TRANSIENT NUMERICAL CODE WITH GRID ADAPTATION FOR GAS COMBUSTION AND DETONATION STUDIES

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Abstract: Combustion, shock waves and detonations in enclosure are implicated in a wide range of applications: knock in internal combustion engines, flame propagation in kerosene tank, pulsed detonation engines. But they also may be related to explosion and hazard when uncontrolled. These phenomena are highly transient and they are managed by heat transfer, fluid mechanics and chemical processes, whose characteristic times are about the order of respectively 1s, 1 ms and 1 μs to few ns. Due to the coupling of these complex phenomenons, a comprehensive study is firstly conducted with a 1-D approach in order to provide a tool with a reasonable computation time (typically less than a night for a simulated time of few hundredths of ms). The equations and the numerical schemes of the code are described in details in this paper. A full set of validation cases is given with analytical and numerical data. Some numerical instability, attributed to the centred scheme, can be found depending on the simulated configuration. Despite this fact, accurate values are obtained. The possibility of initiating a detonation with gaseous reactive mixture in enclosure is seek and the thermal/chemical coupling in gas explosion is investigated. The temperature and rate of increase, the overpressure and the initiation delay are in particular considered.

Nomenclature

c_p	=	Heat capacity
g	=	x coordinate of the gravity
H	=	Total enthalpy
M	=	Molar mass
P	=	Pressure
r	=	Gases constant
R	=	Perfect Gases constant
S	=	Cross Section
T	=	Temperature
t	=	Time
V	=	Velocity
V_i	=	Diffusion velocity of the ith species
Y	=	Mass fractions
x	=	Abscissa along the enclosure
Subscripts		
i	=	species
mix	=	mixture
Greek Letters		
α	=	Thermal diffusivity

λ	=	Thermal conductivity
μ	=	Dynamic viscosity
ρ	=	Density
w_i	=	Net production rate of species i

Introduction

The cool flames and the detonations in enclosure are pretty well known but still some improvements in knowledge can be and need to be brought. These two phenomenons do not seem to be correlated; but they can be strongly linked because a cool flame can notably be observed for detonation in enclosure [1]. The cool flames have been studied in many configurations (microgravity [2-4], in internal combustion engine [5, 6], in rapid compression machine [7, 8], in a reactive flow [9], in enclosure [10-12]) and for various type of fuel (mainly the methane [12, 13], propane [4], butane [3, 14], pentane [7], heptane [7, 8, 15], decane [15], diesel [10] and other hydrocarbon fuel [2, 5, 9, 11]) mostly with air but also with pure oxygen. The cool flames correspond to a low temperature oxidation phenomenon (around 500 K) with a thermal increase of about 200 K, when a typical auto-ignition is encountered for a temperature elevation of 400 K. It is experimentally characterized by a blue light emission due to the chemiluminescence of the formaldehyde [9]. It can appear for concentration lower than the Lower Flammable Limit (LFL) and under the auto-ignition temperature (AIT) [13]. The pressure increase due to this combustion is lower than a factor 2 [13] and elevating the working pressure will facilitate the auto-ignition [14]. The cool flames can be used as a process to produce hydrogen, by mean of methane low temperature oxidation for example [12]. But this phenomenon also needs to be well controlled and understood because it can represent a hazard, for example in polymer production under gas phase. Indeed, the peroxide intermediates accumulate during the low temperature oxidation and this makes the mixture much more reactive and sensible to explosion [14]. Furthermore, it can be a very important step in internal combustion engine because it contributes to evaporation of the fuel but it also facilitates the undesirable auto-ignition process (knock) [8, 16]. Thus, studying the cool flames is directly related to hazard prevention and control.

