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Partnership for Advanced Computing in Europe

High-fidelity Simulation of an industrial swirling Combustor

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Abstract

The proposed project aims to demonstrate the potentials of high-fidelity simulations to predict pollutant emissions and energy efficiency in practical combustion systems. The study is based on the development of advanced numerical simulations to investigate the reacting flow field of an industrial combustor designed and manufactured by E&M Combustion. The focus is given to the assessment of performance measured in terms of thermal power, combustion efficiency, and global emissions, so the SME can make decisions to optimise the system in the future. In particular, the JBM 4.500 G burner has been simulated using large-eddy simulations with a flamelet combustion model. This project has been developed as collaboration between E&M Combustion and the Barcelona Supercomputing Center (BSC) within the SHAPE programme of PRACE.

1. Introduction

In the coming years, the energy industry will face an increasingly urgent need to reduce NO_x levels, with the challenge for the countries to comply with the Paris Treaty on emissions reduction and, on the other hand, the real need in some countries where pollution is already a top-level problem that is directly affecting the health of citizens [1]. This is the case in China, where the government has already set very restrictive emission levels for its large plants and where it is necessary to design burners that are more environmental friendly. Additionally to the reduction on emission levels, these targets need to be achieved with designs that can be manufactured and do not require too much additional costs that make the product less competitive. This trade off in terms of efficiency level, design and manufacturing cost is especially critical for SMEs, where changes in regulations can rapidly put the products out of the market. The fact of having more environment-friendly burners will simply mean that SMEs can compete in certain markets or not. It is possible that in few years, those burner manufacturers that do not reach certain levels in terms of emissions will have to cease their activity because they cannot sell their products anymore.

The market of industrial burners and combustors for energy applications is now demanding higher efficiency in terms of fuel consumption and flexibility of operation, but also on reducing emissions, mainly NO_x [2]. The current state of the art for the design of such systems includes low-order modelling using Reynolds-averaged Navier-Stokes (RANS) or simplified correlations based on global energy balances that allow the adjustment of different parameters. The use of advanced numerical simulations as a tool for design of combustion systems has grown in the last decade as it permits to evaluate the combustion performance of a given burner before the manufacturing process takes place. This strategy can save substantial amount of time and resources in the design process and optimise existing designs at relatively low cost. Nowadays, the availability of computing power has increased with major technological progress in HPC and cloud technologies. Therefore, the use of high-fidelity simulations based on large-eddy simulation (LES) is an advanced numerical approach that can be accessed by the industrial sector at the present time for design and optimisation purposes. The use of these techniques can have an important

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contribution to increase the efficiency and competitiveness of the companies that adopt advanced modelling and simulation techniques in the design process.

In this paper we present a numerical characterisation of the reacting flow field of an industrial swirler combustor manufactured by E&M Combustion using large-eddy simulation. The objective of this work is to investigate the reacting flow field in order to characterise its performance (thermal power, combustion efficiency, and global emissions), so the SME can make decisions to optimise the system in the future. The paper is organised as follows. First, the physical and numerical strategy is described. Second, a description of the burner and operating conditions is detailed along with the computational domain used for the simulations. Then, numerical results of the reacting flow field are included and described. Finally, conclusions and directions for future work are briefly discussed.

2. **Modelling approach**

The modelling approach is based on the low-Mach number approximation of the Navier-Stokes equations for chemically reacting flows [3], [4]. The governing equations include the continuity, momentum, enthalpy equations along with two controlling variables that represent the thermochemical state of the flow, those are mixture faction and progress variable with their corresponding variances. The combustion model is based on the tabulation of laminar premixed flamelets with a presumed-shape probability density function (PDF) to account for turbulence-chemistry interactions [3], [4]. A Favre-filtered description of the governing equations is considered [3]. The governing equations describing the flow field are:

