22nd International Conference on Renewable Energies and Power Quality (ICREPQ'24)
Bilbao (Spain), 26th to 28th June 2024

ISBN: 978-84-09-60656-6

MATLAB Application for determination of 12 Combustion Products, Flame Temperature and Laminar Burning Velocity

R. Cisneros[1] and F. Rojas[1]

[1] Department of Mechanical Engineering
Faculty of Science and Engineering, Pontifical Catholic University of Peru
Av. Universitaria 1801, San Miguel
15088, Lima (Peru)
Phone/Fax number: +51 626-2000

Abstract. The aim of the present work is to contribute to the scientifical community by presenting a simple software tool, MATLAB Application for determining 12 combustion products, flame temperature and laminar burning velocity. The application was developed in the MATLAB App designer for 6 pre-set fuels and 12 combustion products. It is code consist in numerical methods, a variety of conditions and loops evaluation. To summarize, the app will serve as a reference or data source for further experimental or other complex combustion simulation work related because it demonstrates to had similar results compared to some previous studies. Moreover, it has the possibility to use a variety of features and to implement new versions or upgrades for personal purpose needs.

Key words. Burning velocity, combustion products, flame temperature, numerical methods, MATLAB programming.

1. Introduction

In the last decade, industries such as automotive and transport are changing the way we move for more than 30 years, and it is called the electrification era. But at the same time, the idea of developing and doing research related to fuels and their properties is to improve how they performed in all the systems in which they take part so this is a constant requirement for the scientific community. Simulations and numerical studies are the first step for many studies in order to see how the results could be and to analyse and identify the possible differences when an experimental work is being done. Simulation software tools such as Ansys Chemkin, Cantera and programming tools like MATLAB and Python are used for many cases of study and by using them it is possible to observe and have a first view of what is the behaviour of the fuel in a system. In order to mention some fuel combustion properties, the burning velocity, flame temperature and the proportions of products after the combustion process are for many authors and institutions a topic of interest. The aim of the present work is to present an application for determining these properties by using MATLAB and numerical methods. The MATLAB app developer is a powerful tool that let scientists and engineers design applications and at the same time set the necessary boundaries of the process. Moreover, the MATLAB Application methodology was validated in the article 'Determination of 12 combustion products, flame temperature, and laminar burning velocity of Saudi LPG using numerical methods coded in a MATLAB application' [1]. The MATLAB Application is open code source so any user can improve it by adding for fuels, tools or upgrading the code methodology for the calculus process of the properties.

2. MATLAB Application functionality and features

The MATLAB Application functionality and features are described based on the different pre-set fuels and available variables with the different kind of plots to be used. The complete package is possible to be download from https://doi.org/10.5281/zenodo.7894133 [2].

A. *Application main files*

The MATLAB Application consists in the following files:

1) *New_code.m*: Code file that read all the necessary inputs (fuel properties, equivalence ratio, start temperature, work pressure) to perform the iteration process in order to obtain the results (combustion products, flame temperature and laminar burning velocity)
2) *Fractions_Derivatives.m*: Code file that performs each iteration in which the numerical methods (Taylor series, gaussian elimination and newton Raphson) are applied.
3) *MATLAB_Application.mlapp:* App code file that has all the functionality and features of the application deployed in code lines. The initializing parameters are set here.
4) *REACTANTS ENTHALPY.xlsx:* Excel file that contains the properties (CHON elements quantity, enthalpy at 0°, sensitive heat to 298 K, average molar mass) of the fuels set in the application.

5) *DILUENTS ENTHALPY.xlsx:* Excel file that contains the properties (CHON elements quantity, enthalpy at 0°, sensitive heat to 298 K, average molar mass) of the diluents set in the application.
6) *Products.xlsx:* Excel file with the properties (Molar mass, enthalpy and heat at constant pressure) of the 12 products.
7) *Ansys Chemkin Results (0.6-1.7).xlsx:* Combustion products, flame temperature and laminar burning velocity results corresponding to a simulation performed in Ansys Chemkin R2 2022 by using the San Diego Mechanism [3], GRIMMECH 3.0 [4] and RedSD [5] for all the pre-set fuels. These results are used in the application to make further comparation and analysis work of the results.

The mentioned files need to be in the same path folder when the application is started so a MATLAB alert will not appear during the initializing process.

