
# SYSTEMATIC REDUCTION OF A CHEMICAL KINETIC MECHANISM FOR THE COMBUSTION OF DIFFERENT GASOLINE-ETHANOL BLENDS

**Filipe Silva Cota**

**Ramon Molina Valle**

filipe.cotafs@gmail.com

ramon@demec.ufmg.br

Universidade Federal de Minas Gerais – Programa de Pós Graduação em Engenharia Mecânica

Antônio Carlos Avenue, 6627, 31270-901, Belo Horizonte, Minas Gerais, Brazil

**Gustavo Queiroz Hindi**

gustavo.hindi@fcagroup.com

Fiat Chrysler Automobiles LATAM

Contorno Avenue, 3455, 32669-900, Betim, Minas Gerais, Brazil

**Abstract.** *Detailed chemical kinetic mechanisms are capable to characterize complex fuels such as gasoline. However, these mechanisms may consist of hundreds or thousands of species and elemental chemical reactions, which make the use of them impractical in Computational Fluid Dynamics combustion simulations for complex geometries like an internal combustion engine, for instance. The situation is even more complex when working with fuel mixtures, such as Brazilian gasoline type-C, which contains 27% v/v of ethanol. The use of ethanol as a pure fuel or as an additive for gasoline is an approach aiming to reduce the dependence on fossil fuels and to decrease greenhouse gases emission; as a consequence, it is crucial to develop studies aiming to acquire knowledge about the physical and chemical behavior of gasoline-ethanol blends. The objective of this work is to generate a reduced kinetic mechanism capable of representing different blends of gasoline-ethanol through the Direct Ratio Graph method associated with sensitivity analysis. A mechanism containing 1410 species and 6107 elemental reactions was successfully reduced to a skeleton mechanism containing 204 species and 1158 elementary reactions. The resulting mechanisms were validated with experimental data obtained by Mehl, 2011, Marinov, 1999.*

***Keywords:*** *Gasoline surrogate, Ethanol, Kinetic Mechanism Reduction*



Proceedings of the XXXVIII Iberian Latin-American Congress on Computational Methods in Engineering P.O. Faria, R.H. Lopez, L.F.F. Miguel, W.J.S. Gomes, M. Noronha (Editores), ABMEC, Florianópolis, SC, Brazil, November 5-8, 2017.

# 1 INTRODUCTION

The accurate prediction of the combustion behavior in internal combustion engines, via numerical simulation, depends heavily on the kinetic data of the chemical components of fuels used under different operating conditions, Mehl *et al.* (2011). Due to the strong nonlinearity and the fact that the complete fuel mechanism contains hundreds of species and involves thousands of elementary chemical reactions, which requires great computational effort to simulate the system, its use is often impracticable for industrial applications, considering the time required, Curran *et al.* (2011).

The behavior of gasoline combustion follows a complex group of elementary reactions. Due to the great variation on petroleum source, composition and its processing, it is not possible to establish an universal gasoline composition. The use of a mixture of different hydrocarbon species, named as gasoline surrogate, is widely accepted as a simplification method for reproducing the combustion course of gasoline, reducing the computational effort and the investments on composition analysis of each gasoline sample used, Naik *et al.* (2005).

An expressive number of different gasoline surrogate mixtures have been developed by research groups. Naik *et al.* (2005), proposed a surrogate mixture of five components: Isooctane ($C_8H_{18}$), n-heptane ($C_7H_{16}$), toluene ($C_6H_5CH_3$), methyl cyclohexane ($C_7H_{14}$) and 1-pentene ($C_5H_{10}$). Lenhert *et al.* (2005) considered a mixture of Isooctane, n-heptane, toluene, and 1-pentene as a combination capable of representing gasoline on their study.

The simplification of a gasoline composition through the creation of a gasoline surrogate is not sufficiently capable to produce a mechanism small enough to be used in 3D simulation. Therefore, the use of reduced kinetic mechanisms, capable of reproducing the main characteristics of these fuels considering only some key species and reactions involved during combustion is an interesting alternative to reduce the computational effort and the time spent during simulations, Pepiot *et al.* (2008).

Ethanol in Brazil has been used in either blends with gasoline or pure since 1931, but gained more attention in 1975 with the "Pro-Alcohol" program. Later in 2003, with the introduction of the flex fuel vehicles to the national fleet, ethanol gained more space among liquid fuels, Delgado *et al.*(2007). This has happened mainly to reduce the dependency on fossil fuels. On the other hand it presents other benefits, such as: ethanol being a renewable fuel, has better combustion characteristics and its use being capable of reducing some pollutant's emissions, Catapano *et al.*(2016).

The use of blended gasoline-ethanol fuels is an important approach on the reduction on fossil fuel dependence and on the mitigation of greenhouse gases emissions. Some gasoline and ethanol properties are summarized in Table 1. Ethanol has a higher octane number than gasoline, so, the use of gasoline blended with ethanol allows the operation at higher compression ratios, improving efficiency and power output, Bata *et al.* (1989); the flammability and oxygenated characteristic of ethanol are some of the reasons that lead to a reduction of CO and HC emissions, Bata *et al.* (1989) ; due to lower flame temperatures, in comparison with gasoline, lower heat loss to the combustion chamber walls and higher thermal efficiency are expected by the use of ethanol, Owen *et al.* (1995).



