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MODEL FOR CALCULATING THE EMISSION FROM PARTIALLY PREMIXED GAS BURNER EQUIPMENT[1]

Attila MEGGYES and Éva BOSCHÁN*

Department of Heat Engines
Technical University of Budapest
H-1521 Budapest, Hungary

*MOL Plc Oil and Gas Laboratory

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Abstract

Our aim is to construct a computer model for NO emissions for a Bunsen flame by applying kinetic equations describing the formation of NO. Because of difficulties and inaccuracies of the determination of the flameshape, the model primarily suits direct to get a trend of NO_x emission as a function of operating conditions. However, there is a possibility to improve the accuracy of calculation the NO_x emission by validating the model.

Keywords: NO formation, calculation, model, premixed flame.

Introduction

In the ideal case of gas combustion the emissions of CO and NO from a homogeneous combustion may be described by reaction kinetics equations. There are a large number of publications dealing with the calculation of NO formation in turbulent flames. Less attention has been given to the calculation of NO emissions in partially premixed gas flames. However, this occurs most frequently for partially premixed type of flame in domestic gas combustion equipment. This arises from the more complex chemistry of the partially premixed (Bunsen) flame. In constructing a computer model for NO emissions for a Bunsen flame, we have aspired to take into account, and to describe by the means of equations, the structure of the flame by applying kinetic equations describing the formation of NO. Before calculating NO for partially premixed flames it is expedient to give a short review of the burner flame characteristics.

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[1] It was presented at the Anglo-German Combustion Symposium in Cambridge (April 1993).

Structure of Bunsen Flames

It is well known that the Bunsen flame is essentially a double flame where combustion begins in the inner cone and is completed in a thin (approximately 10 μm) 'film' layer along the outer mantle.

Our presumption is that combustion occurs not only along these two surfaces but also in the intermediate space. The space between the two above mentioned cones is rich in fuel. Necessary oxygen can also penetrate into this space by diffusion of the air through the outer surface of the flame, thus creating ideal conditions for combustion. As the diffusion is a slow process, oxygen can only gradually penetrate into this space between the two cones, and for this reason a relatively large volume space of definite form is created between the two conical surfaces.

The space between the two conic surfaces may be understood as an aggregation of elementary units, in each of them following oxidation reactions are continuously under way as can be seen in *Fig 1.*

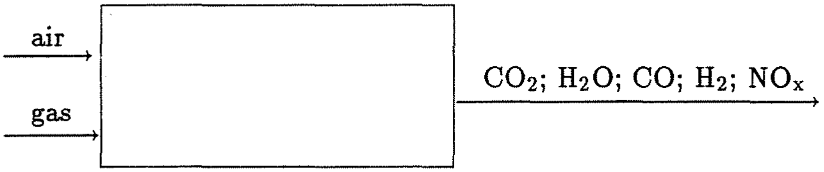

Fig. 1. Simplified combustion reaction in an elementary unit of a Bunsen flame

As a result of this there is a continuous modification:

- of the mass of the elementary unit,
- of the composition of the elementary unit.

The above assumptions are supported by our own measurements and by those of other authors.

Fig. 2 shows the concentrations of components characteristic of the whole, along the axis of the flame, as measured by chromatography.

We have shown the inner and outer cones of the Bunsen flame, along the horizontal axis of the figure, and have also indicated spot results. It can be shown that the concentration of O_2 within the flame is always lower than 1 vol% and that increases to 2 vol% only in the vicinity of the outer mantle. This means that oxygen penetrated into the flame is consumed in oxidation. This observation is supported by the fact that initially high concentrations of H_2 and CH_4 decrease continuously within the flame volume to near zero. Concentration of CO_2 continuously increases with the progress of oxidation, however, diffusion of air and the diluting effect of nitrogen only