B. *Initializing the application*

First, a MATLAB version needs to be installed in the electronic device while at the same time it is necessary to be at least the 2021b version, as it is in this version where the application was developed.

1) *Download and open the MATLAB Application Folder:* The MATLAB_Application.zip has all the previously mentioned files in order to run the application. When starting MATLAB, there is a high possibility that the path folder is not the correct one, so a manual correction is required for the first run.

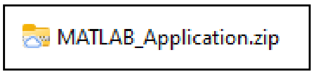

Fig.1. MATLAB Application zip folder available for downloading.

2) *Click on the MATLAB Application icon*

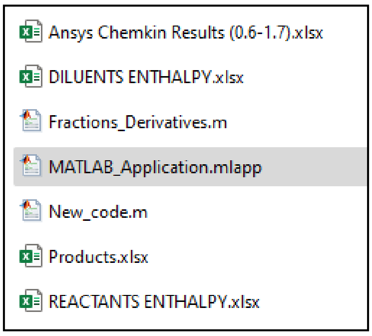

Fig.2. MATLAB Application file.

3) *First view*

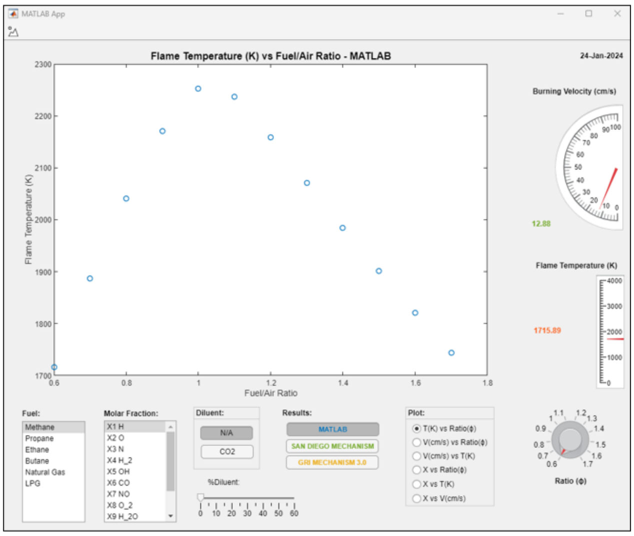

Fig.3. First view of the MATLAB Application once is initialized [1].

C. *Application Main parts*

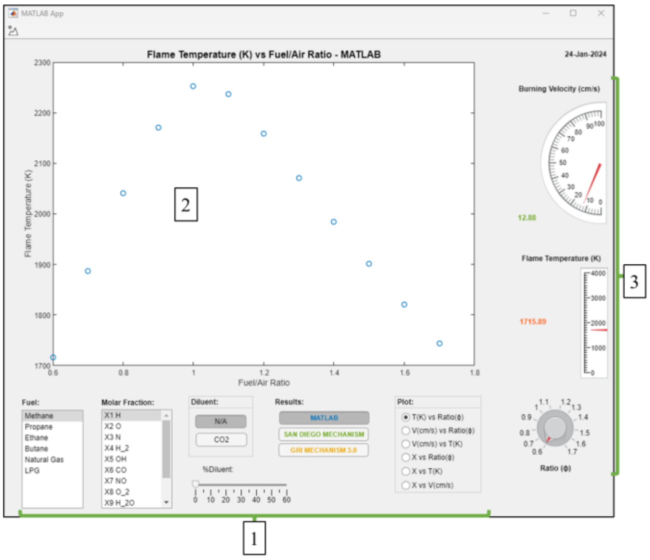

Fig.4. First view of the MATLAB Application once is initialized [1].

1) *Controls zone*: The controls zone is where the results are configurated in order to show the most relevant information for the user.
2) *Plot zone*: The plot zone is where results are shown and is configurated directly by all the selections done in the controls zone.
3) *Results gauges zone:* For this zone, the burning velocity and flame temperature values are shown in two different types of gauges and their value will depend directly on which ratio is selected in the ratio knob.

D. *Features and tools description*

The features and tools are the ones corresponding to the Controls zone identified in Figure 4 as number 1 and Results gauges zone as number 3.

