TOPDEC PROJECT: NEW TOOLS AND METHODOLOGIES FOR THE DESIGN OF NATURAL GAS DOMESTIC BURNERS AND BOILERS

PROJET TOPDEC: NOUVEAUX OUTILS ET METHODOLOGIES POUR LA CONCEPTION DES BRULEURS ET CHAUDIERES DOMESTIQUES A GAZ NATUREL

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ABSTRACT

To satisfy the growing need for natural gas household appliances designed for both the European and world markets, technical constraints that interact, and sometimes conflict with each other, have to be taken into account. To reach this objective, a consortium made of gas companies, a burner manufacturer and academic institutions has developed new Design Tools and methodologies in the form of Design Guidelines, Experimental Methodologies and Computer Codes for the design of burners and boilers. Advanced diagnostic techniques, commercial boilers analysis and modeling of combustion kinetic of natural gas and of reactive flows have been used. After the development of these tools, a real exercise of burner development is currently in progress.

RESUME

Pour satisfaire les besoins croissant d’équipements conçus pour les marchés européens et mondiaux, des contraintes techniques, qui interfèrent et parfois entrent en conflit, doivent être prises en compte. Pour atteindre cet objectif, un consortium constitué de compagnies gazières, d’un fabricant de brûleurs et d’universités a développé des nouveaux outils et méthodologies sous la forme d’un guide de conception, de méthodologies expérimentales et de codes informatiques pour la conception de brûleurs et chaudières. Des techniques avancées de diagnostique, l’analyse de chaudières commerciales et la modélisation de la cinétique de combustion du gaz naturel et des écoulements réactifs ont été utilisés. Après le développement de ces outils, un exercice réel de développement de brûleur est en cours.

CONTEXT AND OBJECTIVES

Household appliances form one of the main application areas of natural gas combustion. The specificity of this application is the use of partially or totally premixed laminar flames. These types of flames are particularly sensitive to gas composition which affects flame stability and pollutant emissions. Such effects should be understood in order to satisfy the growing need for appliances designed for the European and world markets, using a very wide range of natural gas blends. Moreover, technical constraints, which interact, and sometimes conflict with each other, have to be taken into account. As an example, most of the markets require low-NO_x (below 50 mg/kWh), low-noise, compact and low-cost boilers. If the technology exists to design low-NO_x boilers using fully premixed advanced burners, it induces additional costs that are often not acceptable. To reach these objectives, boiler manufacturers need to use Design Tools able to analyze and predict flame stability, pollutant emissions and burner-boiler interactions.

Up to now, few basic studies have been made which address multidimensional laminar partially premixed flames with real natural gas and realistic boundary conditions. A consortium of gas companies (Gaz de France, BG Technology and Gasunie), a burner manufacturer (Worgas) and academic institutions (Centre National de la Recherche Scientifique, University of Heidelberg - PCI, and Imperial College of Science Technology and Medicine) has formulated a project, named TOPDEC. This project is supported by the European Commission in the framework of its Brite EuRam III programme. Its aim is to develop new design tools and methodologies in the form of design guidelines and computer codes for the simulation of burner and boiler performances.

METHODOLOGY

To address the development of efficient Design Tools, a dual approach was undertaken.

Design Guidelines

Measurements in flames of idealized and commercial boilers were made to capture the main basic mechanism of flame stability and pollutant emissions in conditions representative of real appliances. In addition, the methodology of design of domestic boilers was analyzed to identify and quantify the critical parameters influencing the global performance. Furthermore, the characteristics of the boiler components, which influence the boiler behavior, were investigated. From these detailed measurements and analysis, complemented by insights from the modeling, actual Design Guidelines could be derived.

Computer Codes for Burner Design

Recent progresses in numerical simulation techniques and combustion kinetic modeling have opened the way to simulation of practical laminar flames encountered in commercial appliances. Nevertheless, problems remain to be solved. The first one is to derive from a detailed kinetic mechanism of natural gas combustion (not only methane) a simple, although realistic (flame speed, pollutant emissions), reduced mechanism able to be incorporated in a computer code using Computational Fluid Dynamics (CFD) techniques. The second one is to couple this reduced mechanism into a CFD code in an efficient manner to make the resulting design tool usable in an engineering environment.

