

Thermo-acoustic instabilities in turbulent combustion: Pressure influence on partially and perfectly stirred reactors

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Abstract – Laminar flames, perfectly stirred reactors (PSR) and partially stirred reactors (PaSR) are modelled to investigate the interaction between pressure changes and reactions. First it is seen that pressure changes has only minor effects on laminar flames. In a PSR with varying residence time and fixed mass flow and volume, the reaction rate is increased by higher pressure, whereas when the residence time and mass flow is fixed, the reaction rate is not affected. Also in the fixed-volume PaSR, the reaction rate is increased by higher pressure. Some effects of changed mixing time and of changing residence time are investigated.

1 Introduction

Combustion instability phenomena occurring in lean premixed gas turbine combustors remain a major limitation in decreasing NO_x emissions. Such instabilities give rise to pressure fluctuations which cause unstable operation and can lead to early aging or even severe damage of the gas turbine unit. Also, these instabilities pose a serious problem in the case of oxy-fuel combustion. This study is part of an ongoing work on investigation of the physical and numerical behaviour of pressure waves in combustion, cf. last years TLM presentation [11]. Also, experimental studies are included in these efforts, e.g. [5]. The aim is to enable modelling of turbulent combusting flow with such waves. It is related to a larger project on developing technology for power production with reduced CO₂ emissions. One alternative for reduced CO₂ emissions from power production, is a semi-closed O₂/CO₂ gas turbine cycle. These cycles generally impose a lean/stoichiometric combustion with oxygen or oxygen-enriched air as oxidant (“oxy-fuel” combustion). It has been shown [19] that perturbation of

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the fuel-oxygen ratio in near-stoichiometric combustion can lead to unsteady behaviour which can affect the unit integrity and its performance.

The aim of the present study is to analyse the combustion instability phenomena with particular emphasis on the dynamics of reactors. This is motivated by the use and development of Magnussen's Eddy Dissipation Concept for turbulent combustion [14-15,6-9].

This concept is employing a reactor to couple chemical reaction to the turbulent flow.

In the following, some instability mechanisms for lean premixed combustion are briefly reviewed and next a detailed study on the pressure sensitivity of various reactor models is presented. In particular, the study has been carried out on an ozone flame and investigations on the pressure sensitivity are performed in the case of laminar and turbulent flame, with emphasis posed on the constant pressure/constant volume PSR model and on the partially stirred reactor (PaSR) model. The numerical investigation has been carried out with the commercial code CHEMKIN and with the in-house finite-volume-based research code SPIDER.

2 Some instability mechanisms in lean premixed combustion

The coupling between acoustic pressure oscillations and unsteady heat release has been identified ([17]) as the driving mechanism of the thermo-acoustic instabilities although the sources of unsteadiness in the heat release can be very different and case dependent.

One mechanism of instability in lean premixed combustion chambers, which is often cited in literature, is the fluctuating local equivalence ratio [2,12-13]. Fluctuations in fuel/air ratio lead to variations in the reaction rates. The variation in reaction rate determines a variation in the local flame temperature, which causes a variation of the pressure in the combustion chamber. Once the pressure front generated by the variation of local temperature reaches the combustor inlet, it will generate a variation in the mass flow of air, while usually the mass flow of fuel is constant, thus creating a larger variation of the equivalence ratio. If the time lag (time in which the pocket of varied fuel/air ratio mixture reaches the flame front) is approximately in phase with an integer multiple of the acoustic period, then a coupling between the combustion chamber acoustic modes and the heat release fluctuations will exist, and instability will develop.

While the sensitivity of the combustion process to variations of local equivalence ratio is well documented, the sensitivity of the chemical kinetics to acoustical pressure fluctuations is far less well documented. Nonetheless small variations in pressure can significantly change the kinetics of the slower reactions, for example the ones that are responsible for the production or oxidation of the radicals. These variations in the radicals' mass fractions can affect the global reaction rate. Also, these variations in reaction rates can produce a local fluctuation of equivalence ratio. The direct influence of pressure on chemical kinetics is treated in more detail below.

Another possible mechanism is the convective transport of heat leading to periodical extinction-ignition sequences ([4]). The transport of heat in highly turbulent flows with large variations of the velocity field caused by interactions between the larger eddies and by shedding of the vortices can lead to relatively large local variations in temperature, thus affecting the reaction rate.

Also the mechanism of turbulence-induced instability cannot be excluded a priori. In turbulent flames the turbulence convects the reactants towards the flame front and promote the mixing of reactants. Higher level of turbulent kinetic energy will correspond to higher convection rates, leading to steeper gradients at the flame and larger diffusivity losses. But as the turbulent kinetic energy increases, the chemical kinetics can be too slow to generate products at a rate equal to the rate at which the reactants are being supplied. This will lead to lower reaction rate and ultimately to local flame extinction. Unfortunately the mechanism by which a flame induced turbulence production can be triggered by local increases in turbulence level is still unclear and a deeper investigation on the flame induced turbulent production should be seen as a follow-up of the present work.

3 Pressure behaviour of partially and perfectly stirred reactor

3.1 Background

A perfectly stirred reactor is defined as a reactor in which all the species are perfectly mixed and there are no species concentration gradients. This approach is widely used and proved to be satisfactory in a wide range of applications and in particular when the chemical time scales are faster than the mixing ones. However, the response of a PSR to pressure variations is often small and does not allow to predict with sufficient accuracy flames subject to acoustic waves. In this study the effect of pressure variations on a premixed flame was investigated focusing on the effect that they have on both the laminar flame speed and the turbulent burning rate. As a matter of fact, within a limited range of turbulence scale, the turbulent flame velocity can be expressed as[20]

$$v_t = v_l + v' \quad (1)$$

where v' is the root-mean-square velocity fluctuation. This simple relationship outlines that the turbulent burning rate may change both because of variations of the laminar flame speed and of the turbulence.

