26th International Congress of Mechanical Engineering
COBEM 2021
ABCM Associação Brasileira de Engenharia e Ciências Mecânicas
November 22-26, 2021, Virtual Congress, Brazil

COB-2021-0706
SPRAY AND COMBUSTION BEHAVIOR IN A LOCOMOTIVE ENGINE USING DIESEL / BIODIESEL BLENDS: A CRFD ANALYSIS

Daniel do Valle Rotter
daniel.rotter@grad.ufsc.br
Gustavo Zapelini Hackbarth
gustavo.hackbarth@outlook.com
John Adilson Henschel Junior
john.henschel@labmci.ufsc.br
Leonel R. Cancino
leonel.cancino@labmci.ufsc.br
Internal Combustion Engines Laboratory - Joinville Technological Center - Federal University of Santa Catarina - LABMCI/CTJ/UFSC.
Rua Dona Francisca 8300, Joinville, SC, Brazil, CEP 89219-600

Abstract. *The demand for alternative sources of energy has leveraged the use of diesel and biodiesel blends in internal combustion engines, especially in services with high levels of consumption, such as the railway area. This work reports an analysis, based on computational reactive fluid dynamics, of a DASH9-BB40W locomotive engine. The focus was to numerically evaluate the effects of injecting four different diesel-biodiesel blends B0, B10, B20, and B50 (0, 10, 20, and 50% Vol.%). The cylinder, piston, and injector geometric parameters used for simulation were obtained from the engine technical data and then adapted to reproduce the main engine parameters (compression and spray angle, e.g.) in the AVL-FIRE^{TM} ESE manager. The set-up models for the base-case simulation with mixture B0 (100% fossil diesel) were then tuned in terms of combustion, turbulence, and spray parameters to obtain engine power and torque close to the actual operational data of the DASH9-BB40W locomotive. The results show the temperature in the combustion chamber decreases as the percentage of biodiesel blend increases. Also, the higher the biodiesel percentage, the lower the engine power and torque, as expected, because of the reduction in the low heating value of fuel blend as increases the biodiesel content. In terms of emissions, the higher the biodiesel percentage, the lower the soot formation. On the other hand, the lower the biodiesel percentage, the lower the NOx emissions*

Keywords: *Rail Diesel Engine, Computational Reactive Fluid Dynamics, AVL-FIRE^{TM}*

1. INTRODUCTION

Renewable sources of energy and energy efficiency studies have increased in recent years, especially in the transportation sector, where fuel consumption and emissions of polluting gases are higher when it is compared to other areas. This is due to the predominant use of internal combustion engines powered by oil sources. Its bias, in addition to economic, aims to minimize the emissions effects, since biodiesel is an alternative to fossil fuels, which are related to the emission of carbon dioxide (CO_2), the main substance that contributes to the greenhouse effect. Sustainability and energy efficiency studies have increased in recent years, especially in the transportation sector, where fuel consumption and emissions of polluting gases are engineering challenges when dealing with internal combustion engines. In diesel engines, for example, Li *et al.* (2013) studies show that emissions have a severe impact on global warming and tropospheric ozone formation, accounting for much of the environmental damage caused by this thermal machine. The main emissions are CO, CO_2, NO_X, SO_X, and soot formation. It is also known that oil is a limited source and the use of biofuels helps to extend its useful life (Leite and Leal, 2007). Due to the large amount of CO_2 that is released into the atmosphere every day, different ways have been sought to reduce these emissions of this and other polluting gases through alternative fuels that are more respectful of the planet compared to fossil fuels. Biodiesel is already composed of both vegetable oils and animal fats (Mishra and Goswami, 2018). For compression-ignition internal combustion engines (CI-ICE), the most used biofuels are biodiesels and vegetable oils. Several review works can be found in the technical literature, characterizing the different feedstocks, biofuel production process, the vantages and disadvantages, classification by groups as edible, non-edible, animal fats or oils from other sources. (Mishra and Goswami, 2018; Ma and Hanna, 1999; Chozhavendhan *et al.*, 2020). Compression ignition combustion is a very complex process that depends on several factors: (a) the fuel physical and chemical characteristics, (b) the combustion chamber geometry/design, (c) the fuel injection system as well as the spray behavior, among others. The most relevant factor in energy conversion efficiency is the fuel feeding process, which must be fast enough and at the most suitable crankshaft angle, and for that, an efficient injection system is needed, which injects an appropriate amount of fuel mass at high speed and pressure, among other characteristics (Heywood, 1988). In order to improve this process, many researchers have been studying injection strategies, including the main ones: variation in injection pressure, injection rate shaping, injection timing, and multiple injections (Mohan *et al.*, 2013). CI-ICEs also called "diesel engines", are still in improvement process to improve thermal efficiency with the use of biodiesel, however, the growing demand to use fuels from renewable and less polluting sources should lead the transportation industry (Rail, Automotive, or Navy sectors) to invest more and more in adaptations and improvements geared towards to ethanol use. In this scenario, the use of biofuels is promising. Studies on the use of diesel-biofuels blends in compression-ignition internal combustion engines (CI-ICE) have been discussed in recent decades. Lahane and Subramanian (2015) performed an experiment with blends and concluded that the higher the percentage of biodiesel the lower soot values were found. Islam *et al.* (2014) experimentally tested castor biodiesel in a compression-ignition internal combustion engine obtaining equivalent power for the B20 blend with a lower average percentage of change in PM, CO, and HC emissions compared to conventional diesel. However, the use of this alternative fuel has some limitations, such as an increase in the chemical ignition delay, for example, which prevents that the fuel/air mixture burns easily, resulting in a negative impact on the performance of CI-ICEs (Sahin and Durgun, 2009). Therefore, the purpose of this work is to analyze the effects of injecting four different diesel-biodiesel blends B0, B10, B20, and B50 (0, 10, 20, and 50% Vol.%) on the engine performance parameters. The set-up of the engine base-case (B0) was tuned in terms of combustion, spray and turbulence model in order to closer predict the DASH9-BB40W locomotive performance parameters. The base-case set-up was then extrapolated to the B10, B20, and B50 mixtures, and the numerical responses were then compared to the base-case in terms of power, torque, fuel consumption, and emissions (NOx and soot formation). All the numerical simulations were performed using the AVL-FIRE^{TM} ESE software.