Proceedings of the XXXVIII Iberian Latin-American Congress on Computational Methods in Engineering
P.O. Faria, R.H. Lopez, L.F.F. Miguel, W.J.S. Gomes, M. Noronha (Editores), ABMEC, Florianópolis, SC, Brazil, November 5-8, 2017.

**Table 1. Properties of gasoline and ethanol. Heywood (1988).**

| Parameter | Gasoline | Ethanol |
|---|---|---|
| Formula | $C_nH_{1,87n}$ | $C_2H_6O$ |
| Molecular weight ($kg.kmol^{-1}$) | ~110 | 46,07 |
| RON | 91 - 99 | 107 |
| MON | 82 - 89 | 89 |
| Lower heating value (MJ/kg) | 44 | 26,9 |
| Specific gravity ($kg/cm^3$) | 0,72 - 0,78 | 0,785 |

With regard to the consolidation of alternative fuels and the need of numerical simulations to predict the behavior of engines with specific combinations of blends of ethanol in gasoline, the present work aimed to create a reduced kinetic combustion model capable of representing the behavior of gasoline containing a range of ethanol fractions from 0 to 1v/v.

Among the first methods of reducing mechanisms, emphasis should be given to those based on time scale analysis, such as: Computational Singular Perturbation, Intrinsic Low Dimensional Manifolds, and Level of Importance methods. These methods are premised on the elimination of species and reactions, considered as unnecessary based on considerations of quasi-steady-state or partial equilibrium reactions, Terese (2012).

For the quasi-steady-state assumption it is assumed that the rate of consumption of some species overcome the rate of formation of them. The net production rate of the species under this consideration is, therefore, negligible and they would not have a significant influence on the combustion process. Generally, this hypothesis can be applied for intermediate species produced through lethargic reactions and consumed by faster reactions. In a different manner, the partial equilibrium hypothesis is applied for reactions whose reaction rates coefficients', forward and backward, are considerably bigger than the other reactions involved on the combustion process, Terese (2012) and Marzia (2007).

A different approach on the mechanism reduction procedure is the Directed Relation Graph (DRG). This method eliminates unimportant species and reactions by quantifying the coupling between species, attributing to it a coefficient, $r_{AB}$, which represents the error introduced on species A formation rate as a consequence of eliminating species B from the mechanism. The removal occurs if $r_{AB}$ is bigger than a defined threshold, Terese (2012).

The application of sensitivity analysis on mechanism reduction is based on the investigation of the variation in a parameter of interest due to changes in a controlling variable. In the case of this work, the parameter of interest is the ignition delay time; the

controlling variable is changed by removing one by one a fraction of species in the mechanism. The species, and the reactions related to them, which do not have a significant impact in the controlling parameter are removed, Lebedev *et al.*(2012).

This paper proposes the use of the directed relation graph method with sensitivity analysis (DRG-SA) as a tool for the systematic reduction of detailed mechanisms. The DRG-SA method have shown a great potential of generating skeleton models, consisting of the lowest possible number of species and reactions, for the combustion of large hydrocarbon fuels.

As a validation parameter, ignition delay time data obtained experimentally through shock tube analysis was used. The results were then compared to the data obtained in computational simulations for the complete and reduced mechanisms, Mehl *et al.* (2011) and Marinov (1999).

# 2 METHODOLOGY

The methodology proposed was divided into five steps. The first one was the creation of a gasoline surrogate composed by a smaller number of components than the complete gasoline formulation, based on a chemical composition analysis. The second step was the creation of a detailed kinetic mechanism capable of reproducing the characteristics of the surrogate and its blends with ethanol. The next step was the mechanism reduction through the directed relation graph method, by which unimportant species and reactions were removed. The next step was a sensitivity analysis used to achieve a greater reduction by removing species which do not have a significant impact on the simulation of ignition delay time data. The final step was the validation of the obtained mechanism with experimental data for the gasoline surrogate without ethanol addition (E0), and for the ethanol (E100), covering the interval from 0% to 100% of ethanol addition.

The parameter selected to validate the final mechanism was the ignition delay time, $\tau_{id}$. The ignition delay is considered, for engine simulation, as the time elapsed from the start of injection to the start of combustion. The Chemistry tool of the software CONVERGE CFD was used to simulate this parameter. The simulation proceeds by burning the fuel mixture in a constant-volume spherical vessel. The software considers the ignition delay as the time required to a temperature increasing of 400K from its initial value, $T_0$, as shown in Figure 1, Richards *et al.* (2017).



Proceedings of the XXXVIII Iberian Latin-American Congress on Computational Methods in Engineering P.O. Faria, R.H. Lopez, L.F.F. Miguel, W.J.S. Gomes, M. Noronha (Editores), ABMEC, Florianópolis, SC, Brazil, November 5-8, 2017.