The influence of pressure oscillation on the flame was tested using a simple but realistic chemical model. An ozone flame [1] can be represented by a combustion mechanism, which is based on 3 species and 4 reactions. Despite of its simplicity this mechanism behaves in a very realistic manner and has been widely used in the past [18]. The chemical reactions are the following:



Reaction 1 is an endothermic reaction that produces the radical O necessary for the combustion to occur. Reaction 3 is responsible for the most of the oxidation of the radical. The Arrhenius coefficients are the same used by [10].

3.2 Laminar flames: effects of pressure on flame speed

The pressure effect on a laminar premixed flame was investigated for a single step reaction by Zeldovich, who expressed the laminar flame speed as [20]

$$v_L \approx \sqrt{\frac{\alpha}{\tau}} = p^{\frac{n}{2}-1} \exp\left(-\frac{E}{2RT_b}\right)
\tag{3}$$

where α is the diffusivity and n the reaction order. The pressure affects both diffusion and reaction rates. The first and more obvious effect is on the molecular diffusivity, which in this model plays the same role as the energy diffusion: in a first approximation in fact the $\alpha \propto p^{-1}$, and therefore a pressure increase reduces diffusion, slowing down the flame.

The reaction rate is affected by pressure as well. In particular, the first Arrhenius parameter A is known to be pressure dependent ([20]), but for an ozone flame this dependency is relatively small and appreciable only for rather severe pressure variations.

A second effect that pressure might have on the laminar flame speed is to change the temperature of the burnt gases. In fact, higher pressures lead to higher temperatures and thus to a faster flame. In order to study the relative magnitude of these effects the dependency of the laminar flame speed against the pressure was tested. The study was carried out using the commercial package CHEMKIN 3.2 (PREMIX module).

Table 1: Initial condition for the laminar case simulation

| | |
|---------------------------------------|-------------------------|
| Flow rate | 0.1 g/cm ² s |
| Heat Flux | 0 W (adiabatic) |
| Initial Molar Fraction O ₃ | 0.15-0.8 |
| Initial Molar Fraction O ₂ | 0.85-0.2 |
| Initial Molar Fraction O | 0 |
| Initial Temperature | 300 K |
| Pressure | 1 bar |

Preliminary analyses on laminar flames had also been used to check the accuracy of the calculations with comparison with the available literature results [10,18]. Those works do not emphasize the pressure dependency and are mainly focused on variation of the amount of fuel at atmospheric temperature. A synopsis of the boundary and initial condition is reported in Table 1.

The comparison with the available literature data is reported in Figure 1 where flame speed and final gas temperature are plotted versus the equivalence ratio.

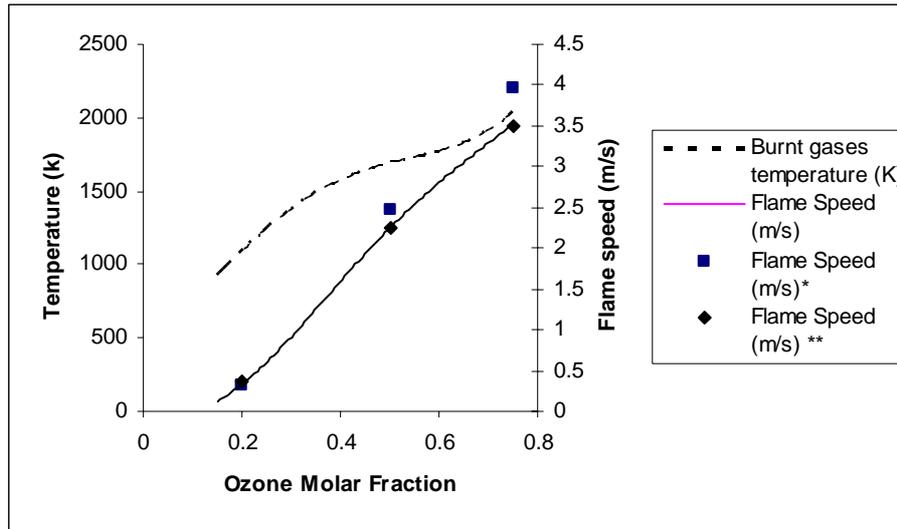


Figure 1. Burnt-gases temperature and flame speed vs. initial O₃ molar fraction. * Data from [10], ** Warnatz's data (from [10])

Figure 1 shows a good agreement with the reference data and also outlines how both flame speed and temperature are drastically influenced by changing the amount of fuel. Figure 2 shows instead how the laminar flame speed for a fixed O₃ molar fraction behaves over a relatively wide range of pressure variations. A synopsis of the boundary condition is reported in Table 2.

Table 2: Boundary condition used for testing pressure dependency

| | |
|---------------------------------------|-------------------------|
| Flow rate | 0.1 g/cm ² s |
| Heat Flux | 0 W (adiabatic) |
| Initial Molar Fraction O ₃ | 0.25-0.75 |
| Initial Molar Fraction O ₂ | 0.75-0.25 |
| Initial Molar Fraction O | 0 |
| Initial Temperature | 300 K |
| Pressure | 1-10 bar |

At low pressures the effect of the increased temperature seems to be dominant and in fact the flame tends to accelerate, but at higher pressures the reduced molecular diffusion plays a key role on the flame speed which is sensibly reduced.

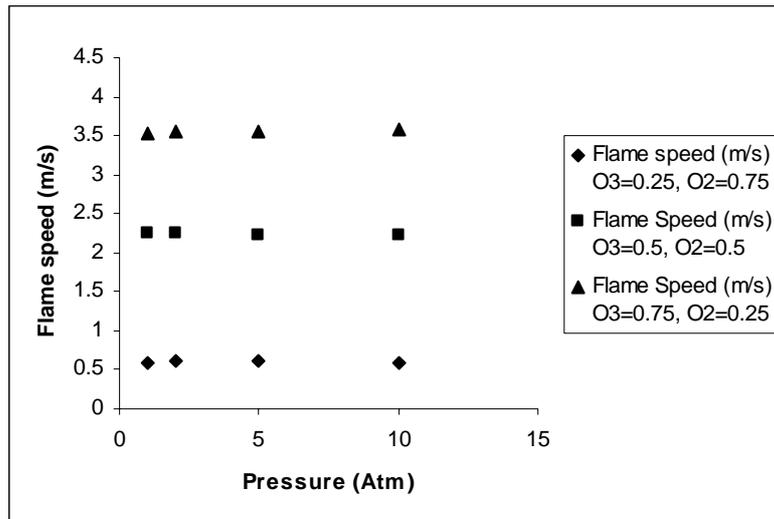


Figure 2. Dependency of the laminar flame speed on pressure

Figure 2 also shows that for a given initial molar fraction the flame speed is only marginally influenced by the pressure. Therefore acoustic pressure waves ($\Delta p/p \approx 2-3\%$) cannot sensibly modify the flame speed and thus the burning rate.

