Proceedings of the International Conference on Industrial Engineering and Operations Management
Dubai, UAE, March 10-12, 2020

Screening Variables using Computer Experiments: An application using a simulated furnace

Nuno Costa
UNIDEMI , CINEA
Escola Superior de Tecnologia de Setúbal-Department of Mechanical Engineering
Instituto Politécnico de Setúbal
2910-761 Setúbal, Portugal
nuno.costa@estsetubal.ips.pt, paulo.fontes@estsetubal.ips.pt

Paulo Fontes
CINEA
Escola Superior de Tecnologia de Setúbal-Department of Mechanical Engineering
Instituto Politécnico de Setúbal
2910-761 Setúbal, Portugal
paulo.fontes@estsetubal.ips.pt

Abstract

Despite advances in computer hardware and software capabilities, the expense of running experiments in computer models of a complex industrial equipment is still a relevant issue. To minimize it, experiments must be statistically designed and critical variables identified using appropriate analysis methods. In the study presented here, several easy-to-implement yet effective data analysis methods were used for identifying the variables that must be measured with more accurate devices and methods to estimate the energy efficiency of a billets reheating furnace. A furnace's simulator was used to perform the experiments and results analysis shows that oxygen percentage in the combustion gases, fuel flow in the burners, and combustion air temperature are critical variables for quantifying furnace's energy efficiency.

Keywords

Audit; Climate; Computer Experiments; Environment; Factorial; Industrial; Screening; Simulation.

1. Introduction

Computer models are increasingly used for maximizing processes' efficiency and products' quality (reliability, durability, performance, robustness, etc.) in a faster, and cheaper way at the design and manufacturing stages. In fact, they allow running experiments which could hardly be possible to perform otherwise, namely when the product or process does not physically exist, the experimentation is time-consuming, too expensive, difficult, risky or even dangerous to be performed. The spectrum of applications ranges from nano (molecular simulations) to mega scale (structural analysis of buildings and bridges) in various science fields, namely in chemistry, toxicology and pharmaceutics, materials, electronics and communication, biotechnology, aeronautics, and so on (Garud et al., 2017).

Despite advances in computer hardware and software capabilities, the expense of running experiments in computer models is still a relevant issue. Single evaluations of stress, thermal, and impact/crash analyses can take hours to days, if not longer. To overtake this inconvenient or hindrance, an alternative has been to run experiments in meta-models or "models of the models". Simulated or computer experiments are becoming increasingly prevalent surrogates for

physical experiments, but practitioners often treat their experiments with simulation models (or "simulators" or "computer codes") very unprofessionally (Kleijnen, 2017). Trial-and-error and brute force practices must not be used because they may neither uncover all the input variables with practical influence on the output variable (response – process or product characteristic under evaluation) nor the functional relationship between input variables and response, and therefore the 'best' settings for input variables.

Many tools for the design and analysis of computer experiments has been put forward in the literature, but there is a strong need for making them more accessible to the practitioners (Garud et al., 2017; Bhosekar and Ierapetritou, 2018). It is known that many practitioners (those who have low background on statistics) do not feel comfortable in using (complex or sophisticated) statistical tools (Sheil and Hale, 2012; Lundkvist et al., 2018), so to choose the experimental design type and the number of experimental runs, to select appropriate methods for data analysis, to implement these methods, and to interpret the results can be daunting (very difficult or even impossible to perform) tasks for practitioners.

To design and analyze computer experiments is more of a science than an art, and it is not a one-time task. It requires critical thinking and not simply some clicks from a mouse (supply a vector of design/input variables to the computer code and obtain a vector of responses/outputs). Moreover, experimenters cannot ignore that the most efficient and widely recommended way to build knowledge about process and/or product is to adopt a sequential experimentation strategy, which may consist of three experimental phases, namely; Screening, Characterization, and Optimization. In some cases, two experimental phases, Screening and Characterization, Screening and Optimization, or Characterization and Optimization are appropriate.

The work reported here focus on screening experimental phase, and a billets reheating furnace simulator is used to run statistically designed experiments. The study objective is twofold: 1) Review and illustrate easy-to-implement data analysis methods for screening (separate dominant variables from the non-dominant ones); 2) identify the factors with practical influence and/or significant statistical effect on the energy efficiency of a billets reheating furnace, so that those factors (input variables) are measured with more accurate measuring devices and methods when real energy audits are performed to that furnace.