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\boldsymbol{u}}) = 0$$

$$\frac{\partial (\overline{\rho}\widetilde{\mathbf{u}})}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}\widetilde{\mathbf{u}}) = -\nabla \overline{p} + \nabla \cdot (\boldsymbol{\tau} + \boldsymbol{\tau}^*)$$

$$\frac{\partial \left(\overline{\rho}\widetilde{h}\right)}{\partial t} + \nabla \cdot \left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{h}\right) = \nabla \cdot \left[\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_t}\right)\nabla \widetilde{h}\right]$$

$$\frac{\partial \left(\overline{\rho}\widetilde{Z}\right)}{\partial t} + \nabla \cdot \left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Z}\right) = \nabla \cdot \left[\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_t}\right)\nabla \widetilde{Z}\right]$$

$$\frac{\partial (\overline{\rho}Z_v)}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}Z_v) = \nabla \cdot \left[\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_t}\right)\nabla Z_v\right] + 2\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_t}\right)\left|\nabla \tilde{Z}\right|^2 - \overline{\rho}\widetilde{\chi}_Z$$

$$\frac{\partial \left(\overline{\rho}\widetilde{Y}_c\right)}{\partial t} + \nabla \cdot \left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Y}_c\right) = \nabla \cdot \left[\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_t}\right)\nabla \widetilde{Y}_c\right] + \overline{\dot{\omega}}_{Y_c}$$

$$\frac{\partial (\overline{\rho}Y_{cv})}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}Y_{cv}) = \nabla \cdot \left[\overline{\rho}\left(\widetilde{D} + \frac{\nu_t}{Sc_t}\right)\nabla Y_{cv}\right] + 2\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_t}\right)|\nabla Y_{cv}|^2 + 2\left(\overline{Y_c\dot{\omega}_{Yc}} - \widetilde{Y}_c\overline{\dot{\omega}_{Yc}}\right) - \overline{\rho}\widetilde{\chi}_{Y_c}$$

where the variables are represented with standard notation [4]. X_Z and X_{Yc} represent the scalar dissipation rates of the mixture fraction and progress variable respectively, while ω_{Yc} is the source term of the progress variable. The scalar dissipation rates are composed by the resolved and unresolved parts, which are given by:

$$\widetilde{\chi}_Z = 2\overline{D}\left|\nabla \widetilde{Z}\right|^2 + \chi_Z^{sgs} = 2\overline{D}\left|\nabla \widetilde{Z}\right|^2 + \frac{C_k}{\tau_t}Z_v$$

$$\widetilde{\chi}_{Y_c} = 2\overline{D}\left|\nabla \widetilde{Y}_c\right|^2 + \chi_{Y_c}^{sgs} = 2\overline{D}\left|\nabla \widetilde{Y}_c\right|^2 + \frac{C_d}{\tau_t}Y_{cv}$$

This modelling approach is valid for technically premixed flames as it allows accounting for local variations of the equivalence ratio and fluctuations of the reaction progress over the mean [3]. A unity Lewis number assumption has been made to simplify the multicomponent transport in the governing equations. The numerical discretisation is based on a low-dissipation numerical scheme using a third-order Runge-Kutta scheme [5].

3. Industrial burner and operating conditions

The EMC's industrial burner JBM 4.500 G is considered for analysis on this work. The burner is designed to operate at low NOx emissions and includes a primary fuel injection from the centreline and pilot injections that are used for flame stabilisation. Details of the geometrical aspects of the burner and combustion efficiency can be found in the technical data reported by EMC [6]. A sketch of the burner is shown in Figure 1, where the fuel injection ports are shown.

