Simulation of Parameters of Locomotive Diesel, Gas Diesel and Gas Engines Using Multi-Zone and One-Zone Models

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Abstract – Modern requirements for reduction of the carbon footprint and toxic emissions of internal combustion engines, as well as their operation cost may be fulfilled by conversion of diesel engines for operation on natural gas. Methane, which is the main component of natural gas, contains by 15% less carbon than diesel fuel, and its heat value is by 15% higher (by mass). Therefore, an engine fed by natural gas may reduce its CO_2 emissions by up to 30% compared to the base diesel engine. The price of natural gas in Russia is almost twice as much less than that of diesel fuel. As locomotive engines often operate 24 hours a day 7 days a week, the gain in fuel costs may be large. Two basic methods of diesel engine conversion for operation on natural gas were analyzed: gas engine and gas diesel (dual-fuel) engine. Simulation of diesel, gas diesel and gas engines for a shunting locomotive was done using the multi-zone AVL FIRE model and one-zone model developed in MADI. The simulation showed that transfer from diesel cycle to gas and gas diesel cycles resulted in considerable decrease in fuel consumption and emissions of particles and NO_x. The gas engine had lower mechanical and thermal stresses compared to diesel and gas diesel versions.

Keywords: conversion of diesel engine; gas engine; dual-fuel engine; engine simulation; one-zone model; multi-zone model; Viebe formula

1 Introduction

Reduction of the carbon footprint to fight the greenhouse effect is a pressing issue of today's world ecological agenda. Conversion of engines for operation on natural gas makes it possible to decrease considerably emissions of carbon dioxide (CO_2). Natural gas produced in Russia contains 95-98% of methane, which has about 15% less carbon compared to diesel fuel. In addition, the heat value of methane is by 15% higher (by mass) than that of diesel fuel. So, if an engine operating on natural gas preserves the same effective efficiency as the base diesel engine, its conversion for operation on natural gas may decrease emissions of CO_2 by 30%. Emissions of nitrogen oxide (NO_x) decrease considerably making it possible to comply with the latest severe ecological standards without mounting a complicated and expensive SCR catalyst. Depending on the method of diesel engine conversion for operation on natural gas, emissions of soot decrease many times or become zero.

For conversion of engines to operate on natural gas, two basic methods are used: spark-ignition gas engine and gas diesel (dual-fuel) engine.

A gas engine may operate on a stoichiometric or lean gas-air mixture. Stoichiometric gas-air mixture ensures a good ignition, stable and complete combustion and low chance of knock origination. The traditional three-way catalyst used on petrol engines may be used for the reduction of three basic emissions of spark-ignition engines: carbon monoxide (CO), hydrocarbons (CH) and nitrogen oxide (NO_x). The basic problem of stoichiometric gas engines is the high temperature of their exhaust gases, which may result in the deterioration of their turbine. Therefore, the power augmentation rate by turbocharging of these engines is limited [1].

Spark-ignition gas engines operating on a lean gas-air mixture usually have a low exhaust gases temperature, which enables high power augmentation by turbocharging and decreases emissions of CO and NO_x. For such engines, an oxidation catalyst to reduce the unburned hydrocarbons is required and the chance of knock origination of lean mixtures is higher. At the Moscow Automobile and Road Construction State Technical University (MADI), a truck diesel engine was converted into a lean-mixture gas engine operating with an air excess coefficient of $\lambda = 1.5$. To preserve the power of the base diesel engine, its original turbochargers were replaced by the models ensuring a higher boost pressure. To comply with the ecological standards, a special catalyst containing rhodium was used to reduce the unburned methane [2].

The main problem of using the gas cycle on medium-speed (locomotive) engines is knock. If the cylinder size and power augmentation increase and when the engine operates on a lean gas-air mixture, the probability of its origination increases. The chance of knock appearance also grows at low engine speeds and transient modes.