2. Study Characterization

To build a billets reheating furnace in a real or reduced scale for experimental purposes is unrealistic, and to run experiments in industrial environment is very difficult, namely due to technical and economic reasons. Thus, the alternative is to develop or use a simulation numerical model (a meta-model) to better understand the furnace behavior under (non)current operation conditions and improving or optimizing their performance. The study presented here is supported on a computer model of an industrial billets reheating furnace. The furnace under study is used to heat cylindrical billets with length between 1.5-1.6 m and diameter between 0.2-0.3 m. The furnace is 22 m long, can heat 10 tons/hour of billets (copper metal alloys) up to 770 ºC, and has a total of 312 burners, whose propane consumption is of 40 kg/h and the thermal power production of approximately 500 kW. The furnace's efficiency was calculated by the ratio between the heat transferred to the billet and the heat released by the fuel's combustion.

Due to the complexity of thermodynamic phenomena inside the furnace and the size of this equipment, the furnace simulator was built by zones. The results presented here were obtained from zone 8 (the penultimate furnace zone), to reduce the computational time for running the planning experiments and because it represents appropriately the furnace operation conditions. In this zone there are 16 burners with a thermal power of 24 kW. The furnace modelling was performed with a commercial software and the simulator (zone 8 of the furnace) validated with values collected in industrial environment.

The variables considered to achieve the study objectives and the test values (current, low, and high levels) associated to them are listed in Table 1. Variables identification and respective test values were defined by senior energy auditors and academic experts in thermodynamics, combustion technologies and processes, and energy management.

Table 1. Input Variables and Settings

Variable		Value		
		Current	Low	High
v1	Fuel Flow in the Burner (kg/s)	0.0011	0.0009	0.0013
v2	O_2 in Combustion Gases (% vol dry)	11	9	13
v3	Combustion Air Temperature (ºC)	275	260	290
v4	Billet Input Temperature (ºC)	730	725	735
v5	Billet Output Temperature (ºC)	745	740	750
v6	Billet Emissivity	0.80	0.72	0.88

3. Design and Analysis of Experiments: Theoretical Framework and Results

Many scientific works provide relevant insights into which design and data analysis method to employ for solving a problem, recommendations for the appropriate use, and how common pitfalls can be avoided in simulated experiments. However, in practice, the type of problem (prediction, feasibility analysis, or optimization) and the problem characteristics may vary in terms of the number and type of decision variables (discrete and/or continuous, quantitative and/or qualitative), and response function shape (degree of non-linearity), as examples. This makes the design and data analysis method selection to the problem at hands very difficult. Unfortunately, there is no single approach to solve all the problems. No one method or design stands out (Bhosekar and Ierapetritou, 2018; Garud et al., 2017; Chen et al., 2006).

The study presented here focus on the so-called screening phase of experimentation, where unreplicated fractional factorial designs with *p* generators and *k* variables (factors) at two levels are often used to establish the 2^{k-p} experiments. In this study, the experiments are unreplicated, because it would not be possible to obtain true replicates of each experimental run with the simulation model used. Running the same input values, it is always achieved the same output (response) value.

A Minimum Aberration Design, namely a fractional factorial of resolution IV with sixteen experiments (2_{IV}^{6-2}) and a minimum number of confounded effects, was adopted to stablish the experimental runs. Variables v5 and v6 were used as generators, with v5 = v1*v2*v3 and v6 = v1*v2*v4, because it was not expected that variables v5 and v6 were the most determinant for the study purpose. The aliased effects structure is presented in Table 2 and the designed experiments are listed in Table 3. Interaction effects between two variables that cannot be estimated separately due to the reduced number of experiments (16 out of 64 experiments), though they could influence the response (energy efficiency), are called redundant effects and are listed in the first row of Table 2. In the second row of this table are presented the alias effects. The energy efficiency values listed in Table 3, expressed in percentage (%), correspond to the results of the sixteen performed experiments.

The analysis of unreplicated fractional factorial designs has been considered an adventure (Hamada and Balakrishnan, 1998; Costa et al, 2013). This is because it is not possible to estimate the true experimental error, and consequently the reliability of the conclusions resulting from the data analysis may not be the most desired. This is particularly true when the sparsity-of-effects principle is not verified, that is, if there are many factors and interactions between two factors that influence the response significantly.