Idealized Boiler

The idealized boiler was developed by Gaz de France and Worgas to mimic the key features of practical appliances while simplifying the problem from a 3 dimensional to a 2D flow (**Figure 1**). The configuration is similar to real boilers equipped with blade burners. Attention was paid to the knowledge and control of the inlet conditions, the air/gas mixture composition, the secondary air flows, and the heat fluxes at the boundaries. It was first characterized by global measurements (stability, total emission levels) for different loads, primary and secondary aerations. It was concluded that the idealized appliance has a similar behavior to practical boilers with respect to correlation between the input and output parameters (**Figure 2**).

Subsequently, detailed measurements were made in the idealized boiler, for different regimes and flame shapes relevant to practical equipment by GDF, BG, PCI and CNRS. Five test cases were defined which span from totally premixed to partially premixed flames that are described in table 1.

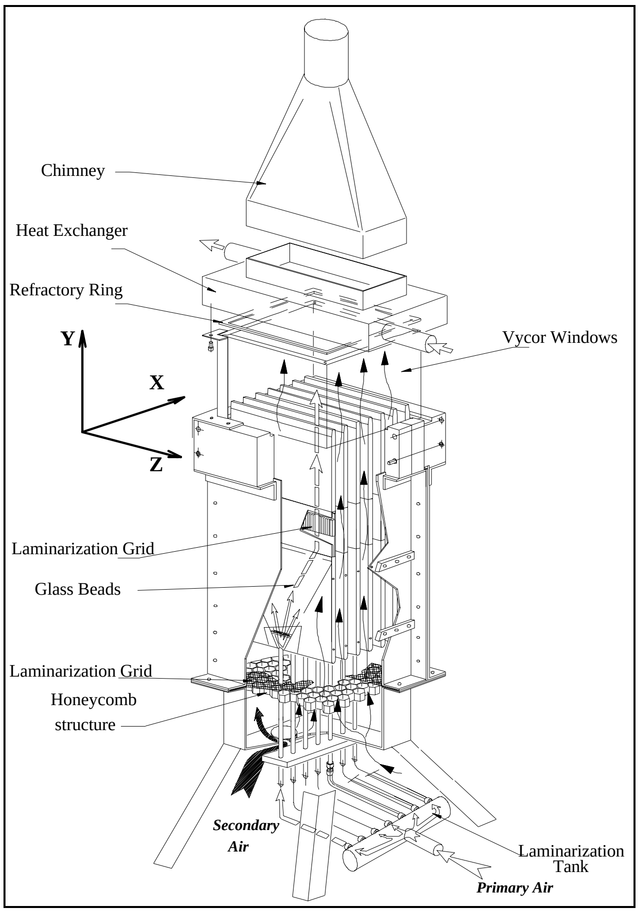

Figure 1: Idealized boiler schematic

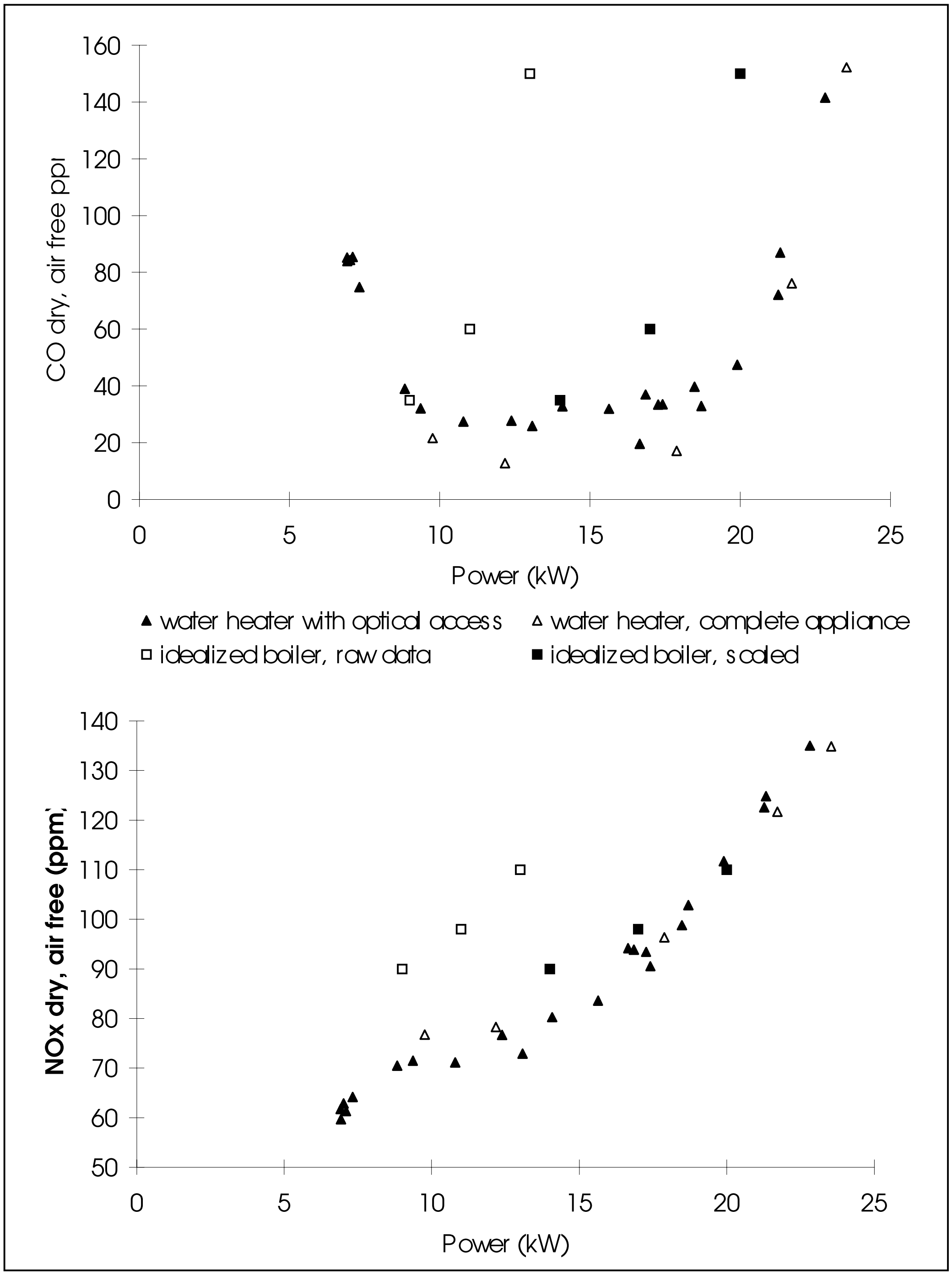

Figure 2: CO and NO_x emissions in idealized and commercial boilers

Bunsen and V-shape flames burning pure methane or natural gas blends have been considered changing primary and secondary aeration and flame shape while keeping constant the thermal load to 10 kW and the total aeration to 1.4. Local temperatures, molecular (CH_4, O_2, CO, CO_2, NO, NO_2), and radical (CH, OH, CN, C_2) species concentrations