The medium-speed Jenbacher 6th series gas engine used for electric power generation has a high power augmentation. It has a high brake mean effective pressure p_e=2.4-2.6 MPa. The engine operates on a very lean gas-air mixture (air excess coefficient λ close to 2.0). For ignition of a lean gas-air mixture, a prechamber with an enriched mixture is used. Here, the natural gas is ignited by a spark plug and then the sprays of burning gas penetrate into the main combustion chamber and ignite the lean mixture. The Miller cycle is implemented to prevent knock. This also improves the effective efficiency up to 49% and reduces NO_x

emissions. To compensate for the losses in volumetric efficiency caused by the early closure of the intake valves in the Miller cycle, a two-stage turbocharging system is mounted [3]. A combination of the Miller cycle with the two-stage charging system is widely used on internal combustion (IC) engines today. As shown in [4], one turbocharger with a high-pressure compressor and a two-stage charging system with two ordinary turbochargers can provide almost the same engine parameters if the p_e value is 2.7 MPa, but only the two-stage charging system can provide much higher engine boosting with the p_e value of 3.2 MPa.

A serious problem of spark-ignition gas engines is knock. The chance of its origination grows with the increase of the cylinder diameter and boost pressure. In gas diesel engines, this problem is not so critical and they may have much larger cylinder size and higher power augmentation.

Gas diesel engines with mechanical fuel supply systems have a low substitution of diesel fuel by gas: the share of diesel fuel is 20-30% at full loads, increases at low loads and reaches 100% at idle mode [5].

The authors of [6] supposed that the need to increase the igniting portion of diesel fuel at low loads was caused by the growth of fuel drops diameter due to the reduction of both the injection pressure and air counter-pressure in the cylinder because the boost pressure decreases at low loads. The ability of the fuel drop to ignite the air-gas mixture diminishes, and more diesel fuel has to be injected at low loads. Therefore, one has to increase considerably the fuel injection pressure.

The latest gas diesel engines are equipped with Common Rail fuel supply systems, which provide a high injection pressure and multiple injections modes. This ensures a good ignition of natural gas by finely atomized diesel fuel sprays and makes it possible to decrease the share of diesel fuel up to 3-5% at full load and keep it pretty small at low loads and idling mode [7, 8]. These engines have a high substitution of diesel fuel by gas, as well as high fuel efficiency and ecological parameters. The only problem is that the injectors of the base diesel engine tend to overheat as just 3-5% of diesel fuel is injected and this volume of the fuel is not sufficient to cool properly the injector nozzles.

The power, fuel efficiency and ecological parameters of gas diesel engines depend on the parameters of the igniting portion of diesel fuel: ignition pressure [9], fuel distribution within the combustion chamber [10], injection rate shape [11], and pressure oscillations in the fuel system [12].

When switching from diesel to gaseous fuel, the volumetric efficiency of the cylinders decreases due to the partial substitution of the air with gas. Calculation results show that the volumetric efficiency decreases by about 10% in a stoichiometric gas engine and by about 6% in the gas-diesel engine operating at the air excess coefficient of $\lambda = 1.5$ [13]. This drop in engine power is to a large extent compensated by a higher heating value of methane compared to diesel fuel.

The performed analysis shows that both the lean mixture spark-ignition gas engine and gas diesel engine can be used for powering of locomotive, though gas diesel engine is preferable in case of the large engine size and high power augmentation.

Conversion of diesel engines for operation on natural gas requires considerable expenses for engine design modification, building of onboard gas storage systems, creation of gas filling infrastructure. Therefore, it is important to evaluate the amelioration of the basic parameters of a diesel engine in case of its conversion for operation on natural gas and deside if these expenses are reasonable.

The goal of this work is to carry out the simulation of operation parameters of diesel, gas diesel and gas versions of the shunting locomotive engine to predict the improvement of its fuel efficiency and ecological parameters, as well as mechanical and heat strains.

2 Methodology

2.1 Simulation Models and Calculation Method

Evaluation of the engine parameters was carried out using simulation results obtained with the well-known multi-zone AVL FIRE model and a one-zone model of diesel, gas diesel, gas engine simulation developed in MADI [14]. The multi-zone AVL FIRE model needs much calculation time, it simulates only compression-combustion-expansion processes and needs boundary conditions: air pressure and temperature at the cylinder inlet, as well as exhaust gases pressure and temperature at the cylinder outlet. The one-zone MADI model is simple and fast in operation. It provides accurate results if it is calibrated by the engine test results. For calculation of the combustion process by the one-zone MADI model, heat release rate parameters of the I.Viebe empirical formula are needed, which may be calculated by the multi-zone FIRE model. Therefore, the following simulation method was used.