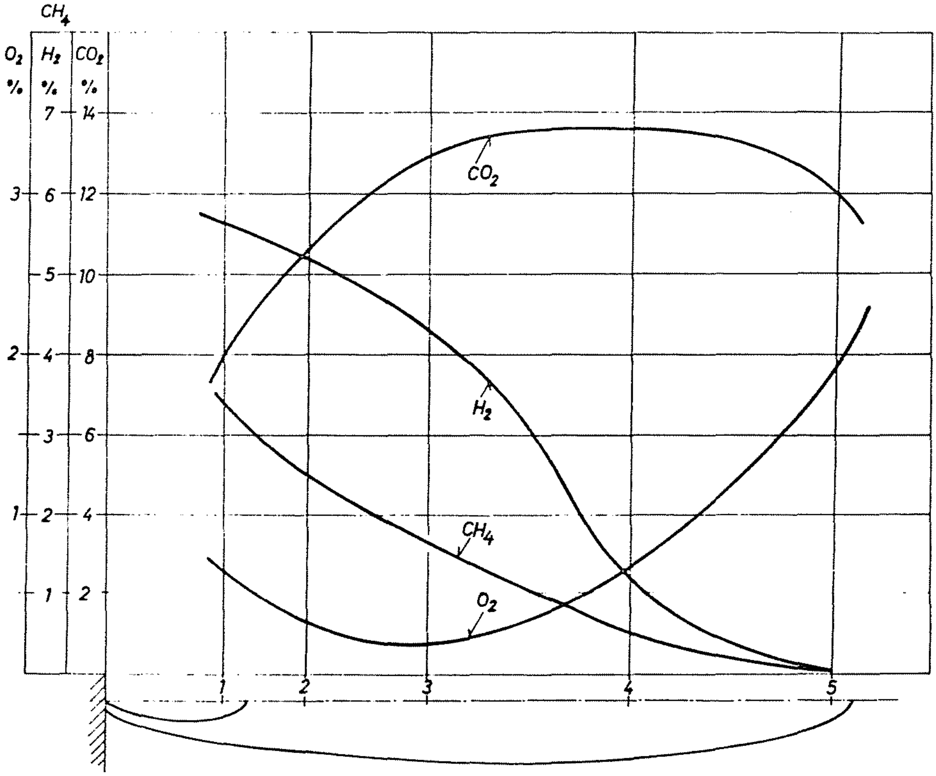

Fig. 2. O_2, CH_4, H_2 and CO_2 concentration in the flame (analysed by gas-chromatography)

begin to decrease near the end of the flame, i.e. formation of CO_2 during combustion will compensate for dilution.

Concentrations of components measured in the direct vicinity of the inner cone show that methane-fuel (corresponding to oxygen to be found in the ratio conditions of premixing) is burnt with the formation of various intermediate products (CO and H_2). The remaining concentration of CH_4 proves that only a part (closely corresponding to the premixing ratio) will participate in combustion. The excessor remainder of the methane-fuel will react in the further parts of the flame.