3.3 Effects of pressure on a perfectly stirred reactor

The species mass balance of an transient perfectly stirred reactor can be written as

$$\frac{dY_k^*}{dt} = \frac{1}{\tau_{res}} (Y_{k,inlet} - Y_k^*) + \omega_k^* \quad (4)$$

The last term is the production of the k -th species and represents the chemical time scale for species k , while the first right-hand-side term rules the mass exchange with the surroundings. The exchange rate is given by the residence time of the mixture within the reactor, which is the only time scale ruling the mass exchange of this model. During this time an intense turbulent mixing action is present. As defined by Eq.4 the PSR does not contain any information about its volume and the kind of thermodynamic process it is subject to. Such information is partially provided by the residence time, which is defined as

$$\tau_{res} = \frac{\rho V}{\dot{m}} \quad (5)$$

Since the mass flow (\dot{m}) is often assumed constant, the residence time and thus the exchange of mass will be limited by the change of density within the reactor which adjusts the residence time and might eventually affect the reaction rate. Hence, through density, pressure can affect the residence time and the reaction rate.

One possible choice is to assume a constant volume reactor. This choice is coherent with many physical reactors and combustion chambers. By doing this, the density is the only quantity limiting the rate of mass exchange with the surroundings and the reactor hosts an isochoric process. Although this concept has been widely used to study several chemical mechanisms and to compare them with experiments, the hypothesis of a fixed volume does not well represent different applications such as internal combustion engines and isobaric reactors.

In the case of a turbulent flow, the concept of PSR is widely adopted. Large-scale turbulence supplies a fixed mass flow rate feeding a reactor that is assumed to be perfectly stirred. The Magnussen EDC model provides such a flow rate in terms of a characteristic time scale. In this case the time scale is kept constant while reactions take place and thus the amount of fresh mixture provided by the surroundings to the reactor does not change. In terms of the above-mentioned residence time, the hypothesis of a fixed flow rate requires the volume of the reactor to change accordingly with the density in order to keep the product ρV (Eq.5) constant. This means that during the reaction, the volume of the reactor may well increase by an order of magnitude. Now, the reactor hosts an isenthalpic and isobaric transformation.

The fixed-volume and freely-varying-volume reactors represent two limiting conditions. However, it is useful to focus on the effects such hypotheses have on the reaction to pressure variations. The first scheme to be tested was the fixed volume reactor; numerical tests were performed using both CHEMKIN 3.2 (PSR module) and Spider. The reaction scheme adopted was the same ozone flame mechanisms tested and validated earlier in the laminar case, the required input are listed in Table 3.

Table 3: Operating condition PSR (cf. Figs. 3-4)

| | |
|---------------------------------------|--------------------|
| Flow rate | 0.12 g/s |
| Heat Flux | 0 W (adiabatic) |
| Initial Molar Fraction O ₃ | 0.25 |
| Initial Molar Fraction O ₂ | 0.75 |
| Initial Molar Fraction O | 0 |
| Initial Reactants Temperature | 750 K |
| Initial Reactor Temperature | 750 K |
| Pressure | 0.5–1.5 bar |
| Initial Residence Time | 10 ⁻⁴ s |
| Volume | Fixed |

The response of the fixed-volume reactor to different pressure levels is reported in Figs. 3–4. As far as reaction rate is concerned, reactions 1 and 3 (Eq.2) at higher pressure occur faster and have a higher peak level, while for lower pressure the reaction is slower. This behaviour depends on how the reaction time is affected by the increased pressure. In fact, since the initial temperature is the same for all pressure levels, the initial density will be different. A

higher initial density will cause a longer residence time in Eq. 5 (as the volume and the mass flow are fixed). In this case the reactants are hosted longer in the reactor and thus reactions have more time to occur. The longer residence time allows more reaction to occur. Therefore a higher reaction rates level can be achieved in a shorter time. This is particularly important for reaction 1 which is the slowest.