1) Calculation of the parameters of the diesel, gas diesel and gas engines by the one-zone MADI model to get the air pressure and temperature at the inlet to the cylinder and the exhaust gases pressure and temperature at the outlet of the cylinder using the approximate values of the I.Viebe heat release rate parameters φ_z and m.

2) Calculation of the compression-combustion-expansion processes of all three engines by the multi-zone FIRE model using parameters of the air at the cylinder inlet and exhaust gases at the cylinder outlet calculated by the one-zone MADI model to get more precise values of the I.Viebe heat release rate parameters.

3) Calculation of the parameters of the diesel, gas diesel and gas engines by the one-zone MADI model using more precise values of the I.Viebe heat release rate parameters calculated by the multi-zone FIRE model.

2.2 Input Data

The comparison of operation parameters of three engines was carried out for the 6-cylinder in-line D200 engine of the chanting locomotive. For calibration of the one-zone MADI model, engine test results of diesel and gas diesel versions of the 6-cylinder in-line Cummins KAMA truck engine were used. The gas diesel engine had a modular gas feeding and electronic control systems developed in MADI, which could be used both on high-speed (truck) and medium-speed (locomotive) engines [7]. The one-zone MADI model for a diesel engine was additionally calibrated by the experimental results of testing the D200 locomotive diesel engine by the locomotive characteristic [15].

Table 1 shows parameters of the base diesel engine: cylinder stroke S, cylinder diameter D, compression ratio ε, as well as engine parameters at the rated mode: brake power N_e, brake mean effective pressure p_e, engine speed n.

Table 1
Parameters of the вase diesel engine

S [mm]	D [mm]	ε -	N_e [kW]	p_e [MPa]	n [rpm]
280	200	14.0:1	870	2.0	1000

Experimental compressor and turbine maps of the turbocharger TK-1020 with centrifugal compressor and axial turbine mounted on the D200 diesel engine were used.

The combustion chamber of the base diesel engine D200 and its gas diesel version is shown in Fig. 1. It can’t be used for the gas engine because of knock. Therefore, the compression ratio was reduced from 14.0:1 to 10.0:1. The value of the over-piston clearance of the base diesel engine (15 mm) was not changed and compression ratio was reduced by increasing the volume of the combustion chamber in the piston head.

The combustion chamber shape was optimized to ensure complete combustion of the gas fuel and minimal toxic emissions. Poor combustion of the gas fuel and formation of unburned hydrocarbons takes place in the over-piston clearance. Therefore, the diameter of the combustion chamber was increased from 156 to 180 mm to obtain the minimal volume of the over-piston clearance and the hemispheric shape was selected as shown in Fig. 2.

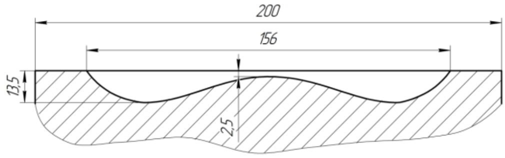

Figure 1
Schematic of the combustion chamber of the diesel and gas diesel engine (compression ratio = 14,0:1)

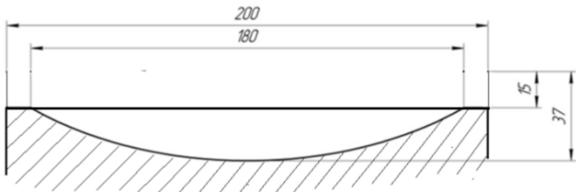

Figure 2
Schematics of the combustion chamber of the gas engine (compression ratio = 10,0:1)

3 Results and Discussions

Calculations of the diesel, gas diesel and gas versions of the D200 locomotive engine were carried out for the rated mode by the multi-zone AVL FIRE model using the boost air and exhaust gases parameters, which were earlier calculated by the one-zone MADI model. The boost air and exhaust gases parameters do not differ much from those obtained after the final calculation by the MADI model indicated in Table 4.

Emissions of NO_x and soot for diesel, gas diesel and gas engines calculated by the multi-zone FIRE model are presented in Table 2.

As can be seen in Table 2, the gas engine produces a minimal amount of NO_x and soot. Compared to the diesel engine, emissions of NO_x are 3.1 times lower and for the gas engine – 13.6 times lower. Soot emissions for the gas diesel and gas engines are very low compared to the diesel engine. Still for the gas engine, they are 1.5 times lower than for the gas diesel engine.