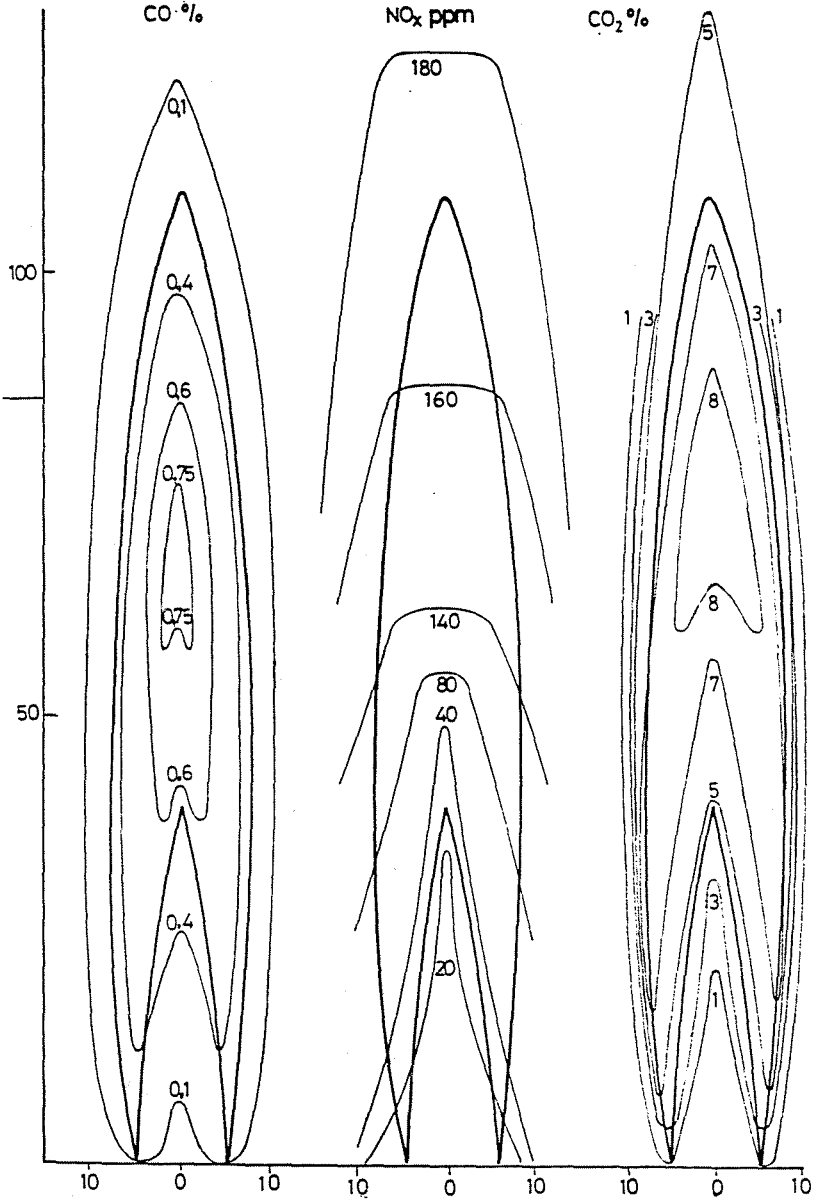

Fig. 3. CO_2, CO and O_2 isoconcentration lines of the flame

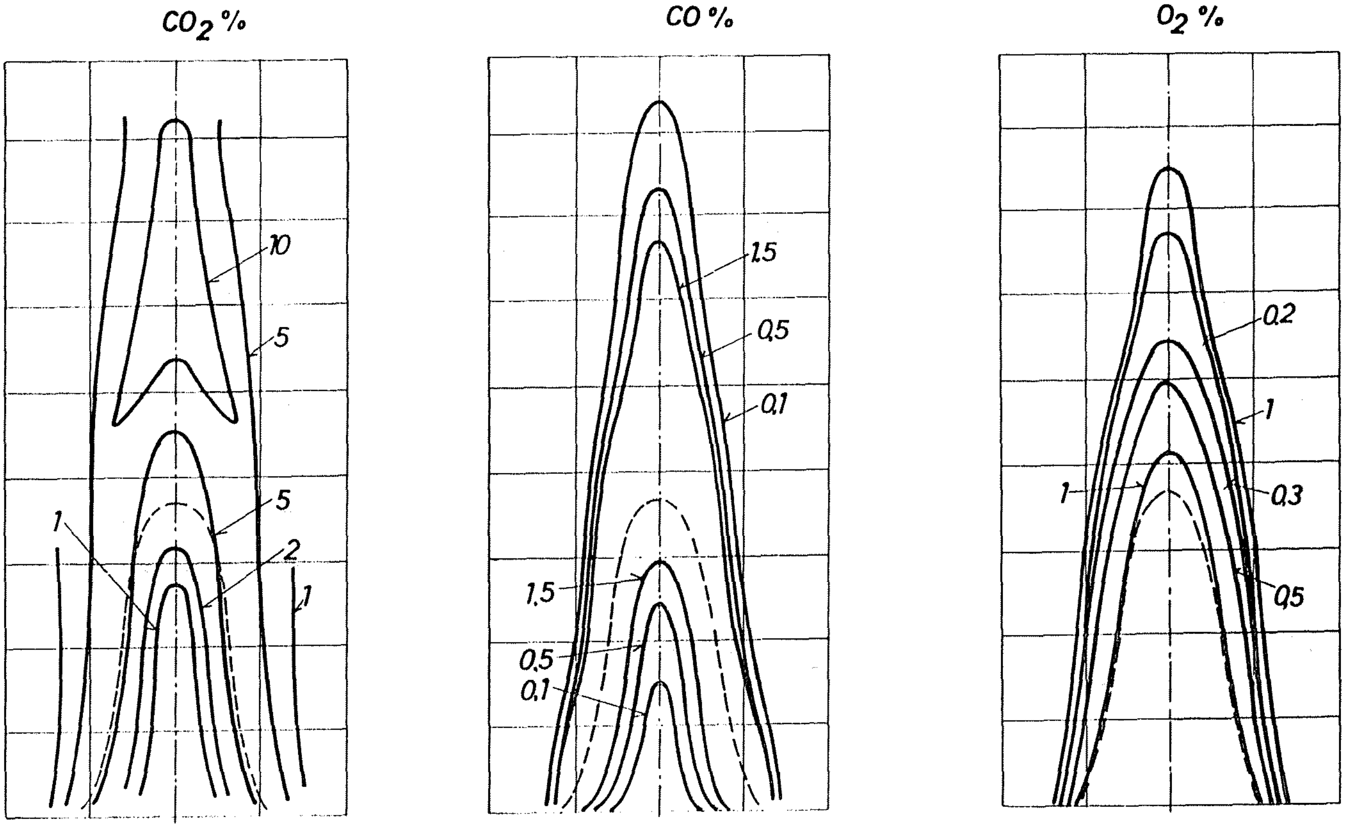

Fig. 4. CO, NO_x and CO_2 izoconcentration lines of the flame

Similar results are reached if we extend measurements from the axis of the flame to the complete flame section (*Figs. 3* and *4*).

As may be seen from *Fig. 4* the concentration of CO remains lower than 1 vol% within the whole volume of the flame while not only CO_2 concentration but also NO gradually increases. Measurements by HESS also show a similar picture as far as CO, CO_2 are concerned while the value of oxygen concentration reaches a maximum of 1 vol%. (*Fig. 3*).

The above is also confirmed by distribution of temperature published by GAYDON (*Fig. 5*).

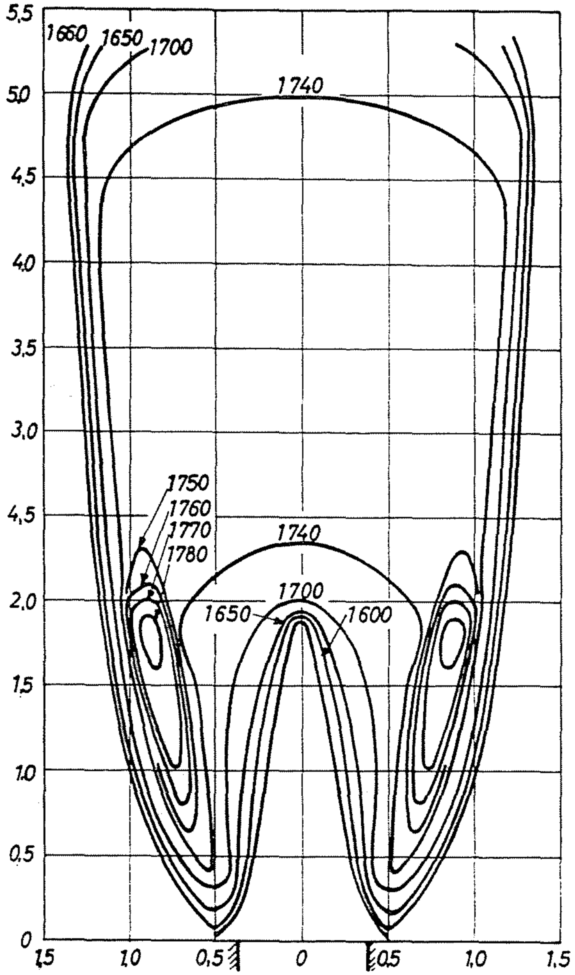

Fig. 5. Temperature distribution for a rich flame

As seen in the figure, temperatures rapidly increase along the inner cone to the maximum flame temperature. Within the flame, temperatures are nearly homogeneous and only begin to decrease rapidly in the near vicinity of the outside cone. Therefore, within the flame near constant (nearly adiabatical) temperatures are predominant.

The phenomenon can be explained in the following way:

A part of the gas, which reacts with the premixed air, is warmed by the combustion up to adiabatic temperature. The remainder gas burns corresponding to the oxygen diffusing into the flame and the combustion process occurs at adiabatic temperature. The combustion continues while the full gas is consumed. The heat transfer in the space between the two cones is negligible, so it can be assumed that the adiabatic temperature is remaining.