2. RAIL ENGINES LITERATURE REVIEW

The current rail freight transport scenario requires high levels of torque and power from engines. For example, according to VALE S.A. (2018), a single train on Carajás Railroad (EFC) must transport more than 45 thousand tons of iron ore in 330 wagons. In this way, locomotives are equipped with large size and medium rotation engines, working with cylinders volume of 11000 cm^3, approximately at compression rates close to 12,7 to 17 and operational rotation between 400 and 1800 rpm (Heywood, 1988). Besides that, it is common to find two or four-stroke engines from 8 to 16 cylinders operating in a range from 700 to 6300 hp (Borba, 2009). In a typical rail engine, there are 8 acceleration points and a consumption rate of more than 700 liters/hour of diesel at full load, resulting in maximum thermal efficiency of close to 40% in this situation. The lower the acceleration point, the lower the efficiency results (VALE, 2018). Looking at these numbers the importance of studies about the subject is noticeable

2.1 The operation of CI-ICE and use of diesel and diesel/biodiesel mixtures

Compression ignition internal combustion engines (CI-ICE), also known as diesel cycle engines are used in vehicles that require high torque, normally applied in road transport vehicles and rail freight transport. The goal of a good diesel fuel, in function of its physic-chemical properties, is to promote the autoignition as fast as possible with high compression rates to achieve high thermal efficiency and lower pollutant emissions. The engine always operates at maximum volumetric efficiency, thus, what is controlled is the amount of fuel mass injected, that the bigger it is, the bigger the torque will be. However, the mass is restricted because of a lean fuel/air mixture for maximum combustion efficiency, avoiding unburned fuel (Heywood, 1988). The diesel engine can run in a two- or four-stroke cycle. Details and a very complete explanation about the strokes for each system can be found in the literature (Heywood (1988); Martins (2013); Brunetti (2012); Merker *et al.* (2012) and references therein). The fuel injection is done with control, in such a way that the exact amount is introduced, and also at the most appropriate angle, so that high combustion efficiency is achieved, high utilization of the work generated, smooth combustion to reduce noise, among other reasons. The quality of fuel ignition is a determining factor for compression ignition engines, which require easy ignition. It is measured by the cetane number – (CN), the property of a fuel that determines its capacity to ignite. Physically, the CN is related to the time between the start of fuel injection and the start of combustion and is called "diesel ignition delay time" (Diesel-IDT). In cases of high CN, the ignition delay is less than for fuel with low CN. The delay implies a shorter firing period, increasing the proportion of incomplete firing and, consequently, a higher specific consumption. This condition is also undesirable because it favors emissions of pollutants such as carbon monoxide (CO) and nitrogen oxides (NO_x), whose formation increases at high temperatures. Larger and more linear carbon chains, as in the case of alkanes and alkenes, have a higher CN because they are more susceptible to fragmentation by temperature, facilitating auto-ignition at lower temperatures (Brunetti, 2012; Heywood, 1988).

3. METHODOLOGY

This work is an exploratory research based on quantitative data used in Computational Fluid Dynamics through Engine Simulation. The geometry model was built using the AVL-FIRE™ ESE - Diesel tool. Soni and Gupta (2017) also used such tool to numerically evaluate the spray dynamics in two piston geometries and for three injection angles using fossil diesel. Karami *et al.* (2020) used the AVL-FIRE™ ESE-Diesel tool to numerically assess the engine performance of a four-cylinder indirect injection diesel engine using diesel/biodiesel mixtures. The main idea of this work is to numerically assess the engine performance parameters using different diesel/biodiesel blends B0, B10, B20, and B50 (0, 10, 20, and 50% Vol.%).

3.1 Geometric and operating parameters for simulation

The first step was to model geometric aspects of a typical locomotive engine based on General Electric's GE 7FDL of DASH9-BB40W manual. Table 1 shows the global geometric parameters of the modeled diesel engine. Based on studies of internal documentation at VALE S.A, (VALE, 2011), and a technical visit to the same company, an ESE-Diesel piston-in-bowl template was adapted for this typical railroad engine as shown in Figures 1 and 2. For constructing the model, the geometric engine parameters of Table 1 and dimensions of Figure 1 were used. Note that the engine has 16 cylinders, but only one was modeled to reduce computational efforts and time. In addition, the axis-symmetrical condition was used, of this form, the piston allows to divide the combustion chamber by the number of injection holes, 8. Thus, only a 45° portion of the cylinder was modeled with a single fuel spray characterized.

Table 1. GE 7FDL geometric parameters used in this work. (VALE, 2011)

Parameter	Description	Parameter	Description	Parameter	Description
Strokes	4	Stroke Length	266.7 mm	Valves	4
Cylinders	16	Compression Ratio	12.7:1	Rod Length	590.50 mm
Configuration	V	Crank Radius	133.35 mm	Piston Bore	228.6 mm

3.2 Numerical model by using AVL-FIRE™

In this work, geometric parameters were collected from real engine injectors and pistons and then used for simulation purposes. Figure 1 shows the main engine geometric parameters from the injector and piston. Note that, for all simulations using diesel-biodiesel blends all the geometric parameters were kept constant, as shown in Figure 2. Figure 1 also shows the values of geometrical parameters used in the numerical approach. Based on studies of internal documentation (VALE, 2011) an ESE-Diesel piston-in-bowl template was created for this typical railroad engine geometry as shown in Figure 2. In order to create the model mesh, the ESE Diesel mesh generator algorithm itself was used which fundamentally respects the concepts of mobile and block-structured mesh. It was possible to create and expand different blocks that accurately described the complex geometries involved, such as spray and combustion chamber, for example, along with crankshaft rotation without losing the sequential indexing of finite volumes within each block. Because of this, it was possible to optimize computational costs and achieve greater reliability in the calculations performed. Initial conditions were inserted into the model. It was adopted the strategy of not contemplating the admission cycle, so simulation begins at the closing of intake valves to reduce computational time. Table 2 shows the initial conditions of the engine at compression cycle at the best engine acceleration point (DASH9-BB40W engine)

Table 2. Initial conditions - DASH9-BB40W engine

Parameter	Description	Parameter	Description	Parameter	Description
Rotation [rpm]	996	Movement wall temp. [K]	570.15	EGR Mass fraction	0.049
Cylinder pressure [Pa]	255000	Fixed wall temp. [K]	470.15	Rotation direction Z	-1
Air temp. [K]	355	Fuel	Diesel-D1	Turbulent kinetic energy [m^2/s^2]	10
Fuel temp. [K]	350	Injected mass [kg]	1.10E-03	Injection duration [ms]	6.35
Swirl [1/min]	2880	Turbulent length scale [m]	0.0045	Crank angle injection start [°]	342

In terms of chemical composition, the fossil fuel "diesel" in the AVL-FIRE™ is composed has an average chemical formula of C7H16, the biodiesel "B10" is C13H24, the "B20" is C14H25O1 and the "B50" is C15H28O1. Note that just for B20 and B50 oxygen is present in the molecular "average" chemical formula. The hydrogen and carbon atom number follows the average composition observed in the literature (Ma and Hanna, 1999; Chozhavendhan *et al.*, 2020).