Table 2
Emissions of NO_x and soot by diesel, gas diesel and gas versions of the D200 engine

	NO_x [g/kWh]	Soot [g/kWh]
Diesel engine	17.742	0.0089
Gas diesel engine	5.743	$5.3492 \cdot 10^{-5}$
Gas engine	1.2945	$3.0173 \cdot 10^{-5}$

3.1 Determination of the Coefficients of the I.Viebe Formula for the Heat Release Rate

Figs. 3, 4, and 5 present the heat release rate diagrams for diesel, gas diesel and gas versions of the D200 engine calculated by the multi-zone AVL FIRE model. The heat release rate diagrams calculated by the I.Viebe formula are superimposed on them. The heat release duration φ_z was calculated as an interval between the start and the end of the heat release process. The heat release law parameter m was determined by combining the curves obtained by the multi-zone AVL FIRE model and the heat release rate curves calculated by the I.Viebe formula.

As m and φ_z coefficients of the I.Viebe formula influence greatly the optimal by fuel efficiency ignition advance angle θ_{ign}, the optimal by fuel efficiency θ_{ign}value was found for every operation mode of each engine and all results presented lower were obtained for the optimal θ_{ign} value.

Analysis of the φ_z and m values demonstrates that the heat release duration is reduced by about 20 crank angle rotation degrees (^{o}CA) after switching from diesel to gas diesel and gas cycles (correspondingly, 70, 36 and 40^{o}CA). This seems reasonable because in a diesel engine, after combustion has already started, fuel injection continues and preparation of new fuel drops for combustion takes some time (fuel drops have to fly away from the injector, disintegrate into smaller drops, evaporate, mix with the air, heat, etc.). In gas diesel and gas engines, the gas-air mixture is already mixed in the intake manifold and in the cylinder during the compression stroke and is ready for combustion, it just needs to be ignited by a spark plug or a small quantity of diesel fuel.

When switching from diesel to gas diesel and gas cycles, the heat release law parameter m increases correspondingly from 0.5 to 1.0 and 2.0, which results in softer combustion and lower noise level and mechanical loads on the engine parts. Diesel noise is largely caused by the “explosion” type ignition of the portion of diesel fuel injected during the ignition delay period. This portion of diesel fuel is the largest in diesel engine, considerably lower in gas diesel engine and is absent in gas engine.

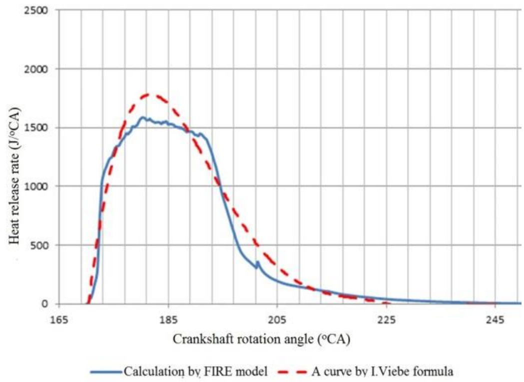

Figure 3
Heat release rate diagram for the D200 diesel engine: φ_z =70°CA, m=0.5

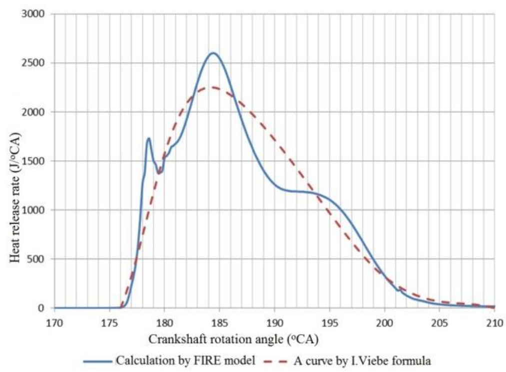

Figure 4
Heat release rate diagram for the D200 gas diesel engine: φ_z =36°CA, m=1

