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Effects of Radicals on Initiations of Detonations in a Pulse Detonation Engine

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Effects of Radicals on Initiations of Detonations in a Pulse Detonation Engine

Abstract (not more than 200 words)

Initiations of detonations are studied. Through numerical experiments it is shown that the initiation is facilitated if hot products from a previous cycle is mixed with the fresh fuel-air mixture. Among other things the hot products consist of free radicals, and the elevated temperature increases the reaction rate of the fuel-air they are mixed with. The effect of adding these hot products are studied through numerical experiments. Simulations of initiations of detonations – both direct and through transitions from deflagrations -- show that the likelihood for a detonation to evolve is greatly enhanced if hot products are initially mixed with the cold fuel-air mixture. By initially removing the radicals from this mixture it is demonstrated that it is the radicals -- and not the elevated temperature -- that is responsible for this effect. The importance of the radicals is also verified through simulations of constant volume explosions. Furthermore it is shown that the state of the hot products and the quantities of radicals, which remains in the engine after the detonation has left the pulse detonation engine and the pressure has decreased to ambient (i.e., the engine is ready for the next cycle), are more than enough to provoke these dramatic changes

Keywords

Pulse Detonation Engine, detonation, deflagration, transition, initiation, chemical kinetics, radicals.

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Radikalers Betydelse vid Initiering av Detonation i en Pulsdetonationsmotor

Sammanfattning (högst 200 ord)

För att öka förståelsen av initiering av detonationer i pulsdetonationsmotorer används numeriska beräkningar. Det visas att de heta gaserna som finns kvar i brännkammaren efter en puls har stor betydelse när detonationen i den följande pulsen ska initieras. Simuleringar där både direkta initieringar och övergångar från deflagrationer studeras visar att sannolikheten för att en detonation ska bildas ökar dramatiskt om heta avgaser blandas med bränslegaserna innan antädningen sker. Det visas vidare att det inte är avgasernas höga temperatur, utan de små mängder radikaler som finns kvar som är ansvariga för denna effekt. Slutligen visas - genom en tvådimensionell simulering där en hel cykel studeras - att de små mängder radikaler som finns kvar i brännkammaren i slutet av cykeln är tillräckliga för att förklara den stora skillnaden i initieringsenergi mellan en motor som opererar i flerpulsmod och experiment där endast en puls studeras (och där inga avgaser finns i blandningen från början).

Nyckelord
Pulsdetonationsmotorn, detonation, deflagration, transition, initiering, kemisk kinetik, radikaler

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Contents

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1 Introduction

One of the key issues regarding efficient opperation of the Pulse Detonation Engine (PDE) in air breathing mode is the initiation of the detonation. Since the thrust of the engine is more or less directly proportional to the frequency, the initiation has to be completed very fast and without use of excessive amounts of energy. For performance reasons and for ease of handling it is also important that the initiation does not depend on exotic fuels or chemical additives to make the fuel-air mixture more sensitive. Typically thousands of Joules are needed to get a Direct Initiation (DI) in a mixture of hydrogen and air. If more conventional fuels are considered (e.g., JP-10), the energy requirement increases even more. It is desirable to operate the engine at a few hundred cycles per second (depending among other things on the size of the engine, and the type of application) and it is obvious that the mentioned energy requirement makes this impossible. One common way to circumvent this issue is to rely on Deflagration to Detonation Transition (DDT) since a deflagration (an ordinary flame) requires substantially less energy to ignite. However, this approach introduces new problems – for realistic fuels the distance to complete the transition are too long for this method to be practical in a PDE.

The two methods of inititaion, DI and DDT, both suffer from a “lack of sensitivity”, i.e., by making the fuel-air mixture more sensitive, reasonable amounts of energy are required to get a successful DI, and the DDT can be completed in an acceptable distance. This can be obtained by adding extra oxygen to the mixture. However, since the extra oxygen has to be carried onboard, the specific impulse of the PDE will be reduced, thereby removing one of the main advantages of the engine.

A different approach to increase the sensitivity of the fuel-air mixture and thereby facilitate the initiation is to use the hot products from the previous cycle. In a PDE operating in multi-cycle mode there will inevitable (unless the combustion chamber is thoruoughly purged) be hot products remaining in the combustion chamber when the fresh fuel-air mixture is injected. Hence the state and the species distribution for that case are going to be different from that of a single shot experiment, where the temperature is ambient and there are no free radicals initially present. The results presented in this paper can explain the relative ease by which detonations can be initiated in a PDE operating in multi-cycle

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mode compared to single shot experiments, see [1, 2, 3]. Consequently, single shot experiments are of limited value when different methods to initiate the detonation in a pulse detonation engine are studied.

The effects of adding hot products to a fresh fuel-air mixture – here hydrogen is used as fuel – are studied in the following cases:

- Constant volume explosions.
- Direct initiations in one dimension.
- Deflagration to detonation transitions in one dimension.

The hot products used in the simulations are obtained through two-dimensional calculations of one pulse of a PDE cycle. The calculations are stopped when the pressure at the front plate has decreased to ambient (the instant when one typically wants to inject fresh fuel in order to keep producing thrust), and the mean values of the state and distribution of species in the combustion chamber at that time are used to specify the hot products.

For the constant volume explosions the initial states and species distributions are varied by mixing different fractions of fresh fuel-air and hot products. Here an ideal mixing is assumed, i.e., the distribution of species and the energy of the mixture is obtained by simply adding the masses and the internal energy of the different species from the cold and the hot gases respectively (of the chosen proportions). A 38 step mechanism is used to model the kinetics. It is shown that the ignition delay time increases several orders of magnitudes if the radicals are initially removed from the hot products, even if they constitute less than one third of one percent of the total mass of the mixture.

The concept of initiations of detonations is studied through the gas dynamic equations in one dimension coupled with the same chemical kinetics as used in the constant volume reactor. In the same way fuel-air is mixed with the products remaining in the PDE after one cycle (and again an ideal mixing is assumed). The effect of the radicals are examined in two different cases:

- A homogeneous mixture of burnt and unburnt media. The mixture is ignited by a deposit of energy at the closed end of the tube. The interesting variable is the critical energy – i.e., the least amount of energy required for a detonation to develop.
- A mixture of burnt and unburnt media, where the fraction between the two varies along the length of the tube. Here the mixture is ignited by hot residual gases, and the variable of interest is the length of the zone over which the composition of the mixture varies. In analogy with the critical energy the least value of the length required for a detonation to develop is here called the “critical length”.

The first case can be seen as a model of direct initiation e.g., by a spark plug, whereas the second case models the transition trough mixing of burnt and unburnt gases as a part of a DDT process. Different authors have shown that a gradient in the induction time is a driving mechanism behind transitions to detonations, and that a certain minimum length of the extension of this gradient is needed if the transition is to be completed with a propagating detonation, see [4, 5, 6]. In this paper this gradient is obtained by mixing cold reactants with hot products in proportions which varies in space (thereby producing a spatial gradient), with the emphasis on the effect of the radicals in the hot products. It is shown that both the critical energy and the critical length can be reduced even if there are only very small amounts of radicals present. This also stresses the importance of using a kinetic scheme which is capable of modeling reactions which includes radicals when problems involving initiations of detonations are treated.

