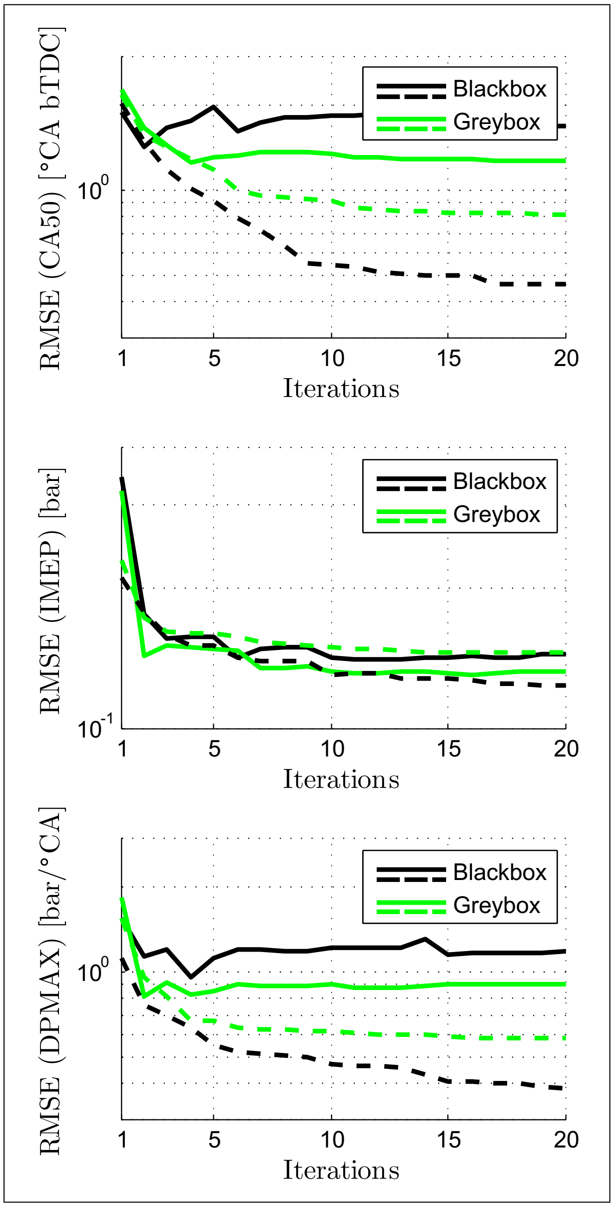

Figure 5. Convergence of the RMSE using blackbox and greybox model depending on validation dataset (solid lines) and on training dataset (dashed lines)

Table 2. Percentile RMSE of the blackbox and greybox model with 20 neurons related to the validation dataset

RMSE/Δ_{max}	CA50	IMEP	DPMAX
Δ_{max}	30 °CA	6 bar	15 bar/°CA
Blackbox	5.6%	2.4%	7.8%
Greybox	4.3%	2.2%	6.1%

Exemplarily, 6 depicts the simulation results for DPMAX. Regarding the training dataset, the model predictions of both models (blackbox and greybox) possess no significant differences. In case of validation dataset the model predictions of the greybox model are closer to the measurement data (between simulation time 1.8 s to 3.5s). Figure 5 illustrates the convergence of the RMSE depending on the network training progress. The iterations correspond to the number of neurons within the LOLIMOT network. It can be seen that the RMSE corresponding to the training dataset (dashed lines) decreases during training process. After a certain number of iterations, the training RMSE converges and the error almost stops decreasing. The RMSE corresponding to the validation dataset converges after a few steps, which indicates an overestimation with regard to the validation measurements. Both types of model (blackbox and greybox) achieve no more improvement of the model quality after approximately 5 iteration steps.

However, it is advisable to select a number of neurons with an almost converged RMSE of the training dataset. In this example, 10 neurons within the neural network can be chosen. For this case the RMSE results are presented in Table 3: Using only 10 Neurons it is possible to reduce the model complexity by the half (20 neurons $\rightarrow$ 10 neurons) without great losses in model quality. Additionally, the greybox model has in this case a higher model generality with regard to the validation measurements.