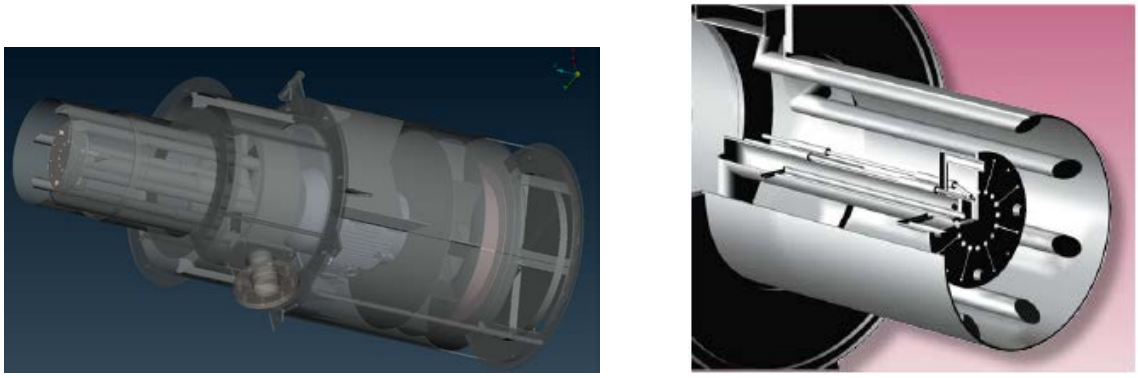

Figure 1: JBM 4500G burner. Left: Full burner. Right: Fuel injection ports.

The operating conditions considered in this study are listed in Table 1 and correspond to the baseline condition at 4.5 MW. The burner is operated at lean equivalence ratio (Φ) and ambient conditions.

Case	Power (MW)	Φ	T (K)	p (bar)	m_{fuel} (kg/s)	m_{air} (kg/s)	W_{fan} (rpm)
# 1	4.5	0.865	298	1	0.07055	1.3864	2000

Table 1: Operating conditions for JBM 4500G burner.

4. Computational domain

The computational domain was simplified in order to reduce the computational cost of the simulation but without a significant loss of accuracy on the results. The upstream locations from Section 3 were removed, but the flow around the electric motor in the middle was considered, as this can influence on the mixing before entering into Sections 2 & 1. Therefore, the computational domain included Sections 1, 2 and 3 along with the combustion chamber. A sketch of the geometry of the burner is shown in Figure 2.

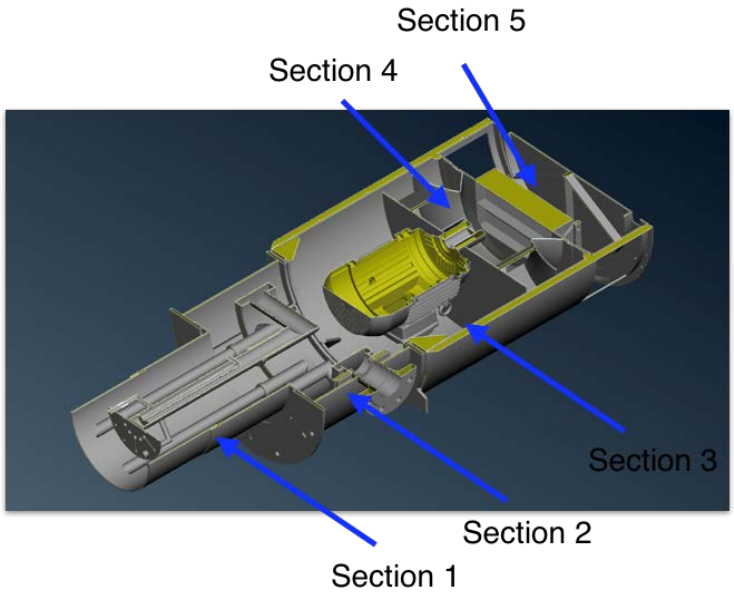

Figure 2: Burner configuration.

A hybrid unstructured mesh composed by tetrahedrons, prisms and pyramids was generated with a total of 48 million elements. The mesh was refined in the region where the fuel enters the domain and where the reacting layers are stabilised. An overview of the mesh is shown in Figure 3. The numerical simulations are conducted with the multiphysics code Alya developed at BSC [7].