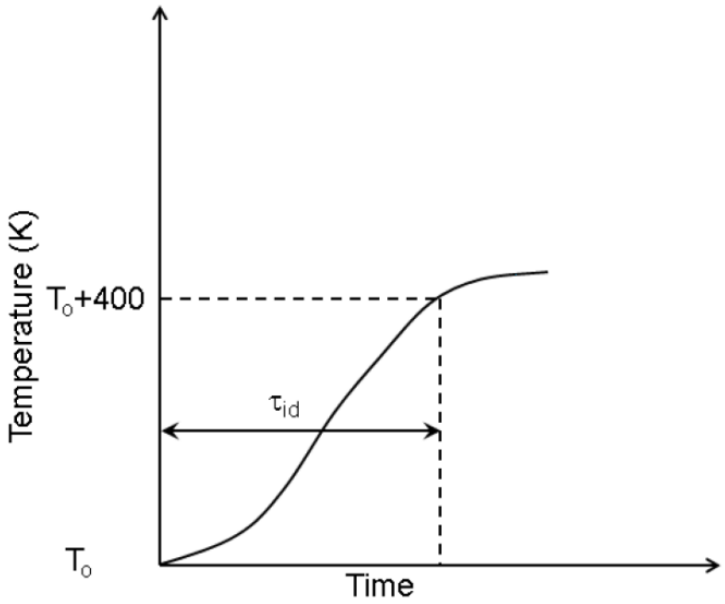


**Figure 1. Ignition delay time calculation in CONVERGE CFD, Chemistry tool, Richards *et al.* (2017).**

The simulations were conducted for pressures of 10, 20, 40 and 80 bar; temperatures from 600K to 1000K; stoichiometric condition; and for blends containing 0% and 100% of ethanol in volume. The samples were named as E0 and E100, respectively.

## 2.1 Fuel composition

For the fuel composition, a chemical analysis was conducted by the Fuel testing laboratory of the Chemical department of the Federal University of Minas Gerais (UFMG). The analysis defined the fractions of Alkanes, Olefins and Aromatics of the fuel through the GS 1000 equipment, according to internal methodology. At this work, following the methodology of Cai *et al.* (2014), a mixture of Iso-octane, n-Heptane, Heptene and Toluene was chosen as a proper gasoline surrogate, representing the fractions of Alkanes, Olefins and Aromatics, respectively. It was decided to use a mixture of Iso-octane and n-Heptane to represent the alkane's fraction, so that it was possible to assure that the theoretical Research octane number (RON) and Motor octane number (MON) were as close as possible to the experimental data obtained for the base fuel. The proportion of Iso-octane and n-Heptane were defined base on Eq.1 and Eq.2.

$$RON_{bf} = \sum_i RON_i x_i \tag{1}$$



Proceedings of the XXXVIII Iberian Latin-American Congress on Computational Methods in Engineering P.O. Faria, R.H. Lopez, L.F.F. Miguel, W.J.S. Gomes, M. Noronha (Editores), ABMEC, Florianópolis, SC, Brazil, November 5-8, 2017.

$$MON_{bf} = \sum_i MON_i x_i \tag{2}$$

Where, $RON_{bf}$ and $MON_{bf}$ are the research and motor octane numbers obtained experimentally for the base fuel, E0; $RON_i$ and $MON_i$ are the theoretical research and motor octane numbers of the component i; and $x_i$ is the mole fraction of the component i.

## 2.2 Mechanism creation

The complete mechanism was divided into a mixture of n-heptane and iso-octane, primary reference fuels (PRF), Toluene, Polycyclic aromatic hydrocarbons (PAH), Heptene, Ethanol and Nitrogen oxides. The detailed kinetic mechanism for the PRF and Heptene mixture was obtained by the research group of Lawrence Livermore National Laboratory of United States, developed by Mehl *et al.* (2009). The PRF mechanism contains 878 species and 3796 elementary reactions.

The toluene oxidation model was adopted from the study of Nakamura (2014). The model consists of 550 species and 2805 elementary reactions. For the Ethanol fraction the mechanism developed by Roehl (2009), was adopted. The mechanism has 38 species and 228 elementary reactions. The Nitrogen Oxides formation mechanism adopted was based on the Lamoureux model (2010) and was also incorporated to the final mechanism.

The individual mechanism were combined using an interactive tool, MechMerge, from the software CONVERGE CFD. This utility is capable to identify repeated species and reactions contained into each model so that the final mechanism does not have species or reactions conflicts.

The final mechanism obtained was composed by 1410 species and 6107 elementary reactions.

## 2.3 Mechanism reduction

### 2.3.1 DRG Method

The concept of creating a skeletal kinetic mechanism consists to identify and remove unimportant chemical species and the elementary reactions associated with them from a complete mechanism.

The DRG method uses a digraph representation, as shown on Figure 2, of the complete kinetic mechanism composed by vertices connected by edges with specific directions. Each vertex represents a species in an elementary reaction of the mechanism; an edge exists between two vertices if the two species represented by them are present in the same reaction.