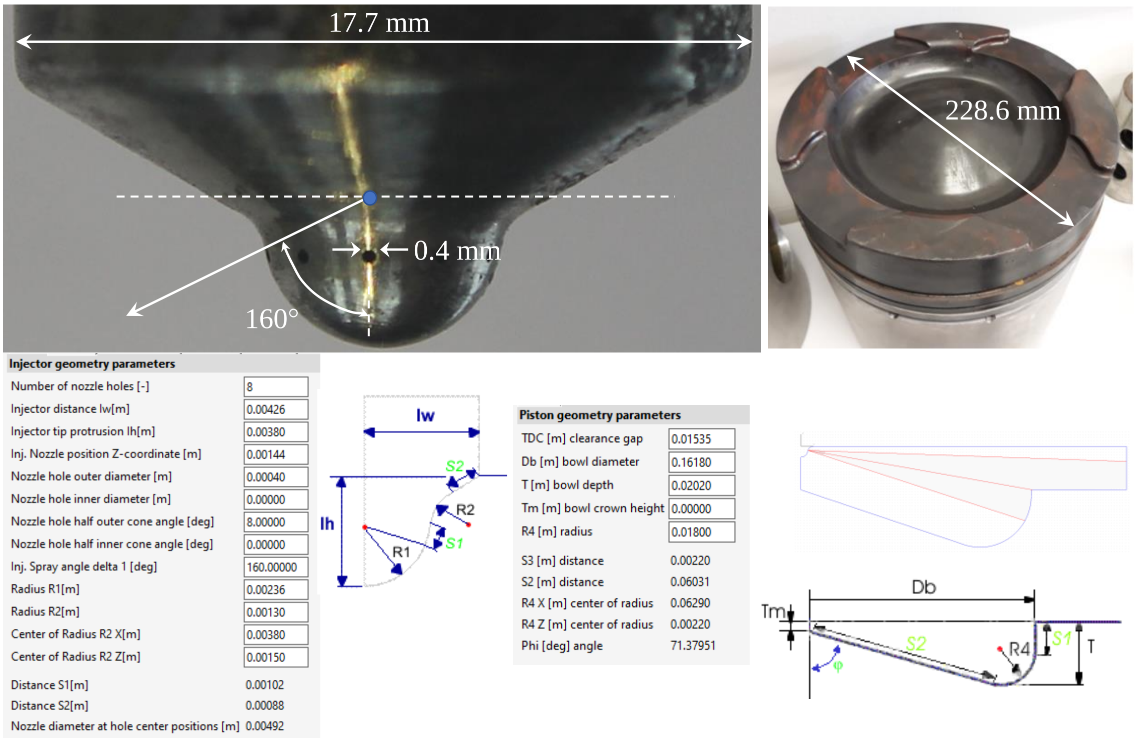

Figure 1. Geometrical parameters used in the numerical approach for injector and piston

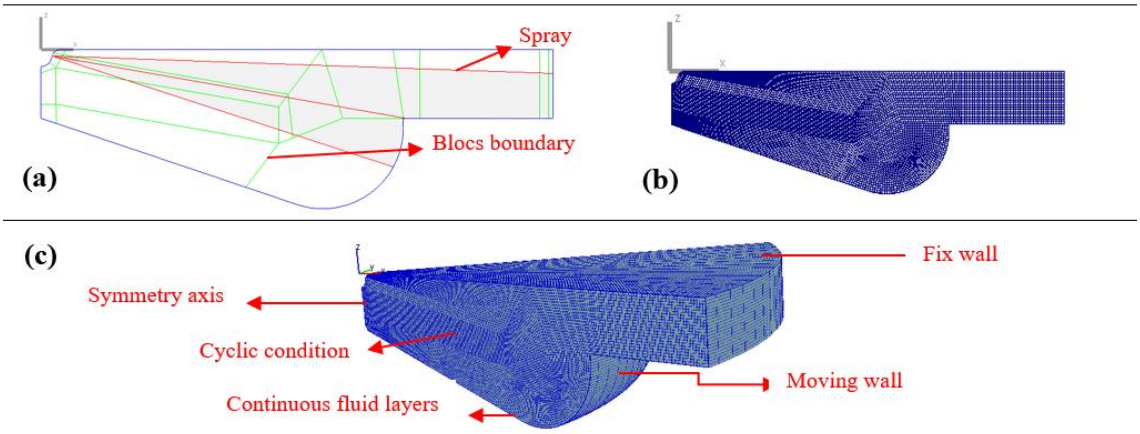

Figure 2. Combustion chamber geometry modeled at top dead center. (a) Block-structured mesh; (b) 2D model; (c) 3D model

3.2.1 The k-zeta-f turbulence model and Wave breakup model

During the combustion process inside the cylinder, an unsteady three-dimensional flow called turbulence occurs. Many mathematical models have been developed to predict the effects of the laminar-turbulence transition. In this work, the four-equation k-zeta-f turbulence model was used to capture the in-cylinder flow. Proposed by Hanjalić *et al.* (2004), this model is a more robust modification of Durbin's elliptic relaxation concept Durbin (1991) that solves the transport equations for the velocity scale ratio instead of the velocity scale, which according to Ramadani *et al.* (2009), improves the stability of the computational procedures. The k-zeta-f turbulence model is widely used in diesel engine simulations due to its robustness for calculations involving meshes with moving boundaries and highly compressed flows, as is the case for the IC engine (Khan *et al.*, 2018). In CFD analyses, in addition to mathematical models to predict the development of combustion and turbulence, a model is still needed to describe the atomization of the fuel spray, that is, how the droplets break up inside the combustion chamber. According to Hossainpour and Binesh (2009), the breakup of the liquid fuel jet plays a decisive role in the evolution of a diesel spray, and it is associated with subsequent processes such as air-fuel mixture formation, auto-ignition, and chemical reactions, which influences efficiency and pollutant formation during engine operation. In a literature review, it is possible to find many proposed models, and for this work, the WAVE breakup model was chosen, which, according to Fu-shui *et al.* (2008), has a good compromise between the complexity of utility and the capability of prediction. The model developed by Reitz *et al.* (1987) considers the stability of a liquid column issuing from a circular orifice into a stationary incompressible gas (Liu *et al.*, 1993). The WAVE breakup model, as pointed out by Turner *et al.* (2012), is based upon the temporal stability analysis of the Kelvin-Helmholtz instability for a liquid jet with an inviscid gas phase, this instability causes aerodynamic stripping of the smaller droplets from the liquid core of the jet.