The examples presented in this paper do not model all aspects of initiations of detonations – the most important one lacking is the mixing process of the hot products with the unburnt gases. However, the examples shown do stress the importance of the hot products – and especially the radicals therein – remaining from the previous cycle when the next detonation is to be initiated. The reduction in ignition delay time, as well as the reduced critical energy and critical length, all indicate that the probability for a detonation to develop is greatly increased if small amounts of radicals are initially present in the solution. For instance, the example where the DDT is studied shows that the structures in the flow field which need to be developed for a detonation to form are reduced if small fractions of radicals are present in the unburnt medium. That is, structures with gradients in the induction time can be generated by turbulence and vorticies, but the extension of these structures are limited (among other things on the Reynolds number and the geometry of the tube) and the increased sensitivity obtained by the presence of the radicals means that these structures can be smaller while still resulting in the development of a detonation. The relationship between the sensitivity of the mixture and the size of the structures can be understood by studying a simplified model; if transport effects are neglected, if only one step kinetics are used, and if a linear mixing region between burnt and unburnt media is assumed, scaling arguments and calculations in one dimension have shown ([5]) that the likelihood for a detonation to develop only depends on the reaction rate, K, and the length of the linear mixing profile, L, through the product KL. This result illustrates that for a given medium a successful transition to detonation can either be obtained by "sensitizing" the medium (increasing K) or by creating larger mixing regions between burnt and unburnt media (increasing L). As stated above, the presence of radicals have a sensitizing effect, and the importance of the product KL explains why the requirement on the size of the structures in the flowfield can be reduced when radicals are initially added to the mixture.

2 Numerical Experiments

The purpose of this study is to use numerical experiments to illustrate the effect of hot products – especially radicals – on combustion processes of relevance to initiations of detonations. The initial distribution of radicals present in the mixture is obtained by mixing the hot products remaining after one cycle with fresh fuel-air. Calculations of one cycle – simulating both the propagation of the detonation in the engine as well as the expansion phase when the pressure at the front plate is reduced to 1 atm – are done to obtain the state and the massfraction distribution in the hot products. The different moments are covered in detail in the subsections below:

- Two-dimensional calculations to obtain the state and distribution of species in the

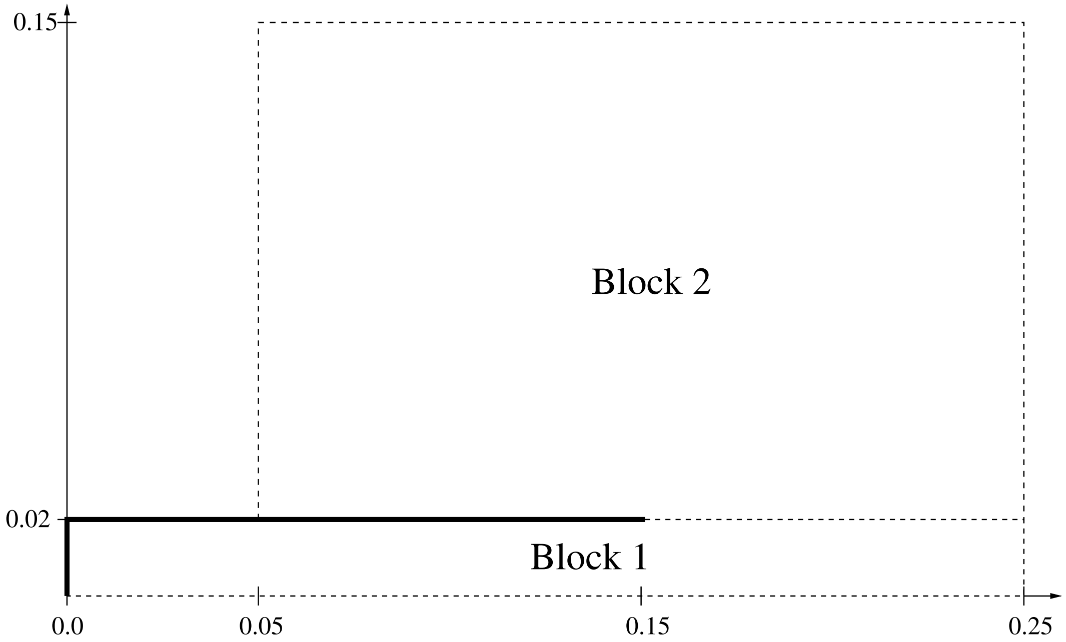

Figure 1: Engine and computational domain.

hot products at the end of one cycle.

- Simulations of constant volume explosions with a varying proportion between the hot products and the fresh fuel-air mixture.
- Calculations of initiations of detonations, both direct and trough transitions from deflagrations.

2.1 Two-dimensional calculation

A multiblock code, Mozart, by J-L Cambier, is used. The engine in the calculation is 4 cm wide and 15 cm long. In order to be able to simulate the exhaust phase accurately and without shock reflections from the external boundaries it is necessary to extend the computational block in the engine to cover not only the engine itself, but also a sufficiently big part of the exterior domain. This is done by extending the computational domain in the engine with 10 cm and adding a block, 20 cm by 13 cm, aligned with the block covering the engine, i.e., two blocks are used (a picture of the layout is shown in figure 1). Note that the symmetry of the problem is used, and only half the engine and only one external block is used in the calculation. Block 1 consists of 20 by 200 cells and Block 2 consists of 40 by 100 cells.

Initially the tube is filled with a stochiometric mixture of hydrogen and air, i.e., the initial mass fractions are: H_2 - 0.0283, O_2 - 0.2265 and N_2 - 0.7452 (initially the mass fractions of the other species are all zero). At the beginning of the calculation the pressure is 1 atm and the temperature is 293 K. This calculation is only used to get the state and the mass fractions of the different species at the end of the first cycle, and hence the detonation

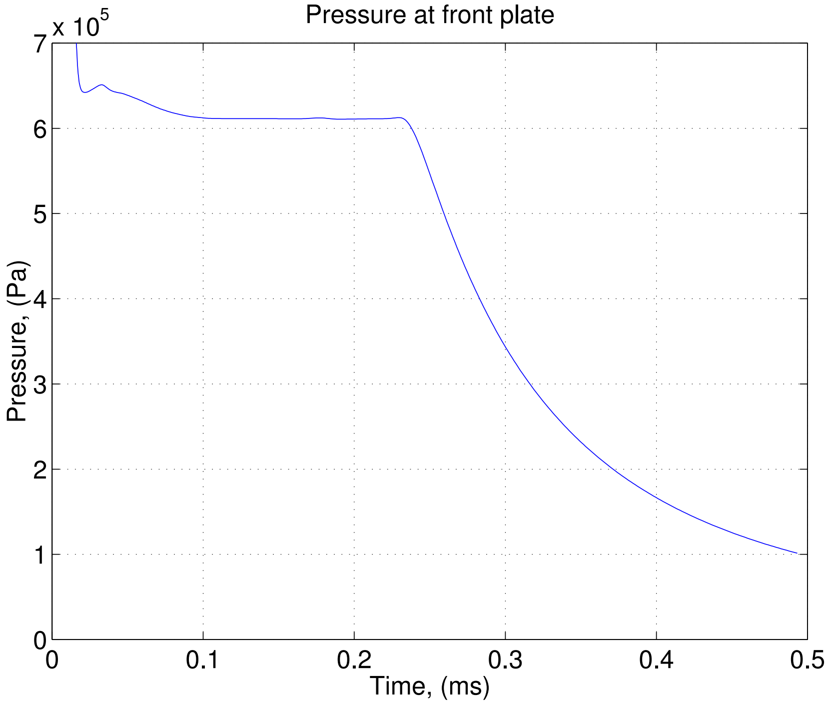

Figure 2: Pressure at front plate during one cycle.