Proceedings of the XXXVIII Iberian Latin-American Congress on Computational Methods in Engineering P.O. Faria, R.H. Lopez, L.F.F. Miguel, W.J.S. Gomes, M. Noronha (Editores), ABMEC, Florianópolis, SC, Brazil, November 5-8, 2017.

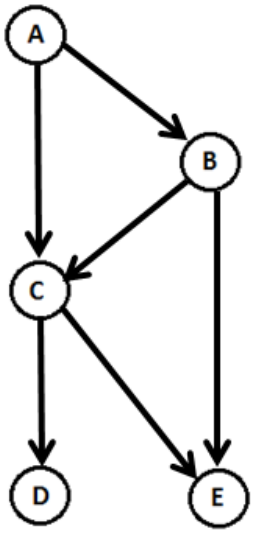


**Figure 2. Schematic configuration of the directed relation graph, Richards *et al.* (2017).**

The DRG method starts by coupling species directly related, species present in the same reaction, which implies that the removal of species B, from the mechanism described in Figure 2, leads to an error to the production rate of species A. This error, $r_{AB}$, can be obtained from Eq. 3.

$$r_{AB} \equiv \frac{\sum_{i=1,I}\left|v_{A,i}\omega_i\delta_{Bi}\right|}{\sum_{i=1,I}\left|v_{A,i}\omega_i\right|} \tag{3}$$

$$\delta_{Bi} = \begin{cases} 1, if\ the\ i^{th}\ reaction\ involves\ species\ B \\ 0, any\ other\ way \end{cases}$$

Where $v_{A,i}$ indicates the stoichiometric coefficient of the species A in a reaction $i$. $\omega_i$ is the difference between the forward and backward reactions, the net rate. The terms in the denominator of Eq. 3, represent the contributions of each reaction to the rate of production of species A. The terms in the numerator correspond to the influence of the reactions which contain the species A and B, notice that when the reaction does not contain both of species, the contribution will be 0.

The analysis starts with a set of major species, the fuel for example. Each major species will have a digraph as shown in Figure 2. The final mechanism will be a combination of all major species digraph.

If the error, $r_{AB}$, overcomes a defined threshold value, $\varepsilon$(cut-off tolerance), the elimination of species B would lead to a considerable error in the rate production of A, therefore, species B must be retained on the skeletal mechanism. There are also the species which are indirectly connected to the major ones. That is the case of species D and E

presented in Figure 2. Species D and E are indirectly connected to species A by intermediately species C and B, respectively. The indirectly connected species are maintained in the final mechanism if they are required for the correct prediction of the production rate of the intermediate species between them and the major species.

During the reduction process, the software CONVERGE calculates all $r_{AB}$ coefficients and then, different values of $\varepsilon$ are imposed and a reduced mechanism is generated for each one of them. One by one, all reduced mechanism are used to create an ignition delay profile, then, the data obtained is compared with the one from the detailed mechanism. The optimum mechanism is chosen as the smallest one with an ignition delay time deviation from the obtained using the detailed mechanism lower than the tolerance defined by the user.

### 2.3.2 Sensitivity Analysis

Once a reduced mechanism is obtained from the DRG method, a sensitivity analysis (SA) is performed in order to reduce even more the mechanism.

Sensitivity analysis can be very time consuming, when it is applied to all species involved in the combustion process, therefore, the methodology used in CONVERGE CFD rearrange the remaining species in the pre-reduced mechanism, obtained after the DRG method, in ascending order of $r_{AB}$ and just a fraction of these species, from the top of the list, is selected to perform the sensitivity analysis. This set of species is call as limbo species. Thus, the species analyzed are those which have the greatest potential to be considered unimportant on the prediction of ignition delay times.

The consequent ignition delay error produced by removing each limbo species from the mechanism is compared with the data obtained for the detailed mechanism and the one obtained from the DRG method, as shown in Eq. 4.

$$\delta_B = \left|\delta_{B,ind} - \delta_{DRG}\right| \tag{4}$$

Where $\delta_{B,ind}$ is the induced error generated by removing of species B regarding the detailed mechanism and $\delta_{DRG}$ is the error of the DRG generated mechanism. The species are then organized in ascending order of $\delta_B$ to remove unimportant species based on it. If this error does not exceed a threshold value defined by the user, the species can be removed.

## 3 RESULTS

## 3.1 Fuel composition

The fuel composition obtained initially for the fuel E0 is presented on Table 2.



Proceedings of the XXXVIII Iberian Latin-American Congress on Computational Methods in Engineering P.O. Faria, R.H. Lopez, L.F.F. Miguel, W.J.S. Gomes, M. Noronha (Editores), ABMEC, Florianópolis, SC, Brazil, November 5-8, 2017.

**Table 2. Base fuel - group composition.**

| Group | Mass fraction |
|---|---|
| Alkanes | 0,3697 |
| Olefins | 0,1780 |
| Aromatics | 0,4523 |

After the proportion between iso-Octane and n-Heptane being determined, the final composition of the E0 and E100 fuels is presented on Table 3.