A very common practice in the analysis of unreplicated fractional factorials is to employ a Normal or "Half-normal" probability plot. In this type of plot, the values of the effects corresponding to the variables (factors) with low contribution to the (average) value of the response tend to be disposed of along a straight line. The effects corresponding to the factors with greater influence on the response, called active or significant effects, are away from that straight line.

This practice was recently criticized by Lenth (2015), who argue that, in some cases, the plot analysis is excessively dependent on the sensitivity and knowledge of the process or product by the analyst so bias in the conclusions taken from the data can be introduced. Many other methods have been proposed and illustrated in the literature. Their performance and usefulness have been also reported in various published works, among which we highlight the works by Hamada and Balakrishnan (1998) and Costa et al. (2013).

Table 2. Aliased Effects Structure

Effect	v1*v2	v1*v3	v1*v4	v1*v5	v1*v6	v3*v4	v3*v6
Alias	v3*v5 , v4*v6	v2*v5	v2*v6	v2*v3	v2*v4	v5*v6	v4*v5

Table 3. Experimental Design and Results

Experiments and Results							
Exp.	v1	v2	v3	v4	v5	v6	Efficiency (%)
1	0,0009	9	260	725	740	0,72	56,1
2	0,0013	9	260	725	750	0,88	51,9
3	0,0009	13	260	725	750	0,88	43,7
4	0,0013	13	260	725	740	0,72	39,2
5	0,0009	9	290	725	750	0,72	57,6
6	0,0013	9	290	725	740	0,88	53,7
7	0,0009	13	290	725	740	0,88	46,5
8	0,0013	13	290	725	750	0,72	41,2
9	0,0009	9	260	735	740	0,88	56,7
10	0,0013	9	260	735	750	0,72	50,6
11	0,0009	13	260	735	750	0,72	42,6
12	0,0013	13	260	735	740	0,88	39,7
13	0,0009	9	290	735	750	0,88	58,2
14	0,0013	9	290	735	740	0,72	52,5
15	0,0009	13	290	735	740	0,72	45,4
16	0,0013	13	290	735	750	0,88	41,7

If practitioners decide or have the chance to use software for data analysis, it is important to have an extreme caution with software features. Some software vendors may claim that they understand the proper experimental protocol, so there are no reasons for worries. They also highlight that if the experimental factors, their levels, and experimental constraints are uploaded in their software, an optimal design we need will be produced to software users and all the necessary analysis to the experimental data will be done by software. Accepting in full these claims is risky. Data analysis software is an extremely important tool; however, it requires intelligent use. Fontdecaba et al. (2014) studied and evaluated five well-known statistical software packages and stated that all packages use different methods and criteria that deliver different results in the analysis of unreplicated factorial designs. Moreover, they show that some of the used methods are clearly incorrect and deliver biased results so methods selection must be carefully made. This is one of the major difficulties felt by practitioners and, unfortunately, one method that performs well in all test conditions has not been found yet. The existing methods perform differently depending on the number and size of the active effects and on existence of abnormalities in the data. Therefore, in the work presented here, and based on results reported by Hamada and Balakrishnan (1998), Costa et al. (2013) and discussions on Lenth's paper (2015), the Al-Shiha and Yang's (Al-Shiha and Yang's, 1999), Dong's (Dong, 1993), and Benski's (Benski, 1989) methods are employed in addition to the popular Half-normal probability plot to identify the factors (location effects- those that affect the mean response) with practical influence or statistical significance in the furnace's energy efficiency.

The multistage stage procedure introduced by Al-Shiha and Yang (1999) uses the test statistic $L_{m,r}$,

$$L_{m,r} = \frac{\sum_{i=m-r+1}^{m} |c_i|^2/r}{\sum_{i=1}^{m-r} |c_i|^2/(m-r)} \tag{1}$$

where m is the number of contrasts, r is the number of potentially active contrasts (estimated by the analyst) and c_i represents the estimated contrasts. When $L_{m,r}$ is larger than a critical value, denoted by $L_{m,r,\alpha}$, the null hypothesis (H_0: *no active contrasts exist*) is rejected, and one can accept that r contrasts are active at the significance level α.The critical values ($L_{m,r,\alpha}$) are available at Al-Shiha and Yang's (2000). Notice that it is recommended to test several r values.