is initiated more or less instantaneously by setting temperature and pressure to 2500 K and 50 atm respectively at five rows of cells neighboring the left boundary (the front plate).

The pressure at the front plate as function of time is displayed in figure 2, and in figure 3 the mass fractions – at the time when the pressure at the front plate has decreased to 1 atm – of the different species are shown. The mass fractions are plotted as functions of x, where x is the coordinate along the length of the engine, at the center of the engine. Also shown, in figure 4, are the pressure and the temperature for the same time along the centerline. Neither the mass fractions nor the pressure or the temperature vary much over the width of the engine, and these plots give a representative picture of the state in the whole engine at the end of the cycle.

The main goal of this paper is to illustrate the drastic influence fractions of hot products – and the small quantities of radicals therein – can have on combustion processes related to initiations of detonation. But due to the approximations used – e.g., the injection of the fresh gases is not simulated, and it is assumed that the mixing between the fresh mixture and the products is complete before the reactions are allowed to start – only a qualitative behavior of these processes can be obtained. Therefore, in order to simplify the calculations, no consideration is taken to the small variations in space, and the distribution of massfractions for the different species is obtained as mean values of the data plotted in figure 3 and is presented in table 1. In the same way a pressure and temperature of approximately 1 atm and 2090 K is obtained from figure 4.

The mixture obtained in this way is used to sensitize the fresh mixture in the different examples below (constant volume explosions and simulations of initiations of detona-

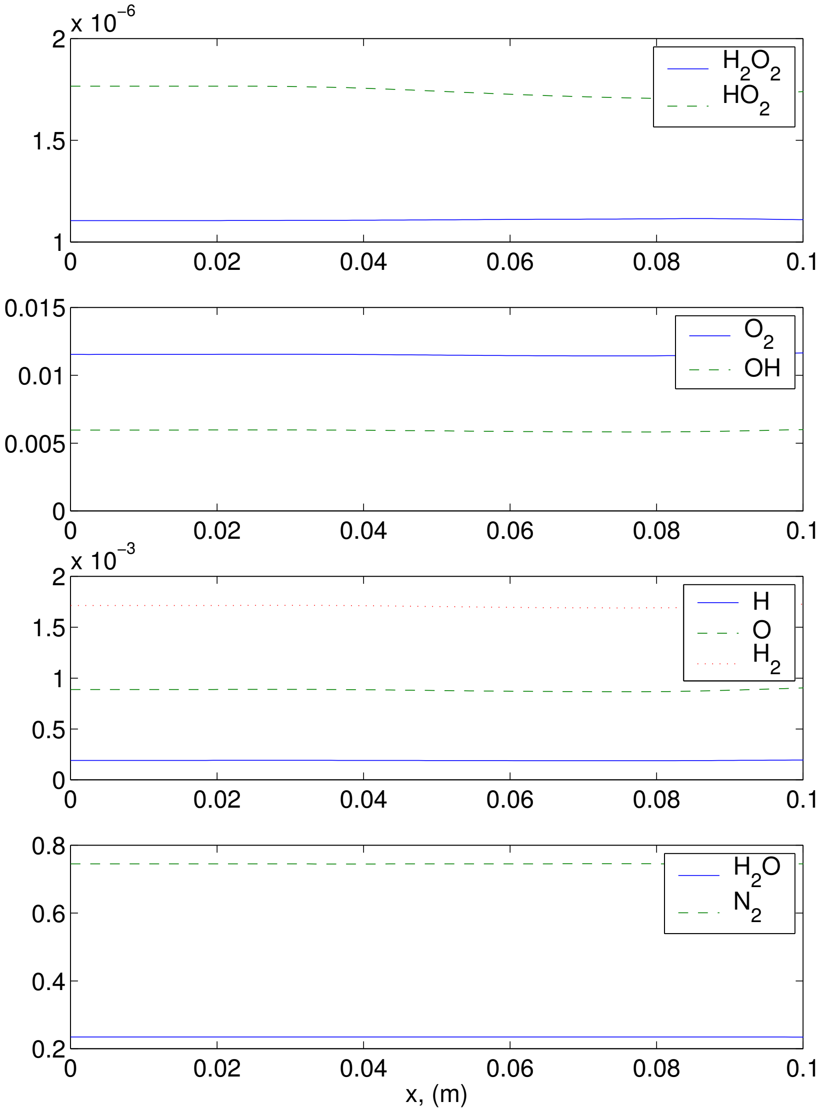

Figure 3: Mass fractions along the center line of the cycle.

O	H	O_2	H_2	OH	H_2O	HO_2	H_2O_2	N_2
$8.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$	0.012	0.0017	0.0060	0.235	$1.8 \cdot 10^{-6}$	$1.1 \cdot 10^{-6}$	0.744

Table 1: Massfraction of species in products at end of the first cycle.

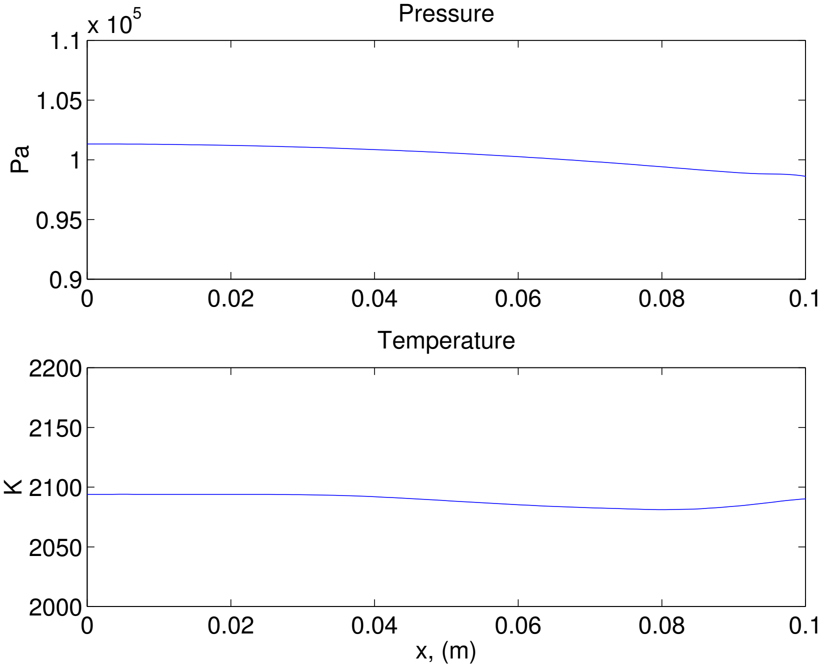

Figure 4: Pressure and temperature along the center line of the tube at the end of the cycle.

tions). For comparisons, calculations are also done where the radicals are removed from the hot products initially as well as calculations using fuel-air without any mixing with the hot products at all. That is, the following media are studied in the different examples:

- The hot products obtained from the two-dimensional calculations described above (i.e., using hydrogen-air as fuel). This medium is called medium A.
- Medium B, the same as above, but with the radicals removed.
- Unburnt fuel (hydrogen-air), i.e., without any radicals and at room temperature, medium C.