1) *Fuel box:* In the fuel box selector, the fuels pre-set and defined in the file REACTANTS ENTHALPY.xlsx appears as options of fuels in order to their results be presented in the plot zone. The MATLAB application had defined the following fuels: Methane, Propane, Ethane, Butane, Natural Gas and LPG.

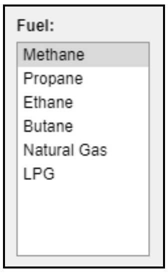

Fig.5. Fuel list box.

2) *Molar Fraction box (Combustion products):* This box allows the user to select between the 12 combustion products that are included in the combustion reaction equation. By default, X1 H (Hydrogen) is selected and in order to see the corresponding plot, on the Plot button list one of options corresponding to molar fraction (X vs.) must be selected.

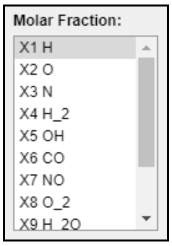

Fig.6. Molar fraction (combustion products) list box.

3) *Diluent box:* The diluent box adds in the combustion reaction equation the elements pre-set, in this case CO_2 is the only configurated to appear and to be selected. N/A is for non aplicable.

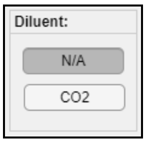

Fig.7. Diluent box.

4) *%Diluent bar:* This tool set the volumetric percentage in the mixture that is for the diluent selected in the diluent box. The bar is able to set a percentage from 0 to 60% (0, 10, 20, etc.).

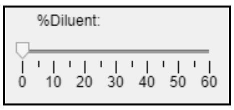

Fig.8. Diluent box.

5) *Results button list:* The results button list allows the user to compare 3 sources of results for the fuels set in the application. For all the fuels except LPG (for interest reasons in other research) the results obtained by MATLAB program, Ansys Chemkin using San Diego mechanism [3] and using GRIMECH 3.0 [4] are available. For LPG the results obtained by MATLAB program, Ansys Chemkin simulation using San Diego mechanism [3] and RedSD mechanism [5] are available.

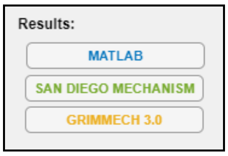

Fig.9. Results button list for all fuels except LPG.

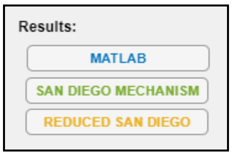

Fig.10. Results button list for LPG.

6) *Plot button list:* The plot button list has included all the possible plots that can be presented in the plot zone (identify in Figure 4 as number 2). The default plot is Flame Temperature (T in K) versus Ratio(ϕ). In order to compare other variables the following plots were added: Burning velocity (V in cm/s) versus Ratio, Burning velocity versus Flame Temperature, Molar Fraction (Combustion product as X) versus Ratio, Molar Fraction versus Flame Temperature and Molar Fraction versus Burning velocity.

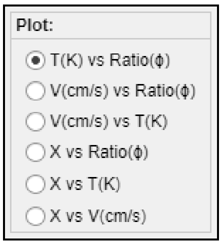

Fig.11. Plot button list.

7) *Burning Velocity Semicircular gauge:* The semicircular gauge shows the burning velocity value in cm/s for the Ratio (ϕ) selected in the knob ratio.

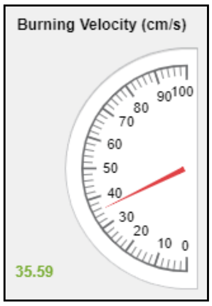

Fig.12. Burning velocity semicircular gauge.

8) *Flame temperature linear gauge:* The flame temperature linear gauge show the falme temperature value value in K for the Ratio (ɸ) selected in the knob ratio.

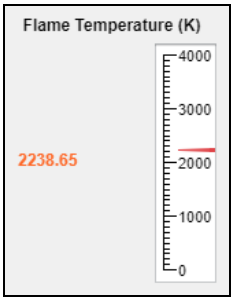

Fig.13. Flame temperature linear gauge.

9) *Ratio knob:* The knob configurate both burning velocity and flame temperature gauges so is possible to see the values for the require ratio.

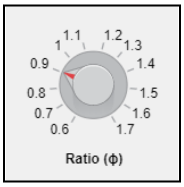

Fig.14. Ratio knob.