Benski (1993) proposed a normality test coupled with an outlier test to identify the active contrasts, and practitioner must proceed to implement the method as follows (Costa and Pereira, 2009):

1) Perform the Olsson's version of the *W'* test of normality,

$$W' = \frac{\left(\sum_{i=1}^{m} z_i c_i\right)^2}{\left(\sum_{i=1}^{m} z_i^2 \sum_{i=1}^{m} (c_i - \bar{c})^2\right)} \tag{2}$$

where $\bar{c}$ is the average of the ordered contrasts or effects c_i, and z_i is the expected standard normal order statistics in a sample of size m. The z_i can be approximated by

$$z_i = \varphi^{-1}(p_i) \tag{3}$$

where φ^{-1} is the inverse normal distribution and $p_i = (i - a)/(m - 2a + 1)$, with

$$a = \begin{cases} 0.275499 + 0.072884(ln(m))^{0.41148}, & 1 < i < m \\ 0.205146 + 0.1314965(ln(m))^{0.226701}, & i = 1, m \end{cases} \tag{4}$$

2) Calculate the significance level (P_1) of W' test,

$$P_1 = exp(C) \tag{5}$$

where

$$C = \frac{(W' - A)/B + 0.0486128}{0.02760309} - ln(100) \tag{6}$$

and $A = 1.031918 - 0.183573(0.1m)^{-0.5447402}$ and $B = -0.5084706 + 2.076782(0.1m)^{-0.4905993}$.

3) If P_1 is not small, go to step five. If P_1 is small ($P_1 < 0.05$), calculate the significance level P_2 of the outlier test (d_F) for any data point outside the interval $[-2d_F, +2d_F]$, where $d_F = F_U - F_L$ is the interquartile range, and F_L and F_U are the first and the third quartiles of c_i. Under normality, P_2 can be estimated as

$$P_2 \approx 0.00698 + (0.4/m) \tag{7}$$

4) Calculate P_C = 2*ln(1/(P1*P2)) and respective significance level, assuming P_C follows a chi-square distribution with four degrees of freedom. If the combined test is rejected at the significance level associated to *Pc*, declare the largest contrast (in absolute value) active, remove it and repeat steps 1 to 4 with the remaining contrasts.

5) Stop. Consider active the contrasts removed in step four (if applicable). Notice that the confidence in claiming that significant effects exist is enhanced when (1 – Pc) is closer to 1 than (1 – P_1).

In Dong's method a contrast c_i is declared active if

$$|c_i| > t_{\gamma; m_{inactive}} \times S_{\text{Dong}} \tag{8}$$

where S_{Dong} is an estimate of the standard error defined by

$$S_{Dong} = \sqrt{\frac{1}{m_{inactive}} \left(\sum_{|c_i| < 2.5 S_0} c_i^2\right)} \tag{9}$$

$m_{inactive}$ is the number of inactive contrasts characterized by $|c_i| \leq 2.5S_0$ among the m contrasts, and the variable $\gamma = \left(1 + 0.98^{1/m}\right)/2$.

4. Results Analysis and Discussion

The graphical representation in a Half-normal probability plot of the experimental results listed in Table 3, as shown in Figure 1, allows us to assume that the variables with the greatest influence in the response are the percentage of oxygen in the combustion gases (v2), the fuel flow in the burners (v1) and the combustion air temperature (v3). The billet emissivity (v6) is not considered a variable with relevant influence on the response, such as Figure 1 suggest, because its effect is aliased with (or is achieved from the combination of) the effects of three variables (v1*v2*v4), namely with the effect of v1 and v2, which are the most influent variables in the furnace's efficiency.