**Table 3. Final fuel composition.**

| Component | Mole fraction | |
|---|---|---|
| | E0 | E100 |
| n-Heptane | 0,1090 | 0,0 |
| isso-Octane | 0,2250 | 0,0 |
| Toluene | 0,4864 | 0,0 |
| Heptene | 0,1796 | 0,0 |
| Ethanol | 0,0 | 0,8810 |
| Water | 0,0 | 0,1190 |

## 3.2 Base mechanism validation

The base mechanism obtained for the gasoline surrogate and its blends with ethanol containing 1410 species and 6107 elementary reactions was validate with experimental data from Mehl *et al.* (2011), for the E0 fuel, and with experimental data from Marinov (1999). The results are presented on Figures 3 and 4.

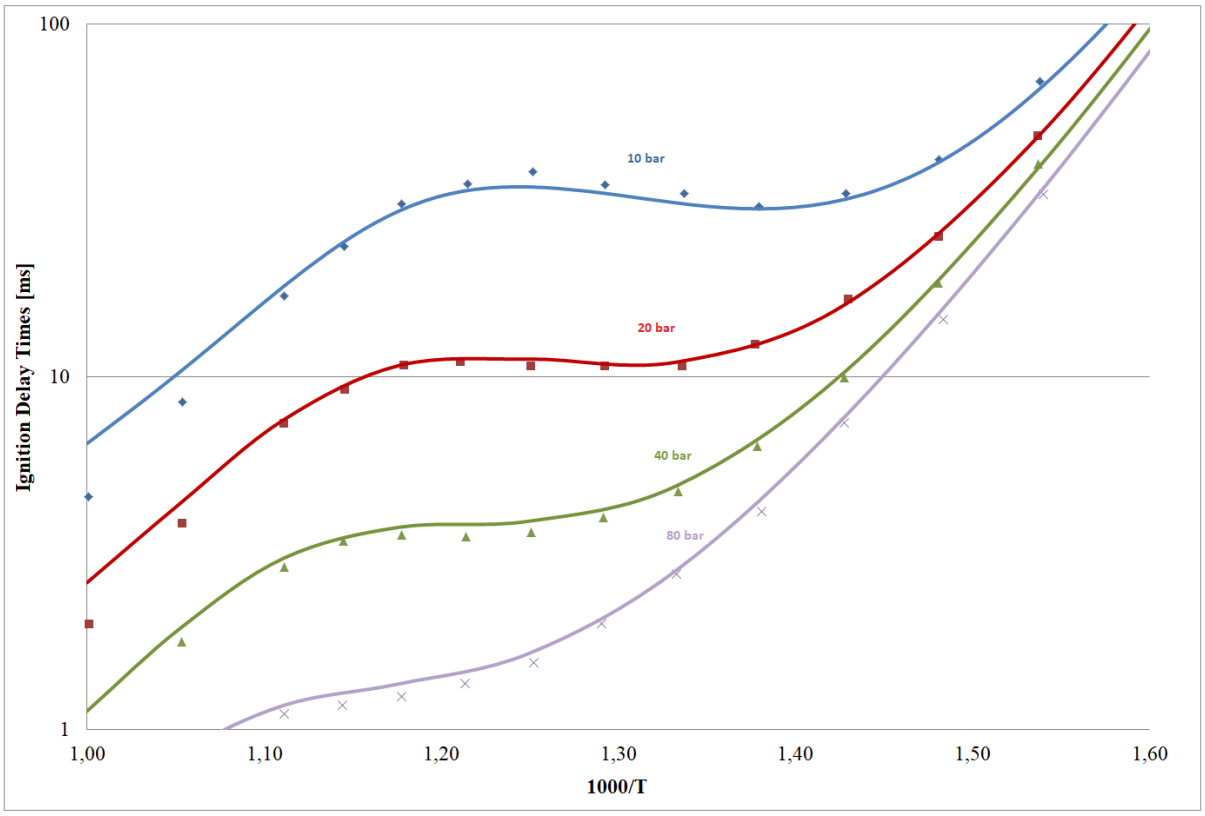


**Figure 3. Ignition delay time data for the E0 fuel simulated with the detailed mechanism. Solid lines: numerical simulation; dashed lines: experimental data.**