have been measured using advanced diagnostic techniques in the idealized boiler. Velocity measured by Particle Image Velocimetry, temperature measured by Fine Wire Compensated Thermocouples and C_2 and OH radicals concentrations imaged by Spontaneous Emission Spectroscopy are presented for the test case #1 (**Figure 3**). For the aerodynamic field, the homogeneity of the secondary air distribution is verified and gradients are identified, along with the laminar nature of the flow. The temperature field shows that the maximum is reached in the region between the premixed reaction zone (inner cone) and the diffusion reaction zone (outer cone). The excited OH distribution shows that the flame is attached to the burner and the maximum located at the burner vicinity, while the C_2 formation is delayed leading to a concentration maximum at the top of the inner cone. From all the detailed measurements collected in a database, a clear understanding of the basic mechanism could be achieved. More details can be found in [1].

Table 1: Test cases for the idealised boiler

Test Case #	Fuel composition			GCV	Power Input	Flame type	Primary Aeration	Second. Aeration	Purpose
	CH_4	C_2H_6	C_3H_8	$kWh/m^3(n)$	kW				
1	0,9	0,06	0,04	11,04	10	Bunsen	0.6	0.8	Conventional boiler with NG blend
2	1	0	0	9,87	10	Bunsen	0.6	0.8	Conventional boiler with pure methane
3	1	0	0	9,87	10	Bunsen	1.4	0	Lean fully premixed flame, no secondary air
4	1	0	0	9,87	10	Bunsen	1.2	0.2	Lean premixed Bunsen flame with secondary air
5	1	0	0	9,87	10	V-shape	1.2	0.2	Lean premixed V-shape flame with secondary air

