Modeling Study of Pulsed and Continuous Detonation in Propane/Air Mixture

D.I. Babushenko, V.I. Kopchenov, P.S. Kuleshov, N.S. Titova, A.M. Starik
Central Institute of Aviation Motors
Moscow, 111116 Russia

1 Introduction

Nowadays, the detonation combustion cycle is considered as promising one for the application in air-breathing and rocket engines. However, until now there exist some important issues that should be carefully investigated. One of them concerns the stability of detonation combustion in practical devices. The other is the provision of detonation initiation with the minor consumption of input energy. One more problem deals with the pollutant formation in detonation engines, because due to high temperature and small residence time in the detonation combustor the emissions of such species as NO and CO can be potentially rather high. In order to resolve these problems, deeper understanding of coupling of gasdynamic and chemical processes is strongly needed.

Analysis, based on CFD simulation of these processes, is one of the widely applied approaches to gain an insight in such complex phenomenon. CFD modeling of detonation, especially in hydrocarbon-fueled combustors, requires the usage of chemical reaction mechanisms enable to describe properly the principle features of ignition and combustion. The computational time strongly depends on the number of species included in the reaction mechanism. Therefore, for 2D and, especially, 3D CFD calculations we can not use the detailed reaction mechanisms comprising for heavy hydrocarbons more than 100 (or even few hundreds) individual species. This dictates a necessity to develop more suitable for CFD simulation kinetic mechanisms involving limited number of mixture components. It should be emphasized that, today, mostly one-step or few-steps quasi-global mechanisms are used for modeling the processes in detonation combustor [1]. However, such mechanisms can not reproduce properly the equilibrium temperature in the combustion exhaust and can be applied only for a very narrow range of temperature, pressure and mixture composition. Therefore, it would be very fruitful to built adequate reaction mechanism more appropriate for modeling of shock induced/detonation combustion for a wide range of parameters.

The current work addresses the development of reduced reaction mechanism appropriate for the description of shock induced / detonation combustion for propane-air mixture and comprehensive analysis of two different detonation modes: (1) pulsed detonation induced by primary shock wave propagating in the tube with constant cross section and (2) detonation combustion in the continuously rotating detonation wave in the annular cylinder channel. Comparative analysis of the prediction ability of developed reduced reaction mechanism and quasi-global mechanism proposed earlier by Basevich et al. [2] for two considered problems is also reported.

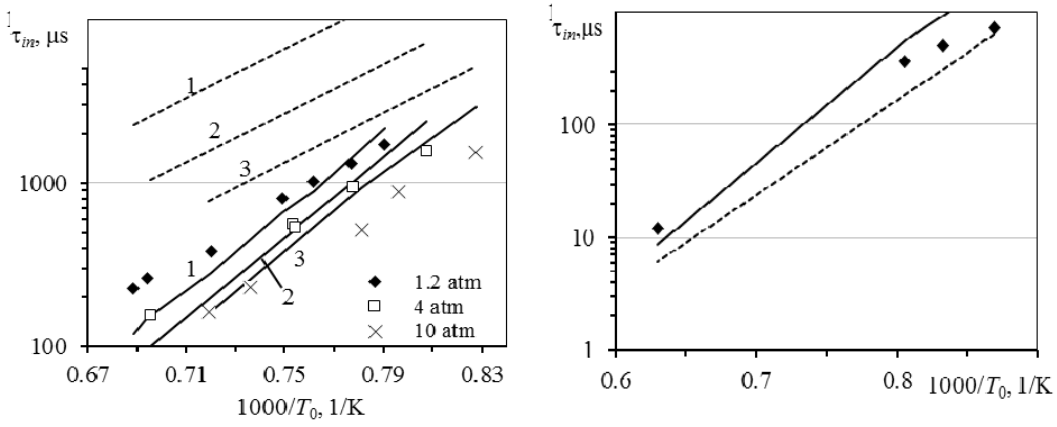
Correspondence to: kop@ciam.ru (V. Kopchenov)