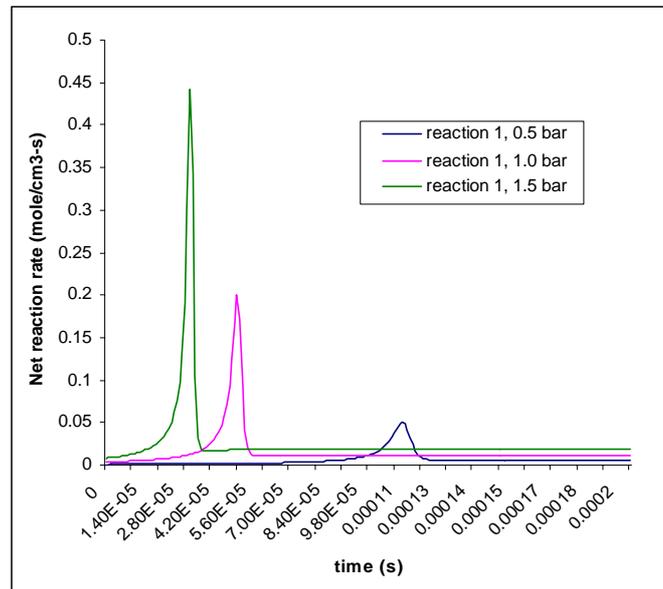


Figure 3. Rates of reaction 1 (Eq.1) at different pressure levels

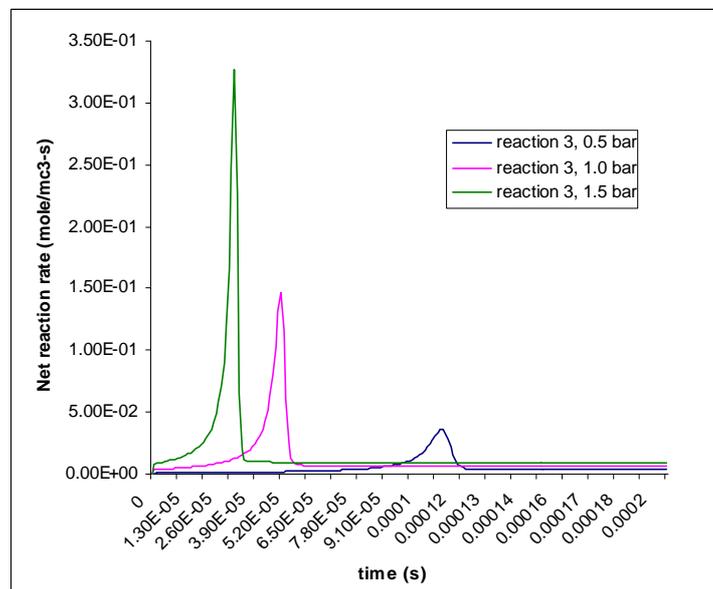


Figure 4. Rate of reaction 3 (Eq.2) at different pressure levels

The PSR as used with Magnussen's Eddy Dissipation Concept (EDC) is based on a residence time determined by the properties of the turbulent flow field, which is locally fixed for each iterative step in the computation. Moreover, the turbulence field is only moderately (or not) affected by the pressure waves. This does not allow the mass flow rate to adjust while

reactions occur. This formulation has no direct link to the pressure except for the dependency on chemistry and molecular diffusion. Both effects have already been tested on laminar flames and previous tests reported above showed them to be negligible in the case of acoustic waves. Therefore a sensible effect of pressure waves (like acoustic waves) on reaction rate and reaction time should not be expected. To investigate this hypothesis, numerical tests were performed using the unsteady PSR recently implemented in Spider. This code, primarily made for 2- or 3-dimensional flow-field modelling, can be run as a reactor model. Then, the reactor of the EDC is solved with specified initial and boundary conditions, but without resolving a flow field outside the reactor. This enables testing of the chemical mechanism as it is implemented in the code, and testing of the reactor model as such. The numerical set up is reported in Table 4.

Table 4: Numerical set up for the isobaric PSR (cf. Figs. 5-7)

| | |
|---------------------------------------|--------------------|
| Heat Flux | 0 W (adiabatic) |
| Initial Molar Fraction O ₃ | 0.25 |
| Initial Molar Fraction O ₂ | 0.75 |
| Initial Molar Fraction O | 0 |
| Initial Reactants Temperature | 750 K |
| Initial Reactor Temperature | 750 K |
| Pressure | 0.5–1.5 bar |
| Residence Time (fixed) | 10 ⁻⁴ s |

Figures 5–7 show that the reaction rates are not sensibly affected by pressure changes in the range of 1 bar, which is fairly wider than what is occurring in combustors affected by acoustic instabilities. Moreover they also outline that the time needed for the reaction to start changes with pressure very little compared with the differences observed in Figs. 3–4.

This last point is probably the most important. When a pressure wave travels along a combustor, the first and most obvious effect is that the density changes and so does the amount of burning mixture. Although this effect can be readily calculated and is already included in the reactor, pressure might have a non-negligible effect on the burning rate and therefore a change in the time to equilibrium should be expected. Experimental evidence [16] show that pressure waves and increases in the heat release are observed and that those phenomena are in phase. The isobaric perfectly stirred reactor with fixed residence time and fixed mass flow cannot be expected to be sensible to these effects.

In summary, the main difference between the two implementations of PSR is the varying vs. fixed residence time. The Chemkin PSR module allows the residence time to be modified by pressure and hence, the reaction rate is affected by pressure changes. In the Spider/EDC implementation of PSR, the residence time is fixed by the turbulence field, and only minor effects of pressure changes are allowed.

