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ON THE EFFECT OF PRESSURE OSCILLATIONS ON DROPLET AUTOIGNITION

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ABSTRACT

The paper discusses the possible interaction between combustion instabilities and induction times of droplets (and sprays) to autoignition. It is shown that acoustic pressure/ temperature oscillations significantly affect the induction times of n-heptane droplets. This may play an additional role in low frequency dynamics and might be the main driver of high frequency dynamics. Experiments on single droplets in an acoustic field were used to validate numerical simulations on the autoignition of large n-heptane droplets. The simulations were then extended towards technical droplet sizes and a gas turbine typical pressure range of 17 bar. It was found that the acoustic-scale changes of the pressure and temperature result in significant changes of the ignition delay. Applying numerical calculations to micro-sized droplets enabled to study the thermo-acoustic effects under conditions approximating real gas-turbines.

The findings reveal the importance of thermo-acoustic effects on ignition processes in the instability-driving mechanisms of combustion and indicate that "acoustics-ignition"- interactions must be taken into account for low-frequency as well as for high-frequency dynamics; this in addition to the flow and mixture perturbations which are well known to drive combustion instabilities in gas-turbines.

INTRODUCTION

Combustion-driven instabilities have an important influence on the performance and noise characteristics of gas turbines. Thermo-acoustic oscillations can increase not only emissions of noise or pollutants such as unburned hydrocarbons or nitric oxides, but can also lead to very high levels of pressure pulsations, resulting in structural damage of the machine. Identified mechanisms capable of driving combustion instabilities include complex flow and flame interactions: fuel feed line - acoustic coupling, equivalence-ratio oscillations, oscillatory vaporization and mixing, oscillatory flame-area variation or vortex shedding.

The design of future burners for combustion of dispersed liquid fuels is aiming for a mostly homogeneous pre-vaporization and premixing of the fuel with air prior to ignition and combustion. This to minimize the emission of nitric oxides generated to the thermal formation mechanism (Zeldovich-Mechanism). The preparation of an air/fuel-premixture ends with the ignition of the ensemble. In case the instant of ignition is altered by pressure oscillations this would lead to an altered local equivalence ratio and thus to an oscillating heat release - one prerequisite for combustion enhanced instabilities. At high pressure/ high temperature conditions as in modern gas turbines, the induction times to hot ignition are in the order of milliseconds. Therefore oscillating ignition delays are generally

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able to explain interactive dynamics in the order of 1 kHz. The effect of acoustic perturbations on droplet selfignition was theoretically predicted by Fachini and Linan [1]. It is shown there that during positive acoustic temperature periods the chemical reaction rate is increased. As a consequence the temperature increases periodically until ignition occurs. In this theoretical study acoustics were assumed to have the potential to promote ignition. The inverse effect of a phase angle dependent delay of ignition was also predicted. This introduces a new feedback mechanism to drive instabilities that cannot be found in literature. This is in addition to the well known aero-acoustic effects on combustion heat release. In order to clarify different aspects of acoustics - ignition interference it is necessary to study the simplified models. At ZARM, Bremen, the effect of acoustic oscillation on single droplet ignition was therefore studied experimentally and numerically.

NOMENCLATURE

t	time
r	radius in spherical coordinates
r_s	coordinate of liquid-gas boundary (droplet radius)
p	pressure
T	temperature
ρ	density
Z	compressibility factor
$\boldsymbol{u}$	velocity
c_{p_i}	heat capacity of specie *i*
μ_i	molecular weight of specie *i*
$\overline{\mu} = \sum \mu_i X_i$	molecular weight of mixture
X_i	mole fraction of specie *i*
Y_i	mass fraction of specie *i*
λ	thermal conductivity
h_i	specific enthalpy of specie *i*
$\overline{h} = \sum h_i Y_i$	enthalpy of mixture
$\dot{w}_i$	rate of production of specie *i* by chemical reactions (mass per volume per time)
A_k, n_k, E_k	coefficients of production-rate of *k*-reaction
$\nu'_{i,k}, \nu''_{i,k}$	stoichiometric coefficients of specie *i* by chemical reaction *k* as an educt and as a product
$\boldsymbol{u}_{Di}$	diffusion velocity of specie *i*
f	fugacity
ϕ	fugacity coefficient
ΔH_v	enthalpy of vaporization
R^0	universal gas constant
$R_i = \frac{R^0}{\mu_i}$	gas constant of specie *i*
φ	fuel-air ratio of mixture
m	mass