2 Kinetic Models and Methodology

The reduced reaction mechanism for high temperature ignition and combustion (T_0>1100 K) of propane-air mixture was built on the basis of detailed reaction mechanism of propane oxidation [3]. This detailed reaction mechanism was carefully validated in the ranges of temperature T_0=680-1900 K, pressure P_0=0.2-30 atm and equivalence fuel to oxidizer ratio ϕ=0.125-2.5. For shortening the number of mixture components, the directed relation graph (DRG) approach [4] was used. The threshold value in this technique was chosen by such a way to ensure the distinction in the values of ignition delay, predicted by the detailed and reduced reaction mechanisms, with given accuracy. Thus, the developed reduced reaction mechanism involves 156 reversible reactions with 27 species: O, O_2, H, H_2, OH, HO_2, H_2O, H_2O_2, CO, CO_2, CH_3, CH_4, C_2H_2, C_2H_3, C_2H_4, C_2H_5, C_2H_6, C_3H_5, C_3H_6, nC_3H_7, iC_3H_7, C_3H_8, HCO, CH_2O, CH_3O, N_2, Ar. This mechanism was validated against the existing experimental data on the ignition delay measured by using the shock tube technique [5, 6] in the C_3H_8/O_2/Ar mixture at different values of T_0, P_0 and ϕ and on the laminar flame speed measured in [7 - 9].

The quasi-global reaction mechanism [2], considered in this work, includes 6 species and 4 reactions, one of them is reversible. The intermediate species H_2 and CO are included in this mechanism alongside with the reagents C_3H_8 and O_2 and products of oxidation CO_2 and H_2O. The rate constants of these quasi-global reactions were fitted so that to describe the experiments [5] on ignition delay of the C_3H_8-O_2-Ar=3.85-19.23-76.92 mixture with ϕ=1, P_0=8.1-14.7 atm in the range of T_0=1200-1430 K.

Figure 1 depicts the measured values of ignition delay τ_{in} as a function of initial temperature T_0 for the C_3H_8-O_2-Ar with ϕ=0.5 and 1 as well as the predictions with the usage of reduced and quasi-global mechanisms. One can see that the quasi-global mechanism reproduces properly the values of τ_{in} only for those conditions where it was fitted to experiment. In the same time, the developed reduced mechanism describes the whole set of experimental data with reasonable accuracy.



a) b)

Figure 1. Ignition delay times in the C_3H_8-O_2-Ar=0.514-5.142-94.344 mixture with ϕ=0.5 and P_0=1.2, 4, 10 atm (curves 1-3, respectively) (a) and in the C_3H_8-O_2-Ar=3.85-19.23-76.92 mixture with ϕ=1, P_0=8.1-14.7 atm (b). Symbols are the measurements [6] (a) and [5] (b); solid and dashed lines are the predictions of reduced and quasi-global [2] mechanisms.

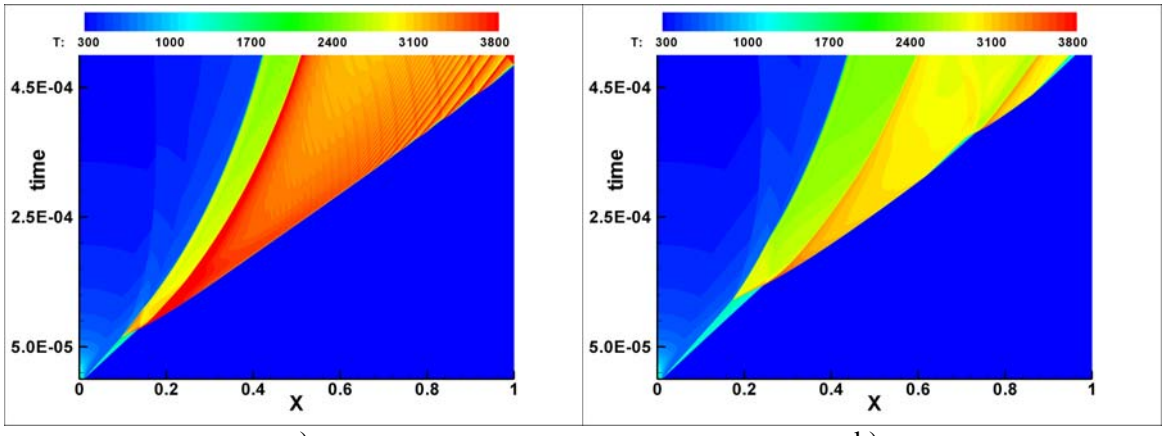
Mathematical flow model is based on the system of two-dimensional unsteady Euler equations for reacting gas mixture. Numerical simulation was performed with the use of the higher order accuracy version of Godunov's method based on the explicit approximation of convective terms and on the implicit approximation of chemical source terms in the equations for species concentrations.

3. Results and discussion

As was mentioned above, analysis was conducted for pulsed and continuous detonation modes.