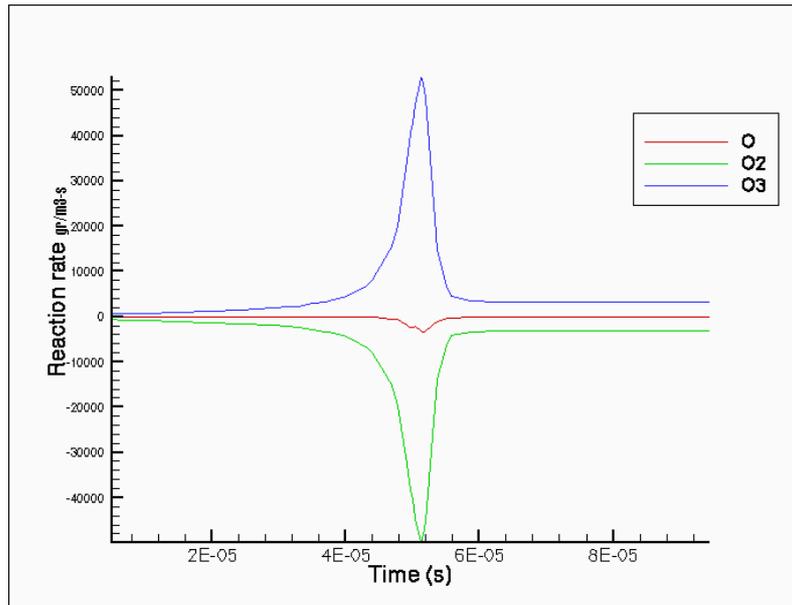


Figure 5. Reaction rate in a PSR with 1.0 bar pressure

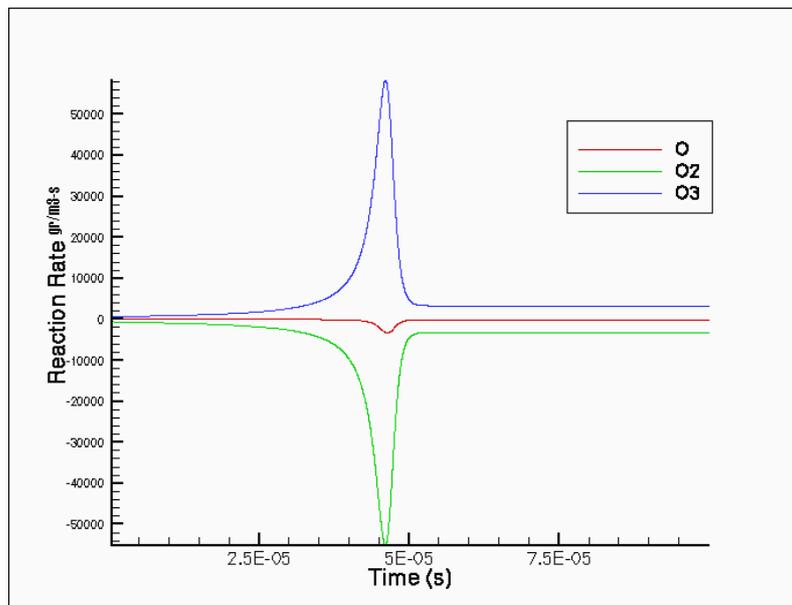


Figure 6. Reaction rate in a PSR with 1.5 bar pressure

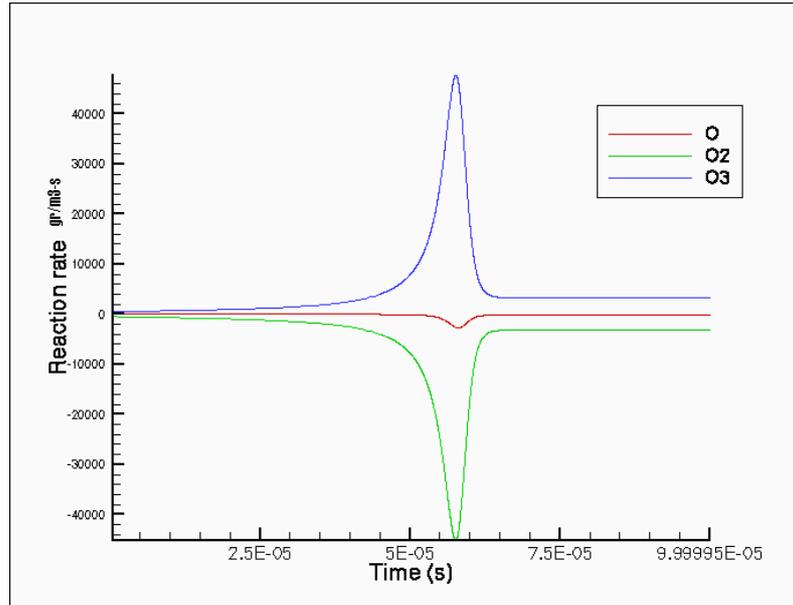


Figure 7. Reaction rate in a PSR with 0.5 bar pressure

3.4 Behaviour of the partially stirred reactor

The partially stirred reactor (PaSR) relaxes the hypothesis of the turbulent mixing action used for the PSR. This is done by adding a second time scale related to the mixing. In this case the reactor is supposed to be constituted by a certain number of perfectly stirred reactors (called particles) interacting with each other ([3]). The way they interact is dictated by the relative magnitude of mixing and residence time: the smaller the mixing time, the greater the interaction. For very small mixing times the PaSR behaves like a PSR.

The unmixedness is defined by Curl's model

$$unmixedness = \frac{1}{1 + \tau_{res}/(3\tau_{mix})} \quad (6)$$

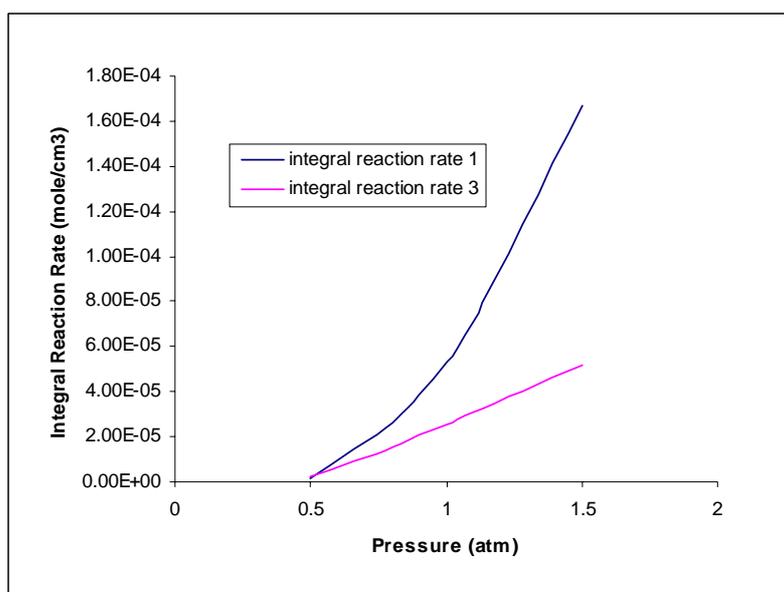
Once again, the effect of the pressure is not explicit, but also in this model the pressure does affect the behaviour of the reactor. The PaSR in fact calculates for each time step the amount of particles flowing through it as $N_c = N \Delta t / \tau_{res}$ where N represents the number of particles present inside the chosen reactor volume and Δt is the time step. In this case, the average residence time is calculated as $\tau_{res} = \langle \rho \rangle V / \dot{m}_0$, where $\langle \rho \rangle$ represents an ensemble average.

When pressure changes so does the density and if the volume V is kept constant the residence time changes and a different number of particles is allowed to enter the reactor.

Tests were performed to understand the way the PaSR behaves for different mixing and residence time and pressure. In this case CHEMKIN 3.2 (PaSR module) was used and the required inputs are listed in Table 5.

