

# Ignition of explosive atmospheres by small hot particles : Comparison of experiments and simulations

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## Abstract

Small hot surfaces can ignite explosive atmospheres in dependence on their temperature and their dimensions. Heating of small particles leading to ignition can be originated by several potential ignition sources like optical radiation, ultrasound or mechanical friction and grinding. The objective of this work is to investigate the ignition capability of single inert particles in dependence on their temperature and dimensions. This is done by a combination of measurements and numerical simulations to ensure valid limit values for the particle temperature. Artificially produced particles of 0.5 mm to 1.3 mm diameter are placed in different explosive atmospheres of hydrogen or different hydrocarbons in air. The inert particles are heated continuously by IR laser light with a specific power. The time–resolved temperature of the particle is measured by two–wavelength pyrometry. The temperatures at which ignition occurs are evaluated with respect to the particle diameter and the mixture composition. The experimental results are compared with numerical simulations using detailed reaction mechanisms. Solving the well–known mass, species and energy equations for spherically symmetrical one–dimensional flames using a time–integration method, ignition temperatures have been determined for selected diameters and mixture compositions.

**Keywords** : ignition source, hot surface, mechanical spark.

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## 1. Introduction

Small hot surfaces can ignite explosive atmospheres in dependence on their temperature and their dimensions. Heating of small particles leading to ignition can be originated by several potential ignition sources like optical radiation, ultrasound or mechanical friction and grinding. Optical radiation and ultrasound heat particles via absorption. Mechanical ignition sources occur when solid surfaces either impinge briefly or rub each other over a longer period of time. Impact, friction and grinding can produce mechanical sparks and hot spots capable of igniting explosive atmospheres.

Mechanical sparks are burning metal particles. Therefore, they are considered as ignition sources due to their high burning temperature compared with the temperature at the contact surface. The relative velocity of the friction partners affects the capability for igniting

the mixture. On the one hand, increasing the velocity increases the temperature of the contact surface, increasing the ignition probability. On the other hand, increasing the velocity leads to increasing turbulence, decreasing the ignition probability. Before the particles start to burn, e.g. during grinding, a lot of particles are separated which do not burn but have a temperature above the auto ignition temperature of the mixture. Thus, which temperature inert particles, i.e. non–burning particles, need to ignite an explosive mixture, is of interest.

The objective of this work is to investigate the ignition capability of single inert particles in dependence on their temperature and dimensions. This is done by a combination of measurements and numerical simulations. Neither of them can be considered as valid standing alone due to uncertainty and statistical influences on the ignition process in the case of measurements and due to necessary

simplifications in the case of numerical simulations. Examining both issues together may allow us to determine the limit values for the particle temperature and may contribute to learning more about the ignition behaviour of small hot surfaces.

The experimental approach used is known from investigations into the ignition capability of optical radiation by Bothe *et al.*<sup>1)</sup> and Welzel *et al.*<sup>2)</sup>. Meanwhile a particle temperature measurement is now possible using a two-wavelength pyrometer. This approach was also used for investigations of mechanical sparks in explosive atmospheres by Proust *et al.*<sup>3)</sup>. Numerical simulations of the ignition process follow the approach described by Maas and Warnatz<sup>4)</sup> using detailed chemistry.

## 2. Experimental

The main part of the experimental set-up is a pressure-relieved glass cylinder (ignition chamber) of 50 cm in height and 15 cm in diameter. A metal ring in the middle of the ignition chamber provides adequate access via windows and openings (Fig. 1).

An artificial particle is fixed with a thin wire on the tip of a lance and is placed in the centre of the ignition chamber. In the case of an explosive gas mixture, two gas flows were continuously mixed. The mixture composition was monitored by an oxygen analyser (Oxymat, Siemens). A vapour/air mixture can be produced by vaporising the combustible liquid into a continuous stream of air. The air flow is controlled by a calibrated flow control unit and the liquid flow by a calibrated dosing pump. Fuel and air were mixed in a heated evaporator coil.

The experiments were carried out in a quiescent gas mixture at ambient pressure and at a temperature of  $325 \text{ K} \pm 2 \text{ K}$  in order to be at the upper limit of the ambient temperature range of explosive atmospheres. Experiments were done with hydrogen, propane, ethylene and pentane (safety characteristic data<sup>5)</sup> see Table 1). The particles were irradiated on opposite sides with defined power for a duration of 20 seconds in each experiment. The particle temperature was measured with a two-wavelength pyrometer (WÜK or SensorTherm, Metis MQ

22). The particle diameter was detected with a CCD camera (Panasonic, WV-BP310 Chip with Canon FD 135 lens) against the background illumination. The measurement was calibrated with reference spheres of a known size. Ignition is recognised by a temperature edge at a  $25 \mu\text{m}$  NiCr/Ni thermocouple above the particle. All data were recorded either directly or via a recording system and processed in a PC.