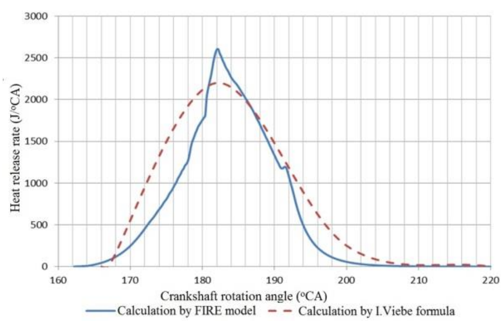

Figure 5
Heat release rate diagram for the D200 gas engine: φ_z =40°CA, m=2

3.2 Comparison of Operating Parameters of the Locomotive Diesel, Gas Diesel and Gas Engines

Comparison of experimental and simulation operation parameters of the D200 by the locomotive characteristic calculated by the one-zone MADI model is presented in Fig. 6 [15]. Here, p_e is the brake mean effective pressure, p_b – boost air pressure, g_e – brake specific fuel consumption, p_z – peak cylinder pressure, G_f – diesel fuel consumption, T_b – boost air temperature. Fig. 6 demonstrates a high convergence of experimental and calculated parameters, both of the diesel engine and its charging system.

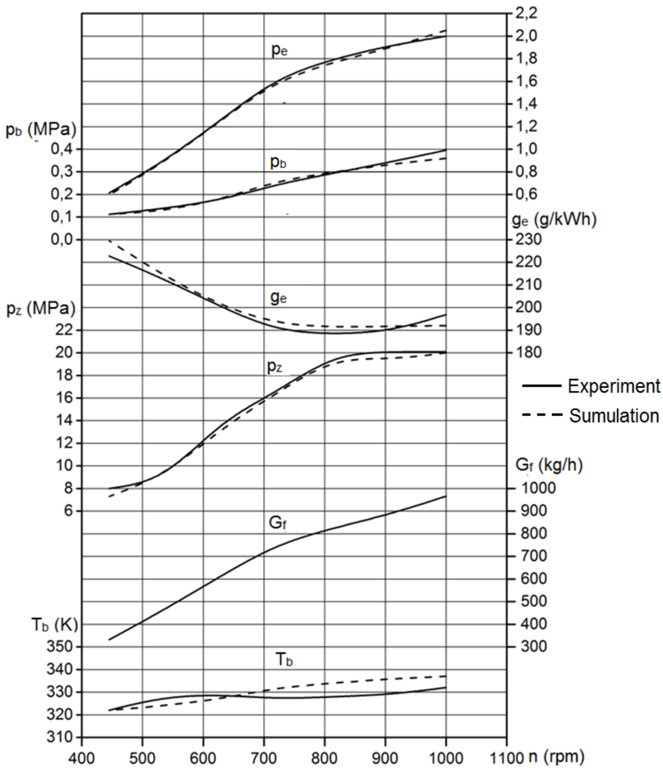

Figure 6

Comparison of experimental and calculated operation parameters of the D200 diesel engine by the locomotive characteristic

To forecast the operation parameters of the locomotive diesel, gas diesel and gas engines, simulation of three engines was carried out at the rated mode by the MADI one-zone model using the Viebe heat release rate parameters calculated earlier by the multi-zone AVL FIRE model. Injection rates of diesel fuel for the diesel engine, gas fuel for the gas engine, gas and diesel fuel for the gas diesel engine were selected so as to get the same rated power 870 kW. For the gas diesel engine, the percentage of the diesel fuel was 5%.

Table 3 presents the basic input data and operation parameters of the engines. The injection rate of diesel fuel G_{df} and gas fuel G_{gas}, parameters of the I.Viebe formula: heat release duration φ_z and heat release mode m, ignition advance angle θ_{ign}, brake specific fuel consumption g_e, indicated efficiency η_i, effective efficiency η_e and air excess coefficient λ.

Table 3

Parameters of the D200 diesel/gas diesel/gas engine at rated mode

Engine	G_{df}	G_{gas}	φ_z	m	θ_{ign}	g_e	η_i	η_e	λ
	[mg/ cycle]	[mg/ cycle]	[°CA]	-	[°to TDC]	[g/kWh]	-		-
Diesel	950	-	70	0.5	16	193	0.488	0.439	1.76
Gas diesel	760	38	36	1.0	6	163	0.499	0.449	1.97
Gas	-	842	40	2.0	12	172	0.469	0.422	2.13