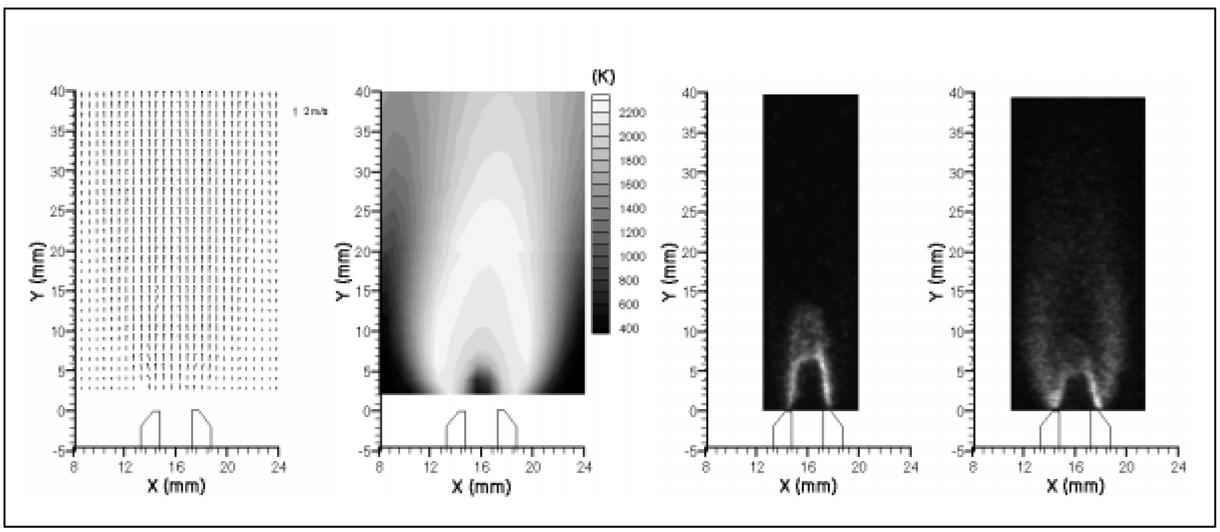

Figure 3: Velocity, temperature, C_2 and OH fields in the idealized boiler (case #1)

Commercial Boilers

These appliances utilize multiblade burners that resemble the idealized two-dimensional burner, but which are essentially three dimensional in nature. In this fashion, the similarities and differences between the idealized and practical cases could be evaluated, and the information obtained will serve for establishing the guidelines. A commercially available, partially premixed, instantaneous hot-water heater was modified for optical access by Gasunie. As a first step, a series of input/output measurements (emissions versus thermal load) intended to ascertain that the modified appliance behaved similarly to the original were carried out. In addition, it was checked, that when properly scaled at the same surface thermal throughput, the NO_x emissions were nearly identical and CO emissions were similar. The difference in scaling behavior is a result from the fact that NO formation is governed mainly by a bulk phenomenon while CO emissions are more influenced by local conditions (**Figure 2**). The distributions of the concentrations of NO and CO and of the temperature were measured by Laser Induced Fluorescence (LIF) and Coherent Anti-Stokes Raman Scattering (CARS). In particular, the effects of mixing between the hot flame gases and the cold secondary air on pollutant formation were studied under realistic conditions of thermal load and limited access of secondary air. The analysis of the results yielded a number of minor differences with the idealized boiler. First, the flames in the practical water heater were substantially less stable than those in the idealized boiler; the practical flames tended to show high-frequency fluctuations ("jitter"). In addition, the CO measurements showed substantial CO concentration between the burner blades (as a result of fuel-leakage), which the measurements on idealized boiler only suggested under fuel-lean conditions. However, none of these observations indicated any real difference in the behaviors of these appliances (**Figure 2**).

The general design and assembly processes of a boiler were considered in terms of different parameters thought to determine the boiler performance. Therefore, a detailed analysis of the manufacturing and development processes was carried out by Worgas to quantify their contribution on the operating conditions and global performance (**Figure 4**). In parallel, to produce design tools of practical use for manufacturers, it is essential to link the Design Guidelines with the manufacturing process and the boiler individual components. These results were incorporated into the Guidelines.

Floor standing and wall mounted boilers, equipped with a burner designed for 8.8 kW of nominal input, have been instrumented with flue gases sample probes, thermocouples and optical accesses for Laser Sheet Visualization by Worgas. All the tests were made with the same nominal power input of about 8.8 kW, varying the secondary air entrainment, the slots pattern and the flue gases obstruction. As an example, the influence of secondary air distribution on the NO_x emissions for different total aerations were assessed (**Figure 5**).