The detonations are also strongly related to industrial explosion and risk. This phenomenon corresponds to a coupling between a supersonic shock wave and a reacting front driven by this wave. It has been deeply investigated and it is now well understood [17] such as the deflagration to detonation transition (DDT). The DDT is a physical change with low induction time that will transform a deflagration (combustion propagating at a subsonic speed) to a detonation. This transition is accompanied by sudden pressure and luminosity increase but with a velocity not greater than half of the Chapman-Jouguet (CJ) detonation velocity [18]. A full review of literature on DDT is given by Oran and Gemzo [19] to analyse its origins. A reactivity gradient (as proposed by Zeldovich et al. [20]), the flame turbulence, the interactions between the shock wave and the flame front are the key factor that control the DDT [19]; even if the two latest are not sufficient alone to initiate a DDT [21]. But the way to practically obtain a DDT is still under study. Indeed, there are some major interests to know how to obtain a DDT, for example in the aerospace application of the Pulsed Detonation Engine (PDE) [22, 23], or to not obtain a DDT, notably for the hazard mitigation (chemical additives can be a solution [24, 25] and dilution of reactant also [26] in that case). This type of study can be conducted in confined or unconfined configuration depending on its aim. For detonations in enclosure, some well-known behaviour can be found in the open literature.

The studies are generally conducted numerically to fasten them and to avoid the safety problems. It is also the most feasible way for fundamental work. The intrinsic parameters of the reactive mixtures (auto-ignition delay, detonation velocity, detonation cell width) [27] can be of interest such as the detonation impact on structures [23, 28-30], the detonation structure in complex geometries and configurations like bends [31], like thin channels with a flame in tulip shape [32, 33], like gaseous bubbles contained in liquid phase [34], like gaseous mixture with solid energetic particles [35].

From a numerical and mathematical point of view, some numerical schemes are developed for such configurations [36-39] and Henrick et al. [40] propose their highly accurate one using Runge Kutta method for time resolution and a fifth order centred one for the space coordinate. Its appears to be accurate and it does not present computational stability problems linked to discontinuities, contrary

to second order centred scheme. The Courant-Friedrichs-Lewy (CFL) number for this scheme is about unity. The Total Variation Diminishing (TVD) schemes are often used because they are stable even when dealing with discontinuities, despite their lower accuracy due to an artificial decrease of the variations in the system [41]. The numerical schemes have been widely tested, on various types of equations and for several purposes [42-45]. The second order centred scheme is known for its high accuracy but it has a poor stability [46].

A way to fasten the numerical simulations is to use a grid adaptation in order to accurately define the area of drastic changes but not the entire mesh. Some methodologies to adapt a grid mesh to the simulated phenomenon are developed, particularly for complex multidimensional geometries that need to be computationally time-reduced [47-49]. Azarenok and Tang [47] propose a grid adaptation with a resolution of both hydrodynamic and chemical part of the reactive flow without decoupling them, as it is often the case to reduce the computation time.

To face the high computational times when simulating complex configurations with chemistry (inherent with detailed chemistry [50, 51]), the studies use some models, which represent the physicochemical phenomena (*how far from reality?*). The modelling of multi-scale phenomenons is notably undertaken and improved [52]. Furthermore, the detailed chemical mechanism are often replaced by tabulated chemistry [53, 54] or by simple few reaction step mechanisms, particularly when dealing with turbulent and 2-D or 3-D configurations [19, 55]. Thus, it is difficult to precisely investigate the reality of phenomena. Because the numerical studies cannot always cope with very complex configurations [56], experimental works can bring explanations. The initiation of the detonation is generally obtained by spark (low energy compared to pyrotechnic system). One of the most advanced benches use synchronised spark to communicate energy, in the most efficient way, just after the propagating shock wave [57]. This allows obtaining a DDT with a lower applied energy than with a single spark and for a shorten distance. The use of obstacles is also a possible way to fasten the DDT [19, 57-59] because of the vorticity effect [60]. The reactivity of the mixture is verified to play a major role on the DDT [61]. Some detonation studies also exist in closed static vessel, mainly for safety interest [23, 62]. Some of these vessels can present a vent [58, 63]. But a fundamental analysis of phenomenons is still very complex with an experimental approach due to the very low spatial scale (few microns) and macroscopically "instantaneous" event (nanosecond order).