E. *Using the app*

An example of application is presented in order to show how the app works. All the tools are used so the effect of these on the plot zone is possible to see. For this case of study, the selected fuel is Natural Gas with 10% of CO_2.

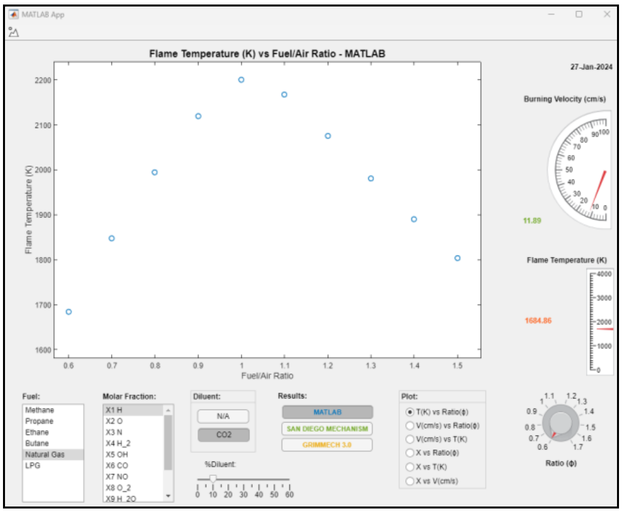

Fig.15. MATLAB Application T(K) vs Ratio plot with Natural Gas and 10% CO_2 as fuel selected.

In order to see the comparation with the other two sources of results, the buttons corresponding to the results simulation using both San Diego mechanism and GRIMMECH 3.0 are selected.

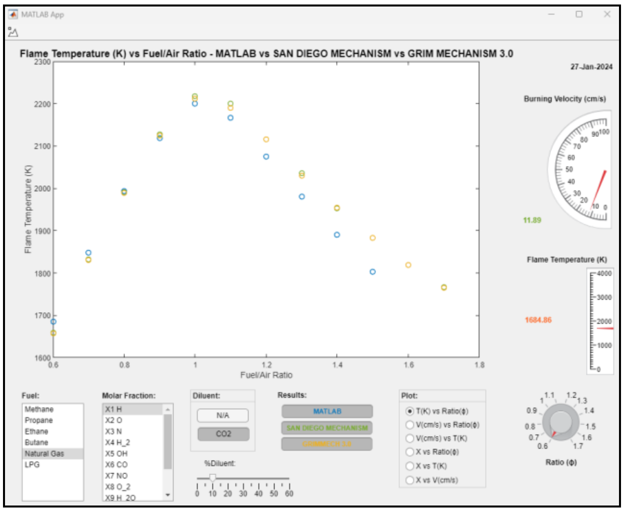

Fig.16. MATLAB Application T(K) vs Ratio plot with Natural Gas and 10% CO_2 as fuel selected with 3 sources of results.

The results corresponding to Burning velocity are possible to be seen by selecting the other 2 type of plots.

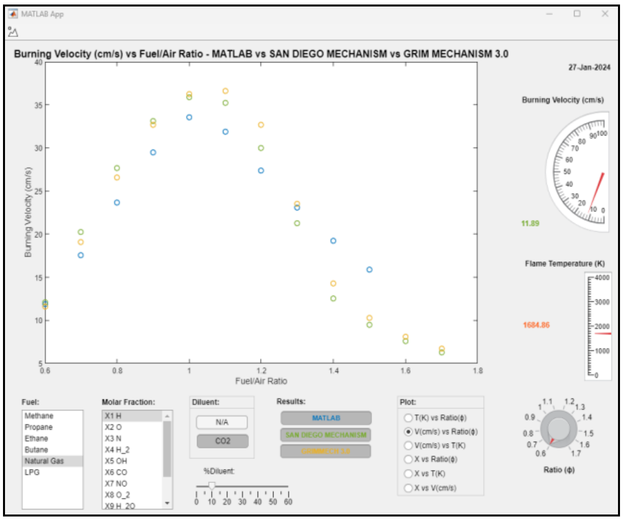

Fig.17. Burning velocity V(cm/s) vs Ratio plot with Natural Gas and 10% CO_2 as fuel selected with 3 sources of results.

For the molar fraction, X10 CO_2 was selected from the molar fraction list.

