**Template for Master Thesis subjects of BruFacE Electromechanical Engineering**

**Title:** Numerical simulation of flameless combustion: validation of combustion models and reduced in a wide range of operating conditions

**Promotor:** Alessandro Parente

**Research Group:** ATM

**Description thesis work:**

Flameless combustion represents a very appealing combustion technology due to its potential of coupling very high combustion efficiency with low NOx combustion emissions. However, due to its young character, the numerical modeling of flameless combustion is still characterized by open research questions, in particular related to the choice of the combustion model and of the kinetic mechanism. In particular, the combustion model should be able to describe the evolution of the system towards perfectly stirred reactor conditions and the kinetic mechanism should be validated at the conditions typical of such combustion regimes, high and homogenous temperatures and enhanced mixing. The aforementioned conditions are seldom verified with existing combustion and kinetic models, as they were developed for conventional combustion regimes. Therefore, the objective of the proposed MFE is that of optimizing the existing combustion models for flameless combustion conditions and to develop appropriate reduced kinetic mechanisms, by means of systematic approaches such as sensitivity analysis and graph theory. The determination of the range of applicability of the reduced mechanisms will be the main outcome of the investigation. The development of the reduced mechanisms will be carried out using kinetic analysis software, DARS by CD Adapco, and the proposed approach will be tested in commercial s well open-source CFD codes (StarCCM+ and OpenFOAM).

**Requirements:** Knowledge of fluid/mechanics and heat transfer. Past experience with CFD codes is an advantage.

**Number of possible students:** 1.

**Assistant/PhD student that will guide the student:** Rafi Malik (PhD student)

**E-mail and tel. contact person(s):** Alessandro.Parente@ulb.ac.be.

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![Figure 1 – Typical Damköhler number distribution in flame and flameless combustion.](image-url)
Template for Master Thesis subjects of BruFacE Electromechanical Engineering

Title: Implementation of the Eddy Dissipation Concept for turbulent combustion in the commercial code Fine/Open by NUMECA International.

Promotors: Alessandro Parente, Francesco Contino

Research Group: ATM (ULB), MECH (VUB)

Description thesis work:

Combustion processes can be simulated by solving the Navier-Stokes equations for multi-species reacting flows. The approach is general for the simulation of laminar combustion processes. For the simulation of turbulent combustion processes in the RANS context, the turbulence chemistry interaction (TCI) has to be modeled. In the eddy-dissipation modeling (EDM) approach the TCI is modeled assuming fast chemistry and that the mixing is the rate limiting process. The combustion process is ideally modeled using global one- or two-step reaction mechanisms, which obviate the need for stiff-chemistry solvers. The EDM approach implemented is versatile and can be used for the simulation of both premixed and non-premixed combustion processes. The method has however the disadvantage that a tuning of the empirical constants to the particular application might be required to attain results of satisfactory quality. The Eddy-Dissipation Concept represents a generalization of the EDM approach and can be used in conjunction with detailed reaction mechanisms. Based on an existing EDM approach, the Eddy-Dissipation Concept will be implemented in FINE/Open. To determine the chemical source terms, the method requires however an integration of the chemical source terms over the eddy turnover time. Since detailed reaction mechanisms usually are numerically very stiff, the integration of the chemical source terms will be carried out using a dedicated ODE solver. To speed up the method, In-Situ Adaptive Tabulation method will be used. The method will be verified on elementary flames and validated on industry-like combustor test cases. The thesis could be coupled to a stage, this is the solution preferred by the company.

Requirements: Fluid mechanics, numerical methods, CFD, programming language: C++.

Number of possible students: 1.

Assistant/PhD student that will guide the student:

For thesis in cooperation with industry:

Name company: NUMECA International

Name, e-mail address, tel. contact person industry: Jan E. Anker, jan.anker@numeca.be

E-mail and tel. contact person(s): Alessandro.Parente@ulb.ac.be, fcontino@vub.ac.be.
**Template for Master Thesis subjects of BruFacE Electromechanical Engineering**

**Title:** Reduced-order combustion models for combustion applications.

**Promotors:** Alessandro Parente, Francesco Contino, Axel Coussement

**Research Group:** ATM (ULB), MECH (VUB)

**Description thesis work:**

The detailed simulation of combustion processes still represent a challenging task, due to the high number of equations involved in the numerical modeling of common fuels. The simulation of a fuel as simple as methane would require, in fact, 53 species transport equations in addition to continuity, momentum and energy. The detailed mechanism for methane oxidation is characterized by 53 species involved in 325 reactions. Efforts for reduction are then needed. Within this context the ATM department at ULB and the Mechanical Engineering Department at VUB investigated the development of reduced-order combustion models based on the use of Principal Component Analysis and other techniques, which identify the most important parameters controlling a reaction process, providing a significant reduction of the CPU time associated to the numerical simulations. The objective of the present Master’s Thesis is to validate this method for a wide range of fuels and operating conditions. The Master’s Thesis will be carried out in the framework of a project funded by the American Department of Energy, in collaboration with the University of Utah, USA.

![Figure 2 – Sketch of model development process based on Principal Component Analysis.](image)

**Requirements:** Knowledge of fluid/mechanics and heat transfer. Programming experience in MATLAB and C++ is also required.