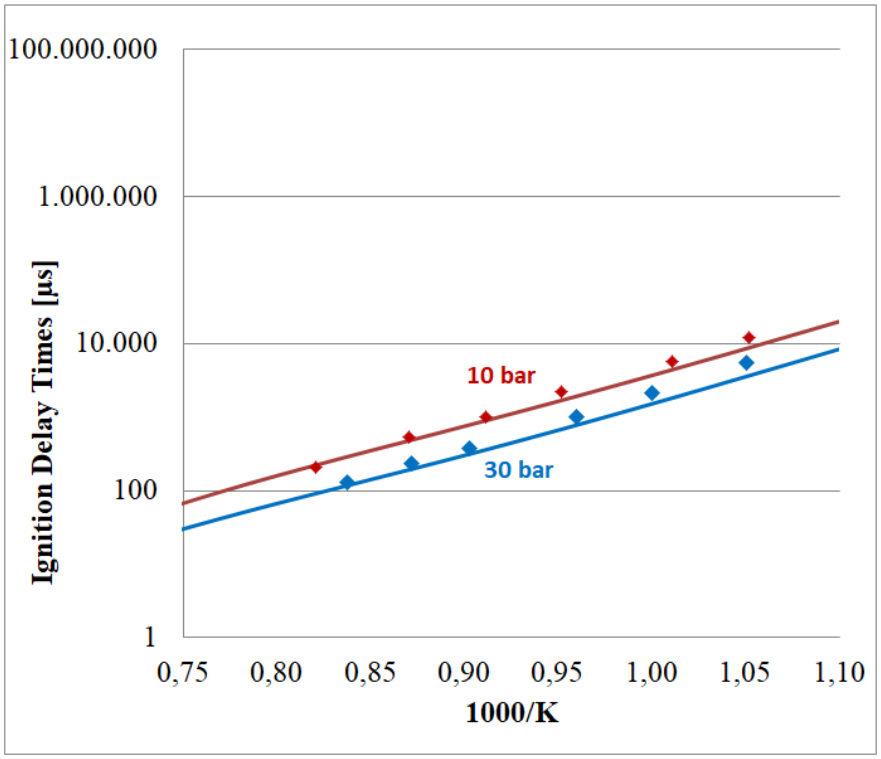


**Figure 4. Ignition delay time data for the E100 fuel simulated with the detailed mechanism. Solid lines: numerical simulation; dashed lines: experimental data.**

The results for both, E0 and E100, showed a great correlation with the experimental data from Mehl *et al.* (2011) and Marinov (1999), respectively. For the E0 simulations the model has a bigger deviation at intermediate temperatures close to the negative temperature coefficient and for higher temperatures. The deviations became smaller as the pressure was increased.

## 3.3 Reduced mechanism validation

The reduced mechanism accomplished consists of 204 species and 1158 elementary reactions. The results for the simulations with the reduced mechanism are presented on Figures 5 and 6.

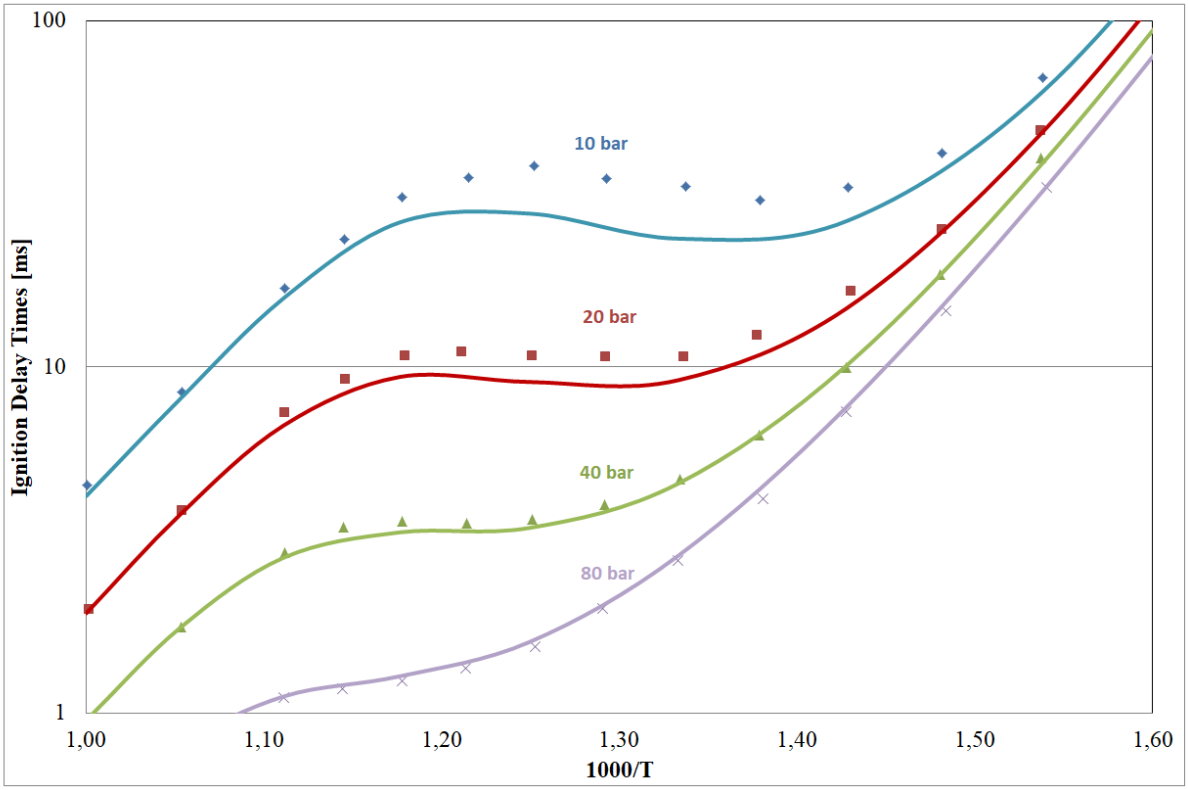


**Figure 5. Ignition delay time data for the E0 fuel simulated with the reduced mechanism. Solid lines: numerical simulation; dashed lines: experimental data.**