In the different cases below, mixtures AC and BC as well as C alone are studied. The different mixtures are obtained by assuming that a fraction, α, of the burnt gases (either A or B) is mixed with the unburnt gases (C). If the burnt state is denoted by superindex b and the unburnt state by u, the following hold for the masses for the different species of the mixture between burnt and unburnt:

$$m_i = \alpha m_i^b + (1-\alpha) m_i^u = \alpha \rho^b V Y_i^b + (1-\alpha)\rho^u V Y_i^u \tag{1}$$

$$\rho_i = \frac{m_i}{V} = \alpha \rho^b Y_i^b + (1-\alpha)\rho^u Y_i^u \tag{2}$$

$$Y_i = \frac{\rho_i}{\rho} = \frac{\alpha \rho^b Y_i^b + (1-\alpha)\rho^u Y_i^u}{\sum_{i=1}^{N}(\alpha \rho^b Y_i^b + (1-\alpha)\rho^u Y_i^u)} = \frac{\alpha \rho^b Y_i^b + (1-\alpha)\rho^u Y_i^u}{\alpha \rho^b + (1-\alpha)\rho^u}. \tag{3}$$

prod.	temp.	pres.	O	H	O_2	H_2	OH	H_2O	HO_2	H_2O_2
50%	580	$1.1 \cdot 10^5$	$1.2 \cdot 10^{-4}$	$2.6 \cdot 10^{-5}$	0.20	0.025	$8.4 \cdot 10^{-4}$	0.033	$2.5 \cdot 10^{-7}$	$1.5 \cdot 10^{-7}$
60%	690	$1.2 \cdot 10^5$	$1.7 \cdot 10^{-4}$	$3.7 \cdot 10^{-5}$	0.18	0.023	0.0012	0.046	$3.5 \cdot 10^{-7}$	$2.1 \cdot 10^{-7}$
70%	850	$1.2 \cdot 10^5$	$2.4 \cdot 10^{-4}$	$5.2 \cdot 10^{-5}$	0.17	0.021	0.0016	0.064	$4.9 \cdot 10^{-7}$	$3.0 \cdot 10^{-7}$
80%	1072	$1.2 \cdot 10^5$	$3.5 \cdot 10^{-4}$	$7.5 \cdot 10^{-5}$	0.14	0.018	0.0024	0.092	$7.1 \cdot 10^{-7}$	$4.3 \cdot 10^{-7}$

Table 2: Temperature, pressure and massfraction at the beginning of the calculaton.

In these equations m_i and ρ_i are the mass and density of specie i, V is the volume, $\rho = \sum_{j=1}^{N} \rho_i$, N is the number of species involved and $Y_i = \rho_i/\rho$ is the mass fraction of specie i.

The energy, E, for the mixture is given by

$$\frac{E}{V} = \alpha \rho^b e^b + (1-\alpha)\rho^u e^u \tag{4}$$

where e is the specific energy. Here it is assumed that the mixing occurs under constant volume, and hence the temperature can be obtained from the equation

$$g(T) = \sum_{i=1}^{N} \rho Y_i e_i(T) - \frac{E}{V} = 0, \tag{5}$$

where e_i is the specific energy for species i of the mixture. This can be solved iteratively by the secant method:

$$T^{n+1} = T^n - \frac{T^n - T^{n-1}}{g^n - g^{n-1}} g^n \tag{6}$$

or

$$T^{n+1} = T^n - \frac{(T^n - T^{n-1})\left(\sum_{i=1}^{N} \rho Y_i e_i(T^n) - \frac{E}{V}\right)}{\sum_{i=1}^{N} \rho Y_i e_i(T^n) - \sum_{i=1}^{N} \rho Y_i e_i(T^{n-1})}. \tag{7}$$

Finally, the pressure of the mixture can be obtained from

$$p = \rho R_u T \sum_{j=1}^{N} \frac{Y_j}{W_j}. \tag{8}$$

2.2 Constant Volume Explosion

Here constant volume explosions in mixtures of hot products and fresh fuel-air are studied. Four different cases – where α (the fraction of the burnt gases) is varied from 50% to 80% – are treated. The initial temperature and pressure as well as the massfractions for the different mixtures are shown in table 2. In order to illustrate the effect of the radicals the calculations are also done with the radicals removed (i.e., O, H, OH, HO_2 and H_2O_2). The total mass of the volume is slightly reduced by this, but, as can be seen from table 2, not very much. Of the radicals the dominating specie is OH, but in none of the cases considered its mass fraction is larger than a quarter of a percent (and since the rest of the radicals constitute even smaller mass fractions, the total mass of the volume is not