3.2.2 The Coherent Flame Model (ECFM-3Z)

It should be noticed that this model follows the principles of mass, momentum, and energy conservation in a finite domain of control volumes. These are fundamental features of ESE-Diesel, also known as the finite volume method. Also, sub-models recommended by AVL-FIRE™ (2017) and published and used for other authors in the literature, (Soni and Gupta, 2017), were used to describe important phenomena involved such as combustion (ECFM-3Z), spray droplets (Wave), drag (Schillar Naumann), evaporation (Dukowicz), cylinder wall interaction (Wall Jet 1), NO formation (Extended Zeldovich) and soot formation (Kinetic Model). The 3-zone ECFM combustion model is based on turbulent flame surface density equations, which allows for the approximate construction of the local properties of the gases inside the combustion chamber. For application in Diesel models, the model description is separated into three different mixing zones: A fuel zone, a fresh air zone with residual gases, and a mixing zone where the ECFM model is applied (Colin and Benkenida, 2004). This approach to the combustion model in diesel engines is due to the fact that the fuel injection does not happen in a pre-mixed way, leading to a reaction that is known as diffusion flame, where the fuel and air are separated by a thin layer where the reaction occurs and knowing that diesel engines are fired through auto-ignition, a small pre-mixed region must be formed inside the combustion chamber that will undergo the auto-ignition due to the increase in pressure and temperature inside the combustion chamber, thus requiring three different regions to describe the reaction (Colin and Benkenida, 2004). Each element is divided into three zones where the state of the gas mixture is represented in 2D space, in addition to being described as a function of the reaction progress. The combustion reaction must take place in the region where the equations are governed by the ECFM model. Thus assuming that the reaction time in this zone is much less than the time required for the diffusion process, it is determined that the diffusion combustion is completely controlled by the mixture of fuel and oxidant, thus the separation of the two phases, ignition and combustion makes the model extremely suitable for computer simulation cases of diesel engines (Mobasheri, 2015).

3.3 Mesh independence test

In order to check the mesh independence, four meshes were built. The aspect ratio was used as mesh size control for this purpose. Figures 3(a) and (b) shows the results. The brake mean effective pressure (BMEP) was choose as the target parameter for this mesh independence test, however, all the engine-specific output data follow the trend of BMEP for all the meshes tested in this work. The numerical simulations were performed for all meshes, in a computer with 8 cores, 3.4 GHz processing and 32 GB of RAM, which lasted around 24 hours (each simulation / average time for all meshes). Figures 3(a) and (b) pointed out the mesh size (Mesh 3) to be used for all the simulations ($\sim$ 590000 cells).

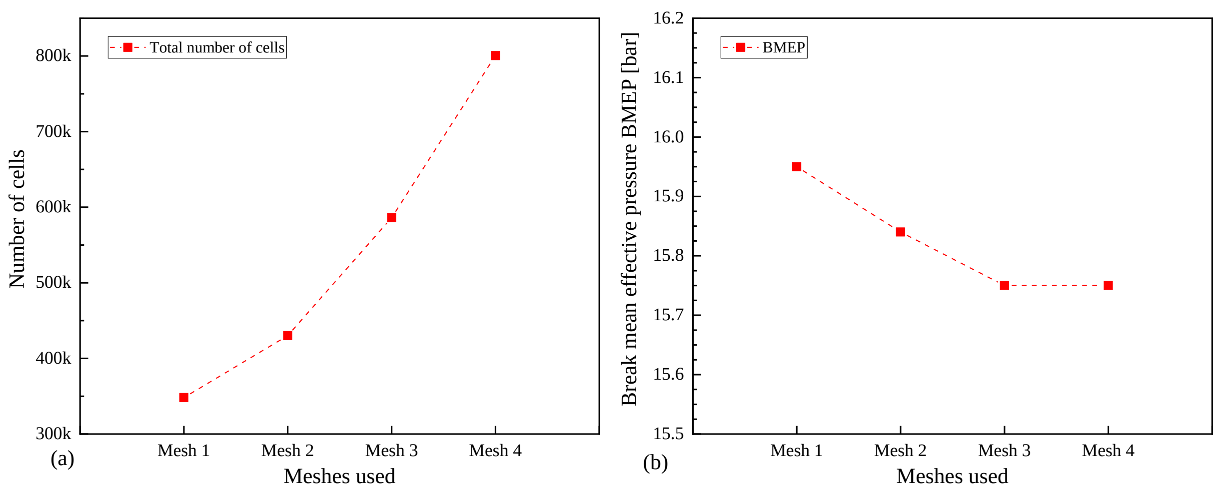

Figure 3. Mesh independence test (a) Number of cells in each mesh, (b) The brake mean effective pressure BMEP [bar] behavior

4. Results and discussion

4.1 Mean Effective Pressure, Indicated Power and torque, Specific Fuel Consumption and Indicated Thermal Efficiency

Table 3 shows the numerical predictions for Diesel/air mixture. The air/fuel ratio and stoichiometric ratio estimated was 1.77, according to Borba (2009), the stoichiometric ratio of GE-7FDL diesel engines is not less than 1.3 at full load, and may increase according to the operation of the turbochargers and injection system. Comparing Table 3 and 4, it can be seen that the effective mean pressure and indicated power of Diesel/air mixture are 15.55 bar, and 144.09 kW, the values are within the range of maximum and minimum values found in locomotive 'A', which qualify the present work. To search for the best diesel/biodiesel blend, four fuel injection points were simulated and the engine performance was then compared to the diesel fuel engine operation. Figure 4 shows the numerical predictions.