**Number of possible students:** 1.

**Assistant/PhD student that will guide the student:** Rafi Malik (PhD student)

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Template for Master Thesis subjects of BruFacE Electromechanical Engineering

Title: Development of a combustion chamber for gas-turbine applications

Promotors: Alessandro Parente and Patrick Hendrick

Research Group: ATM

Description thesis work:

The ATM department is very active in the field of gas turbines and novel combustion technologies, i.e. flameless combustion and micro-mix. Within this framework, the feasibility of novel combustion concepts for gas turbine is under investigation, for applications related to the micro-cogeneration of heat and power. The objective of the proposed MFE is to develop a conceptual prototype of a combustion chamber for a micro gas turbine using advanced Computational Fluid Dynamic tools. The study will in particular focus on the analysis of the combustion regime, the minimization of the pollutant emissions (CO and NOx) and the maximization of the combustion efficiency. The proposed work will be carried out within a project granted to the ATM department by the Walloon Region (NANOCOGEN+) and it profits from interaction with a CFD company based in Brussels, NUMECA. The numerical simulations will be carried with the NUMECA software FINE/Open and they will be benchmarked against reference CFD codes such as FLUENT.

![Figure 3](image)

Figure 3 – Combustion chamber operation in flameless combustion (left) and example of miniaturized combustion chamber for micro gas turbine (right).

Requirements: Knowledge of fluid/mechanics and heat transfer. Past experience with CFD codes is an advantage.

Number of possible students: 1.

Assistant/PhD student that will guide the student: Valentina Fortunato (PhD student)

For thesis in cooperation with industry:

Name company:

Name, e-mail address, tel. contact person industry:

E-mail and tel. contact person(s): Alessandro.Parente@ulb.ac.be, patrick.hendrick@ulb.ac.be
Template for Master Thesis subjects of BruFacE Electromechanical Engineering

**Title:** Numerical simulations of a glass furnace

**Promotor:** Alessandro Parente and Francesco Contino

**Research Group:** ATM (ULB), MECH (VUB)

**Description thesis work:**

The production of glass is an energy intensive process where a specific mixture is molten in big furnaces. These furnaces generally work 24/7 and modifications or developments are very difficult. Therefore, the role of computational fluid dynamics (CFD) appears of paramount importance to analyze the different aspects related to furnace operation and modifications, e.g. switching to a new fuel, adjusting the fuel air ratio, etc.

This Master's thesis can only be selected in conjunction with a stage/training to be performed at AGC. This should be done by first contacting Prof. Francesco Contino or Prof. Alessandro Parente. During the training, the student will develop the required expertise to simulate combustion problems with OpenFOAM. Then, the Master's thesis will focus on the numerical modeling of an existing combustion experimental rig, to compare the results obtained with OpenFOAM to experimental data as well as to previously obtained CFD results (with Fluent). This step might also be extended to an industrial furnace at the end of the thesis.

![Flame issuing into a glass melting furnace.](image)

**Figure 4 – Flame issuing into a glass melting furnace.**

**Requirements:** Knowledge of fluid/mechanics and heat transfer. Past experience with CFD codes is an advantage.

**Number of possible students:** 1.

**For thesis in cooperation with industry:**

- **Name company:** AGC

- **Name, e-mail address, tel. contact person industry:** Sylvain Drugman, R&D Project Leader, AGC Glass Europe (sylvain.drugman@eu.agc.com)

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**Title:** Validation of computational tools for fire propagation inside heated and ventilated rooms

**Promotor:** Alessandro Parente

**Research Group:** ATM

**Description thesis work:**

The objective of the proposed research is that of validating numerical tools such as FDS (Fire Dynamics Simulator) and FireFOAM to model fire propagation in the fields HVAC (heating, ventilation, and air conditioning) applications.

The available propagation models will be tested to predict temperature distribution inside rooms, in different configuration, forced convection, no ventilation, and presence of energy sources. The results will be compared to literature data and benchmark to already validated codes.

![Figure 5 – Simulated temperature distribution inside a room subject to a confined fire.](image)

**Requirements:** Knowledge of fluid/mechanics and heat transfer. Past experience with CFD codes is an advantage.

**Number of possible students:** 1.

**For thesis in cooperation with industry:**

**Name company:** Tractebel Engineering

**Name, e-mail address, tel. contact person industry:** Isabelle Hendrickx, Tractebel Engineering - isabelle.hendrickx@gdfsuez.com

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Template for Master Thesis subjects of BruFacE Electromechanical Engineering

Title: Optimization of two-equations turbulence models for ABL flows using uncertainty quantification

Promotor: Alessandro Parente

Research Group: ATM

Description thesis work:

There is an increasing interest in the application of Computational Fluid Dynamics (CFD) to the quantification of fluid flow in the lower atmosphere at the mesoscale, for weather prediction and wind resource assessment, and in the lower troposphere at the micro scale, where the highly turbulent atmospheric boundary layer (ABL) interacts directly with the human environment. Simulation of atmospheric flows at the meso and micro scales over both flat and complex domain is necessary for the estimation of wind loads on buildings and building heating requirements, to predict wind turbine loadings and for the optimal design of wind farms, to predict and evaluate the production and transport of pollution in the atmosphere and to perform micro-climate studies. The simulation of ABL flows is generally performed using commercial CFD codes with RANS turbulence modeling, applying the standard k–ε model. A novel approach has been recently proposed in the ATM department, consisting in the modification of the turbulence model and wall function formulation to retrieve an overall consistent treatment of the ABL, under different stratification conditions. The methodology has been demonstrated for the simulation of ABL flows over flat and complex terrains, and around buildings.

The present project aims at investigating the potential of turbulent zonal modeling for such problem, in combination with Uncertainty Quantification techniques. The objective of the study is that of identifying the parameters mostly affecting the results and to propose an optimized model, by comparing the numerical simulations to high-fidelity experimental data from the literature. The numerical simulations will be carried out with the commercial CFD software FLUENT.

Figure 6 – Velocity field around a single building (left), a mountain (center) and a group of buildings (right)

Requirements: Knowledge of fluid/mechanics and heat transfer. Past experience with CFD is a plus.

Number of possible students: 1.

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