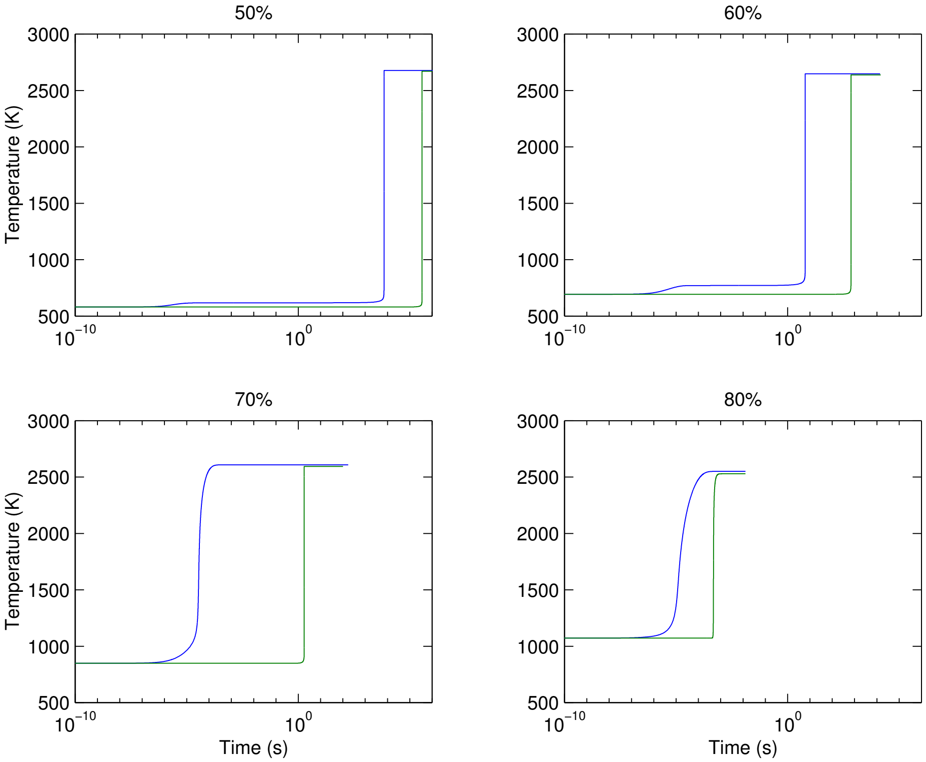

Figure 5: Constant volume explosion, blue:with radicals, green:radicals removed

altered much by removing them). The temperature obtained from these calculations is plotted as a function of time in figure 5. From these plots the ignition delay time can be estimated, and as evident the radicals have a significant influence on this time. For the case where $\alpha = 70\%$ the difference is almost five orders of magnitude. Apart from the effect of the radicals for a fixed α, it can also be seen that the ignition delay time is significantly reduced if the fraction of hot products is increased (this is probably an effect of the increased temperature which follows from a larger fraction of hot products in the mixture). However, for the cases where the radicals are kept in the volume (which is the most physically relevant) the difference in ignition delay time between the two cases with the largest fraction of hot products (70% and 80%) is small.

Since these calculations do not model waves of any kind (e.g., pressure and shock waves can of course not be modeled by a zero-dimensional code, where only a set of ordinary differential equations are solved) the result per se can not give any information regarding transitions to detonations. But since a relevant kinetic scheme is used the chemistry is captured reasonably well, and the results do suggest that phenomena involving initiations of detonations will be influenced by the presence of hot products and radicals.

2.3 Transition to Detonation

The focus of this paper is to illustrate the importance of radicals being initially present in the flow field, and in order to do so the mathematical model of the physical problem is simplified. For example, only one-dimensional calculations are used, and transport effects are not simulated, i.e., except for numerical artifacts neither heat conduction, diffusion of species nor viscous effects are simulated. Neither the injection of hydrogen-air nor the mixing of these gases with the products are simulated. There are two reasons for doing this: it lessens the demand on the computational power required, and it serves as a mean to isolate – and make more clear – the effects of the radicals. Therefore, the results obtained are only valid within the context of the current mathematical model, and further studies are needed to be able to predict the physical behavior when the moments mentioned above are included to the model. For instance, since the transport effects are excluded deflagrations (ordinary flames) can not be simulated, and the first phase of the DDT – where the acceleration of the flame is important – can not be simulated.

Furthermore, the parameter space to investigate is obviously very big (infinite), and the parameters that have been used in the sections below have been chosen since the results produced when they are used clearly illustrate the importance of the radicals.

2.3.1 Direct initiation

The initiation is simulated by letting the computations start with a higher energy content at a small part of the initial flow field at the left end of the computational domain (the closed end). This is done both for a mixture of burnt and unburnt (AC) where 40% unburnt and 60% burnt is used, and for unburnt only (C). The energy added is 6 MJ/m^3, and it is added at the first millimeter of the one-dimensional computational domain (e.g., if a three-dimensional domain of cross section 5 by 5 cm were considered and if the extra energy were added over the whole front plate with a depth of 1 mm the total energy added would

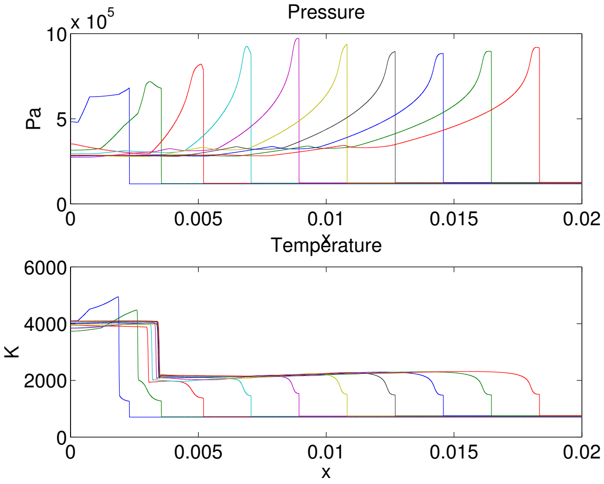

Figure 6: Subsequent plots of temperature and pressure after initiation in a mixture of burnt and unburnt, with the final graph at $t_{end} = 0.012$ ms.

be about 15 Joules). The length of the computational domain is 2 cm, the number of cells used is 20,000, the CFL-number is 0.16 and the computations continue until $t = 0.012$ ms when burnt and unburnt is used and until $t = 0.018$ ms when the initiation is simulated in unburnt only. Different final times are used since a detonation-like wave develops in the first case – which is considerably faster than the decaying shock wave that develops in the second case – and it is desirable that the waves do not leave the computational domain.

The results from the two different cases are shown in figures 6 and 7. Here temperature and pressure profiles are plotted for different times in order to visualize the movement of the fronts. The main difference is that when the AC mixture (burnt and unburnt) is used, a wave develops which can be characterized as a detonation since the shock wave and the reaction zone are tightly coupled, and that a quite high peak pressure is obtained. The normal ZND-peak value is not reached because the detonation propagates in a medium with a lower than usual energy content (60% of it is burnt). When mixture C (unburnt only) is considered it is obvious that the energy applied is not sufficient to initiate the detonation, instead a decaying shock wave is formed. The difference can also be seen in figure 8 where the maximum pressure in the flow field as a function of time is plotted. As can be seen the pressure drops steadily to about 3.5 atm in the unburnt only mixture, and there are no indications of a transition to a detonation taking place under the time of the calculation.

Simulations have also been done using the mixture of burnt and unburnt but with the radicals removed (in the same way as described in section 2.2). The results from these calculations have the same essential features as those for simulations in unburnt only, namely the coupling between the shock wave and the zone of reaction required for a successful initiation is never achieved, and insted a decaying shock wave is developed. Due to the close resemblance, the results from these calculations are not shown.