Table 3. Global operation parameters - Numerical predictions

Run case	Mean Effective Pressure [bar]	Indicated Power [kW]	Indicated Torque [Nm]	Air-Fuel Ratio (λ)	Specific Fuel Consumption [kg/kWh]	Indicated Thermal Efficiency
Diesel	15.55	144.09	1381.44	1.77	0.2299	0.37

Table 4. Averaged measured parameters, per piston - Dash 9 BB40W - locomotive 'A'. (VALE, 2011)

	Mean Effective Pressure [bar]	Indicated Power [kW]
Average	15.79	154.17
Maximum	16.96	169.27
Minimum	14.13	140.88

In Figures 4(a), (b), (c), and (d) the horizontal dot gray lines represent the engine performance parameter of the engine using diesel fuel, see tables 3 and 4 for numerical/experimental values. Figures 4(a), (b), and (c) show that increasing the biodiesel percentage decreases brake mean effective pressure (BMEP), indicated power and indicated torque of the engine. Also, Figure 4(b) shows that the higher the biodiesel percentage, the higher the brake-specific fuel consumption (BSFC). The decrease of these engine parameters occurs because of the reduction in the low heating value of the fuel blend as increases the biodiesel content.

4.2 Spray development and temperature fields

Figure 5 shows the spray behavior for diesel, from 704° CA to 707° CA, in terms of average drop diameter. The numerical simulation shows that as spray penetrates, the Wave breakup model acts, of this form as the drops going into the combustion chamber, undergoes heat and mass transfer making the diameter decrease and releasing fuel (diesel) in vapor phase promoting the mixture with and of this form allowing the thermodynamics and kinetics conditions for mixture autoignition (premixed combustion phase).

Figure 6 shows the temperature fields at 720° CA (Top Dead Center) for diesel with 702° CA fuel injection point (upper figures), comparing to the temperature fields at 720° CA (Top Dead Center) of diesel/biodiesel blends with four fuel injection points (696°, 698°, 700°, and 702° CA). It is clear that coming back the injection point, the gas temperature at TDC is higher.

4.3 Temperature fields, NO, and Soot formation

As the spray is developing, pressure and temperature are also in evolution. Figure 7 shows the temperature and fresh gas-phase temperature fields (upper part) for the 710° CA, when a portion of diesel already in the vapor phase has mixed with air and started the combustion process (Figure 5 shows the spray behavior till 707° CA). Note that in the fresh gas-phase temperature, the domain around the spray is $\sim$ 611 K surpassing the diesel vaporization temperature at that pressure condition ($\sim$70 bar). Those conditions of pressure and temperature promote the NO and soot formation, as observed in Figure 7 (bellow part of the figure).

Figure 8 shows the differences in terms of emissions, (a) NO and (b) soot formation, for all four diesel-biodiesel blends, and for all the fuel injection points. It can be observed in Figure 8(a) the higher percentage of biodiesel, the higher the Mean NO mass fraction presents. Differences in Physic-Chemical characteristics of biodiesel and the temperature inside the combustion chamber are responsible for the increase of NO formation. On the other hand, Figure 8(b) shows that the higher percentage of biodiesel, the lower mean soot mass fraction, following the experimental observations of several works reported in the literature Karami *et al.* (2020); Lahane and Subramanian (2015)

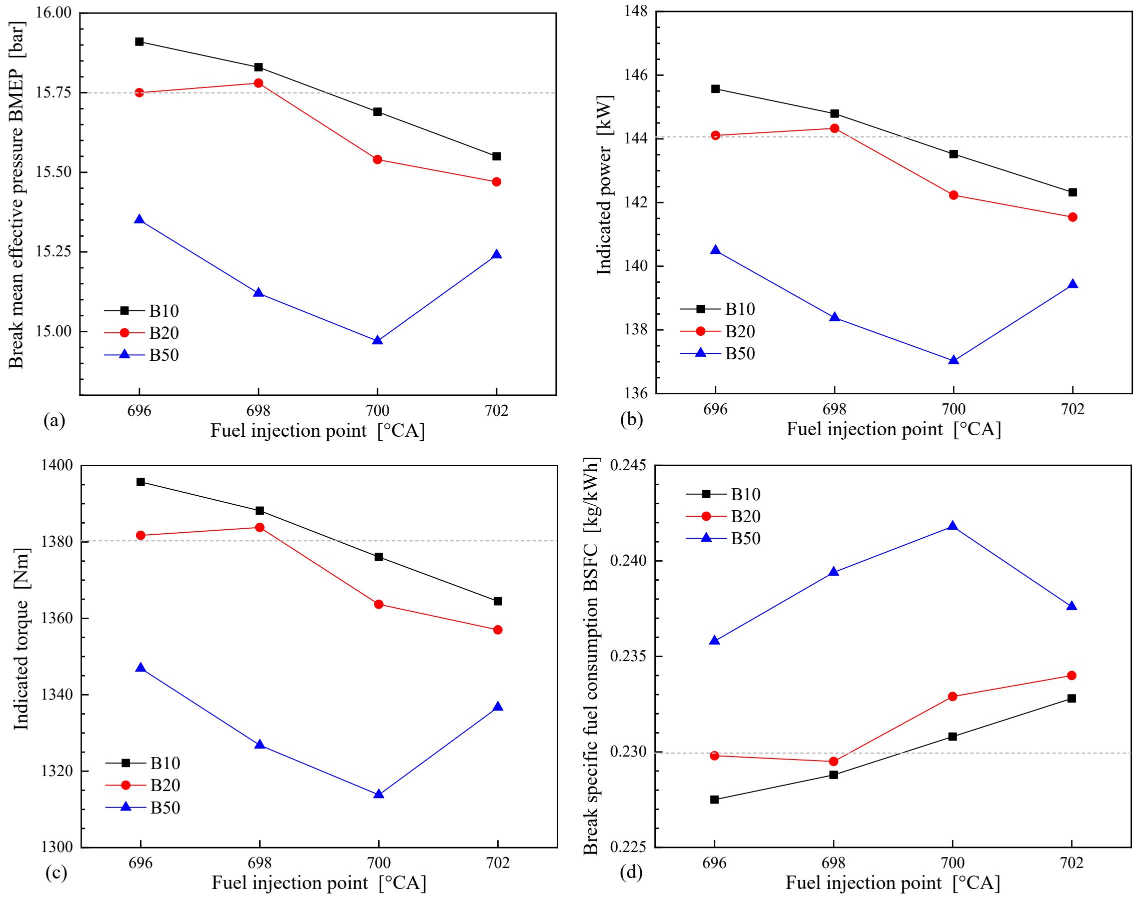

Figure 4. Diesel/biodiesel blends B10, B20 and B50 performance parameters: (a) Break mean effective pressure, (b) Indicated power, (c) Indicated torque and (d) Break specific fuel consumption, for the four fuel injection points investigated in this work.