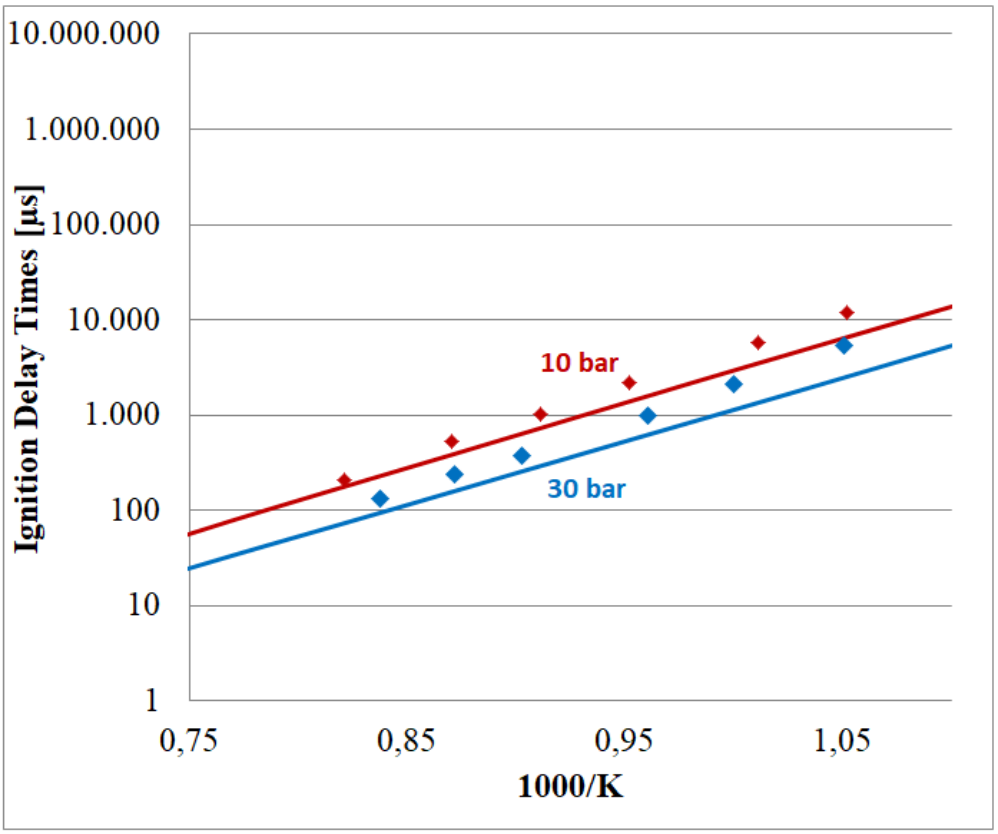


**Figure 6. Ignition delay time data for the E100 fuel simulated with the reduced mechanism. Solid lines: numerical simulation; dashed lines: experimental data.**

The results obtained with the reduced mechanism have a good correlation with the experimental data for the fuel E100 for the different pressures and temperatures tested. However, for the fuel E0 the correlation for intermediate temperatures, close to the NTC, was not so good for the pressures of 10 bar and 20 bar. For bigger pressures the model has shown a better agreement, indicating that its use is limited for those conditions.

## CONCLUSIONS

The detailed mechanism has shown a great agreement with the experimental data. However, its use at 3D simulations is limited, once its size requires a big computational effort. The reduced chemical kinetic mechanism obtained has shown a good correlation with the experimental data from Mehl (2011) and Marinov (1999), especially for low and high temperatures for pressures under 20 bar. For pressures between 40 bar and 80 bar the simulation results had a great agreement with the experimental data for all temperatures tested.

## ACKNOWLEDGEMENTS

The authors would like to thank Fiat Chrysler Automobiles (FCA) for financial support and stimulate the technological development on the automotive sector in Brazil.

## REFERENCES

Bata, R.M, Elord, A.C, Rice, R.W. (1989). *Emissions from IC engines fueled with alcohol–gasoline blends: a literature review*. Transactions of the ASME. 111: 424-431.

Blouza, A., Coquel, F., Hamel, F. (2000). *Reduction of linear kinetic systems with multiple scales*. Combust. Theory Modelling, 4: 339-362.

Cai, L., Pitsch, H. (2014). *Optimized chemical mechanism for combustion of gasoline surrogate fuels*. Combustion and flame, 162(5), 1623-1637.

Catapano, F., Sementa, P., Vaglieco, B.M. (2016). *Air-fuel mixing and combustion behavior of gasoline-ethanol blends in a GDI wall-guided turbocharged multi-cylinder optical engine.* Elsevier. Renewable Energy. 96: 319-332.

Curran, H.J., Gaffuri, P., Pitz, W.J., Westbrook, C.K. (2011). Lawrence Livermore National Laboratory, Livermore, CA 94551.