Assumptions Used in Elaboration of the Model

In elaborating this model we have made some assumptions that are summarized below.

a) Combustion commences in the approximately 10 μm thick film layer along the surface of the inner cone, where an air-fuel mix closely corresponding to the conditions of premixing is to be found. A quantity of fuel corresponding to the concentration of oxygen is consumed here, the rest of the fuel flows on further unchanged. The following quantities of fuel are consumed in the space between the two cones in direct proportion to the diffusion of oxygen. This increases the material consumed in combustion and decreases the concentration of fuel. This process continues until fuel is totally consumed, this occurs in the thin reaction layer of the outer cone. The principle of the process may be seen on *Fig. 6.*

   As shown on the Figure, the unconsumed fuel continually decreases, while at the same time the part consumed in combustion shows a corresponding continual increase. The mass and correspondingly the volume of material shows continuous increase corresponding to the diffusion of air (oxygen).

b) Along the inner cone the temperature corresponds to the adiabatic temperature of combustion. The process in the further elementary units is also of an adiabatic nature.

c) We neglect transfer of heat in the processes taking place in the space between the two cones.

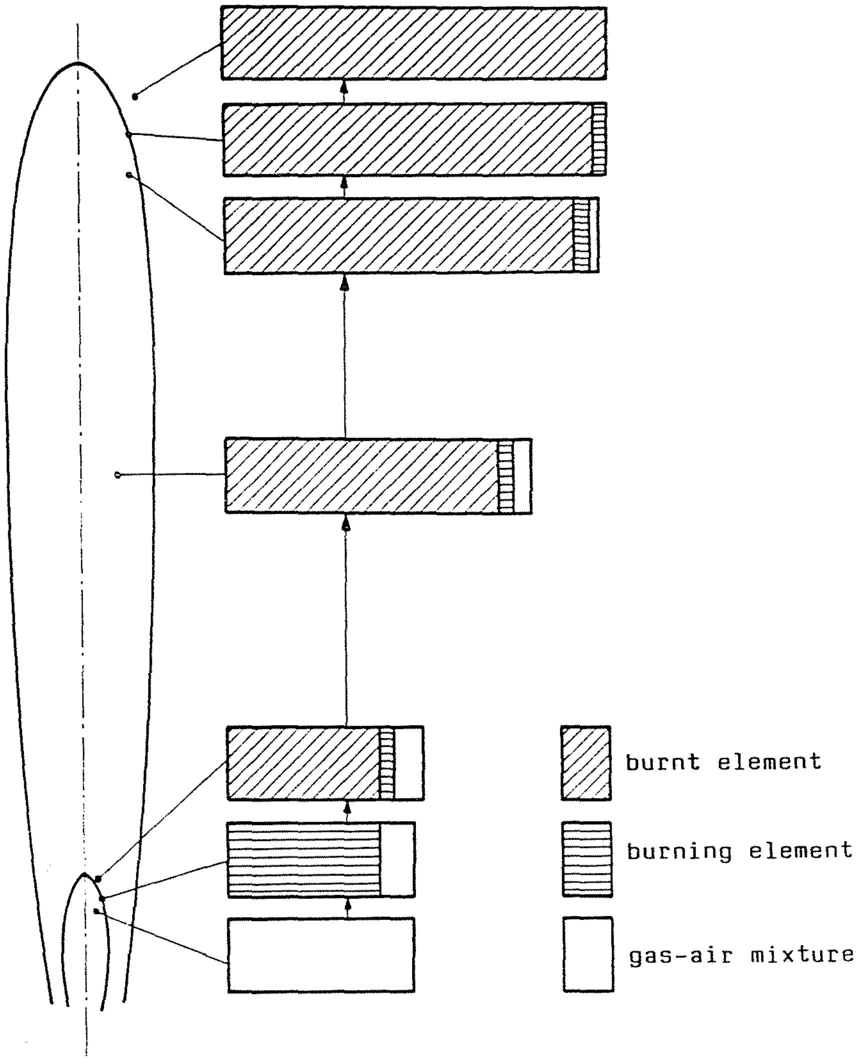

Fig. 6. Different elements in the flame

d) Division of the several elements of the flame into material consume in combustion material in the process of combustion and non-combusted parts is arbitrary. In reality there exists a mixture of all these parts.

e) In calculating formation of NO it is most important to determine the time of residence of the several elements at any given point. Above and beyond a knowledge of the geometry of the flame (outer and inner cones) it is therefore necessary to determine the quantity of the mix and its temperature. The quantity of mix along the surface of the inner cone is given by the conditions of premixing along the outer cone and may be determined from the conditions of stoichiometry. In the space between the two cones the diffusion of oxygen is continuous in direct proportion with conditions.