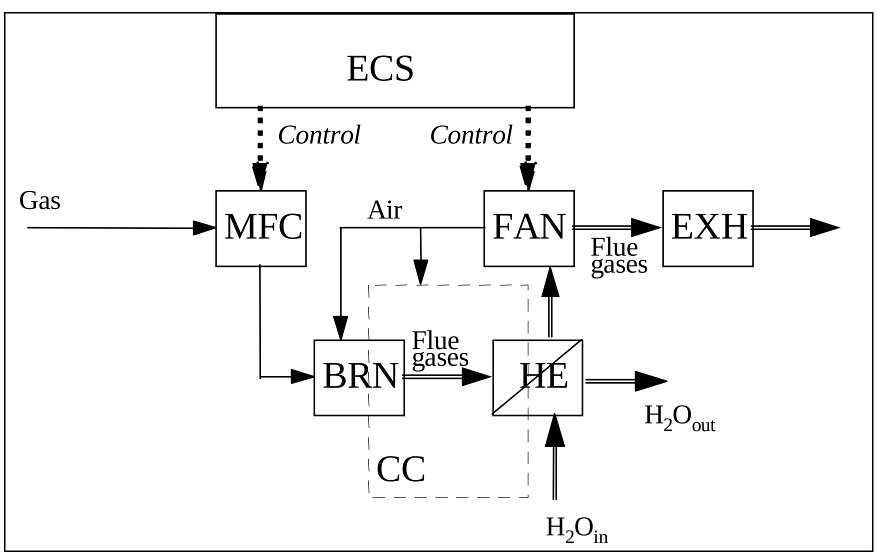

Figure 4: Boiler system schematic (ECS: Electronic Control System; MFC: Mass Flow Controller; EXH: Exhaust; BRN: Burner; HE: Heat Exchanger; CC: Combustion Chamber)

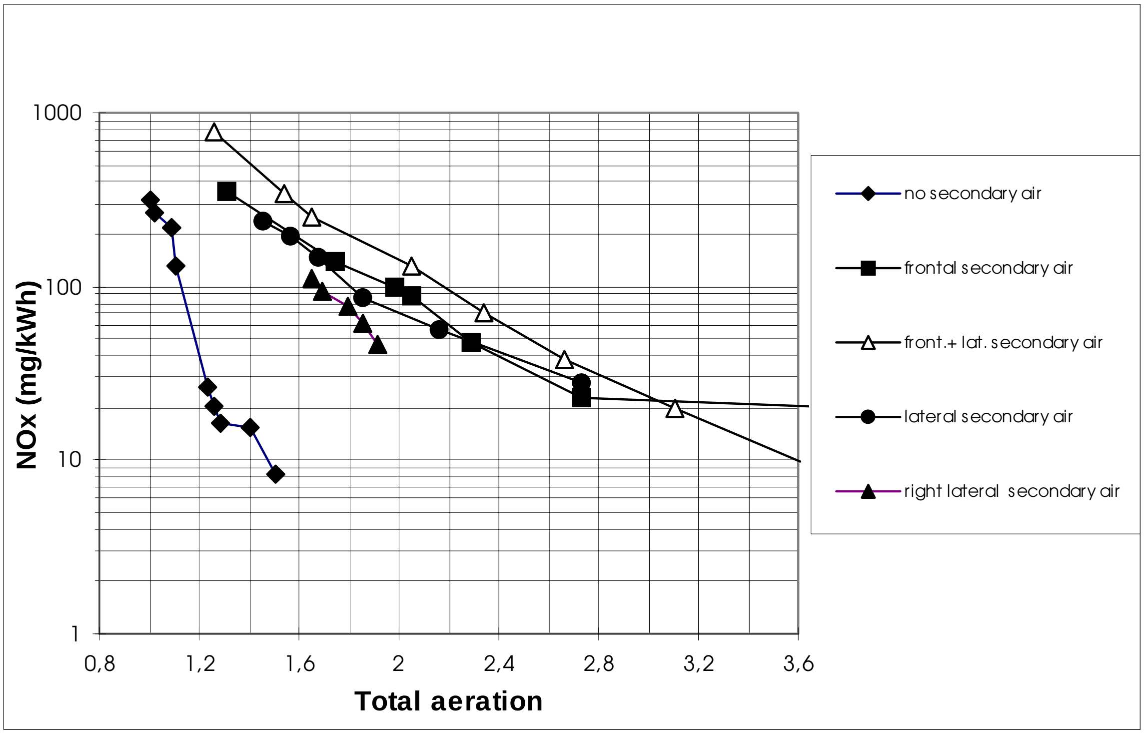

Figure 5: NO_x emissions in a wall-mounted boiler as a function of total aeration and secondary air distribution.

DEVELOPMENT OF BURNER DESIGN GUIDELINES

These guidelines feature correlations and trends, which are based on scientific knowledge acquired during the project. They should be provided in a form suitable for design engineers.