The explosions in open or closed vessels are also related to the previous phenomena because it is characterized by flame ignition or auto-ignition, by flame propagation and by overpressure. This can conduct to strong impact on the structures and on the direct environment. Then a DDT is also possible and when it appears, the above comments on detonation and hazard are applicable. Some studies, similar to detonation, can be conducted for explosion, i.e. deflagration. For example, the ignition point location influences the strength of the explosion [64]. A complementary study could also focus on the flame propagation in adjacent compartments, for which the orifice size between two vessels acts directly on the flame propagation and on the strength of explosion [65, 66]. Numerous study are available on this point to evaluate the relationship between the overpressure and the initial one before explosion initiation [17], the flame propagation as a function of ignition point and the vent position [67]. Studying the combustion, fundamentally [68, 69] or in applied configurations, is of great interest in all of the above mention configurations and general or specific advances are welcome. For example, considering the radiation in heat transfer can reduce by up to 30 % the computed ignition delay for fuel droplet evaporating configuration [70]. The flame quenching can be analysed depending on the heat losses at the wall [71]. Thus the configuration (adiabatic, isothermal,…) is of importance. It has to be noticed how the obstacles influence a freely propagating flame in a reactor [72, 73]. Such results have to be kept in mind to well conduct the present study. On a practical and applied interest, these accurate and fundamental approaches finally allow proposing some macroscopic laws to evaluate the hazard of a configuration in order to mitigate it or to prevent it. The overpressure of an explosion is often a parameter estimating the risk [74-81].

Regarding an enclosure, the cool flames, the gas explosion, the DDT and the detonations are all related to a complex coupling between fast or slow chemistry with hydrodynamic of the fluid, shock waves, interaction with wall, heat transfer at boundaries of the vessel. The characteristic times of these phenomenons are highly incompatible. This is particularly true for detonation and DDT, which are due to physical and chemical interactions with spatial and temporal scale of several orders of magnitude. Thus, investigating fundamentals aspects of these phenomena is facilitated by a numerical approach.

This is the way retained in this paper, whose purpose is to present a new computation code for simulating and furthering the understanding of all above phenomenons encountered in enclosure. The aim is to officially document the code validation and to propose some examples of its use.

Equations of the numerical simulation

The computation program, realized in Fortran language, considers an one-dimensional closed geometry in Cartesian coordinates between two infinite plates. The number format is the double precision. The simulation is written conservatively in transient regime with Partial Differential Equations and it handles compressible reactive flow with detailed chemistry. A combustion mechanism suitable for low and high temperatures is required for the fuel under study. The equations are discretized in space with finite differences using an Eulerian second order centred scheme [46]. They are implicitly solved in time with a fourth order Runge Kutta method [1]. A convergence criterion (relative variation lower than one percent) is applied to each of the computed physical quantities to ensure the good reliability on the numerical values at each time step. The physical and chemical phenomenons are separated and a time step is applied independently to the resolution of them both. The initial conditions needed for the computations are the initial distribution profiles of temperature, pressure, velocity and chemical concentrations. The boundary conditions are the one of an adiabatic, non catalytic and impermeable closed reactor. Thus, the variations in temperature and density (and hence in pressure) are equal to zero, such as the ones of chemical concentration. The velocity gradient at the boundaries is chosen to be equal to zero but several other possibilities have been investigated (linear and parabolic decrease). The grid is adapted automatically as a function of thermal gradients in the enclosure. This adaptation can also be applied depending on other physico-chemical quantities.

It is chosen to study simple configurations, with detailed chemistry but without modelling. Thus, the turbulence is not considered but this allows not disturbing the fundamental and real behaviour of phenomenons by the call to models that will approximate them at various space scales. In enclosure, the flame front is shown to become turbulent after few milliseconds, which is a time much higher than the characteristic one of detonation [82]. This allows considering a laminar flame for DDT studies.

A solver is used to take detailed chemistry into account. It only needs to give the common reaction data such as the pre-exponential factor and the activation energy for each chemical reaction related to the species combustion of interest. Thanks to the solver, the net production (or consumption) rate for each chemical compounds is known and this allows taking it into account in the energy equation and the species continuity equation for the transport consideration. The chemical transport processes, corresponding to laminar flow, are considered (diffusion, viscosity, Soret effect). The Dufour effect is considered when computing the temperature.