Table 5: Operating condition for the PaSR

| | |
|---------------------------------------|--|
| Flow rate | 0.12 g/s |
| Heat Flux | 0 W (adiabatic) |
| Initial Molar Fraction O ₃ | 0.25 |
| Initial Molar Fraction O ₂ | 0.75 |
| Initial Molar Fraction O | 0 |
| Initial Reactants Temperature | 750 K |
| Initial Reactor Temperature | 750 K |
| Pressure | 0.5–1.5 bar |
| Residence Time | 5·10 ⁻⁵ s, 5·10 ⁻⁴ s |
| Mixing time | 10 ⁻⁵ s |
| Volume | Fixed |
| Number of particles | 8001 |

**Figure 8. Pressure dependency of the integral reaction rate of the PaSR**

A first insight on the sensibility of the PaSR on pressure is given in Fig. 8. In this case the residence time was 10^{-4} s and the mixing time 10^{-5} s. The graph shows the two main reactions of the ozone flame. Reaction 1 is the decomposition of O₃ forming the radical O, while reaction 3 is the production of the final product O₂ by oxidation of O. The two reaction rates behave in a quite different way. The first reaction is in fact more accelerated by the pressure increase, while reaction 3 behaves almost linearly. This can give an interesting clue about the operation of the reactor. Reaction 1 is in fact the time-limiting mechanism: Once the radical O has been produced it will be quickly consumed. Since the first reaction requires more time to be completed, the increased number of particles has a stronger (and non-linear) effect on it. Nonetheless it is not just the integral reaction rate which is changing, but also the time needed

for the reaction to start. As appears in Fig. 9, when pressure increases, the rate of reaction 1 (as well as 3) becomes faster and larger.

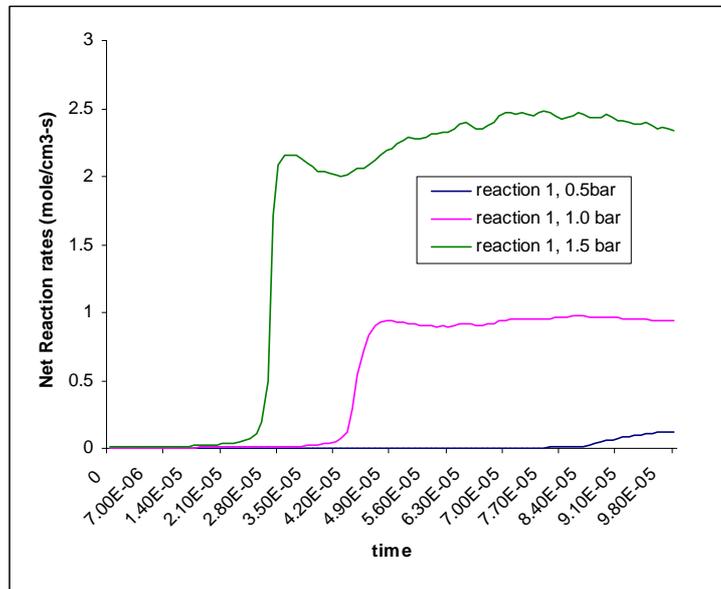


Figure 9 Rates of reaction 1 (Eq.2) at different pressure levels, mixing time 10^{-5} s.

In the limit of very low pressures (0.5 bar) the reaction does not even have time to begin. Compared with the PSR results plotted in Fig. 3, the PaSR shows similar time scales but different behaviours. It is in fact worth to note how the interaction between the particles slows down the reactions. In this case in fact mixing is limited by the mixing time scale and thus reactants are only partially stirred. The effect is that reactions do not occur simultaneously within the reactor leading to a longer time required to reach equilibrium.

The final temperature and the final composition reached by the reactor are strongly affected by the actual pressure. In this respect the residence time is too short to achieve equilibrium, and therefore the temperature variations are larger than what would be expected in an equilibrium case. Figure 10 shows how the dependency of temperature on pressure is much higher at low pressure where equilibrium is far from being reached. In this case the mixing time was equal to 10^{-5} s, the residence time was 10^{-5} s, and the unmixedness 0.23 (Eq.6).

For pressures above 1 bar, the dependency is less sensible. These results confirm that in the case of the ozone flame, pressure does affect both reaction and temperature. However, it remains to be investigated whether such an effect is only related to the residence time, and thus to the number of particles flowing through the reactor, or has some connections with the mixing time and thus to the interaction between the particles. This is definitely a key point, because it might suggest whether a second time scale, and therefore all the problems linked to its definition, is really needed. In order to clarify this aspect, additional tests were performed by varying the mixing time from 10^{-6} to $5 \cdot 10^{-5}$ seconds and keeping all other parameters, including pressure, constant. The list of the parameters kept constant is reported in Table 6.

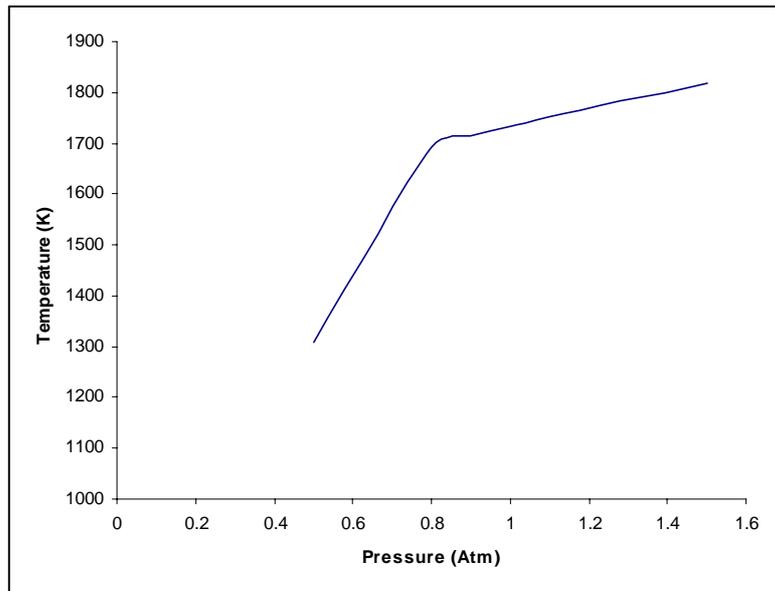


Figure 10. Final temperature vs. pressure

Table 6: PaSR parameters for the mixing time sensibility test

| | |
|---------------------------------------|--------------------|
| Flow rate | 0.12 g/s |
| Initial Molar Fraction O ₃ | 0.25 |
| Initial Molar Fraction O ₂ | 0.75 |
| Initial Molar Fraction O | 0 |
| Initial Reactants Temperature | 750 K |
| Initial Reactor Temperature | 750 K |
| Pressure | 0.5–1.5 bar |
| Residence Time | 10 ⁻⁴ s |
| Volume | Fixed |
| Number of particles | 8001 |