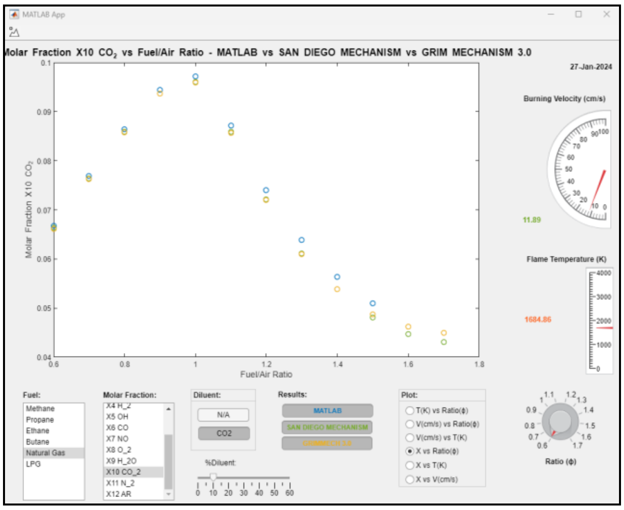
Fig.18. X10 CO_2 molar fraction vs Ratio plot with Natural Gas and 10% CO_2 as fuel selected with 3 sources of results.

3. Comparation of the MATLAB Application versus other studies

The MATLAB Application numerical methodology was validated and analysed in the article 'Determination of 12 combustion products, flame temperature, and laminar burning velocity of Saudi LPG using numerical methods coded in a MATLAB application' [1]. For this case of study, the comparation of results for the laminar burning velocity demonstrate the MATLAB application determined the experimental results more accurately, from 0.7 to 1.4 of the equivalence ratios compared to Ansys Chemkin simulations taking B. Yang [3] as the experimental result reference [1].

Table I. - LPG laminar burning velocity compared studies [1].

WORK	TYPE OF STUDY
MATLAB Application	Numerical methodology in MATLAB
San Diego mechanism	Numerical simulation in Ansys Chemkin
RedSD mechanism	Numerical simulation in Ansys Chemkin
B. A. Alfarraj et al. [6]	Experimental – Modified Bunsen burner method
B. Yang [7]	Experimental – Constant Volume Bomb Method
Huzayyin et al. [8]	Experimental – Constant Volume Chamber Method
Ahmed Sh. Yasiry et al. [9]	Experimental – Constant Volume Chamber Method
Miao, et al. [10]	Experimental – Constant Volume Chamber Method
Chakraborty et al. [11]	Experimental – Flat Flame Burner Method

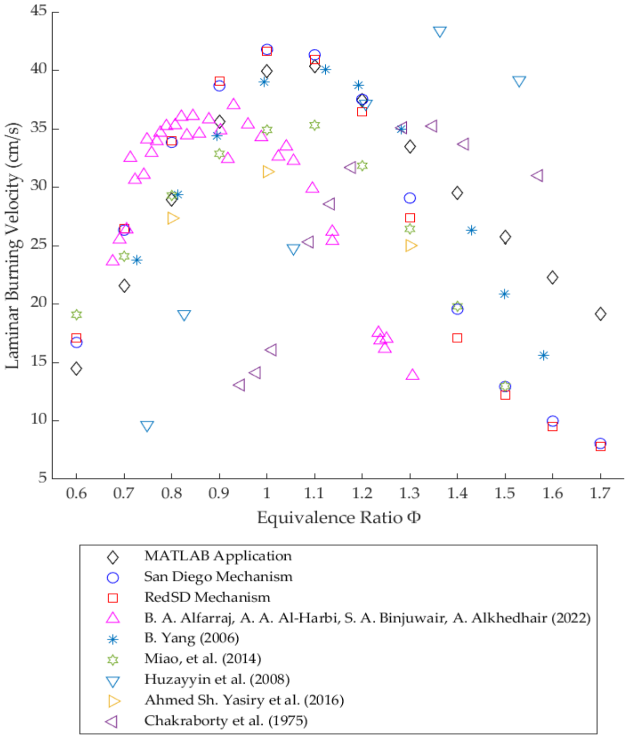

Fig.19. Burning velocity (cm/s) results comparation between all the studies [1].