3.1 Pulsed detonation induced by shock wave

Following scheme of shock-induced detonation wave propagating in the tube was considered. The tube with the length of 1 m is closed on the left end. The initiation section of 0.01 m length located near the closed end is filled by nitrogen. The main operational part of the tube is filled by a stoichiometric propane-air mixture with P_0=1 atm and T_0=300 K. In the initiation section, the pressure and temperature are increased, and after breakdown of arbitrary discontinuity the strong shock wave propagates to the open end of the tube and, at some conditions, the detonation wave forms. The problem of primary shock wave and detonation wave initiation is solved by using 1D approach.
Shown in figure 2 are the temperature fields in x-t plane predicted by quasi-global and reduced kinetic mechanisms. As is seen, shock induced combustion occurs in both cases with the ignition at the hot side of contact discontinuity that results in the formation of primary detonation wave. The main detonation wave arises at some time instant t_d as a result of the interaction of primary detonation wave with leading shock. However, the values of t_d predicted with the use of quasi-global and reduced kinetic mechanisms differ notably. So, for conditions considered, quasi-global mechanism predicts $t_d=7\cdot10^{-5}$ s, and reduced mechanism gives $t_d=1.2\cdot10^{-4}$ s. The temperature and pressure behind the detonation wave are equal to 4100 K and 66 atm in the case of using quasi-global mechanism and to 3000 K and 48 atm, respectively, upon usage of reduced mechanism. It is worth noting that these results were obtained with the 50 μm size cells of computational grid in longitudinal direction. In this case, Zel'dovitch-Neumann-Döring (ZND) structure is resolved. The "stripped" structure is well observed in figure 2a. Such a structure is connected with the periodical time variation of the distance between the leading shock wave and the leading edge of the heat release zone. It is worth noting that the characteristic scale of the oscillations obtained upon the computations with quasi-global reaction mechanism is essentially smaller than that predicted by reduced mechanism (see figures 2a and 2b). It should be emphasized that the values of averaged velocity of detonation wave front predicted by quasi-global and reduced kinetic mechanisms differ only slightly (approximately by 60 m/s), while the magnitude of averaged velocity of detonation wave is equal to 2020 m/s (in the case of using reduced mechanism).



a) b)

Figure 2. Temperature fields: (a) prediction of quasi-global mechanism; (b) prediction of reduced mechanism.

3.2 Continuous rotating detonation

We considered continuous rotating detonation in the annular coaxial channel. Its radial dimension is much smaller than those in the azimuth and axial directions. In this case, the flow can be modeled using 2D approach. The combustion in the continuously rotating detonation wave (CRDW) was simulated at the fixed stagnation conditions in the collector from which the premixed stoichiometric propane-air mixture was injected into the combustor. The combustion products were exhausted into environment with low back pressure. The geometry of combustor was chosen identical to the device utilized in the experiments reported in [10]. It should be noted that there exists the difference in the experimental conditions [10] and the computational problem formulation considered in the present work. In experiments, the fuel was injected into the air flow at the entrance of combustor, and fast mixing of fuel and air was supposed to occur in the real combustor.

For the simulation, the following values of stagnation pressure and temperature in the collector were chosen: P_0=12 atm, T_0=640 K, and the back pressure was equal to 1 atm. Within 2D approach, the axial and circumferential lengths of the model combustor were equal to 0.57 m and 0.909 m, respectively. Boundary conditions at the combustor entrance were taken in line with the recommendations of [11] on the basis of the installation of the system of micro-nozzles. The computation runs were performed with varying ratio of exit and throat areas of micro-nozzles (K_s).

The comparative analysis of flow characteristics computed with the use of reduced and quasi-global mechanisms were performed. The computations showed that for the regime with regular continuously rotating detonation wave the difference in the combustion characteristics predicted with the use of both reaction mechanisms is small. So, the values of detonation wave velocity differ approximately by 4.5%, the maximal values of temperature at the combustor exit differ by 3.5%. The difference of the values characterizing the rise (from the entry to exit cross section) of longitudinal component of impulse (averaged in time and in circumferential direction) does not exceed 6%.

However, the distinction in the predictions of quasi-global and reduced mechanisms becomes significant near the boundary of the existence of CRDW. For this flow regime at K_s=1.1, the reduced mechanism predicts the appearance of regime with irregular rotating detonation wave. During the rotation of detonation wave, the length of the wave front can vary. It should be noted that this numerical solution was obtained using the flow fields for the case K_s=1.5 as initial data. The obtained novel multiply repeating cyclic regime is illustrated by the temperature and pressure fields depicted in figure 3.