EXPERIMENTAL FACILITY

The experiments were carried out in the Bremen drop tower in a microgravity environment during 4.74 seconds of free fall of the experiment in a vacuum chamber of 110 m height. This was to ensure mostly spherical conditions with no drop-off of cold dense fuel vapor or buoyancy acting to hot precursor reaction gases (absence of natural convection). The experimental facility allows the investigation of the ignition of a large single droplet under variable pressure and temperature conditions of the ambient gas. The suspended fuel droplet with initial diameter of 0.7 mm is placed in a furnace, two opposite walls of which are motor-driven pistons. The scale of the oscillation of gas parameters in the furnace corresponds to that in real gas-turbines under condition of a thermo-acoustic resonance. In the present work parameters of the ignition of a single n-heptane droplet under mean pressure (p_0) up to 5 bar and temperature 700 K was examined at sound level up to 180 dB.

Fig. 1 shows the outer appearance of the experimental set-up installed within the pressure tight drop capsule (dismantled).

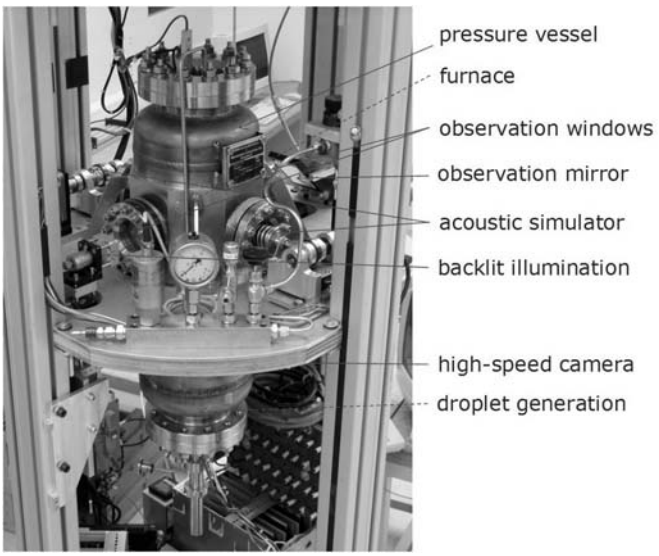

Figure 1. EXPERIMENTAL SETUP MOUNTED IN A DROP TOWER TEST RIG

Fig. 2 depicts schematically the experiment core and its principle of operation. After release of the drop vehicle from 110 m elevation, the prepared suspended droplet is rapidly

lifted into the furnace. The lifting device also closes the furnace at its arrival position. Then the pistons are activated in counteracting motion. This simulates the situation of a droplet in the pressure anti-node of a standing sound wave field.

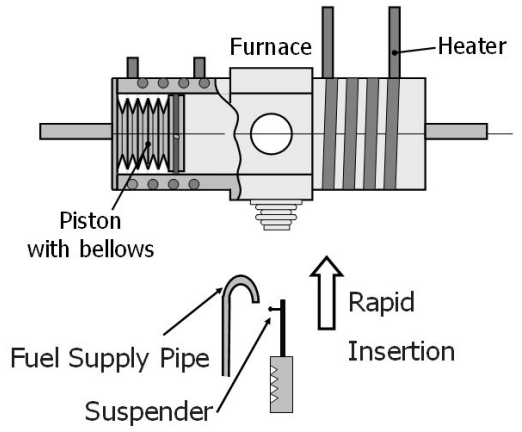

Figure 2. SCHEMATIC OF THE EXPERIMENT CORE AND THE EXPERIMENT PROCEDURE

NUMERICAL MODEL

The computational model is 1-dimensional and is subjected to the following assumptions: low velocities of the gas - no pressure gradient; Temperature gradient is sufficiently small – no thermal diffusion; no radiative heat transfer; no invasion of the gas into the liquid phase; no chemical reactions in the droplet; the surface tension is neglected as it influence is assumed to be minor for higher pressures.

A complex reduced reaction mechanism for n-heptane with 62 steps (437 elementary reactions, 92 species in total, 25 steady-state species) was included in the numerical simulations. This reaction model was developed by the Institut für Technische Mechanik at RWTH Aachen within the "Development and Research Program on Pollutant-Reduced COmbustion Systems". In the chemical kinetics, special attention was paid to the low-temperature reaction branch and the balance between low- and high-temperature reactions. Details can be found in [2]. The reaction mechanism was optimized and validated by comparison with numerous experimental studies on droplet ignition in quiescent ambience throughout the recent years [2-8]. For this study the model was enhanced by the introduction of a movable oscillating outer boundary.