Due to shock waves study, it is important to consider the fluid as compressible. Thus, the continuity equation is given by Eq. 1. The fluid velocity is given by Navier-Stokes equation (Eq. 2) for which gravity is considered, even if it plays a negligible role in the presented configurations. The temperature is computed thanks to the energy equation (Eq. 3), in which chemistry terms appear notably. The pressure is then deduced by the perfect gases law (Eq. 4), which is also introduced directly in the preceding equations when applicable. After resolution of chemistry with a detailed kinetic scheme, the species continuity equation (Eq. 5) enables computing the transport properties with a multicomponent diffusion [90]. The viscosity and the thermal conductivity of the fluid are also calculated [90]. The butane can be the fluid of study because its combustion is well-known [91, 92] and various data can be found, such as the flame velocity or the self ignition delay. The methane will also be considered.

$$\frac{\partial(\rho)}{\partial t} = -\frac{\partial(\rho.V)}{\partial x} \qquad (1)$$

$$P = \rho.\left(\frac{R}{M_{mix}}\right).T \quad \text{with} \quad M_{mix} = \frac{1}{\sum \frac{Y_i}{M_i}} \qquad (2)$$

$$\frac{\partial(\rho.V)}{\partial t} = -\frac{\partial(\rho.V^2)}{\partial x} - \frac{\partial P}{\partial x} + \frac{4}{3}\frac{\partial}{\partial x}\left(\mu\frac{\partial V}{\partial x}\right) + \rho.g \tag{3}$$

$$\frac{\partial(\rho.H)}{\partial t} = -\frac{\partial(\rho.V.H)}{\partial x} + \frac{\partial P}{\partial t} + \frac{4}{3}\mu\left(\frac{\partial^2 V}{\partial x^2}\right) + \frac{\partial}{\partial x}\left(\lambda.\frac{\partial T}{\partial x}\right)$$
$$- R.T.\sum\left(-\frac{1}{M_{mel}}\left[\frac{\partial V_i}{\partial x}\times\frac{\partial(\rho.Y_i)}{\partial x} + V_i\times\frac{\partial^2(\rho.Y_i)}{\partial x^2}\right]\right)$$
$$- \frac{\partial T}{\partial x}\times\sum\left(C_{p,i}.\rho.\frac{V_i}{T}\frac{\partial T}{\partial x} - V_i\frac{\partial(\rho.Y_i)}{\partial x}\right) \tag{4}$$

$$\frac{\partial(\rho.Y_i)}{\partial t} = -\frac{\partial(\rho.V.Y_i)}{\partial x} + \rho w_i + \frac{\partial}{\partial x}\left(V_i\frac{\partial(\rho.Y_i)}{\partial x}\right) \tag{5}$$

The present numerical code has been validated using several comparison data and this is presented in the following section.

Validation and test of the code

Several validation test cases have been studied to ensure the reliability of the code (uniform gas explosion, flame propagation, shock wave, detonation). Analytical and numerical data are used in that way (some of them coming from the open literature). Each term of the equations has been first separately validated, like: the thermal conductivity, the chemical heat production, the viscous friction and the chemical diffusion (in the equation energy). The multi-component diffusion and the production rate of the species equation have also been validated, such as the contribution of the pressure and the density gradients of the momentum equations. An analytical validation has also been carried on the transient heat transfer. For each of the validation cases, the mass conservation is checked and the internal energy also (when no chemistry is considered). The thermal conductivity was checked with a two regions enclosure filled by nitrogen at temperatures of 600 K in the first half of the reactor and 300 K in the second one. The grid adaptation is not used in this case. The final temperature is found to be exactly the analytical one, even at the last digit. The transient thermal conductivity of the system has been validated with classical analytical formula for such configuration (Eq. 6). The enclosure is filled in by nitrogen at 300 K and the left wall of the reactor is heated at 1000 K.