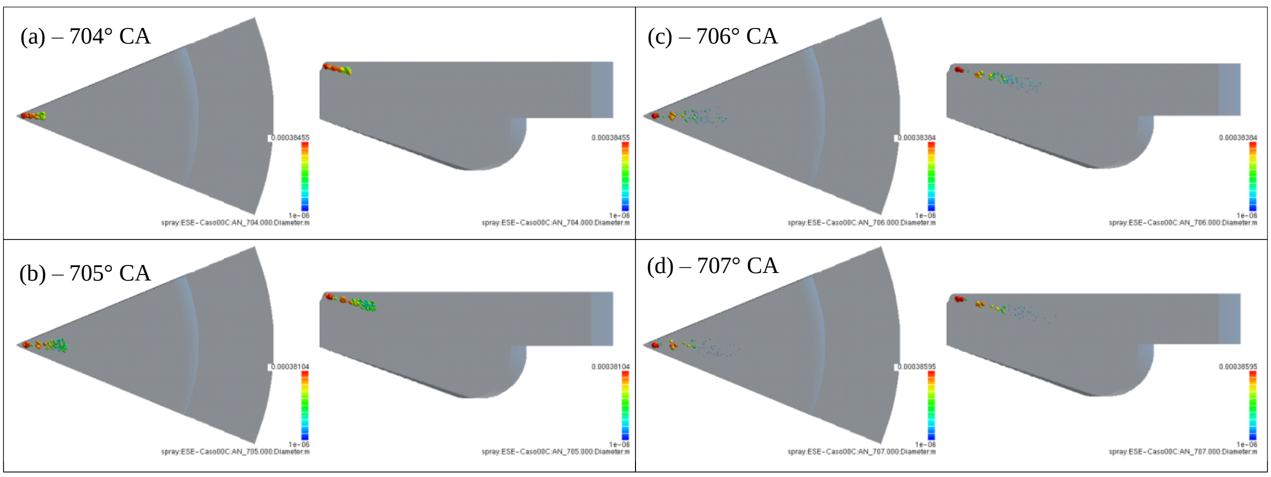

Figure 5. Spray behavior from 704° CA to 707° CA, Diesel / air mixture

5. CONCLUSION

Modern compression engines can run with high blends however, the physic-chemical properties of the fuel are modified by adding biodiesel to diesel, which affects the development of the injection spray and engine efficiency, then the efficiency of internal combustion engines is directly related to fuel consumption and the reduction of pollutant gases, which can be controlled by optimizing injection system parameters such fuel injection point. If there is a change in the

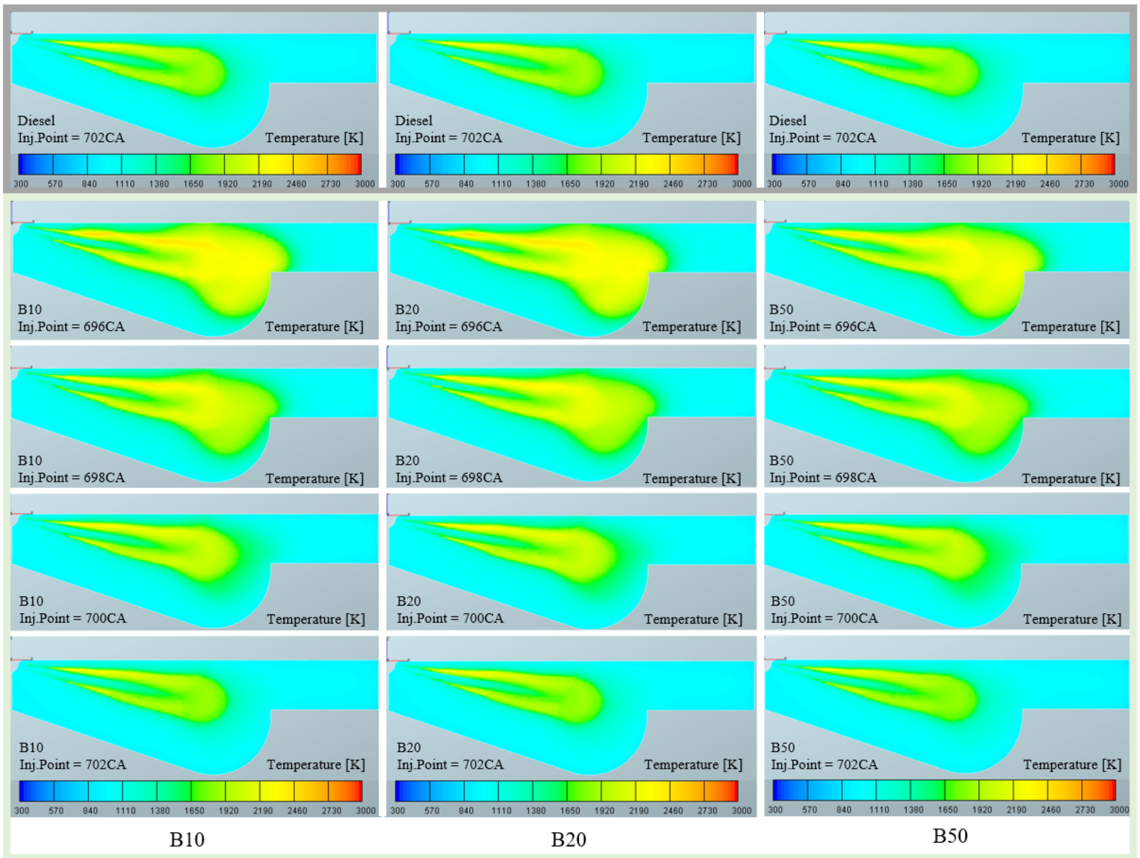

Figure 6. Temperature fields at 720° CA (Top dead center) for diesel with 702° CA (upper figures) and for diesel / biodiesel blends B10, B20 and B50 with 696°, 698°, 700° and 702° CA