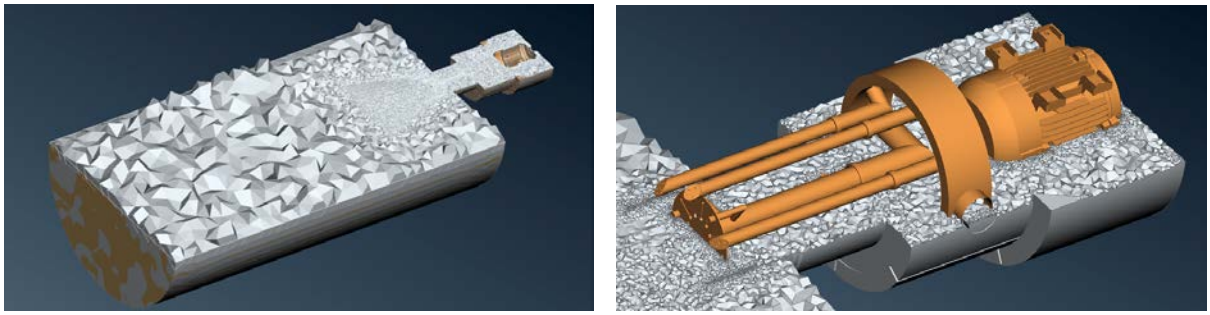

Figure 3: Hybrid mesh.

5. **Results**

The results section is divided into two parts. First, a description of the mixing process is introduced where fuel and air are injected at the operating conditions, but without considering the ignition. These simulations are used to provide an overview of the mixing process and the aerodynamics performance of the burner to evaluate the quality of the design. Second, the fuel is ignited as it occurs in practical applications and the reacting flow field is described. This simulation was conducted in the supercomputer MareNostrum IV with 35 nodes (1680 cores) spending about 150,000 CPU hours.

5.1. Non-reacting simulation: mixing process.

Numerical results of the mean velocity and mixture fraction fields are shown in Figure 4 for analysis. The velocity field shows the formation of the central recirculation zone (CRZ) along the centreline caused by the angular velocity induced by the swirler. The distribution of fuel in the mixture fraction plot shows the rich layers located in the CRZ and the uniform fuel distribution placed in the backflow region. These simulations permit the calculation of pressure losses along the combustor and are of primary importance in the design process.

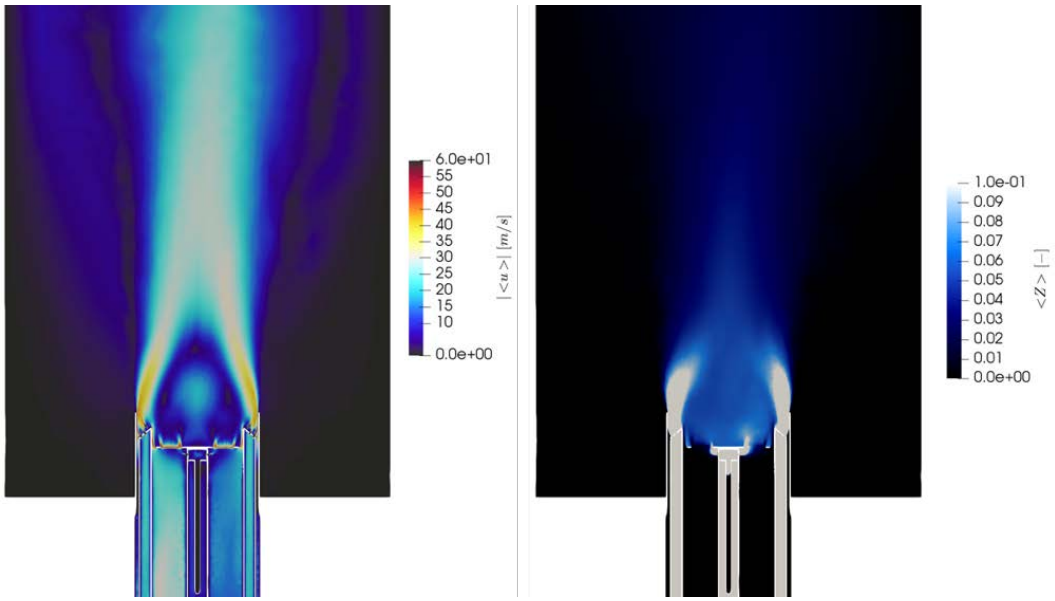

Figure 4: Time-averaged velocity module (left) and mixture fraction (right) fields at central plane.