$$T_{x,t} = T_{x=0,t} + \left(T_{x=0,t} - T_{x,t=0}\right)\times erf\left(\frac{x}{2\sqrt{\alpha.t}}\right) \tag{6}$$

where $T_{x,t=0}$ is the initial temperature in the system, $T_{x=0,t}$ the constant temperature of the left wall.
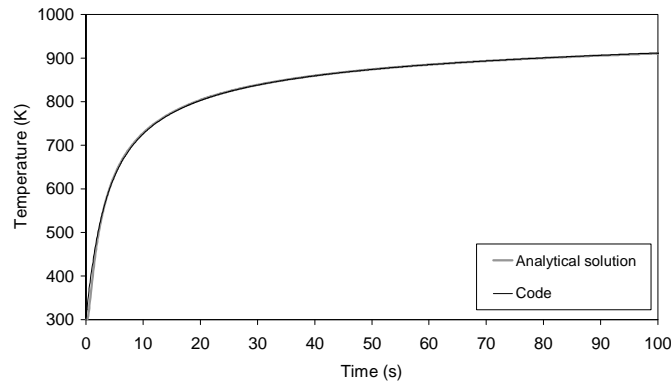

Figure 1. Time evolution of the temperature near the left wall.

The time evolution of the fluid temperature in the enclosure, near the left wall for example (Figure 1), is in perfect agreement with the analytical solution (even for the last numerical digit).

A shock wave propagation in pure nitrogen has been computed. The reactor (300 K) is divided in two regions, the left third with 0.2 MPa and the right two third with 0.1 MPa. At the initial time, a wave propagates from the frontier between the two regions and toward the low pressure region. In close agreement with the analytical formula for such configuration, the temperature of the wave is 319 K (gas compression at the wave front) and 266 K (gas expansion at the back of the wave), the pressure is 0.138 MPa and the velocity is 84 m.s^{-1}. The final pressure of the reactor is 0.133 MPa which is equal to the analytical one. What can be mentioned are the numerical instabilities on all the computed physical quantities such as the pressure (Figure 2). This is due to the centred second order scheme, which is used due to its recognised high accuracy. A convergence criterion to limit the variations of the physical quantities between two time steps is employed to cope with this problem. Such numerical instabilities should be eliminated because they could propagate and also conduct to high discrepancies on the chemistry point of view.
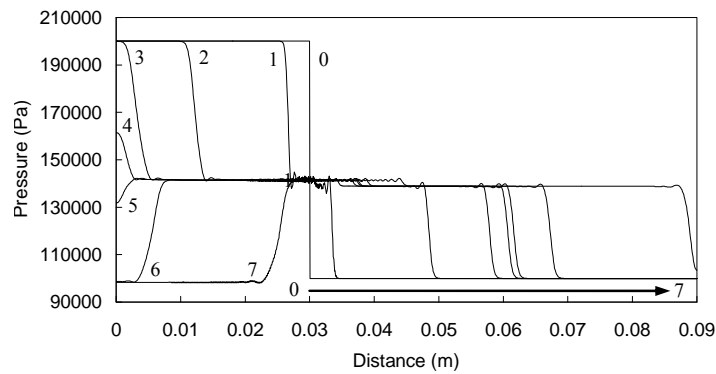

Figure 2. Pressure inside the enclosure for different times: 0-t=0 s, 1-t=10.3 μs, 2-t=52.7 μs, 3-t=79.1 μs, 4-t=87.1 μs, 5-t=89.7 μs, 6-t=105.6 μs, 7-t=158.6 μs.
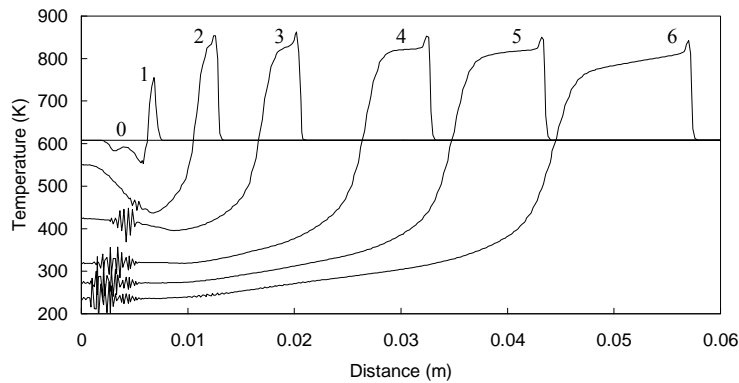

Figure 3. Temperature computed for 400 space steps at different times: 0-t=0 μs, 1-t=2.0 μs, 2-t=10.0 μs, 3-t=19.8 μs, 4-t=35.6 μs, 5-t=49.6 μs, 6-t=67.6 μs.