Figure 11 shows the final temperature as a function of the unmixedness for 3 pressure levels. It appears that the unmixedness plays only a secondary role in terms of the final temperature, and that its general effect is to quench the flame. Except for the low pressure case (0.5 bar) where the reason for the lower temperature is to be attributed to the extreme slowness of the flame compared with the residence time, mixing is always affecting the flame marginally. This leads to the conclusion that although mixing may affect the flame final temperature, such an effect is small compared to the one induced by pressure. The difference between the effect of pressure and unmixedness (Fig.12) can also be shown by observing how the reaction rates changes for different mixing times at a given pressure (in this case 1.5 bar).

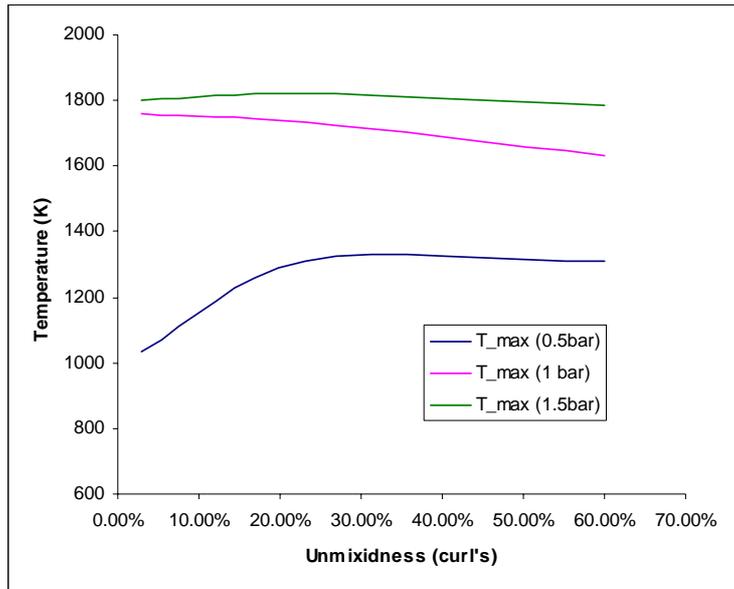


Figure 11. Effect of unmixedness (Eq.6) on temperature

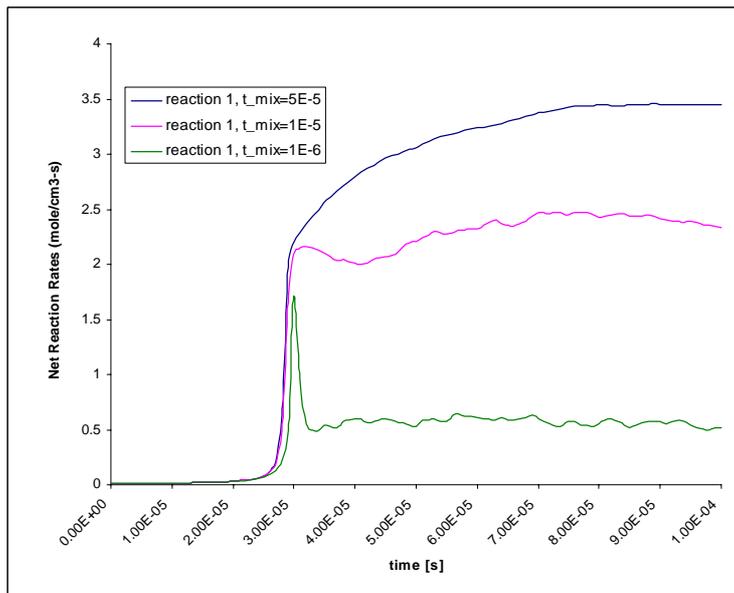


Figure 12. Effect of mixing time, pressure 1.5 bar

From Fig. 12 it is clear that the reaction rate is modified by the mixing scale, but the time for the reaction to start is not affected, and this is why the final temperature reported in Fig. 11 is not changing as much as in Fig. 10.

The results reported in Figs. 10–11 seem to suggest what is really affecting the flame when pressure changes. Since the single particles behave exactly like a perfectly stirred reactor and the PSR with a fixed volume is sensible to pressure fluctuation, the effect must be due to the convection and not to the mixing. Tests on the mixing scales proved the mixing time to affect

reactions differently compared with pressure, while on the opposite the effect of the residence time is quite similar. Figure 13 shows how pressure affects the rate of reaction 1 for three different residence times.