Grid refinement studies have been performed, covering the range of grid sizes from $dx = 3{\cdot}10^{-4}$ m to $dx = 1{\cdot}10^{-5}$ m (the finest grid size is used in the calculations whose

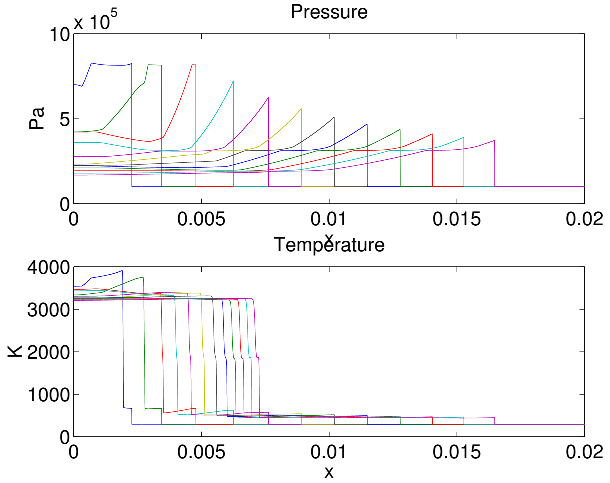

Figure 7: Subsequent plots of temperature and pressure after initiation in unburnt only, with the final graph at $t_{end} = 0.018$ ms.

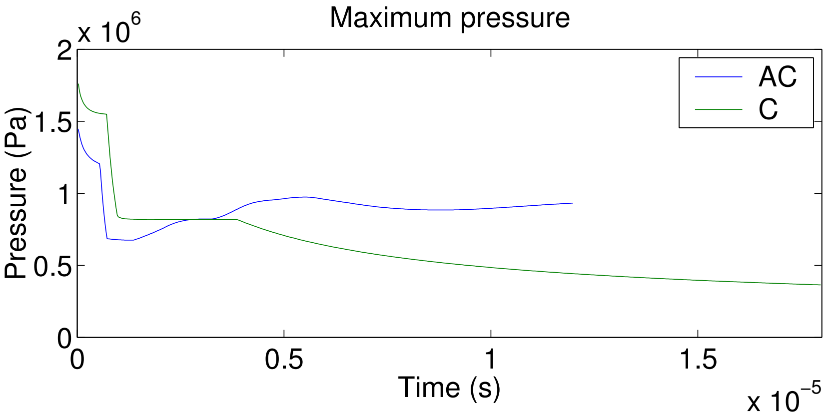

Figure 8: Difference in maximum pressure between initiation in a mixture of burnt and unburnt (AC) and unburnt only (C).

results are presented above). As the grid is refined the fronts become sharper and the peak pressures increase slightly, but the important conclusion is valid for all grid sizes, i.e., a detonation develops in the mixture of burnt and unburnt but not in unburnt only. Hence, the results from the grid refinement study are not presented.

The question of whether the detonation that develops in the mixture of burnt and unburnt will continue as a detonation when passing over an interface – either a gradual or a discontinuous one – to unburnt only is important, but is left to future studies.

2.3.2 Deflagration to Detonation Transition

One of the most important processes behind a DDT is the "convective explosion", [5, 7]. It has been shown that this process can be responsible for building up the high pressures needed for the transition to detonation to be completed, [4, 5, 6]. The convective explosion is not driven by diffusion, instead the main mechanism responsible is a spatial gradient in the source term in the equations of species. Since the temperature and the composition of species varies over the gradient, the explosion limit will be reached at different points in space at different times (see e.g., section 2.2). Therefore an apparent wave will be produced (apparent in the sense that the speed of this wave can be infinite if there is no gradient and the explosion limit is reached simultaneously for all points in space). It is this apparent wave that is called convective explosion (or reaction wave or fast flame). The transition have a chance of beeing successful if the speed of this convective explosion is comparable to the speed of sound in the medium, since then pressure waves originating from the first point that reaches the explosion limit will be augmented when the explosion limit at a neighboring point is reached simultaneously as the passage of the original pressure wave. The convective explosion can only propagate as long as there is a gradient in the induction time, and if a sufficiently high pressure is built up during the indicated process a detonation will develop in the medium outside of the domain in which the initial gradient exist. In a DDT in a fresh fuel-air mixture, turbulence and vortices are developed as the flame accelerates. These structures are responsible for the mixing between the hot, burnt gases and the fresh mixture which eventually produces the gradient in the induction time. In the light of the results from sections 2.2 and 2.3.1 it is reasonable to believe that this process will be affected if hot products and radicals from a previous cycle are present in the chamber already before the flame is ignited.

In this paper neither the details of the injection, the mixing of the gases nor the propagation of the flame and turbulence are simulated. Instead an initial distribution consisting of two parts, with constant states and constant species compositions, connected by a linear profile is chosen, see figure 9. That is, the events leading to the gradient in the induction time is not simulated even though it is reasonable to believe that this part of the DDT will also be greatly affected by the hot products present in the fluid from the beginning. The linear profile is chosen since more detailed information is lacking and a linear profile is the simplest way to specify a gradient in the induction time. However, the events occuring after the gradient has developed are simulated accurately in the present study. In a future study the effect of different shapes of the initial gradient will be treated.

The two constant states in the initial profile consist of fresh fuel-air (C) mixed with burnt gases obtained from the two-dimensional calculation described in section 2 (both

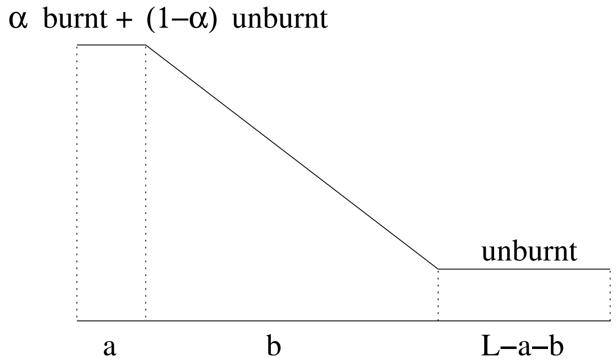

Figure 9: Initial distribution.

with radicals, A, and with the radicals removed, B). The fraction between the hot and the cold media are chosen in such a way that the temperature in one of them (the one containing the largest portion of burnt gases) is sufficiently high to induce more or less instantaneous reaction (see section 2.2 to get an estimate of the times involved). Here the high temperature zone is placed at the left end, where also a wall condition is enforced, and consequently the reaction starts in the vicinity of the left boundary.

In the calculations the "hot" (left) side is defined as

$$m_i^c = \alpha m_i^b + (1-\alpha) m_i^u, \tag{9}$$

and in the calculations a specific value – $\alpha = 0.75$ – has been used.

The ease by which a detonation can develop depends both on the mixture itself (i.e., its composition and its thermodynamic state) and on the structures in the flow field (emanating from dynamic effects). As pointed out above, the development of these structures is not simulated in this study, but by changing the length of the part of the initial data where the induction time varies – b in figure 9 – it is possible to use one-dimensional calculations to get an estimate of the size of the turbulent mixing region required for a detonation to develop. Therefore it is possible to quantify the sensitivity of the mixture (here meaning how easy it is for the detonation to develop) by obtaining the minimum value of b for which a detonation develops. In table 3 data for calculations with varying b are displayed. For these calculations the spatial resolution has been kept the same ($dx = 0.0003$).