4. Future improvements and upgrades

Future improvements were detected in order to make the MATLAB Application more flexible, easy to use and faster in processing the different implemented tools. Some of the improvements and upgrades that are being on working progress are:

1) *Resume the excels*: Currently there are different excels that are needed in order to make the application run, so it is better for the code and app to have just one source of information.
2) *Enter new fuels and their properties by the app*: In order to make an easy implementation of new fuels, the next upgrade will introduce a new screen for the entering of new fuels to the program by the user and it would not be required to enter to the excel manually and set the fuel properties.
3) *Results button list:* For the next upgrade, the buttons will be removed and a multiple-choice list will be added in replacement.
4) *Enter new results sources by the app:* For the entering of other kind of results like experimental or simulation ones, the app will have a new screen so the user will be able to define the new points or charge directly a new file in order to add the data to the results one.
5) *Percentage Diluent bar:* The bar will be configurate for the manual setting of the diluent percentage, including one or two decimals.
6) *Knob Ratio:* Similar to the percentage diluent bar, the knob ratio will be configurate for manual setting of the ratios that were evaluated.

5. Conclusion

The MATLAB Application functionality, tools and previous validation were presented. To summarize, is a free powerful tool for all the science community and with a clear development potential that could be done by any user in order to improve the whole package for their research needs. Moreover, with the future upgrades mentioned, the limitation of only 3 sources for comparation, few ratios and percentage of dilution, the analysis and applications of the app will get a remarkable improvement.

Acknowledgement

Thanks are due to the DFI of the Pontificia Universidad Católica del Perú that, through the annual competition for applied research projects CAP PUCP 2021, financed research PI0735.

References

[1] R. F. Cisneros and F. J. Rojas, "Determination of 12 Combustion Products, Flame Temperature and Laminar Burning Velocity of Saudi LPG Using Numerical Methods Coded in a MATLAB Application," Energies (Basel), vol. 16, no. 12, p. 4688, Jun. 2023, doi: 10.3390/en16124688.

[2] R. Cisneros and F. Rojas, “MATLAB Application.” Lima, May 04, 2023. doi: 10.5281/zenodo.7894133.

[3] “Chemical-Kinetic Mechanisms for Combustion Applications.” Accessed: Nov. 29, 2022. [Online]. Available: https://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html

[4] GRI-Mech 3.0, The Gas Research Institute, http://www.me.berkeley.edu/gri_mech/

[5] S. M. Kumaran, D. Shanmugasundaram, K. Narayanaswamy, and V. Raghavan, “Reduced mechanism for flames of propane, n-butane, and their mixtures for application to burners: Development and validation,” Int J Chem Kinet, vol. 53, no. 6, pp. 731–750, Jun. 2021, doi: 10.1002/kin.21477.

[6] B. A. Alfarraj, A. A. Al-Harbi, S. A. Binjuwair, and A. Alkhedhair, “The Characterization of Liquefied Petroleum Gas (LPG) Using a Modified Bunsen Burner,” Journal of Combustion, vol. 2022, 2022, doi: 10.1155/2022/6977930.

[7] B. Yang, “Laminar Burning Velocity of Liquefied Petroleum Gas Mixtures,” Loughborough University, Loughborough, 2006.

[8] A. S. Huzayyin, H. A. Moneib, M. S. Shehatta, and A. M. A. Attia, “Laminar burning velocity and explosion index of LPG-air and propane-air mixtures,” Fuel, vol. 87, no. 1, pp. 39–57, Jan. 2008, doi: 10.1016/j.fuel.2007.04.001.

[9] A. Sh Yasiry and H. A. Shahad, “An Experimental Study for Investigating the Laminar Flame Speed and Burning Velocity for LPG International Journal of Thermal Technologies,” 2016. [Online]. Available: http://inpressco.com/category/ijtt/

[10] J. Miao, C. W. Leung, Z. Huang, C. S. Cheung, H. Yu, and Y. Xie, “Laminar burning velocities, Markstein lengths, and flame thickness of liquefied petroleum gas with hydrogen enrichment,” Int J Hydrogen Energy, vol. 39, no. 24, pp. 13020–13030, Aug. 2014, doi: 10.1016/j.ijhydene.2014.06.087.

[11] S. K. Chakraborty, B. N. Mukhopadhyay, and B. C. Chanda, “Effect of inhibitors on flammability range of flames produced from LPG/air mixtures,” 1975. doi: 10.1016/0016-2361(75)90022-8.