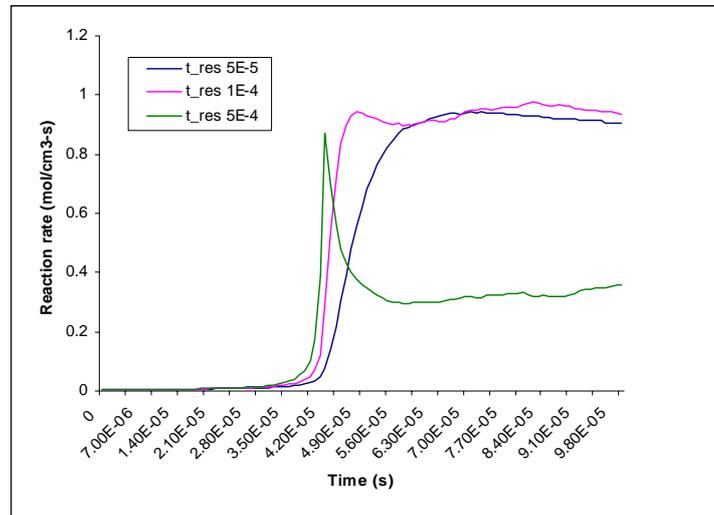


Figure 13. Effect of the residence time on reaction 1 (Eq. 2)

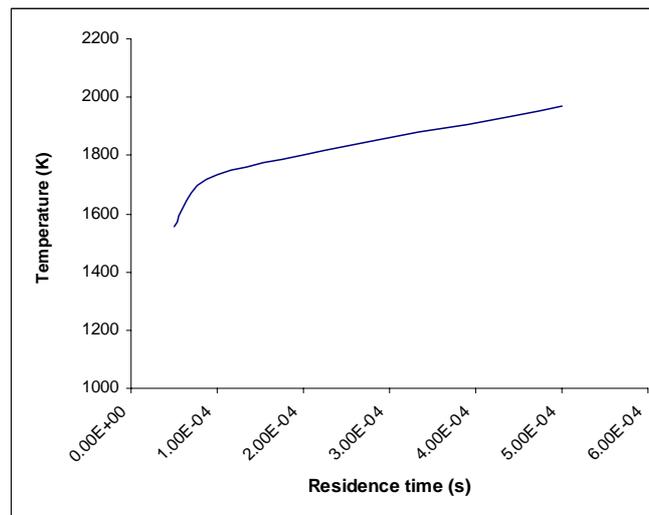


Figure 14. Effect of the residence time on the final temperature

As a matter of fact, increasing the residence time is equivalent to increasing the pressure: in both cases there are less new particles entering the reactor and more time for the reaction to occur, which explains the higher temperature reached by the reactor (Fig. 14). Reaction 1 is also slightly faster.

3.5 Considerations on reactor models

The tests on the laminar premixed flame outline that acoustic waves cannot sensibly affect chemical kinetics and molecular diffusion. Flame speed, reaction rate and final temperature require in fact huge pressure variations in order to show appreciable responses.

Turbulent flames are often computed assuming the main flow to feed, by means of a turbulence cascade, “local” reactors where reactions take place. These reactors are based on the concept of a continuously stirred reactor which is often adopted for studying chemical mechanisms and for modelling devices used in the chemical industry. However the reactors used in many chemical plants are often characterized by a fixed volume reactor, while in the case of turbulent flames the reactors volume can expand without further constraints.

The fixed and variable volume PSR are two limit approaches: however, their behaviour suggests that linking pressure waves to the response of the PSR requires some kind of hypothesis about the volume of the reactor. Although the idea of a fixed volume PSR seems not to be a feasible assumption for turbulent combustion modelling with pressure waves, it must be considered that during the dilatation the reactor encounters some resistance from the outside that might affect its change of volume. In this respect the assumption of isenthalpic transformation needs probably to be relaxed since the reactor must use part of its energy to compress the surrounding flow, and thus the constant pressure assumption may be nullified and the volume might not be allowed to freely expand any longer.

In order to understand whether some additional information is needed to take into account pressure variation effects, perfectly and partially stirred reactors have been also investigated. In this case the PaSR was the fixed volume reactor which includes most of the features of the PSR and behaves in the same manner in terms of pressure changes. The main difference is the mixing time, which is a second time scale and requires the use of a PDF to be determined. However before undertaking extended analyses of a PaSR it is worth to verify whether it is really needed for treating combustion instabilities. In this respect the mixing time proved to play an important role in terms of reaction rate, but such a response is not related to pressure variation and might therefore be neglected in a first stage of the investigation. Moreover the final temperature reached by the reactor is not deeply influenced by this scale.

4 Concluding Remarks

In the present work some instability mechanisms in turbulent lean premixed flames are overviewed. The interaction between pressure and reaction rate is analysed in the case of laminar premixed flames and turbulent premixed flames.

The tests on the laminar premixed flame confirm that acoustic waves cannot sensibly affect chemical kinetics and molecular diffusion. Flame speed, reaction rate and final temperature require in fact huge pressure variations in order to show appreciable responses.

Turbulent flames are often computed assuming the main flow to feed, by means of a turbulence-reactor interaction (in EDC: a cascade model), “local” reactors where reactions take place. These reactors are based on the concept of a continuously stirred reactor which is often adopted for studying chemical mechanisms and for modelling devices used in the chemical industry. However the reactors used in many chemical plants are often characterized by a fixed volume reactor, while in the case of turbulent flames the reactors volume can expand without further constraints.

The fixed and variable volume PSR are two limit approaches: however, their behaviour suggests that linking pressure waves to the response of the PSR requires some kind of hypothesis about the volume of the reactor. Although the idea of a fixed volume PSR seems not to be a feasible assumption for turbulent combustion modelling with pressure waves, it must be considered that during the dilatation the reactor encounters some resistance from the outside that might affect its change of volume. In this respect the assumption of isenthalpic transformation needs probably to be relaxed since the reactor must use part of its energy to compress the surrounding flow, and thus the constant pressure assumption may be nullified and the volume might not be allowed to freely expand any longer.

Further work has to be focused on the development of a reactor type in which the volume occupied by the fine structures adjusts itself according to the surrounding environment thermodynamical state, thus providing a better coupling between the pressure and the reactor behaviour.

In order to understand whether some additional information is needed to take into account pressure variation effects, perfectly and partially stirred reactors have also been investigated. In this case the PaSR was the fixed volume reactor which includes most of the feature of the PSR and behaves in the same manner in terms of pressure changes. The main difference is the mixing time, which is a second time scale and requires the use of a pdf to be determined. However before undertaking extended analyses of a PaSR it is worth to verify whether it is really needed for treating combustion instabilities. In this respect the mixing time proved to play an important role in terms of reaction rate, but such a response is not related to pressure variation and might therefore be neglected in a first stage of the investigation.

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