The particles consist of an absorber material most effective for the used radiation wavelength<sup>2)</sup>. They were manufactured from a suspension of iron oxide black, ceramic glue, ethanol and distilled water. The coating is brought onto a tungsten wire step-by-step in thin layers under a microscope. After each step the particles are dried carefully by hot air until alcohol and water are evaporated completely. Residues of these substances lead to the rapid destruction of the particle during the heating procedure. Tungsten wire is chosen as an incombustible base material because of its high melting temperature and its mechanical stability at high temperatures. This allows us to use a  $25 \mu\text{m}$  wire minimising heat loss via the fixation.

For heating, a cw Nd:YAG laser (Chromatron Laser Systems, Berlin) with an emission wavelength of 1064 nm is used. The maximum output power is 10 W. The working range is 50–2000 mW. The laser beam is split into two parts (5% and 95%, Fig. 1). The weaker part impinges on the reference power meter with an angle of  $90^\circ$  measuring the total power of the laser. The optical main path leads to the optical bench enclosing the ignition chamber. Here, the laser beam is split into two equal parts in order to irradiate the particle on both sides. Therefore, the second part of the beam is guided around the ignition chamber. The two beams were led via 100% mirrors onto the power meters to measure the power difference between the inlet and the outlet representing the power absorbed by the particle. The angle between the inlet and the outlet beam is approx.  $5^\circ$ . Applying the laser beam to the particle causes a nearly constant temperature rise at the particle and leads to a steady state after approx. 2.5 s depending on the laser power and the particle diameter.

Figure 2 shows the optimal irradiation of the particle. The pyrometer and the laser beam were well adjusted and mechanically fixed in their positions. A rough adjustment of the particles can be done via the CCD camera. Subsequently, they have to be adjusted with a manual adjustment device individually in all three spatial axes (see Fig. 1). This is achieved, firstly, when the particle is in the focus of the pyrometer leading to maximum temperature under steady state conditions. As a second criterion, the power measured shows a minimum when the particle absorbs the maximum of both parts of the laser beam. After an ignition has occurred, readjustment of the particle is necessary because of its fixation by a very thin wire and its movement during the explosion.

The temporal resolution of the pyrometer ( $1 \mu\text{s}$ ) does not significantly influence the measurement uncertainty. In case of the correct placement of the particle, the temperature measured by the pyrometer can be

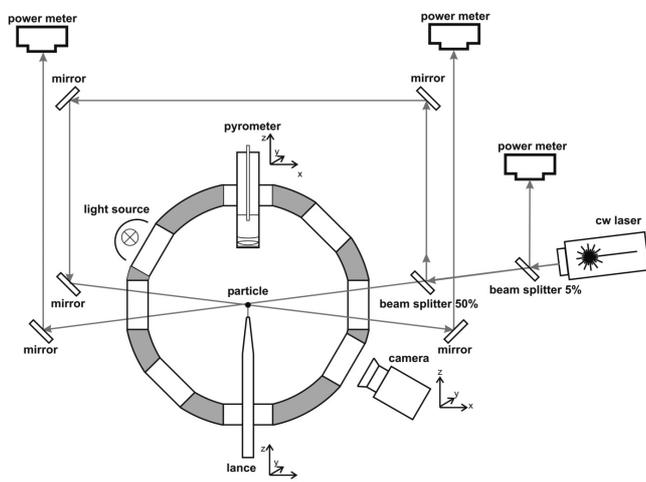
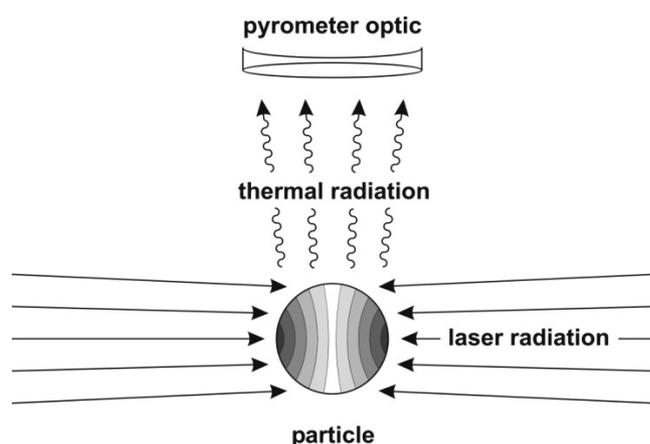


Fig. 1 Experimental set-up with laser beam paths, particle lance and instrumentation (dimensions and angles are not to scale).