The results obtained in the idealized and commercial boilers were analyzed by all the TOPDEC Consortium partners and gathered to obtain a comprehensive description of the phenomena governing flame stability, flow behavior and pollutant formation in domestic boilers. In particular, the combinations of primary and secondary aeration, the relative velocities and distributions of primary mixture and secondary air, the influence of these parameters on NO_X and CO emissions, and the effects on flame structure revealed by the diagnostic and modeling studies were analyzed to assess the effects of the variations of these parameters on boiler performance. A preliminary version of the Design Guidelines and the experimental methodologies is now available and should be validated during a real exercise of burner development.

CFD TOOLS

Modeling of Natural Gas Combustion and NO Formation Kinetics

For most of the studies dedicated to practical burner modeling, natural gas was assimilated to methane. Few studies on natural gas blends [2] have shown the importance of minor species in natural gas flames, especially for predicting flame stability and key radicals on the route to NO formation by the prompt and thermal channels. Advanced reduced kinetic mechanisms, which feature the chemistry of methane, higher hydrocarbons and NO, have been developed by ICSTM from a detailed C/H/N/O reaction scheme containing 73 chemical species and 503 reactions previously developed for combustion of methane-ethane type mixtures [3]. It is consisting of 15 steps and is capable to accurately reproduce levels of key radicals such as CH and HCCO and shows good agreement (**Figure 6**) compared to experimental measurements from [4]. A key difference compared to previous reduced mechanisms is that the present mechanism incorporates the full effects of the C_2-chain and thus works well also under rich combustion conditions. The inclusion of the C_2-chain in also important in the context of an accurate modeling of the prompt NO channel and the destruction of NO through the interaction with hydrocarbon fragments.

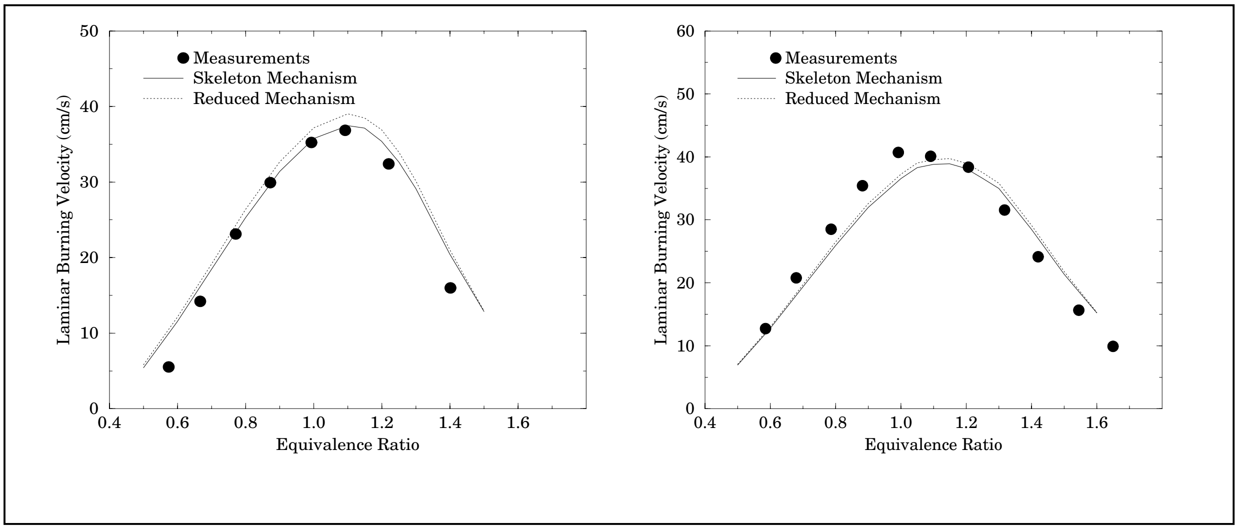

Figure 6: Computed laminar burning velocities for methane-air (left) and ethane-air (right) mixtures and experimental data from [4]