It should be noted that it is problematic to determine the inner and outer flame cones (mantles) in case of the interaction of several flames, especially in such cases when diffusion of air (oxygen) from the outside (from the side or from under the flame) is impeded. In such cases, this would result in a wide variety of 'outer' flame surfaces, the geometrical measurements of which are not even approximately known. In such cases the dimensions of the flame and the times of residence of material may be entered into the programme from the results of some measurements.

Description of the Model

The model has been developed for calculation of the NO emissions of partially premixed flames. This was achieved by a modification of our programme for homogeneous turbulent flames taking into consideration the special properties of partial premixed flames. This software package and results obtained from its application were demonstrated by authors on the 1989 '14. Deutscher Flammentag'. The modified programme consists of four parts:

a) Selection of initial data. The type of gas (G20, G25, G30) should be defined, also the extent of premixing, the parameters of gas and air (pressure, temperature, moisture content).

b) Determine the combustion process. The characteristics of the burner equipment should be entered (geometrical dimensions), and also the characteristics of the process of combustion (degree of premixing, recirculation, water injection, etc.) With the application of an approximation formula the geometrical dimensions of the partially premixed flame are determined.

c) Calculation of the cooling process. The calculation programme determines an approximate formula describing the cooling cycle on the basis of the given burner equipment and combustion process for the different points of the combustion apparatus to determine temperature values at these points.

d) Calculation of production of pollutants. By the application of reaction kinetics equations, we determine thermo nitrogen oxides for the combustion and cooling cycles, for every element in the cooling cycle (along the inner cone surface, in the space between the two cones, and along the mantle of the outer cone).
The algorithm of the software is shown on *Fig. 7.*

The determination of the burning process is rather problematic. In the first place the partially premixed flame shape has to be calculated. There are several state of the art formulae known. According to trial calculations, describing the partially premixed flame from two interpenetrating cones leads to an adequate result. The calculation is carried out by equations found in the dissertation of HESS.

The most difficult problem is to define the exact size of the orifice. In the first step of computation, a series of the orifices has been considered as one unit.

Results

We completed several trial runs to determine the applicability of the proposed software. In the first place calculations were carried out for cases where we had measurement data at our disposal. Initially, we controlled whether the calculated results showed the same trends as measured data. The most suitable data for this purpose are calculations of NO emissions as a function of premixing and load. The problem of prime importance for us was to determine the accuracy of trends. When this gave favourable results, we continued calculations for cases where we had at limited data on the combustion equipment and its operation. This had to serve as a basis for the calculation of measured emissions. Measurements were made by the CETIAT Institute (France) and these followed our calculations. Our experience may be summarized as follows.

a) The most difficult task is to define the shape of the flame from calculation and match it to the observed shape. This in turn effects the calculated NO emission. At the same time even with an application of the simplified formula for determining the form of the flame, satisfactory results were obtained for NO emissions from the point of view of determining trends.

b) *Fig. 8* shows calculated formation of NO in relation to the retention time in the flame of natural gas and LP.
According to results of calculations the degree of NO emissions increases together with the increase of time of residence within the flame.