The shock wave propagation has also been studied in pure oxygen and compared to the open literature [92]. It appears that the dynamic of the wave is slightly different from validation data. The shock wave reaches the position 0.05 m after about 60 μs (Figure 3), instead of 120 μs. Even if the initial conditions between the two calculations may differ (due to the interpolation between the two initial pressure regions), this needs to be carefully analysed. At this time, it is assumed to be due to the computation steps and to the numerical scheme. Furthermore, the numerical instabilities are shown to be very important and not in an acceptable range. A short peak just behind the shock wave appears. This is clearly due to the centred scheme.

The coupling between the hydrodynamic and chemical resolutions has been investigated to evaluate the possible sources of error, compared to what a Direct Numerical Simulation (DNS)

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approach should give for a result. A methane-air explosion (mass fractions of 0.055 CH_4 + 0.21 O_2 + 0.735 N_2) is computed in an initially uniform enclosure (concentrations, temperature of 1000 K and pressure of 0.1 MPa). When the thermal activity and the dynamic one are simulated, the chemistry is supposed to not evolve during one time step. The largest is the time step, the biggest is potentially the loss of accuracy due to the variables separation. This is what is shown on this case when comparing the results to 0-D chemistry (Figure 4). The thermal discrepancy is reduced by an order of magnitude 2 when decreasing the time step from 26.5 µs to 0.1 µs. This exemplifies the fact that dynamic and chemistry are highly linked and that the separation of the variables should be carefully used. A variation criterion should be used from now to limit the chemical gradient between two time steps.
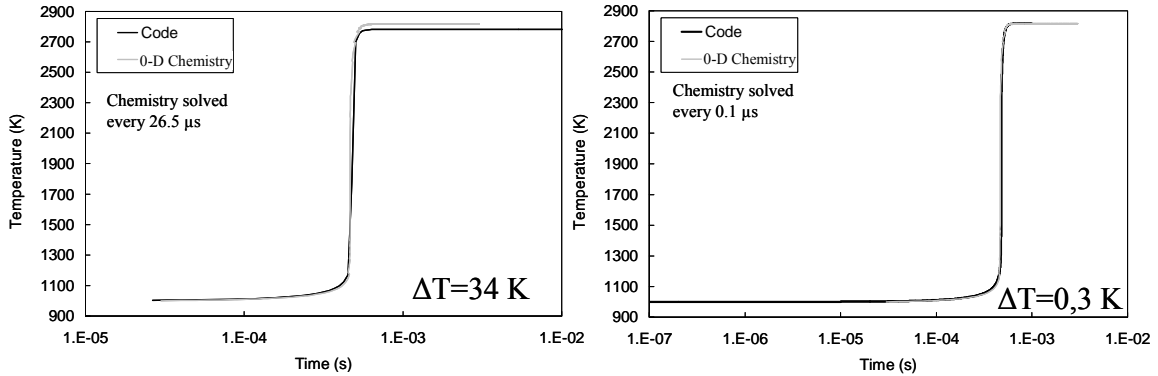

Figure 4. Thermal accuracy depending on the time step for a Methane-Air explosion. Comparison to pure chemistry solver in 0-D configuration.

Combustion and explosion

It is well-known that a detonation appears for a strong reactivity gradient in the fluid. This corresponds to a thermal gradient or to a fuel concentration one for example. But the open literature is very scarce on how to practically obtain a DDT, numerically speaking [83] more than experimentally [84-88]. One of the aims of the present numerical program is to investigate how to obtain a DDT in the shorter distance and with the simplest system. Some solutions are already proposed like obstacles [89] or shape of the reactor but none is based on heat transfers. Starting from the work of Frolov et al. [57], who experimentally used a succession of spark along the reactor to obtain a DDT, it is decided to numerically investigate the combined effect of the temperature and the chemistry before working on complex DDT and detonation cases.