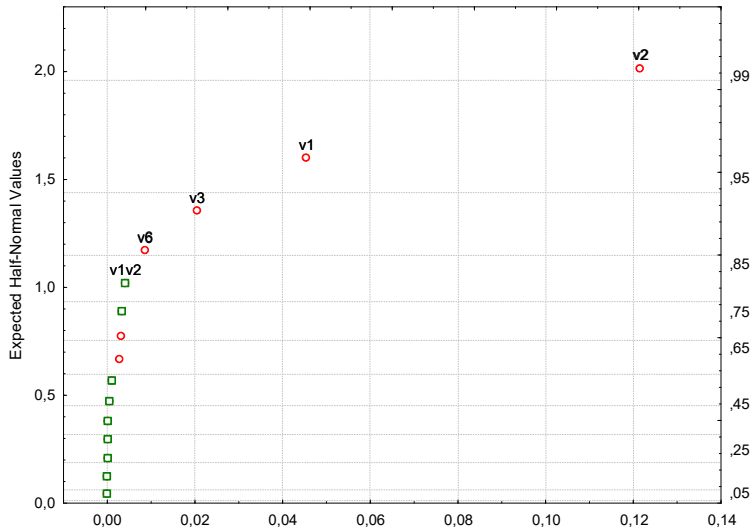

Figure 1. Half-Normal Probability Plot

Al-Shiha and Yang's method analysis corroborates the interpretation made to Figure 1. Only the variables v2, v1, and v3 are statistically significant (their effects are active) at a significance level α = 1%, with $L_{15,3} = 3095.3 > L_{15,3,1\%} = 19.8$; $L_{14,2} = 119.9 > L_{14,2,1\%} = 19.2$; $L_{13,1} = 40.5 > L_{13,1,1\%} = 19.9$.

Dong's method, with $S_{Dong} = 0.0021$, $m = 15$, and $m_{inactive}=12$, confirms that v2, v1, and v3 are statistically significant.

Benski's method also identifies v2, v1, and v3 as statistically significant variables. The remaining ones are not influential or statistically significant (see Table 4).

Table 4. Benski's method Results

Variable	W'	P_1	$\pm 2d_F$	Pc
v2	0.5177	8.5×10^{-7}	0.0077	34.75
v1	0.6087	1.7×10^{-6}	0.0073	33.27
v3	0.6961	3.3×10^{-6}	0.0081	31.77
Others	0.8445	6.7×10^{-6}	0.0036	30.24

To obtain an indication of the best level for these three variables, the mean values of each variable were calculated at the high and low levels separately, and the highest value of this mean was selected so that the energy efficiency of the furnace is the highest possible. In this case, the efficiency will be higher when v2 is at low level, v1 is at low level, v3 is at high level and all other variables are kept at low level for technical-economic reasons.

To validate the data analysis, a confirmatory experience was performed using the computer model and an efficiency value equal to 57.8% was obtained. This result confirms that a rigorous measurement of the three aforementioned variables to adequately quantify the energy efficiency of the furnace under study is required.

5. Conclusion

As the trend in technology favors a shorter product development cycle and a quicker reaction to market opportunities, shorter-duration non-sequential experiments will become more popular in engineering. However, practitioners (engineers, researchers, …) cannot ignore that valid and practical conclusions drawn from experimental studies depend to a large extent on the way how the data were collected. To try out many settings of an input variable in a "what if" scenario or testing many variables simultaneously in an unstructured way to achieve a specified objective are counterproductive practices. To appropriately plan and run statistically designed experiments is a more structured, faster, cheaper, and reliable practice for that purpose at the systems design and manufacturing stages.

The operation and the energy efficiency maximization of systems supported on user's empirical knowledge is an unsustainable practice. Thus, even when it is not possible to perform experiments in industrial environment, due to technical, economic, lack of resources, or other reasons, running statistically designed experiments in a computer model and analyzing the results with tested and validated methods is an efficient approach for maximizing the systems performance.

This study shows that fractional factorial designs and easy-to-implement methods for screening are alternatives to more sophisticated approaches for designing and analyzing results from computer models. Al-Shiha and Yang's, Dong's, and Benski's methods are structurally different, efficient, and easy-to-implement in Excel by those who are not experts in statics and computation. Moreover, they can supplement or replace the popular Half-normal probability plot. In this case study, all the analysis methods lead to the same conclusion so one can assume their result confidently.

In this study a computer model of a billets reheating furnace was used, and it was possible to conclude, only with 16 out of 64 experiments, that the percentage of O_2 in the combustion gases (v2) is the variable with the greatest influence on the furnace's energy efficiency. Its effect is 2.5 times higher than that of fuel flow in the burners (v1) and 6 times higher than that of combustion air temperature (v3). The monitoring and measurement as accurate as possible of the v2 value is determinant in the furnace's energy efficiency evaluation, but a similar approach is required to variables v1 and v3. Results analysis provides evidence that v2 and v1 should be set at the low level, while v3 should be set at the high level. All the other variables must be set at low level. For future work, it is suggested further studies to identify the optimal value for v1, v2 and v3. To validate the presented results to other furnace zones is also recommended.