In figure 10 the maximum pressure over the whole computational domain as a function of time is plotted for the different cases, and by looking at the peak value of the pressure from this plot it is obvious that a detonation develops if $b \geq 0.25$. The detonation propagates substantially faster than the decaying shock wave resulting from an unsuccessful DDT. Therefore – in order to keep the detonation within the computational domain the computations for $b = 0.25$, $b = 0.30$ and $b = 0.45$ (where a detonation do develop) end at $t = 0.325$ ms instead of at $t = 0.70$ ms as is the case for those calculations where no detonation develops. The results from the calculations with $b = 0.45$ and $b = 0.10$ are shown in figures 11 and 12. In these two figures pressure and temperature profiles are plotted for subsequent times. Note that in order to better capture the peak values different scales are used for both temperature and pressure in these two figures (the peak pressure

Data for DDT calculations							
	With radicals						Without radicals
L (m)	0.60	0.60	0.60	0.60	0.60	0.60	0.60
a (m)	0.02	0.02	0.02	0.02	0.02	0.02	0.02
b (m)	0.10	0.15	0.20	0.25	0.30	0.45	0.45
#cells	2000	2000	2000	2000	2000	2000	2000
CFL	0.001	0.001	0.001	0.001	0.001	0.001	0.5
t_{end} (ms)	0.70	0.70	0.70	0.325	0.325	0.325	1.5
DDT?	no	no	no	yes	yes	yes	no

Table 3:

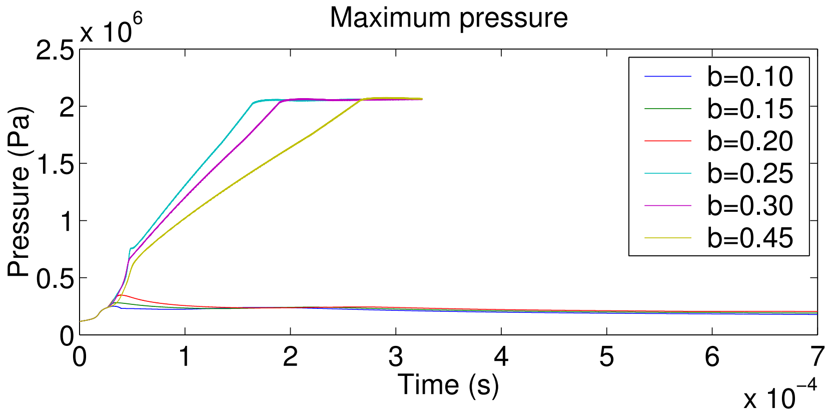

Figure 10: Difference in maximum pressure between successful and unsuccessful transition in a mixture of burnt and unburnt (with the radicals retained).

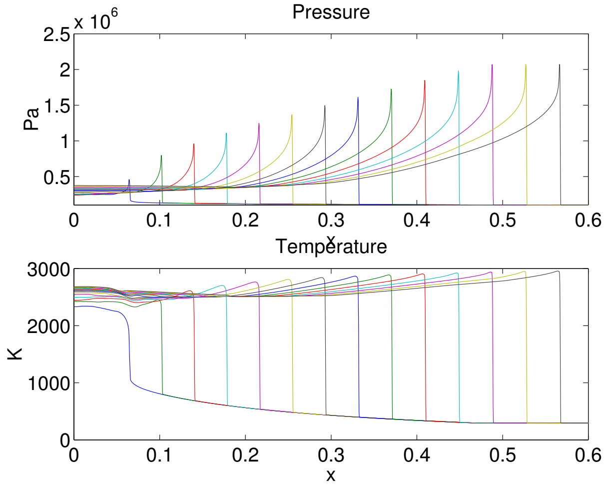

Figure 11: Plots of temperature and pressure with $b = 0.45$ and $t_{end} = 0.325$ ms

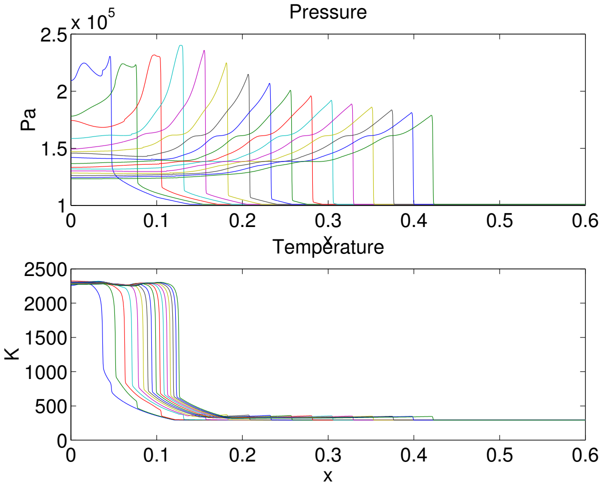

Figure 12: Plots of temperature and pressure with $b = 0.10$ and $t_{end} = 0.70$ ms

is about ten times higher in the first of them). When a detonation is developed it can easily be identified by the emerging ZND-spike and by the tight coupling between this spike and the release of energy (manifested by the distinct increase in temperature). This is illustrated in figure 11 where a detonation develops for the case when $b = 0.45$. When a detonation does not develop a shock wave "runs away" from the zone where the main part of the energy is released, and the necessary coupling between the two never occurs. This scenario is shown in figure 12 where the results from calcultions with $b = 0.10$ are displayed. As pointed out earlier the simulations do not model propagation of flames, and the entity propagating as a distinct increase in temperature behind the shock wave in figure 12 is instead an illustration of a convected explosion. As explained above, a convected explosion can only exist as long as there is a gradient in the induction time (or if there is a continuous regeneration of this gradient – as is the case in a propagating detonation). This can be clearly seen in figure 12. Here the shock wave is too weak to generate the required gradient, and in the absence of transport effects the speed of the convective explosion is continuously reduced (which can be seen from the diminishing distance between the front of two consecutive time plots when the convective explosion "runs out of gradient").

The remaining cases with radicals listed in table 3 yield results very similar to those described above. That is, the results obtained when $b = 0.15$ and $b = 0.20$ are similar to those when $b = 0.10$ (shown in figure 12), and the solutions obtained with $b = 0.25$ and $b = 0.30$ have the same essential features as the successful DDT obtained with $b = 0.45$ (and shown in figure 11). None of these cases are therefore displayed.