As shown in Table 3, for the gas diesel and gas engines, ignition starts closer to the top dead center (TDC) due to a shorter heat release duration φ_z. The value of θ_{ign} for the gas engine is higher than for the gas diesel engine because the gas engine has a higher value of the I.Viebe parameter m. Compared to the diesel engine, the value of g_e for the gas diesel engine is by 15.5% lower and for the gas engine – by 11% lower basically due to a higher heat value of methane, but also partly due to a shorter heat release duration φ_z. The values of η_i and η_e are similar for the diesel and gas diesel engines and are by relatively 4% lower for the gas engine. The gain in the value of g_e is not so high for the gas engine because it has a reduced compression ratio. For the same reason, the values of η_i and η_e for the gas engine are by 4-6% lower than for the diesel and gas diesel engines. The value of λ for the gas engine is by 7% higher than for the gas diesel engine and by 17% higher than for the diesel engine due to a higher exhaust gases temperature T_t caused by a lower compression ratio, which results in a higher turbocharger rotor speed as shown in Table 4.

Table 4 shows the charging system parameters: boost pressure p_b, turbine inlet pressure p_t, boost air temperature T_b, exhaust gases temperature T_t and turbocharger rotor speed n_r. The values of compressor and turbine efficiency are not shown because they are similar for all three engines.

As can be seen in Table 4, for the gas engine, the values of p_b, p_t, T_b are higher than for the diesel and gas diesel engines because the gas engine has a higher value of T_t. which results in a higher value of n_r.

Table 4
Parameters of the charging system of the D200 diesel, gas diesel and gas engines

Engine	p_b	p_t	T_b	T_t	n_r
	[MPa]	[MPa]	[K]	[K]	[rpm]
Diesel	0.287	0.241	339	801	30287
Gas diesel	0.282	0.238	338	792	30035
Gas	0.314	0.259	341	815	31668

Table 5 shows parameters, which characterize mechanical and thermal loads of the engines: peak combustion pressure p_z, maximum pressure rise rate $(dp/d\varphi)_{max}$, which indicates the noise level, temperature resulting from the heat exchange T_{res}, average heat transfer coefficient for the cycle α_{av} and the product $T_{res} \cdot \alpha_{av}$, which characterizes the thermal factor of the engine.

Table 5
Parameters of mechanical and thermal loads of the D200 diesel/gas diesel/gas engine

Engine	p_z	$(dp/d\varphi)_{max}$	T_{res}	α_{av}	$T_{res} \cdot \alpha_{av}$
	[MPa]	[MPa/°]	[K]	[W/m^2·K]	[kW/m^2]
Diesel	18.4	0.801	1110	759	842.5
Gas diesel	18.2	0.799	1100	752	834.7
Gas	14.4	0.555	1040	705	733.2

As seen from Table 5, parameters of mechanical and thermal loads of the diesel and gas diesel engines are close. The value of p_z does not exceed the limit for this engine, which is 20 MPa. Compared to the diesel engine, parameters of mechanical and thermal loads of the gas engine are lower: p_z – by 22% which indicates lower mechanical loads, $(dp/d\varphi)_{max}$ – by 35% which indicates lower mechanical loads and noise level and the product $T_{res} \cdot \alpha_{av}$ – by 13% which indicates lower thermal factor.

Conclusions

1) Simulation by the AVL FIRE multi-zone model provided coefficients of the I.Viebe formula for the heat release rate, which are needed for engine simulation by the one-zone MADI model. For the locomotive diesel, gas diesel and gas engines, the heat release duration φ_z was 70, 36 and 40°CA and the heat release law parameter m was 0.5, 1.0 and 2.0 correspondingly.

2) Simulation by the AVL FIRE model showed that compared to the diesel engine, the gas diesel and gas engines have, correspondingly, 3.09 times and 13.7 times lower NO_x emissions. Emissions of soot of the gas diesel and gas engines are close to zero.

3) Simulation by the MADI model demonstrated that compared to the diesel engine, the gas diesel engine and gas engine have, correspondingly, by 15.5% and 11% lower brake specific fuel consumption. The indicated and effective efficiency

of the gas diesel engine is by 4% higher due to a shortened heat release duration, and of the gas engine – by 6% lower due to a lower compression ratio, despite a shortened heat release duration. Mechanical and thermal loads of the gas engine are lower than in the diesel and gas diesel engines because of its lower compression ratio.

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