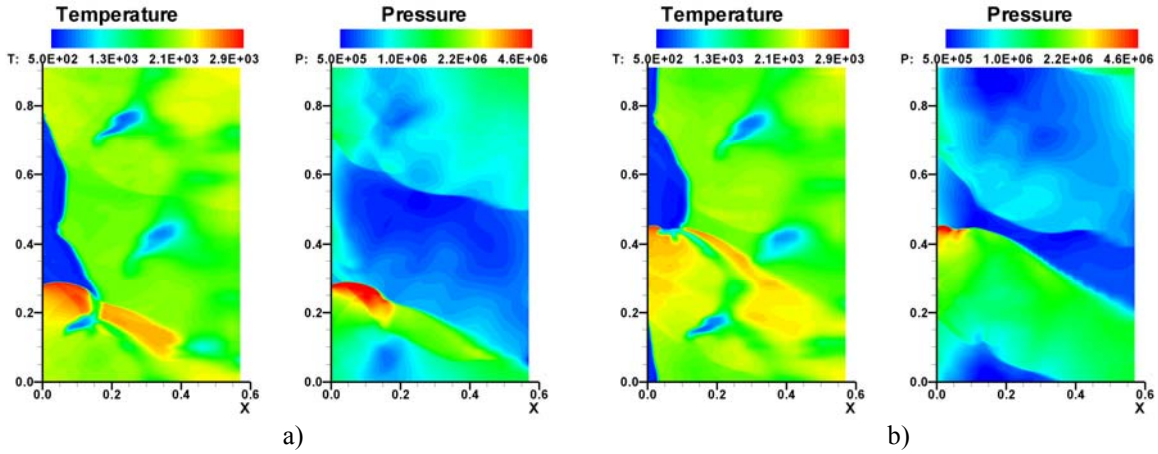


Figure 3. Temperature and pressure fields at time instances when maximal (a) and minimal (b) lengths of detonation front is achieved

At the same time, quasi-global mechanism predicts that the breakdown of detonation wave occurs at the nine turn of its evolution after starting. The temperature and pressure fields for some sequential

time instances preceding to the detonation wave breakdown computed with the use of quasi-global mechanism are shown in figure 4.