The following set of equations is applied and solved:

Liquid phase:

equation of state $$p = \rho Z \frac{R^0}{\mu} T \qquad (1)$$

mass conservation $$\frac{\partial \rho}{\partial t} + div(\rho \cdot \boldsymbol{u}) = 0 \qquad (2)$$

energy conservation

$$\rho c_p \left(\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T \right) = div(\lambda \nabla T) + \frac{\partial p}{\partial t} \qquad (3)$$

Gas phase:

equation of state $$p = \rho \frac{R^0}{\bar{\mu}} T \;;\quad \bar{\mu} = \sum \mu_i X_i \qquad (4)$$

mass conservation $$\frac{\partial \rho}{\partial t} + div(\rho \cdot \boldsymbol{u}) = 0 \qquad (5)$$

components conservation

$$\rho \frac{\partial Y_i}{\partial t} + \rho \boldsymbol{u} \cdot \nabla Y_i + div(\rho Y_i \cdot \boldsymbol{u}_{Di}) = \dot{w}_i \qquad (6)$$

energy conservation

$$\rho \sum c_{pi} Y_i \left[\frac{\partial T}{\partial t} + u \cdot \nabla T \right] - \frac{\partial p}{\partial t} + \sum h_i \dot{w}_i + div(-\lambda \nabla T) + \\ + \rho \sum c_{pi} Y_i u_{Di} \cdot \nabla T = 0 \qquad (7)$$

Maxwell-Stefan model for multi-component diffusion

$$\nabla X_i = \sum_{j \neq i} \frac{X_i X_j}{D_{ij}} \left(\boldsymbol{u}_{Dj} - \boldsymbol{u}_{Di} \right) \qquad (8)$$

chemical reactions – concentration rate

$$\dot{w}_i = \mu_i \sum_{k_{reaction}} \left(\nu''_{i,k} - \nu'_{i,k} \right) A_k T^{n_k} e^{-\frac{E_k}{R^0 T}} \prod_{j_{species}} \left(\frac{X_j p}{R^0 T} \right)^{\nu'_{j,k}} \qquad (9)$$

Boundary conditions

Center of the droplet – point of symmetry ($r = 0$)

no heat flux $$\left. \frac{\partial T}{\partial r} \right|_{r=0} = 0 \qquad (10)$$

no mass flux $$\boldsymbol{u}|_{r=0} = 0 \qquad (11)$$

Liquid-gas phase boundary ($r = r_s(t)$)

temperature equilibrium $$T_l \big|_{r=r_{s-}} = T_g \big|_{r=r_{s+}} \qquad (12)$$

fugacity equilibrium

$$f_i^l \big|_{r=r_{s-}} = f_i^g \big|_{r=r_{s+}} .., \; f_i = X_i \cdot \phi_i \cdot p \qquad (13)$$

mass conservation

$$\rho_l \left(u_l - \dot{r}_s \right) \big|_{r=r_{s-}} = \rho_g \left(u_g - \dot{r}_s \right) \big|_{r=r_{s+}} = \dot{m} \qquad (14)$$

components conservation

$$Y_i^l \cdot \dot{m}\Big|_{r=r_{s-}} = Y_i\left(\dot{m} + \rho_g \cdot \boldsymbol{u}_{Di}\right)\Big|_{r=r_{s+}} \quad , \quad Y_i^l = \delta_{i,\,fuel} \qquad (15)$$

energy conservation

$$-\lambda_l \cdot \nabla T_l\Big|_{r=r_{s-}} + \dot{m} \cdot \Delta H_v = -\lambda_g \cdot \nabla T_g\Big|_{r=r_{s+}} \qquad (16)$$