In order to illustrate the importance of the radicals they are simply removed from the initial solution in the same way as described in section 2.2. When doing this, the reactions are substantially slowed down, and there are no indications of a transition to detonation occuring. The same initial profile as in figure 11 is used ($b = 0.45$), but for this case the final time of the calculations is 1.5 ms which is more than four times longer than required for a successful transition when the radicals are retained. During the calculations the maximum pressure in the solution does not increase, but instead drops from about

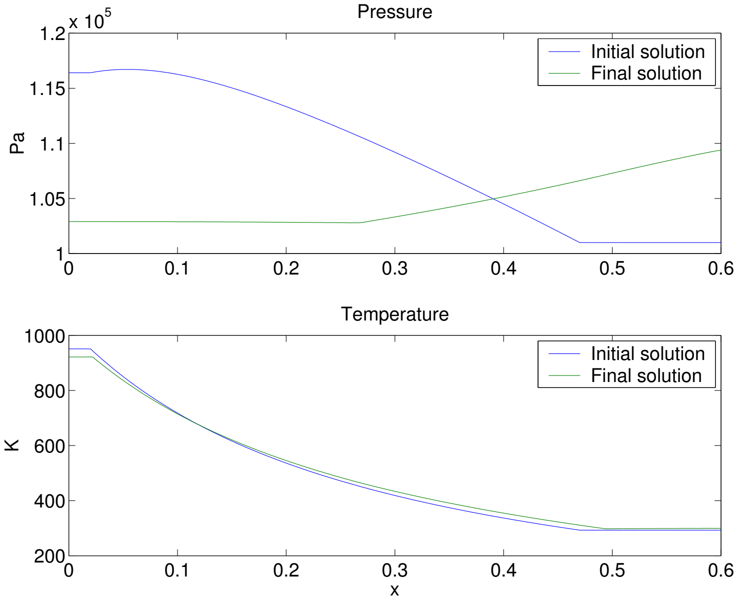

Figure 13: Plots of temperature and pressure from simulations when the radicals have been removed from the mixture. $b = 0.45$, $t = 0$ ms and $t = 1.50$ ms.

1.2 atm to 1.1 atm. The profiles of the pressure and temperature for the initial and final solutions are plotted in figure 13. As can be seen the removal of the radicals lowers the sensitivity of the mixture to the extent that there are no noticable heat release during the the calculation. Hence, the conclusions in sections 2.2 and 2.3.1 can be applied to DDTs as well, i.e., the very small quantities of radicals in the burnt gases have a dramatic influence on transitions to detonations.

As already pointed out the results above have all been obtained with the transport effects removed from the model (because this makes the calculations notably faster, and because it is believed that the transport effects are of lesser importance in the last phase of the DDT simulated here). Therefore it is not obvious that grid convergence can be obtained, see [8]. A refinement study has nevertheless been performed. Two cases have been chosen, one with $b = 0.45$ m and $L = 0.6$ and the other with $b = 0.90$ and $L = 1.1$. The first of these is the same as the one plotted in figure 11, and in both cases the radicals are retained (since no major events take place in the simulations when the radicals have been removed, it is reasonable to believe that grid convergence are much easier to obtain then). It turns out that a dramatic change in the solution occurs if the grid is sufficiently refined. When 64,000 cells are used in the first case and when 128,000 are used in the second case there is a separation between the shock wave that is building up and the zone where the heat is released. This is shown in figure 14 where the maximum pressure over time at each point is plotted. The point of separation is spotted by an abrupt decrease in pressure preceded by rather severe instabilities. The drop in pressure is explained by the fact that when the shock wave and the reaction zone become separated there is no mechanism to support an increasing pressure, and the strength of the shock wave can only decrease. The calculations for the different grid sizes for the two problems have the same

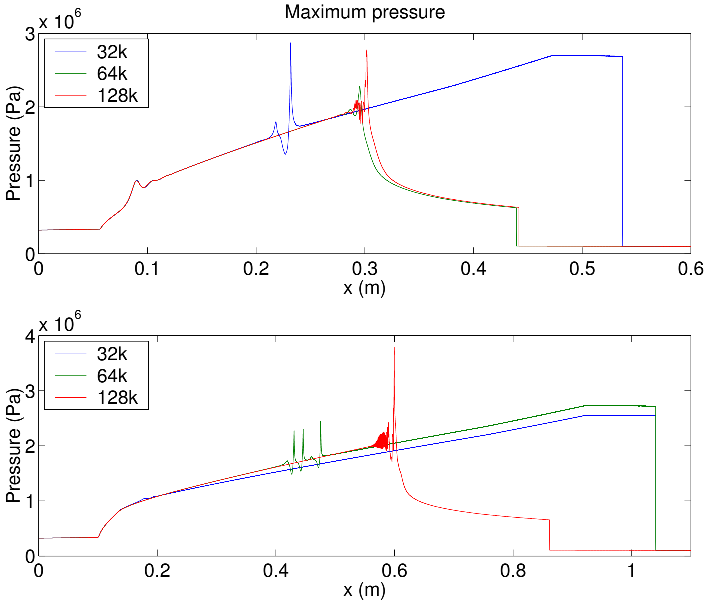

Figure 14: Plots of maximum pressure with $b = 0.45$ m (top) and $b = 0.90$ m (bottom) under grid refinement.

final time ($t = 0.325$ ms when $b = 0.45$ m and $t = 0.55$ ms when $b = 0.90$ m). Since the speed of the decaying shock wave is significantly lower than the developing detonation the shock wave will not reach as far as the detonation (which can be seen in the plots). Even though there are no DDT for the finest grids, a later transition can not be completely ruled out. It is also clear that the results will be affected by keeping transport effects and by adding turbulence modeling to the calculations. Further studies are needed to claifify this behavior.

The number of grid points in these refinement studies make the computations very time consuming. For example, the calculations on the finest grids above take over 24 hours to complete on 18 processors on a PC-cluster built up of nodes running at 2 GHz.

3 Conclusions/Discussions

The problem of initiating the detonation in an air breathing pulse detonation engine is studied. This problem has to be solved in an efficient manner using practical fuels before this type of engine will be in more general use. Here it is hypothesized that radicals remaining from the previous cycle has an important role when the consecutive detonation is to be initiated.

The effect of mixing hot products with fresh fuel gases is studied through numerical experiments. The hot products used in the simulations are obtained from a two-dimensional calculation of one cycle in a pulse detonation engine, including the blow down phase. These hot products are mixed with the fresh fuel gases (hydrogen-air) in different proportions. In none of the cases studied do the radicals constitute more than one third of a percent of the total mass. The significance of the radicals are demonstrated by doing the calculations both with included and excluded radicals in the initial mixture. Under the context of the mathematical model used in the simulations it is shown that the presence of radicals:

- significantly reduce the ignition delay time for constant volume explosions,
- facilitate direct initiations, and
- reduce the demand on the size of the structures in the flow field required for a successful deflagration to detonation transition.

It can be concluded that the remnants of hot products in the engine when one cycle is finished is of great importance when the detonation in the next cycle is to be initiated. The results also show that the main reason for this is the presence of the small fractions of radicals – and not the elevated temperature – in the hot products. From these conclusions it can be deduced that

- Single shot experiments are of limited value when methods to initiate a detonation in a pulse detonation engine is studied.
- It is essential to have a model capable of handling radicals when initiations of detonations are studied numerically.

In order to lessen the demand on the computational power required and to isolate the effect of the radicals certain simplifications have been introduced in the mathematical model. For instance, the initiations have only been studied in zero (constant volume explosion) and one dimensions, and the transport effects have been removed from the model. This means that neither the initial acceleration of the flame nor the injection and mixing of the fuel-air with the hot products have been simulated. These effects are important, and can hopefully be treated in a future study. However, the results obtained do explain the dramatic reduction in energy required to initiate a detonation in a pulse detonation engine operating in multi-cycle mode compared to initiations in a quiescent mixture in a shock tube, see [1, 2, 3].

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