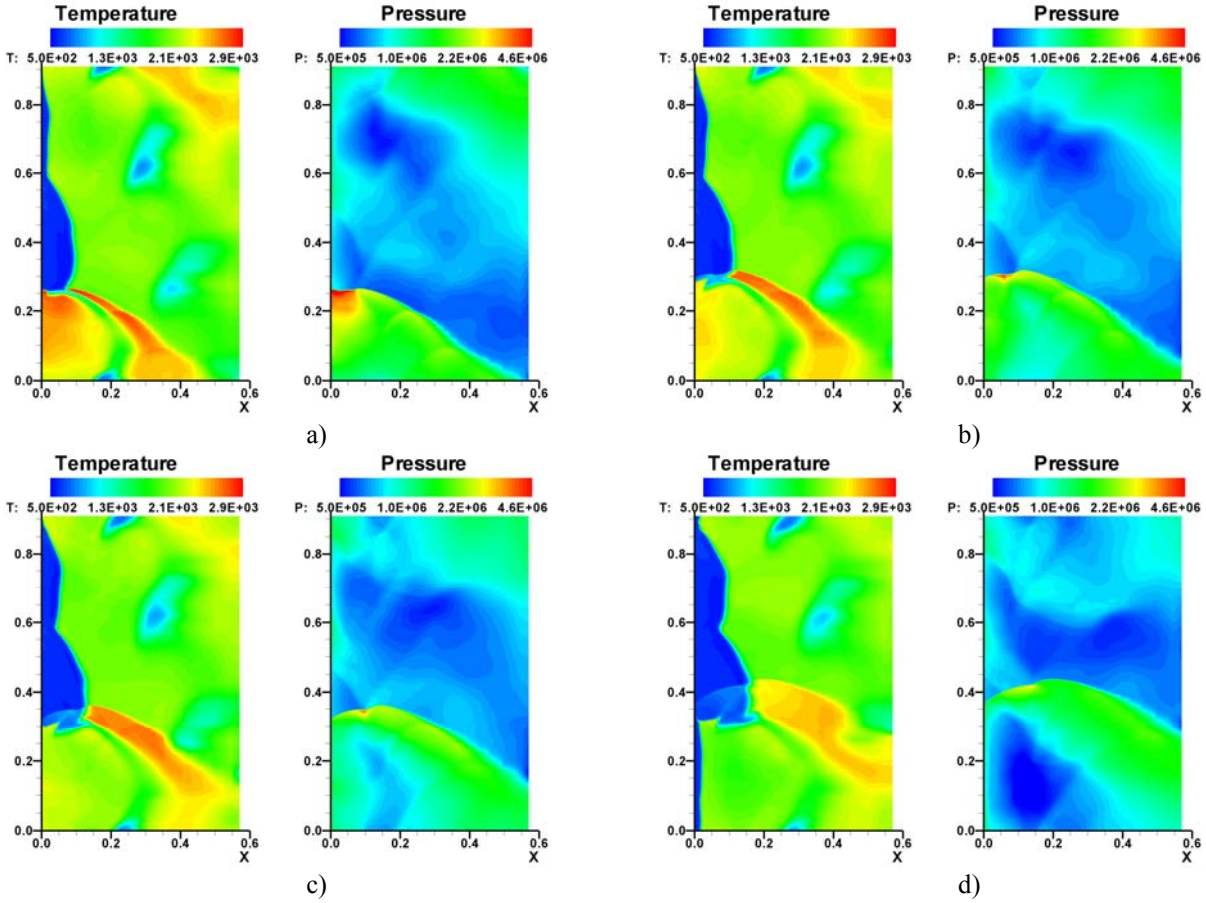


Figure 4. Temperature and pressure fields for sequential time instances (a) – (d) preceding to the breakdown of detonation front

4 Conclusion

The reduced reaction mechanism for high temperature (T>1100K) ignition and combustion of propane-air mixture has been developed. This mechanism possesses higher prediction ability compared to proposed earlier quasi-global mechanism and applied for numerical simulation of detonation combustion. The flow regimes with pulsed shock-induced and continuous rotating detonation combustion have been analyzed with the usage of reduced and quasi-global mechanisms. It was shown that the influence of the applied reaction mechanism on the predicted characteristics of detonation combustion can be essential, especially, at the stages of detonation initiation and detonation wave breakdown, where kinetic effects are the most important. To describe properly these regimes it is needed to apply the reaction mechanisms that enable to reproduce principal features of ignition and energy release during combustion with reasonable accuracy.

5 Acknowledgments

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References

[1] Frolov SM, Ivanov VS. (2010). Combined flame tracking-particle method for numerical simulation of deflagration-to-detonation transition. In: Deflagration and Detonation Combustion. Ed. G.D. Roy and S.M. Frolov. Moscow: Torus Press: 339.

[2] Basevich VYa, Frolov SM. (2006). Overall kinetic mechanisms for modeling multistage selfignition of hydrocarbons in reacting flows. Rus. J. Chem. Phys. 25(6): 54.

[3] Titova NS, Kuleshov PS, Starik AM (2011). Kinetic mechanism of propane ignition and combustion in air. Combust. Explos. Shock Waves. 47: 249.

[4] Lu T, Law CK. (2005). A directed relation graph method for mechanism reduction. Proc. Combst. Inst. 30: 1333.

[5] Burcat A, Lifshitz A, Scheller K, Skinner GB. (1971). Shock-tube investigation of ignition in propane-oxygen-argon mixtures. Proc. Combust. Inst. 13: 745.

[6] Penyazkov OG, Ragotner KA, Dean AJ, Varatharajan B. (2005). Autoignition of propane-air mixtures behind reflected shock waves. Proc. Combst. Inst. 30: 1941.

[7] Kwon S, Tseng LK, Faeth GM. (1992). Laminar burning velocities and transition to unstable flames in $H_2/O_2/N_2$ and $C_3H_8/O_2/N_2$ mixtures. Combust. Flame. 90: 230.

[8] Vagelopoulos CM, Egolfopoulos FN. (1998). Direct experimental determination of laminar flame speed. Proc. Combust. Inst. 27: 513.

[9] Sun CJ, Sung CJ, He L, Law CK. (1999). Dynamics of weakly stretched flames: Quantitative description and extraction of global flame parameters. Combust. Flame. 118: 108.

[10] Bykovskii FA, Zhdan SA. (2013). Continuous spin detonation. Novosibirsk: Siberian Branch of the Russian Academy of Sciences. 423 p.

[11] Zhdan SA, Bykovskii FA, Vedernikov EF. (2007). Mathematical modeling of a rotating detonation wave in a hydrogen-oxygen Mixture. Combust. Explos. Shock Waves. 43: 449.