The test case defined by the table 1 shows a maximum temperature evolution in time, which is qualitatively and quantitatively satisfying (Figure 5). The first temperature increase (from 620 K to about 870 K) is due to the shock wave propagating from the left to the right of the enclosure with a velocity higher than 900 m.s^{-1} (the sound speed is about 600 m.s^{-1}). During the time noted t_1 (from 0 to 65 µs), the temperature slightly decreases (due to a pressure decrease). The temperature and pressure rise for the shock reflection on the right wall lasts about 5 µs. This second thermal increase (about 300 K) is not followed by explosion because the autoignition delay for methane-air stoechiometric mixture is about 30 µs. Because of the gas expansion after the propagating shock wave, the spontaneous combustion is not observed. A noticeable thermal decrease is observed (lower than 100 K), which is probably not physical in this adiabatic configuration. This case has been also computed with pure air. The maximum of temperature in the enclosure also decreases during the propagation of the shock wave.

The time (noted t_2) before reflection on the left wall (45 µs) is lower than the time needed by the wave in the opposite way (65 µs). This is due to the temperature of the firstly shocked mixture, in which the reflected wave propagates with a Mach number of about 2. On the left wall, the gases reach a temperature of about 1450 K (after a time noted t_3, i.e. about 3 µs). At this temperature, the autoignition delay is lower than 1 µs and the explosion appears. It can be noticed that four thermal increases appear on the figure 5. The first one ($1.28.10^8$ K.s^{-1}) is due to the shock in initial gases, the second one ($1.2.10^8$ K.s^{-1}) is due to the reflecting wave, the third one corresponds to t_3 ($1.17.10^8$ K.s^{-1})

and the last one to the explosion (5.10^8 K.s^{-1}), i.e., to the chemical impact. This one is noticeably more important (factor 4) than dynamical impact on temperature.

For another computation (Figure 6), the initial temperature of the enclosure has been increased from 620 K (autoignition delay largely higher than several tenths of second) to 1000 K (delay of about 460 µs) to observe the chemical activity of the reactive mixture. The shock firstly increases (at a rate of $4.6.10^9$ K.s^{-1}) the temperature up to 1410 K near the initial pressure gradient. Then the wave propagates in fresh mixture and brings the gas to this temperature for which the autoignition delay is about 1 µs. This allows the shocked mixture to react and a combustion appears slowly ($4.8.10^7$ K.s^{-1}) back to the pressure front. The thermal increase is up to 1850 K. The reflection on the right wall makes the temperature rising 2680 K ($4.4.10^8$ K.s^{-1}) before flowing back in burned gases. The thermal increase rate is larger for the dynamical impact than for the chemical one (one or two order of magnitude) compared to the case with a temperature of 620 K, for which the inverse trend is observed (factor 4). The difference between these two cases is very thin because the fluid temperatures are 1410 K and 1450 K before combustion. This highlights the strong interaction between chemistry and dynamics, particularly when their characteristic times are close enough.

Table 1. Configuration of explosion test case computed with fixed grid of only 100 points.

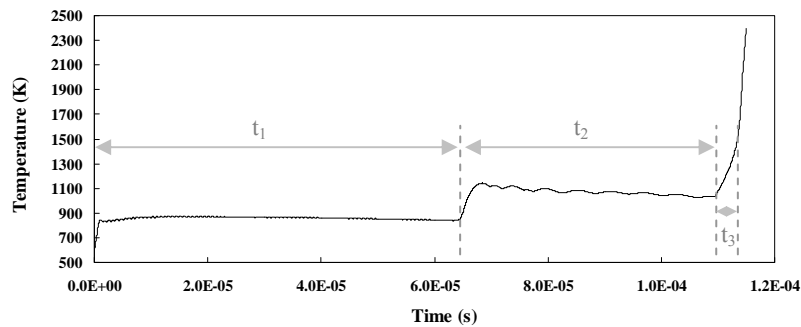| Parameter	Value
Enclosure length	0.06 m
Mixture composition	$0.735 N_2 + 0.21 O_2 + 0.055 CH_4$
Initial temperature	620 K
Region 1: 0-0.003 m, initial pressure	1 MPa
Region 2: 0.006-0.06 m, initial pressure	0.42 MPa
Region 3: : 0.003-0.006 m, initial pressure	Linear interpolation
Initial velocity	0.