**Table 1** Safety characteristic data of the combustibles<sup>5)</sup>.

Safety characteristics		Hydrogen	Ethylene	Propane	n-Pentane
Ignition temperature AIT	[°C]	560	440	470	265
Minimum ignition energy MIE	[mJ]	0.017	0.082	0.24	0.28
Maximum experimental safe gap MESG	[mm]	0.29	0.65	0.92	0.93
Lower explosion limit LEL	[%]	4.0	2.4	1.7	1.4
Upper explosion limit UEL	[%]	77.0	32.6	10.9	7.8
Stoichiometric composition	[%]	29.5	6.5	4.0	2.6

**Fig. 2** Adjustment of the particles for heating and temperature measurement.

interpreted as the average surface temperature of the particle. The measurement uncertainty is well within  $\pm 5\%$  of the measured value including small deviations from optimal adjustment, deviations from spherical shape and the measurement uncertainty of the pyrometer itself considering the particle material. This uncertainty is represented by the error bars in the following figures in order to demonstrate significant differences between the measured temperatures. But, as shown in Fig. 2, the particle temperature distribution on the particle surface is not constant. How the measured average particle surface temperature is related to the relevant ignition temperature for different mixtures will be discussed later.

The mixture composition is measured at the outlet of the ignition chamber after due flow time and is within  $\pm 0.3$  vol.-% of the given values. The particle diameter measurement is calibrated with an ideal steel sphere and is within  $\pm 2\mu\text{m}$ . The particles are handmade and, thus, it is not possible to prepare particles of the intended size and spherical shape. The particles were used for experiments when their diameter deviation in the object plane of the camera was within  $\pm 6\%$  of the intended value. When this criterion is met, the particle is considered as spherical. According to increasing practical experience the effective dimensions of most of the particles used are much closer to the nominal values (Table 2).

### 3. Simulation

The ignition process at a hot particle and the subsequent flame propagation were represented by means of a one-dimensional numerical model. A spherical

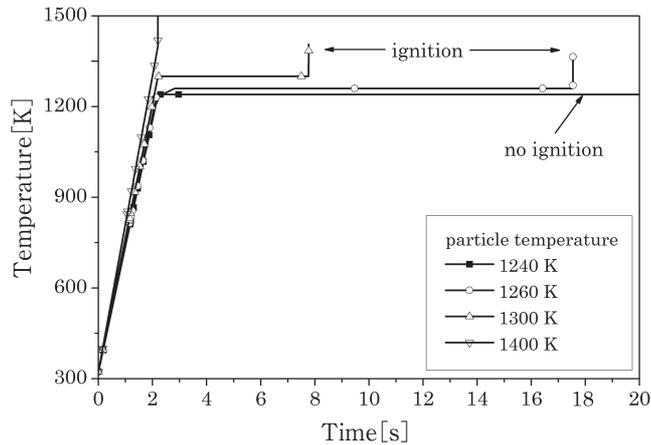
**Table 2** Diameters of the particles used for the data presented here.

Nominal particle diameter	Diameter tolerance	Particles used	
		min.	max.
1300 [ $\mu\text{m}$ ]	1222 1378	1292	1314
1000 [ $\mu\text{m}$ ]	940 1060	958	1056
750 [ $\mu\text{m}$ ]	705 795	712	772
500 [ $\mu\text{m}$ ]	470 530	485	518

geometry of a closed vessel with an outer radius of 40 mm was applied. The conservation equations for total mass, momentum, species mass and energy were solved to examine the autoignition process and the flame propagation numerically as described by Maas and Warnatz<sup>4)</sup>. Furthermore, a detailed multi-species transport model was used to solve the conservation equations. The ideal gas law was applied to relate the state functions of pressure, temperature, and volume.

Calculations were done for different combustible gases in air with varying mixture compositions. Therefore, detailed reaction mechanisms were used consisting of 9 chemical species and 37 elementary reactions for hydrogen/air by Maas and Warnatz<sup>4)</sup>, 34 species and 295 reactions for ethylene/air and propane/air by Chevalier<sup>6)</sup>, and 138 species and 883 reactions for pentane/air. This specific reaction mechanism also includes a detailed description of low temperature oxidation.