Acknowledgements

This work was supported by AuditF project Lisboa-01-0247-FEDER-017980.

References

Al-Shiha, A., Yang, S., A multistage procedure for analyzing unreplicated factorial experiments, *Biometrical Journal*, Vol. 41, nº. 6, pp. 659-670, 1999.

Al-Shiha, A., Yang, S., Critical Values and Some Properties of a New Test Statistic, *Biometrical Journal*, Vol. 42, nº. 5, pp. 605-616, 2000.

Benski, C., Use of a Normality Test to Identify Significant Effects in Factorial Designs, *Journal of Quality Technology*, Vol. 21, nº. 1, pp. 174-178, 1989.

Bhosekar, A., Ierapetritou, M., Advances in surrogated based modeling, feasibility analysis, and optimization: A review, *Computers and Chemical Engineering*, Vol. 108, nº. 1, pp. 250-267, 2018.

Chen, V., Tsui, K., Barton, R. and Meckesheimer, M., A review on design, modeling and applications of computer experiments", *IIE Transactions*, Vol. 38, nº. 4, 273-291, 2006.

Costa, N. and Pereira, Z. Decision-Making in the Analysis of Unreplicated Factorial Designs, *Quality Engineering*, Vol. 19, nº. 3, pp. 215-225, 2007.

Costa, N., Pires, R. and Fontes, P., On the selection of significant variables from unreplicated factorial designs, *International Journal of Productivity and Quality Management*, Vol. 12, nº. 2, pp. 161-180, 2013.

Dong, F., On the identification of active contrasts in unreplicated fractional factorials, *Statistica Sinica*, Vol. 3, nº. 1, pp. 209-217, 1993.

Fontdecaba, S., Grima, P. and Tort-Martorell, X., Analyzing DOE With Statistical Software Packages: Controversies and Proposals, *The American Statistician*, Vol. 68, nº. 3, pp. 205-211, 2014.

Garud, S., Karimi, I. and Kraft, M., Design of computer experiments: A review, *Computers and Chemical Engineering*, Vol. 106, nº. 2, pp. 71-95, 2017.

Hamada, M., Balakrishnan, N., Analyzing Unreplicated Factorial Experiments: A Review with Some New Proposals, *Statistica Sinica*, Vol. 8, nº. 1pp. 1-41, 1998.

Kleijnen, J. (2017). Design and Analysis of Simulation Experiments: Tutorial. In: Tolk A., Fowler J., Shao G., Yücesan E. (eds) Advances in Modeling and Simulation. pp. 135-158, Springer, Cham.

Lenth, R., The Case Against Normal Plots of Effects, *Journal of Quality Technology*, Vol. 47, nº. 2, pp. 91-97, 2015.

Lundkvist, P., Bergquist. B. and Vanhatalo, E., Statistical methods – still ignored? The testimony of Swedish alumni, *Total Quality Management & Business Excellence*, in press, DOI: 10.1080/14783363.2018.1426449, 2018.

Sheil, J., Hale, D., The 'Democratisation' of Statistics: Parastatisticians in Manufacturing, *Quality and Reliability Engineering International*, Vol. 28, nº. 5, pp. 524-534, 2012.

Biographies

Nuno Costa is an Adjunct Professor in the Department of Mechanical Engineering at Setubal College of Technology, Setúbal, Portugal. He has a PhD in Industrial Engineering from NOVA School of Science and Technology (FCT NOVA), Portugal. Dr Costa has various publications in indexed journals and conferences, has published book chapters, and has acted as reviewer for indexed journals and conferences. He holds five international awards, has participated in research projects and is a member of CINEA and UNIDEMI research units. His research interests include quality engineering, operations and quality management, simulation, optimization, maintenance and reliability. He is member of IAENG and ISEA.

Paulo Fontes is a Coordinating Professor in the Department of Mechanical Engineering at Setubal College of Technology, Setúbal, Portugal. He has a PhD in Mechanical Engineering (Instituto Superior Técnico, Portugal) in the area of CFD modeling of combustion processes in industrial boilers. Dr. Fontes has participated in research projects and is a member of CINEA, a research unit of Instituto Politécnico de Setúbal. His research interests include thermal energy processes, namely combustion and numerical simulation of this processes.