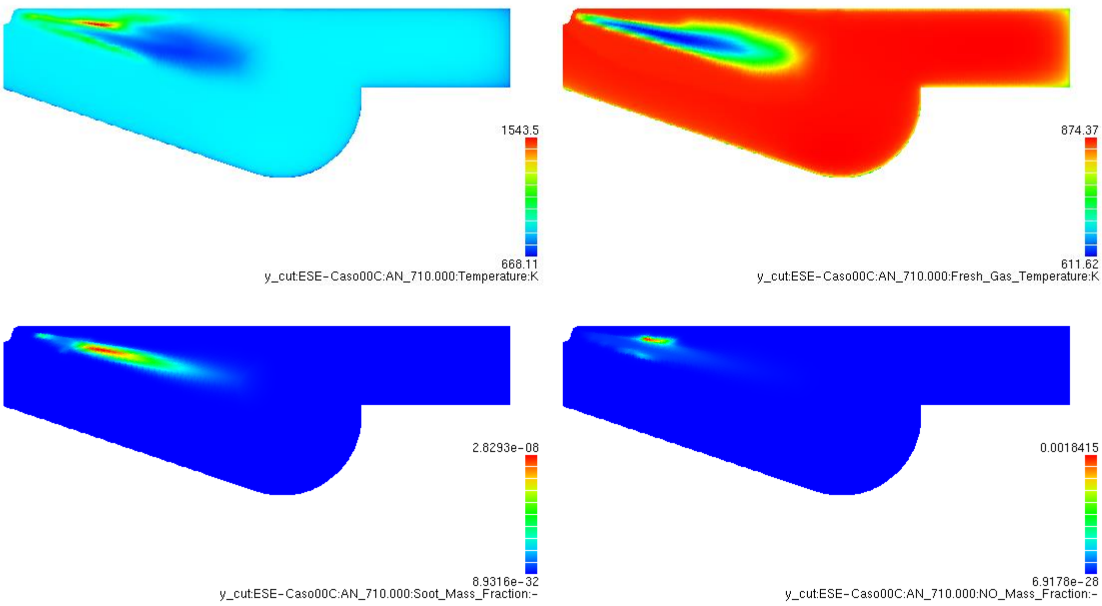

Figure 7. Temperature, NO and Soot fields at 710° CA, Diesel / air mixture

characteristics of the spray, then there is a deviation of behavior from what was intended as ideal in the engine's plan. Considering that the fuel costs for rail freight are remarkably high, any efficiency improvement in the engines is beneficial. In this way, several considerations can be made from the numerical results of this work: (i) Figures 4(a), (b), and (c) shows that all the simulated points above (or close to) the gray dot line represent good conditions or comparable engine

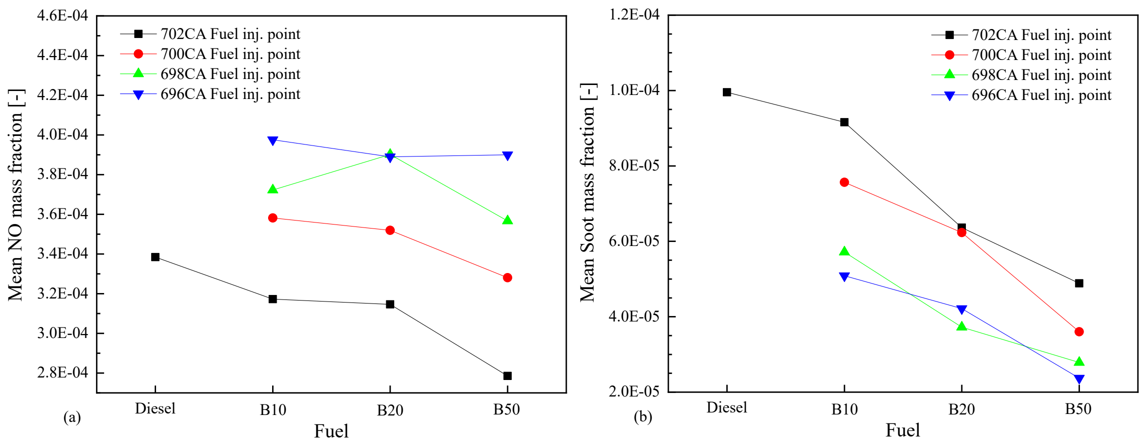

Figure 8. Diesel and diesel/biodiesel blends (a) Mean NO mass fraction and (b) Mean soot mass formation numerical predictions at exhaust valve open

operation conditions to the fossil diesel engine operation, especially the B20 diesel/biodiesel blend that shows a close behavior in terms of brake specific fuel consumption Figures 4(d), adopting a fuel injection point close to 698° CA. (ii) Figure 6 shows that the fuel injection point can be "moved" backward 4° CA improving the combustion behavior without penalizing the emissions in terms of high pressure and temperatures reached in the combustion chamber before the TDC. (iii) Figure 8 shows that numerical simulations performed in this work using the fuel database of AVL-FIRE™ reproduce numerical results comparable to the experimental ones reported in the literature.

6. ACKNOWLEDGMENTS

The authors would like to acknowledge the AVL-AST University Partnership Program (UPP) for the use and support of AVL-AST software. All the support from VALE S.A along the development of this research work is also highly appreciated. The support of the UFSC Joinville TI team (Mr. Kleber Carlos Francisco.) is also appreciated.

7. REFERENCES

AVL-FIRE™, 2017. “Engine simulation environment diesel – ese diesel”. ESE Diesel Manual.

Borba, J.L., 2009. *Mecânica de Locomotivas*. PUC Minas Gerais.

Brunetti, F., 2012. *Motores de combustão interna: volume 1*. Blucher, São Paulo, 3rd edition.

Chozhavendhan, S., Singh, M.V.P., Fransila, B., Kumar, R.P. and Devi, G.K., 2020. “A review on influencing parameters of biodiesel production and purification processes”. *Current Research in Green and Sustainable Chemistry*, Vol. 1-2, pp. 1 – 6. ISSN 2666-0865. doi:https://doi.org/10.1016/j.crgsc.2020.04.002.

Colin, O. and Benkenida, A., 2004. “The 3-Zones Extended Coherent Flame Model (Ecfm3z) for Computing Premixed/Diffusion Combustion”. *Oil & Gas Science and Technology*, Vol. 59, pp. 593–609. ISSN 1294-4475. doi:10.2516/ogst:2004043.

Durbin, P.A., 1991. “Near-wall turbulence closure modeling without “damping functions””. *Theoretical and computational fluid dynamics*, Vol. 3, No. 1, pp. 1–13.

Fu-shui, L., Lei, Z., Bai-gang, S., Zhi-jie, L. and Schock, H.J., 2008. “Validation and modification of wave spray model for diesel combustion simulation”. *Fuel*, Vol. 87, No. 15, pp. 3420–3427. ISSN 0016-2361. doi:https://doi.org/10.1016/j.fuel.2008.05.001.