In the numerical simulations, a particle of variable diameter was placed in the centre of the vessel. Within 2.5s it was heated to a given maximum particle temperature. An additional temperature rise of 100K inside the gas phase within 100s was considered as an ignition. The maximum particle temperature is varied in steps of 20K until ignition is obtained. Therefore, the particle temperature in the case of no ignition is in general 20K below the particle temperatures for ignition. As can be seen in Fig. 3, a particle with a diameter of 1000 $\mu\text{m}$  and a maximum temperature of 1240K cannot ignite a 4.0 vol.-% pentane in air mixture. However, the same particle with a temperature of 1260K leads to ignition after approx. 17s. Increasing the maximum particle temperature to 1300K decreases the time until ignition occurs. If a maximum particle temperature of 1400K is chosen (Fig. 3), the examined gas mixture ignites even before the maximum



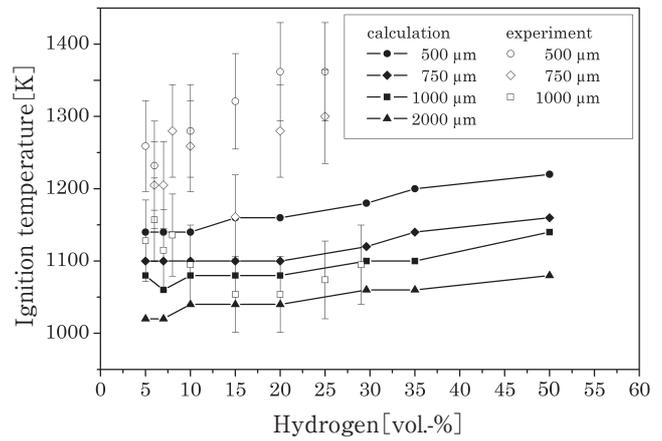
**Fig. 3** Simulation of the temporal evolution of the maximum gas phase temperature using different particle temperatures (4.0 vol.-% pentane, particle diameter  $1000\ \mu\text{m}$ ).

particle temperature has been reached.

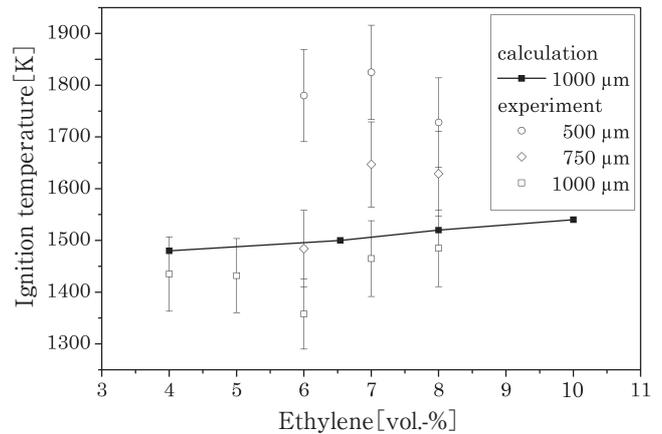
#### 4. Results

The ignition temperature is the minimum evaluated from several experiments or heating curve records at the time when ignition is recognised. This value is related to a specific mixture composition and a nominal particle diameter. The maximum temperature in the case of no ignition (steady state temperature of the heating curve) is about 100 K, sometimes 150 K above the ignition temperature under the same conditions due to the statistical influences of the ignition process. Such a difference between the lowest temperature for ignition and the highest temperature for non-ignition demonstrates that the ignition temperature which has been found is sufficiently close to the limit. The numerical results cannot show this difference because of the systematic approach and, therefore, the missing statistical influences. As stated above, the lowest numerically determined temperature for ignition is just above the highest temperature for non-ignition considering the temperature steps.

Welzel *et al.*<sup>2)</sup> have reported that the critical conditions for the ignition of hydrogen atmospheres by inert absorbers were near the lower explosion limit (Table 1). Consequently, experiments and calculations for hydrogen were carried out for a wide range of mixture compositions with emphasis near LEL using particles with diameters of  $500\ \mu\text{m}$ ,  $750\ \mu\text{m}$  and  $1000\ \mu\text{m}$  (Fig. 4). Measurements and numerical simulations are in good agreement for  $1000\ \mu\text{m}$  particles considering the measurement uncertainty. The lowest ignition temperature measured is 1054 K at a hydrogen concentration of 15 vol.-%. The lowest ignition temperature obtained by calculation is 1060 K at 7 vol.-%. The highest temperature without ignition measured at 15 vol.-% was 1157 K (not shown in Fig. 4). The calculations show a slight increase of the ignition temperature with hydrogen concentration and a considerable increase with decreasing particle diameter. The experimental results also show an increase with particle diameter, but, this is considerably stronger compared to the calculation results.