Outer boundary ($r = r_{max}(t)$) (Acoustics only - no changes of fuel-air ratio)

pressure continuity $$p = p_{out}(t) \qquad (17)$$

no heat flux $$\left.\frac{\partial T}{\partial r}\right|_{r=r_{\max}} = 0 \qquad (18)$$

no mass flux $$\mathbf{u}\big|_{r=r_{\max}} = \dot{r}_{\max} \qquad (19)$$

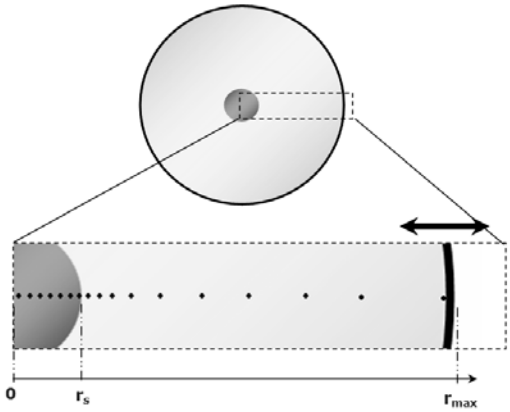

Figure 3. SCHEMATIC OF THE NUMERICAL GRID AND THE BOUNDARIES

RESULTS AND DISCUSSION

Fig. 4 shows the comparison between experimental and numerical results on the induction time to hot ignition of single n-heptane droplets of initial diameter of 0.7 mm, an ambient temperature of 700 K, at mean pressure of 3, 4 and 5 bar and under the influence of an acoustic pressure change in the range of 100 mbar. The lower section of the diagram shows the temporal evolution of the highest temperature occurring somewhere around the droplet. The curves stand for the numerical results while the symbols represent the experimental results of the moment of hot ignition. It can be seen, that the induction time is shortest at 5 bar and longest at 3 bar and that in all cases an exothermal cool flame ignition precedes the hot ignition.

The full lines and the points stand for results in quiescent ambience with no acoustic perturbation while the dotted lines and triangles represent the acoustically perturbed ignition. The upper section of the diagram depicts the type of acoustic perturbation. For these experiments it was assumed, that the effect of acoustics on ignition is largest if the frequency is just the inverse of the unperturbed induction time. Therefore the frequency was chosen to reach the maximum or minimum acoustic pressure at the moment of expected ignition of the unperturbed case. The figure shows that a comparably small pressure rise of 100 mbar shortens the induction time and a pressure drop of the same magnitude prolongs the induction time. However, experimental and numerical results are in satisfying agreement.

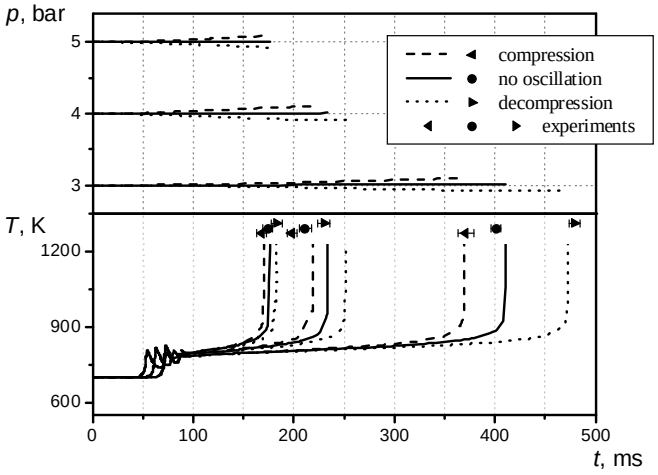

Figure 4. COMPARISON OF EXPERIMENTAL AND NUMERICAL RESULTS ON THE IGNITION OF SINGLE N-HEPTANE DROPLETS (d_{ini} = 0.7 mm) UNDER SPHERICAL CONDITIONS

As pressure is not a factor in the chemical mechanisms the effect of acoustics can only be attributed to the corresponding temperature changes. Therefore the simulations were then conducted within the pressure range of stationary gas turbines and these led to results as shown in Fig. 5. Here the initial droplet diameter is reduced to 100 µm. The ambient pressure and temperature are set to 17 bar and 750 K respectively. The overall fuel/ air-ratio, represented through the relation between the initial radius of the droplet and the radius of the calculation domain is set to ϕ = 0.5 and is thus lean. The acoustic pressure changes are now of approx. 0.65 bar corresponding to approx. 180 dB of effective sound pressure. The frequency is set to 500 Hz. This was done to test the effect of high frequencies on the ignition and it is evident how the initial phase affects the total induction time.

The full line indicates the unperturbed induction time. The figure shows, that the total induction time is shortened by approx. 5 % when the induction time ends during a compressive period while it is prolonged into the next compressive period if the pressure (and thus temperature) is

lowered at the moment when ignition would happen under unperturbed conditions.