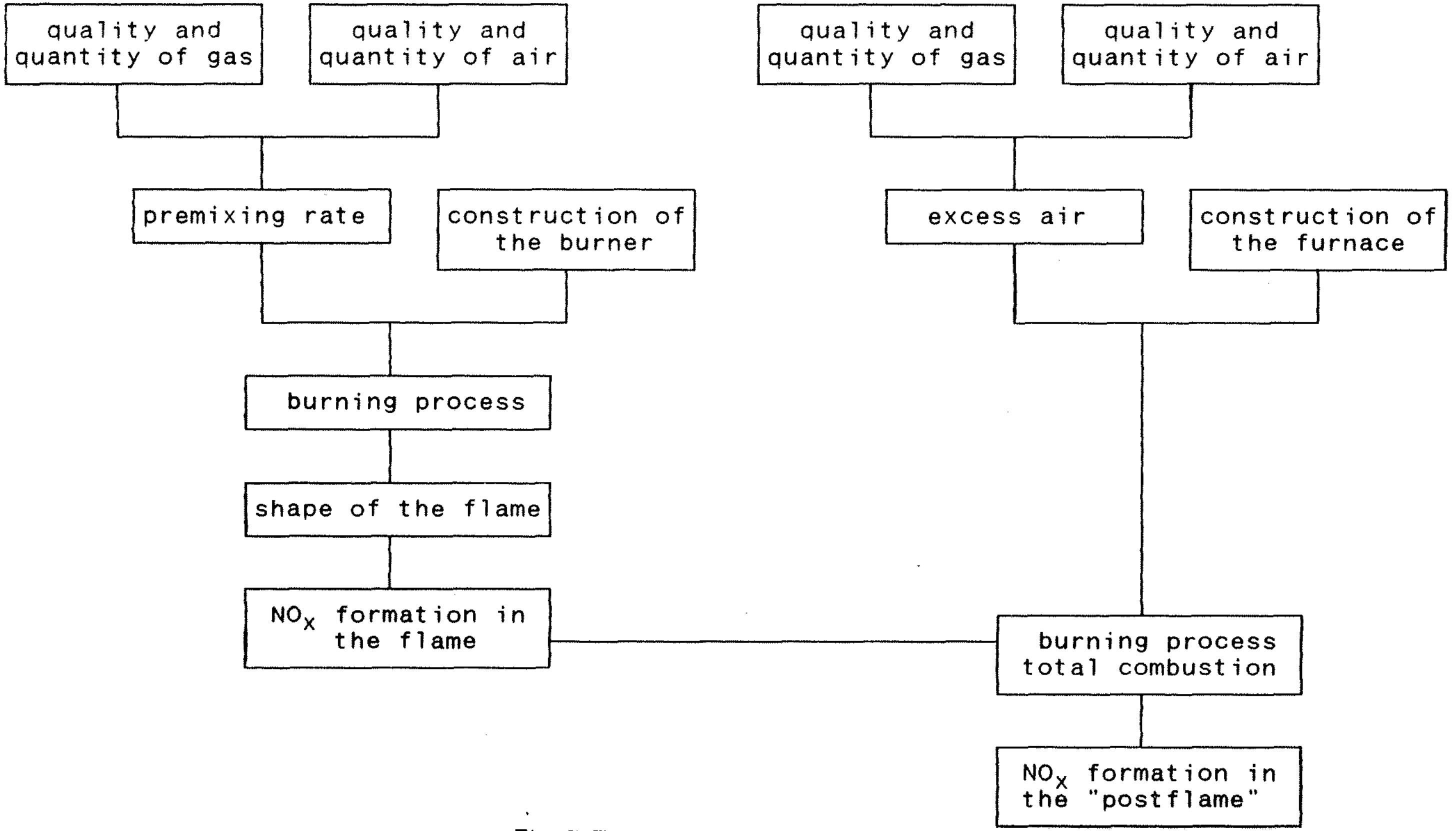

Fig. 7. The algorithm of the software

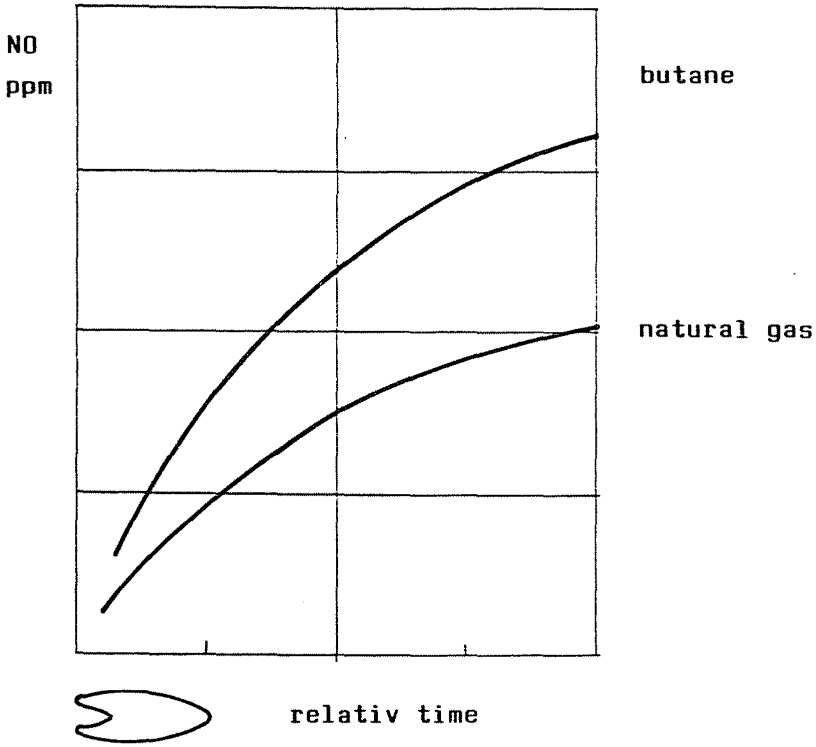

Fig. 8. Calculated NO emission by natural gas and LP

c) Calculated NO emission as a function of premixing is shown on *Fig. 9.* In agreement with model computation formation of NO in the flame considerably decreases with increase in premixing. Calculated relative decreases follow the measured values of relative decrease of emission.

d) Data computed for premixed burners are shown in *Table 1.*
Measurements were made on a small domestic boiler operating with two partial premixed atmospheric burners.
The calculated values from the first calculations showed a high degree of divergence from measured data, although trends of change were in close agreement. Divergences resulted from the calculated flame dimensions being considerably different from visually measured values. If we calculated with the real flame dimensions the software gave satisfactory results.

e) In the interest of approaching real conditions, the software package is capable of calculating a correction formula for real flame dimensions

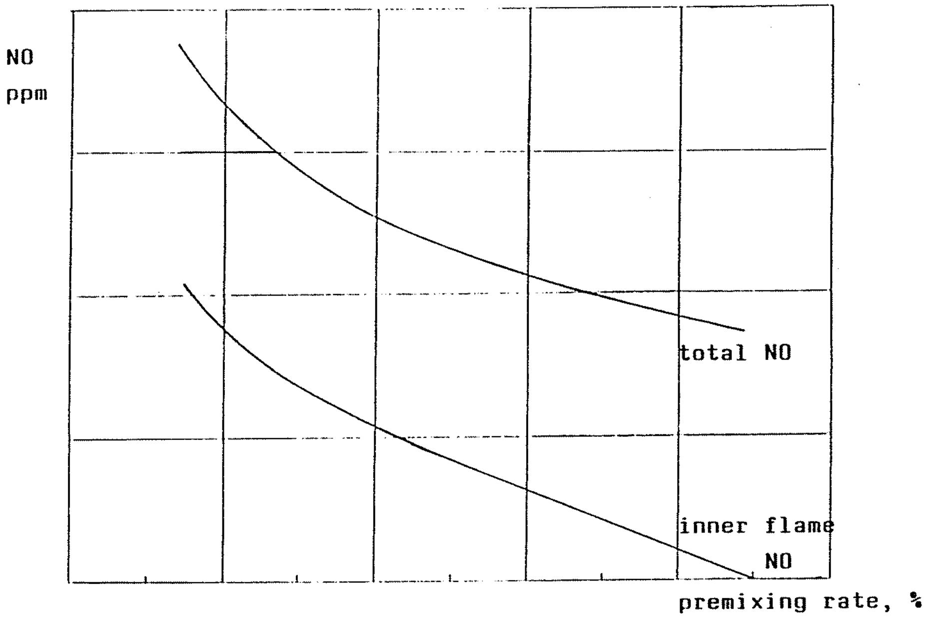

Fig. 9. The calculated NO (total and that formed in the flame)

Table 1

The calculated and the measured NO_x emission for a partly premixed burner

load kW	gas quality	premixing rate, %	excess air, %	NO_x emission, ppm measured	 calculated
20.0	G20	66	54	120	128
15.7	G20	65	86	113	124
20.9	G25	67	45	87	97
21.6	G30	48	38	209	216
21.6	G31	59	44	184	178

from measured burner characteristics and at least one measurement of NO emissions for validating the model. After this resultant NO emissions for other operational conditions may be calculated with an accuracy of 10–20 %.

Summary

Because of difficulties and inaccuracies of the determination of the flameshape, the model primarily suits direct to get a trend of NO_x emission as a function of operating conditions. However, there is a possibility to improve the accuracy of calculation of the NO_x emission, by introducing into the programme measured NO_x values. From the measured values, the program calculates a factor for calculated and measured flame shapes, that may be applied subsequently. The practical application of the programme, used to calculate changes of NO emissions, has proved highly successful in following changes due to the modification of the mechanism of a partially premixed burner.

Acknowledgement

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