Delgado, R.C.O.B., Araujo, A.S., Fernandes Jr., V.J. (2007). *Properties of Brazilian gasoline mixed with hydrated ethanol for flex-fuel technology.* Fuel Process. Technol. 88: 365-368.

Gauthier, B.M., Davidson, D.F., Hanson, R.K.(2004). *Shock tube determination of ignition delay times in full-blend and surrogate fuel mixtures*. Elsevier. Combustion and Flame. 139: 300-311.

Heywood, J. B. (1988). *Internal Combustion Engine Fundamentals (1$^{st}$ edition)*. Education, McGraw-Hill.

Lamoureux, N., Desgroux, P., Bakali, A.E., Pauwels, J.F. (2010). Experimental and numerical study of the role of NCN in NO formation in low pressure CH4-O2-N2 and C2-H2-O2-N2 flames. Combustion and Flame 157 – 1929-1941.

Lebedev, A., Okun, M., Chorkov, V., Tokar, P., Strelkova, M. (2012). *Systematic procedure for reduction of kinetic mechanisms of complex chemical processes and its software implementation*. Journal of Mathematical Chemistry. 51: 73-107.

Lenhert D.B., Cernansky NP, Miller D.L. (2005) *Oxidation of large molecular weight hydrocarbons in a pressurized flow reactor.* Proceedings of the 4th Joint Meeting of the U.S. Sections, Philadelphia.

Marinov N.M.. (1999). *A detailed chemical kinetic model for high temperature ethanol oxidation.* Int. J. Chem. Kinet. 31: 183–220.

Marzia, B., Fiammetta, C., Laurent, D. (2007). *Quase-steady-state approximation for reaction-diffusion equations*. Bulletin of the Institute of Mathematics Academia Sinica. Vol. 2, N°4: 823-850.

Mehl, M. Curran, H. J., Pitz, W. J., Westbrook, C. K. (2009). *Chemical kinetic modeling of component mixtures relevant to gasoline.* European Combustion Meeting, Vienna, Austria.

Mehl, M., Pitz W.J., Westbrook, C.K., Curran, H.J. (2011). *Kinetic modeling of gasoline surrogate components and mixtures under engine conditions.* Elsevier. Proceedings of the Combustion Institute. 33: 193-200.

Naik, C., Pitz, W., Westbrook, C., Sjöberg, M. et al.. (2005). *Detailed Chemical Kinetic Modeling of Surrogate Fuels for Gasoline and Application to an HCCI Engine*. SAE Technical Paper 2005-01-3741.

Nakamura, H., Darcy, D., Mehl, M., Tobin, C.J., Metcalfe, W.K., Pitz, W.J., Westbrook, C.K., Curran, H.J.. (2014). *An experimental and modeling study of shock tube and rapid compression machine ignition of n-butylbenzene/air mixtures.* Combustion and Flame 161 - 49-64.

Owen, K., Coley, T. (1995). *Automotive fuels reference book".2nd ed. Society of Automotive Engineers*, Inc., USA.

Pepiot-Desjardins, P., Pitsch, H. (2008). *An efficient error-propagation-based reduction method for large chemical kinetic mechanism.* Elsevier. Combustion and Flame. 154: 67-81.

Richards, K. J., Senecal, P. K., Pomraning, E. (2017). CONVERGE Manual (v2.4), Convergent Science, Inc., Madison, WI.

Rohl, O., Peters, N. (2009). *A Reduced Mechanism for Ethanol Oxidation.* Institut fur Technische Verbrennung RWTH Aachen University. Aachen, Germany.

Soares, L. d. B., Alves, B. J. R., Urquiaga, S., & Boddey, R. M. (2009). *Mitigação das emissões de gases efeito estufa pelo uso de etanol da cana-de-açúcar produzido no Brasil*. Embrapa Agrobiologia-Circular Técnica (INFOTECA-E).

Tan, J. Y., Bonatesta, F., Ng, H. K., & Gan, S. (2016). *Developments in computational fluid dynamics modelling of gasoline direct injection engine combustion and soot emission with chemical kinetic modelling*. Applied Thermal Engineering, 107, 936-959.

Terese, L. (2012). *Chemical Kinetics. Chapter 4: Model reduction techniques for chemical mechanisms*. Department of Energy and Process Engineering. Norwegian University of Science and Technology. Norway.

**Definitions/Abbreviations**

| | |
|---|---|
| $r_{AB}$ | Introduced error from B to A. |
| $\tau_{id}$ | Ignition delay time. |
| $\mathbf{T_0}$ | Initial temperature. |
| $v_{A,i}$ | Stoichiometric coefficient of species A in a reaction i. |
| $\omega_i$ | Net reaction rate |

| | |
|---|---|
| $\delta_B$ | Induced error |
| $\varepsilon$ | Cut-off tolerance |
| **DRG** | Direct relation graph |
| **SA** | Sensitivity analysis |
| **CTM** | Mobility Technology Center |
| **PAH** | Polycyclic aromatic hydrocarbons |
| **PRF** | Primary reference fuel |
| **RON** | Research octane number |
| **MON** | Motor octane number |
| **x** | Molar fraction |