As amplitude and frequency remain unchanged this gives rise to the assumption that in case of higher frequencies the last period prior to ignition is by far more important than the periods before. In order to verify this, four different cases were compared. Fig. 6 shows the effect of a continuous oscillation compared to an oscillation that stops prior to the last period and compared to an oscillation that only performs the last period. All of them are related to the unperturbed droplet ignition. The initial and ambient conditions remain unchanged.

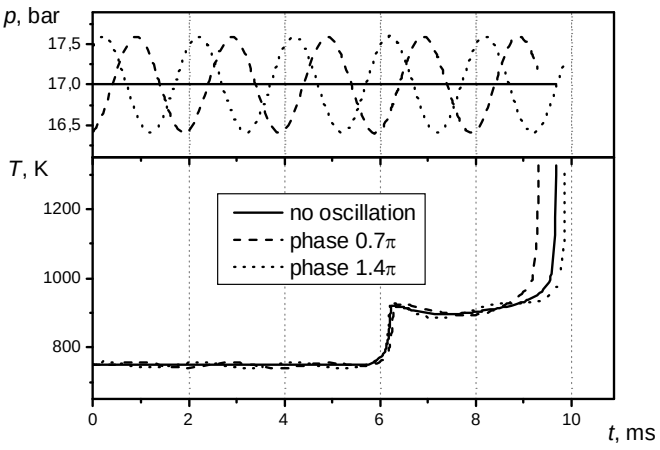

Figure 5. EFFECT OF INITIAL PHASE ON THE INDUCTION TIME OF A 100 µm DROPLET AT 17 bar AND SOUND PRESSURE OF 180 dB

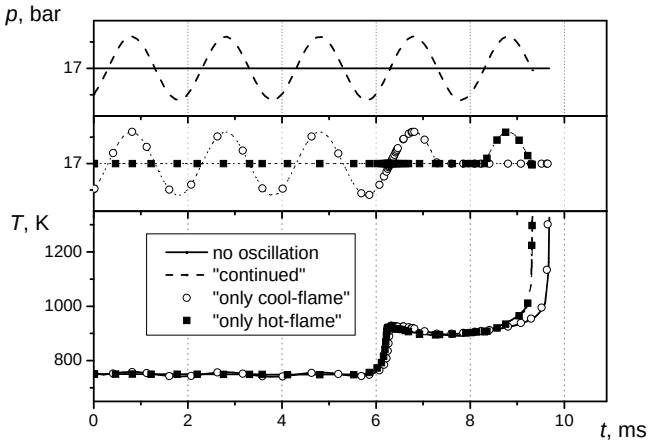

Figure 6. NUMERICAL EXPERIMENT REVEALING THE IMPORTANCE OF AN ACOUSTIC PERTURBATION AT OR AROUND THE MOMENT OF IGNITION

It can be seen that the total induction time is almost identical for a continuous oscillation (dashed lined) and the case where the droplet is subjected to only the last compression period. And as expected an oscillation that stops before the last compression period affects the total induction time only slightly and results in an induction time that is comparable to quiescent conditions. The legend´s text also indicates that the latter case with small influence is an acoustic perturbation acting to the cool-flame only while the very effective single pulse near the end of the induction time affects the hot-flame only.

To what extent the phase angle affects the induction time of an n-heptane droplet under these conditions is shown in Fig. 7.

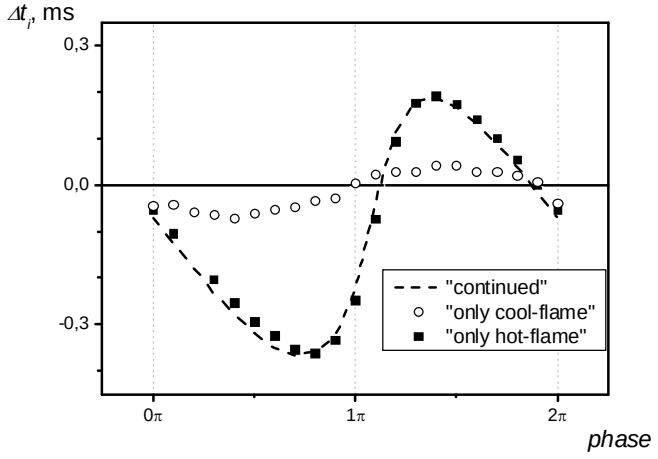

Figure 7. EFFECT OF INITIAL PHASE ANGLE ON THE TOTAL INDUCTION TIME

The shortening effect through compression under these conditions is almost twice as large at maximum as the delaying effect of a decompression. The effect of an oscillation that only happens during the cool-flame period and stops prior to ignition affects the total induction time by only 20% compared to the effect of the acoustic pulse near the end of the induction time or the continuous oscillation.