Table 3. RMSE of the blackbox and greybox model with 10 Neurons

RMSE/Δ_{max}	CA50	IMEP	DPMAX
Δ_{max}	30 °CA	6 bar	15 bar/°CA
Blackbox	6.1%	2.4%	8.1%
Greybox	4.5%	2.2%	6.1%

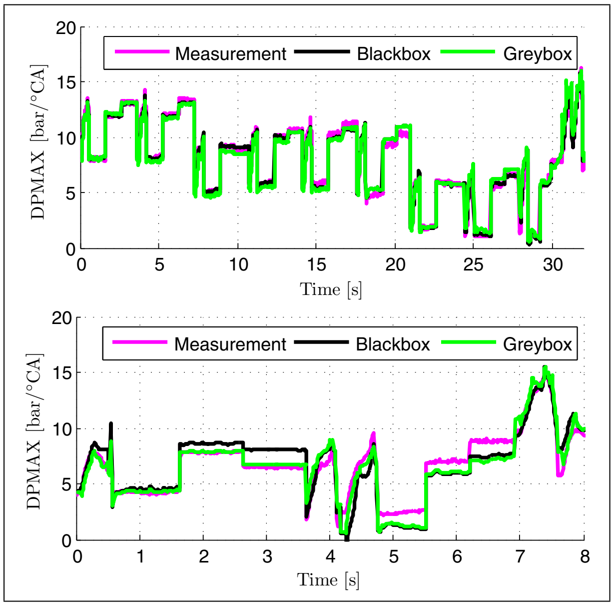

Figure 6. Blackbox compared to greybox predictions regarding training (above) and validation (below) datasets

4. CONCLUSIONS

In this paper, an approach to extend a blackbox combustion model by use of the scalar dissipation rate was introduced. Here, the dissipation rate was identified by an analytic expression based on an exponential function. To integrate the dissipation rate into the blackbox model a calculation of characteristic numbers was necessary. With the new greybox structure of the combustion model it was possible to reduce the model error and improve its prediction capability. Without any information losses, the blackbox model input EGR was replaced by the physical input. EGR was then only used to calculate the scalar dissipation rate. Thereby the model error decreased. Because of the less model error a complexity reduction of the neural network is possible. This fact was shown by analyzing the convergence of the model RMSE and identifying a greybox model with 10 instead of 20 neurons. One topic to be researched in future is to apply the represented method (greybox modeling) on a combustion process with multiple injection strategy. Furthermore, the pollutant emissions have to be considered meaning that greybox models for engine-out emissions have to be identified.

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References

[1] DREWS, P. ; ALBIN, T. ; HESSELER, F.-J. ; PETERS, N. ; ABEL, D.: Fuel-Efficient Model-Based Optimal MIMO Control for PCCI Engines. In: *Proceedings of the 18th World Congress, August 28 - September 2, 2011 Milano (Italy)*, 2011

[2] DREWS, P. ; ALBIN, T. ; HOFFMANN, K. ; VANEGAS, A. ; FELSCH, C. ; PETERS, N. ; ABEL, D.: Model-Based Optimal Control for PCCI Combustion Engines. In: *AAC 2010, IFAC-Symposium Advances in Automotive Control, 12. - 14. Juli, 2010 Mnchen*, 2010

[3] NELLES, O.: *Nonlinear System Identification*. Springer-Verlag Berlin Heidelberg, 2001

[4] PETERS, N.: *Turbulent Combustion*. Cambridge University Press, 2000

[5] PITSCH, H.: *Modellierung der Zuendung und Schadstoffbildung bei der dieselmotorischen Verbrennung mit Hilfe eines interaktiven Flamelet-Modells*, RWTH Aachen, Diss., 1998

[6] WILLIAMS, F.A.: Recent advances in theoretical descriptions of turbulent diffusion flames. In: *Turbulent mixing in nonreactive and reactive flows*. Plenum Press, New York, 1975

[7] ZWEIGEL, R. ; HESSELER, F.-J. ; ABEL, D. ; BOGDANIC, M. ; HORSTMANN, M. ; KRATZSCH, M.: Entwurf und Optimierung von steuergertetauglichen Vorsteuerungen aus lokal-linearen Neuro-Fuzzy Regelstreckenmodellen. In: *AUTOREG 2011, Baden-Baden 2011*, 2011