Development of CFD Based Design Tools

For basic research purposes, 1D laminar flame codes are widely used (i.e. PREMIX code). They are very helpful to analyze the combustion behavior of a fuel and are widely used among the scientific community to validate combustion kinetic schemes against experimental data obtained in low-pressure (flat) laminar flames. Of course, they are not incorporating features needed to design a practical burner of a domestic boiler. For computer simulation of multidimensional combusting flows, several commercially available 3D codes, running on workstations, are able to predict the flow in bar burner system of domestic boilers (PHOENICS, FLUENT, CFX, ESTET, etc.). Nevertheless, none of these codes has the capability to use a complex chemistry for combustion and has been validated against experimental data in such a configuration. They have been designed for general purpose in industry and most of the current improvements are targeted towards fluid mechanics and heat transfer. Predicting multidimensional laminar premixed reactive flows implies the coupling of 3D flow calculation with a detailed chemistry. In the flames concerned, chemistry is very important: the flame position and shape must be calculated with great accuracy because they are strongly related to the heat transfer with the burner, which influences the temperature field and, consequently, the combustion kinetics, flame stability and final composition of the exhaust gas. Moreover, relatively complex phenomena such as hydrogen atom recombination near the burner surface have to be considered. Such a chemistry-flow coupling for multi-dimensional gaseous fuel combustion has not yet been made in a commercially available code, only in 2D research code [5].

Modeling work, using recent scientific knowledge related to laminar combustion and the reduced kinetic mechanism described above, were used and implemented into commercially available CFD codes. Two CFD codes were used, one developed jointly by BG and Mantics Numerics (COBRA) and one developed by Electricité de France and use by GDF (ESTET). COBRA, that had already the capability of handling reduced chemical kinetics, was enhanced to give global results to the user like CO, CO_2 and NO concentrations at the fire box exit. ESTET was coupled with the GDF kinetic library BISCUIT, resulting in a specialized version of the ESTET code, called ESTET-CC for Complex Chemistry (**Figure 7**). These efforts have, together with experimental data obtained in the idealized boiler, resulted in two numerically validated tools (**Figure 8**). A specific attention has been paid to the methodology of use of such numerical Design Tools to ensure the efficiency of computations related to manufacturers needs and to the ease of use.

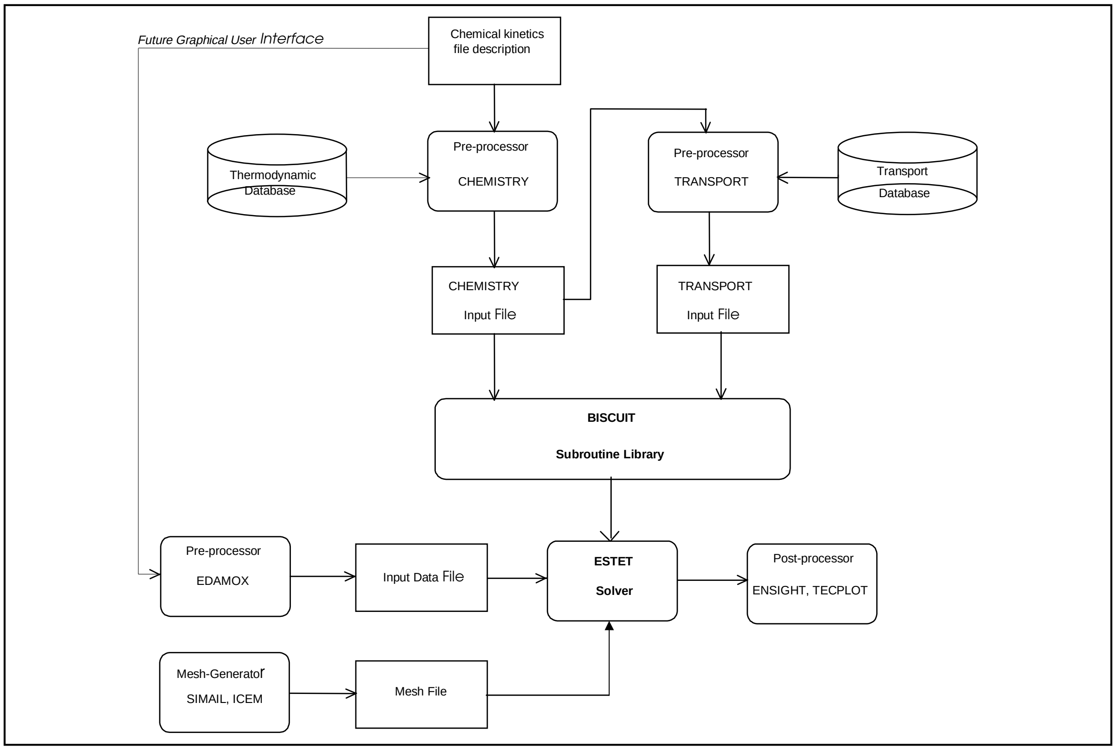

Figure 7: General structure of the BISCUIT library - Integration into the ESTET-CC code