Fig. 8 displays the effect of the acoustic pressure on the total induction time. For the same conditions as before, the curves show the effect of a continuous wave or a hot-flame pulse respectively. An acoustic pressure of $\Delta p = 0.12$ bar complies with 160 dB and $\Delta p = 0.65$ bar stands for approx. 180 dB. It can be seen that the larger the acoustic pressure becomes the larger is the potential shortening of induction time while the potential prolongation at the related phase angle is much less dependent on acoustic pressure.

For 180 dB ($\Delta p = 0.65$ bar) Figure 9 shows the relation of a change of induction time and the phase angle for different frequencies. This again validates the initial assumption of the effect being strongest for frequencies near the inverse of the induction time. The phase angle of the compression phase close to ignition is most significant, as the moment of ignition

follows the phase shift of the rising edge (last quarter period) until it is too soon for ignition to occur. Under these circumstances ignition jumps to the next rising edge and becomes delayed compared to the unperturbed case. Therefore a frequency in the range of the inverse of the unperturbed induction time has the largest potential to promote “Induction Induced Instabilities”.

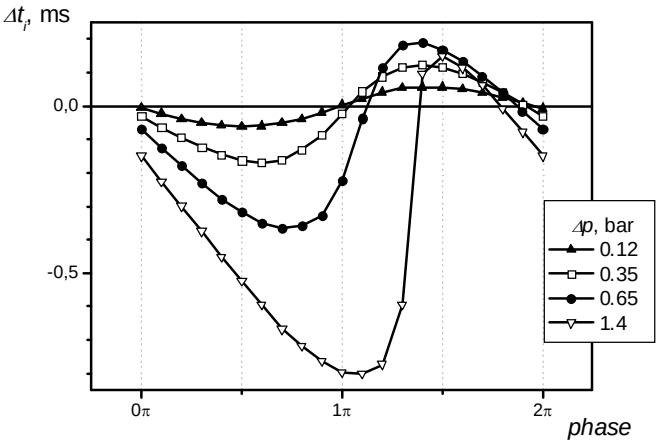

Figure 8. DEPENDENCY OF CHANGE OF INDUCTION TIME FROM PHASE ANGLE AND SOUND PRESSURE

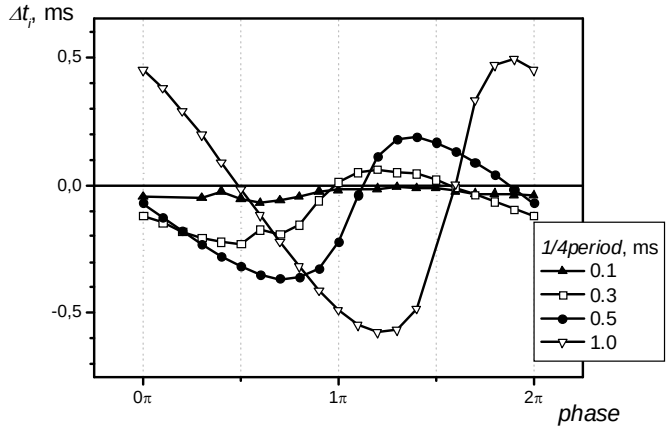

Figure 9. DEPENDENCY OF CHANGE OF INDUCTION TIME FROM PHASE ANGLE AND FREQUENCY

CONCLUSION

The experiments as well as the simulation results give rise to the assumption that acoustics can significantly affect the induction time of droplets and sprays. As an acoustic wave induced compression close to the moment of autoignition affects the induction time far more than the periods before, the induction time may be affected by any occurring instability. Therefore low frequency dynamics, known to be an interaction between combustion and a resonance of the confinement may also be affected by changes of induction time. High frequency dynamics in contrast may mainly be explained by an interaction between a confinement eigen-frequency and induction time. As a premixed burner (partially - or fully premixed) operating with liquid fuels is sensitive to alterations in induction time, the effect of acoustics might be the difference between a stable flame in the combustion chamber and a flashback into a premixing region. This all the more as the induction time of an only partially prevaporized system is shorter than that of a single phased gaseous system. The results however justify this assumption and show an urgent need for further experimental and numerical investigations.

ACKNOWLEDGMENTS

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