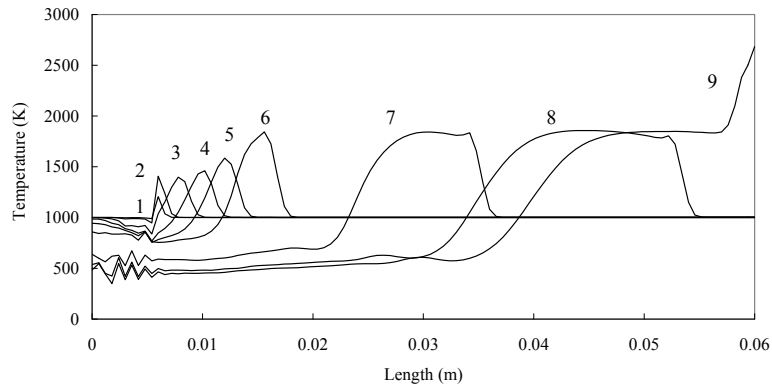Figure 5. Time evolution of the maximum temperature in the enclosure.

Figure 6. Spatial evolution of temperature at different time steps (1-t=0.4 µs, 2-t=0.9 µs, 3-t=2.9 µs, 4-t=4.9 µs, 5-t=6.9 µs, 6-t=9.9 µs, 7-t=24.9 µs, 8-t=39.9 µs, 9-t=47.4 µs). Numerical instabilities are visible.

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Conclusion

The numerical simulation is presently the most feasible way for understanding very complex and fundamental phenomena such as cool flame and detonation and their applications, like knock or detonation for propulsion applications. It allows accessing in details some physical and chemical characteristic that are somewhat difficult or impossible to measure experimentally (reacting gas composition, flame front thickness, flame and wave speeds, pressure and temperature, residence time and others characteristic times of phenomenons). A new computation code has been presented with its validation and its capacity to provide new understanding of such specific phenomena. A one-dimensional approach has been chosen because it is considered to be sufficient to adequately investigate them. It allows obtaining "rapidly" results of simulation. An adaptive grid is employed to well represent strong gradients and discontinuities with a reasonable number of mesh points, about one thousand. A chemical kinetic solver with detailed kinetic mechanism is used to accurately account for reactive flow and the coupling between chemistry and the dynamic flow; between a flame and a shock wave for example. The geometric configuration is the one of an enclosure with the dimensions freely given by the user. Other configuration could be considered with adapted boundary conditions.

The results of numerical simulation have been compared to analytical and numerical data, some are from the literature. An overall good agreement is obtained on the test cases. The shock wave is well described such as the thermal conductivity. The chemistry presents a good behaviour but it needs to be well coupled to dynamics to ensure a good accuracy (0.3 K degrees). The effect of temperature on the reactivity of the mixture has been studied to evaluate the possibility of the code. The ability to obtain and describe a deflagration propagating in methane-air mixture is shown. Nevertheless, some errors have been found (multidiffusion, strong density gradient, numerical instabilities…) and they still need to be solved. The numerical stabilities are attributed to the numerical scheme. The accuracy of the code is not in the range of few degrees with complex reactive test case and that needs to be corrected.

However, the code is shown to be a promising tool notably to numerically investigate detonations in enclosure, even if it still need some improvement. The future work will focus on the possibility to obtain detonation by adjusting the temperature profile of the reactive gases in the closed vessel. The next code improvements could be to allow different boundary conditions (heated enclosure, catalytic wall,…) and to adapt the code to cylindrical and spherical geometries, potentially multidimensional. A comparison to a code which does not separate physical and chemical variables could be also interesting to evaluate the discrepancies of both methods.

Acknowledgements

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