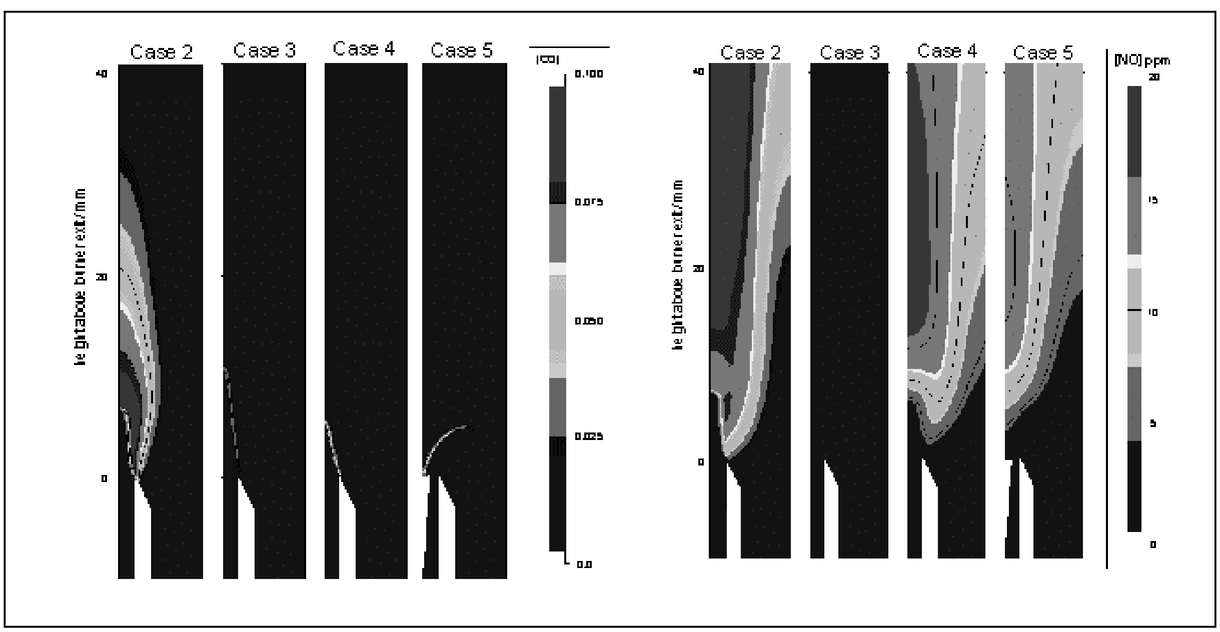

Figure 8: Computed maps of CO (left) and NO (right) for test cases # 2–5 obtained with COBRA code

EVALUATION OF DESIGN TOOLS

In order to assess the benefit of the new tools and methodology, a real exercise featuring the development/improvement of a commercial burner is currently made by Worgas, GDF and BG. A conventional Bunsen-type burner and a V-shape flame burner are being improved using the Design Guidelines and the CFD tools. The targeted specifications are given in **Table 2**. The tools are expected to be further optimized as a result of this exercise. At the end of the latter, the benefits obtained by using the tools in improving the design of practical appliances will be compared to their costs.

Table 2: Specifications for the burner to be developed in the real exercise

Power input	~ 25 kW net
Efficiency	93%
Emissions	CO < 100 mg/kWh
	NOx < 50 mg/kWh
Gas Type	G20, G21, G231
Modulation	30% ÷ 100%
Noise	< 50 dbA (1m distance)

CONCLUSION AND PERSPECTIVES

An idealized household boiler was designed, build and characterized. The results show that its reproduces commercial domestic boilers behavior with a simplified geometry and a better control of the boundary conditions. Detailed measurements were made in both idealized and commercial household boiler flames which highlighted the key mechanisms of combustion control in such appliances.

Two CFD computer codes are being enhanced to extend their capability to simulation of household boiler flames in an engineering environment and to offer a user-friendly interface for the burner designer. Good results were obtained in terms of trend predictions of flame shape, stability and NO emissions.

From the detailed measurements, burner/boiler development analysis and some simulation results, guidelines were derived. These Design Guidelines, in the form of a book, help the designer in analyzing the results of prototype tests and provide key parameters to adjust to meet design specifications such as CO and NO emissions. In addition, a methodology of use of in-flame measurement techniques is given.

The evaluation of these tools (Design guidelines and CFD codes) during a real exercise is on progress. At the end of the project, planned for beginning of 1999, these Design Tools will be made available to the gas industry.

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