Hanjalić, K., Popovac, M. and Hadžiabdić, M., 2004. “A robust near-wall elliptic-relaxation eddy-viscosity turbulence model for cfd”. *International Journal of Heat and Fluid Flow*, Vol. 25, No. 6, pp. 1047–1051. ISSN 0142-727X. doi:https://doi.org/10.1016/j.ijheatfluidflow.2004.07.005.

Heywood, J.B., 1988. *Internal Combustion Engine Fundamentals*. McGraw-Hill, New York.

Hossainpour, S. and Binesh, A., 2009. “Investigation of fuel spray atomization in a di heavy-duty diesel engine and comparison of various spray breakup models”. *Fuel*, Vol. 88, No. 5, pp. 799–805. ISSN 0016-2361. doi:https://doi.org/10.1016/j.fuel.2008.10.036.

Islam, M.S., Ahmed, Abu Saleh amd Islam, A., Abdul Aziz, S., Xian, L.C. and Mridha, M., 2014. “Study on emission and performance of diesel engine using castor biodiesel”. *Journal of Chemistry - Hindawi Publishing Corporation*, Vol. 2014, p. ID451526. ISSN 2090-9063. doi:10.1155/2014/451526.

Karami, R., Rasul, M.G. and Khan, M.M.K., 2020. “Cfd simulation and a pragmatic analysis of performance and emissions of tomato seed biodiesel blends in a 4-cylinder diesel engine". *Energies*, Vol. 13, No. 14. ISSN 1996-1073. doi:10.3390/en13143688.

Khan, S., Panua, R. and Bose, P.K., 2018. "Combined effects of piston bowl geometry and spray pattern on mixing, combustion and emissions of a diesel engine: A numerical approach". *Fuel*, Vol. 225, pp. 203–217. ISSN 0016-2361. doi:https://doi.org/10.1016/j.fuel.2018.03.139.

Lahane, S. and Subramanian, K., 2015. "Effect of different percentages of biodiesel–diesel blends on injection, spray, combustion, performance, and emission characteristics of a diesel engine". *Fuel*, Vol. 139, pp. 537–545. ISSN 0016-2361. doi:https://doi.org/10.1016/j.fuel.2014.09.036.

Leite, R.C.C. and Leal, M.R.L.V., 2007. "O biocombustível no brasil". *Novos estudos CEBRAP*, pp. 15 – 21. URL `http://www.scielo.br/scielo.php?script=sci_arttext&pid=S0101-33002007000200003&nrm=iso`.

Li, T., Liu, Z.C., Zhang, H.C. and Jiang, Q.H., 2013. "Environmental emissions and energy consumptions assessment of a diesel engine from the life cycle perspective". *Journal of Cleaner Production*, Vol. 53, pp. 7 – 12. ISSN 0959-6526. doi:https://doi.org/10.1016/j.jclepro.2013.04.034.

Liu, A., Mather, D. and Reitz, R., 1993. "Modeling the effects of drop drag and breakup on fuel sprays". *SAE Technical Paper 930072*, p. 17. doi:10.4271/930072.

Ma, F. and Hanna, M.A., 1999. "Biodiesel production: a review". *Bioresource Technology*, Vol. 70, No. 1, pp. 1 – 15. ISSN 0960-8524. doi:https://doi.org/10.1016/S0960-8524(99)00025-5.

Martins, J., 2013. *Motores de combustão interna*. Publindústria, Porto, 4th edition.

Merker, G.P., Schwarz, C. and Teichmann, R., 2012. *Combustion Engines Development: Mixture Formation, Combustion, Emissions and Simulation*. Springer, Berlin.

Mishra, V.K. and Goswami, R., 2018. "A review of production, properties and advantages of biodiesel". *Biofuels*, Vol. 9, No. 2, pp. 273–289. doi:10.1080/17597269.2017.1336350.

Mobasheri, R., 2015. "Analysis the ECFM-3Z Combustion Model for Simulating the Combustion Process and Emission Characteristics in a HSDI Diesel Engine". *International Journal of Spray and Combustion Dynamics*, Vol. 7, pp. 353–371. ISSN 1756-8277. doi:10.1260/1756-8277.7.4.353.

Mohan, B., Yang, W. and kiang Chou, S., 2013. "Fuel injection strategies for performance improvement and emissions reduction in compression ignition engines—a review". *Renewable and Sustainable Energy Reviews*, Vol. 28, pp. 664 – 676. ISSN 1364-0321. doi:https://doi.org/10.1016/j.rser.2013.08.051.

Rafidah, R., Mamat, R., Yusof, T. and Abdullah, A., 2012. "Influence of fuel temperature on a diesel engine performance operating with biodiesel blended". *International Journal of Advanced Science and Technology*, Vol. 43, pp. 115–126.

Ramadani, K., Kelterer, M., Pecnik, R. and Sanz, W., 2009. "Application of the zeta-f-turbulence model to steady transitional flow". In *European Conference on Turbomachinery Fluid Dynamics and Thermodynamics*. pp. 119–130. ISBN 978-3-85125-036-7.

Reitz, R. *et al.*, 1987. "Modeling atomization processes in high-pressure vaporizing sprays". *Atomisation and Spray technology*, Vol. 3, No. 4, pp. 309–337.

Soni, D.K. and Gupta, R., 2017. "Numerical analysis of flow dynamics for two piston bowl designs at different spray angles". *Journal of Cleaner Production*, Vol. 149, pp. 723 – 734. ISSN 0959-6526. doi:https://doi.org/10.1016/j.jclepro.2017.02.142.

Turner, M., Sazhin, S., Healey, J., Crua, C. and Martynov, S., 2012. "A breakup model for transient diesel fuel sprays". *Fuel*, Vol. 97, pp. 288–305. ISSN 0016-2361. doi:https://doi.org/10.1016/j.fuel.2012.01.076.

VALE, 2011. "Dados da locomotiva dash9-bb40w". Internal Documentation VALE S.A. - General Electric.

VALE, 2018. "Estrada de ferro carajás: o caminho onde passa a nossa riqueza - http://www.vale.com/brasil/pt/initiatives/innovation/carajas-railway/paginas/de-fault.aspx". Internal Documentation VALE S.A.

8. RESPONSIBILITY NOTICE

The authors are solely responsible for the printed material included in this paper.