5.2. Reacting simulation

The reacting flow have been initiated by igniting the fuel within the flammability range and left running until the flow is adapted to this condition. The residence time has been obtained based on the averaged axial velocity to be t_{RES} = 2 s, so the combustor is assumed to operate in stable mode after this time. The flame dynamics can be distinguished by the iso-contour of stoichiometric mixture fraction shown in Figure 5. After 4s, when the flow could be assumed to be stationary, the flow field is time-averaged for 2.2s to obtain statistics. The results of the time-averaged velocity and temperature are shown in Figure 6. The results indicate that additional simulation time is required to obtain fully converged statistics as the mean values are not axisymmetric in the downstream part of the burner, and this is left as a future work. It can also be observed that the flame is stabilised by the central recirculation zone, its length is of about 1 m. These are challenging conditions for conducting high-fidelity numerical simulations.

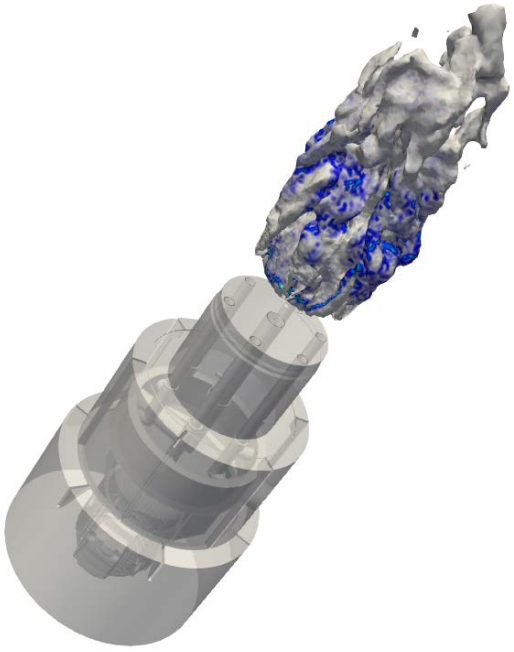

Figure 5: Iso-contour of stoichiometric mixture fraction coloured by progress variable source term at t = 4.6 s after ignition.

The simulations can also provide distributions of pollutant emissions as CO, CO_2, NO_x or precursors for soot formation, as polycyclic aromatic hydrocarbons (PAHs). Figure 7 shows some snapshots of primary pollutants generated in industrial combustors. The plot shows that CO is produced at the upstream regions, and it is then oxidised before it exits the combustion chamber. The CO_2 is formed in the central part and it is emitted at the exit, as it is one of the main combustion products. NO_x is formed primary at the regions of high temperature, which mainly correspond to the burning conditions close to stoichiometry.

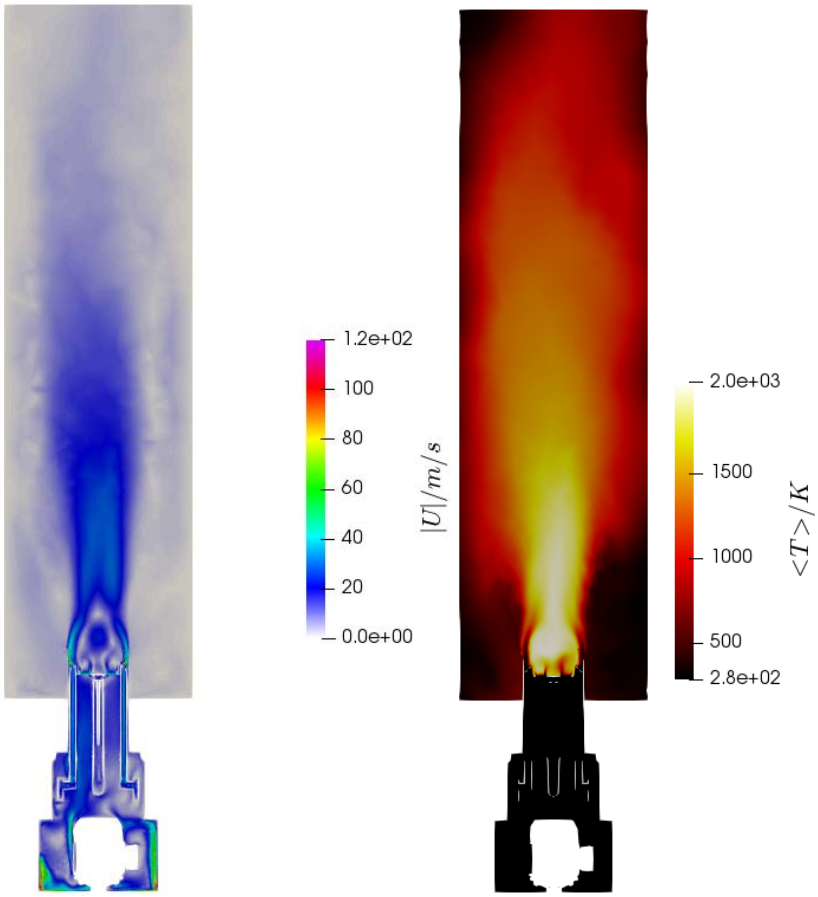

Figure 6: Time-averaged velocity module (left) and temperature (right) fields at central plane.

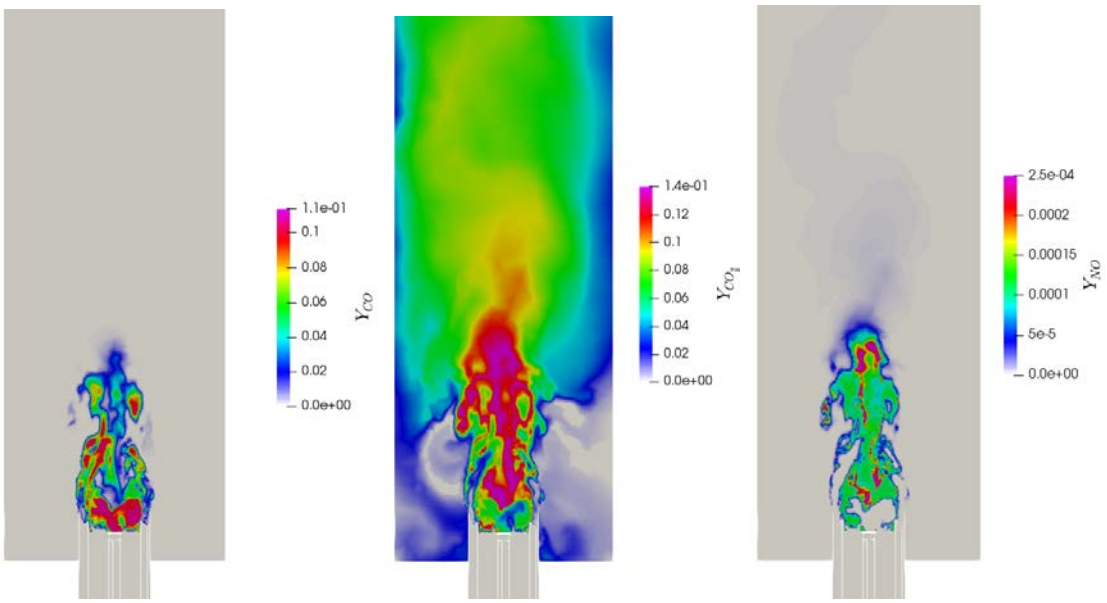

Figure 7: Snapshots of mass fractions of different pollutants at t = 4.5 ms after ignition at central plane. Left: YCO, middle: YCO2 and right: YNO.

6. Conclusions and Outlook

This paper is the result of a SHAPE project where our aim was to demonstrate the ability of LES to characterise the reacting flow field of an industrial combustor. The modelling approach is based on LES featuring a low-dissipation numerical scheme along with a combustion model based on flamelet modelling, which allows the

solution of complex geometries with detailed chemistry with an affordable computational cost. The results outlined in this paper correspond to the baseline condition of the burner including both the aerodynamic and combustion studies. The computational framework shows a great potential for pollutant predictions and design optimisation. The outputs of this SHAPE project will be highly valuable for a better understanding of the performance of the JBM 4.500 G burner produced by EMC and for a further optimisation of its design. Further collaboration between BSC and EMC is expected to evaluate potential design optimisations in the future.

Acknowledgements

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