**Fig. 4** Ignition of hydrogen/air atmosphere by particles of different diameters.



**Fig. 5** Ignition of ethylene/air atmosphere by particles of different diameters.

The increase of the ignition temperature with hydrogen content is so small that a clear tendency of the measured values cannot be expected, i.e., the results are not in contradiction to the results of Welzel *et al.*<sup>2)</sup>

Figure 5 illustrates the results for ethylene. Experiments were carried out with particle diameters of  $500\ \mu\text{m}$ ,  $750\ \mu\text{m}$  and  $1000\ \mu\text{m}$ ; calculations only for  $1000\ \mu\text{m}$  with mixture compositions around the stoichiometric composition. As in the hydrogen measurements, the numerical simulations agree quite well for  $1000\ \mu\text{m}$  particles. The lowest ignition temperature measured is 1358 K at a concentration of 6.0 vol.-% which is about 300 K above that for hydrogen. The lowest ignition temperature obtained by calculation is 1480 K at 4.0 vol.-%. The highest temperature without ignition measured at 4.0 vol.-% was 1485 K (not shown in Fig. 5). Again, the calculations result in a minor increase of the ignition temperature with ethylene concentration. The experimental results show a dependence on the particle diameter similar to that of hydrogen (Fig. 3).

Numerical simulations for propane/air mixtures were performed for a set of particle diameters and with mixture compositions in the region of the stoichiometric composition (Fig. 6). Initially, experiments were done with a  $1000\ \mu\text{m}$  particle diameter. Again, measurement results and numerical results show acceptable agreement. The lowest ignition temperature measured is 1555 K with 3.4

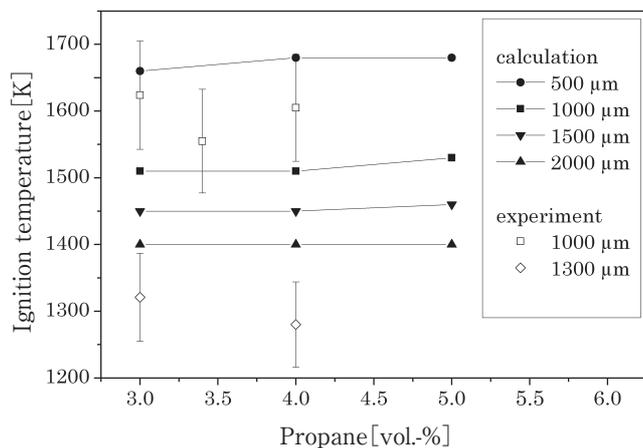


Fig. 6 Ignition of propane/air atmosphere by particles of different diameters.

vol.-% propane. The lowest ignition temperature obtained by calculation is 1510 K at 3.0 and 4.0 vol.-%. The highest temperature without ignition was 1703 K measured for 3.0 vol.-% mixture (not shown in Fig. 6). The calculations show no significant increase of the ignition temperature with concentration, but, once again a major increase with particle diameter. The numerical results concerning ignition temperature in dependence on particle diameter are in consistency with the results for hydrogen and ethylene (Figs. 4, 5).

It was difficult to apply temperatures of 1600 K and more to the particles because they are not able to withstand such high temperatures. They turned oval or melted, and craters were formed on the surface. Due to the fact that smaller particles require higher temperatures for ignition, an adequate number of successful experiments with smaller particles was not achievable. Hence, additional investigations for propane/air mixtures were performed with 1300  $\mu\text{m}$  particles. With the same total laser power applied, the particle temperature rises and the maximum particle temperature of a 1300  $\mu\text{m}$  particle is lower compared with a 1000  $\mu\text{m}$  one. Again, the difference of approx. 300 K between the ignition temperatures measured for 1000  $\mu\text{m}$  and 1300  $\mu\text{m}$  is much larger than the difference of approx. 60 K between the ignition temperatures calculated for 1000  $\mu\text{m}$  and 1500  $\mu\text{m}$ .

Ignition temperature of pentane/air mixtures was calculated between 2 and 5 vol.-% for 1000  $\mu\text{m}$  particles (Fig. 7). The results show an opposite dependence on the mixture composition compared to the other combustibles. This is confirmed by calculations for 2000  $\mu\text{m}$  particles. Experimental and numerical results verify again the acceptable agreement for 1000  $\mu\text{m}$  particles. The lowest ignition temperature measured is 1522 K at 2.5 vol.-%. The lowest ignition temperature obtained by calculation is 1150 K at 5.0 vol.-%. The highest temperature without ignition was 1783 K measured for 2.5 vol.-% mixture (not shown in Fig. 7).

Figure 8 shows the ignition temperature in dependence on the particle diameter for explosive hydrogen and propane atmospheres obtained from the numerical simulations. It demonstrates a significant difference

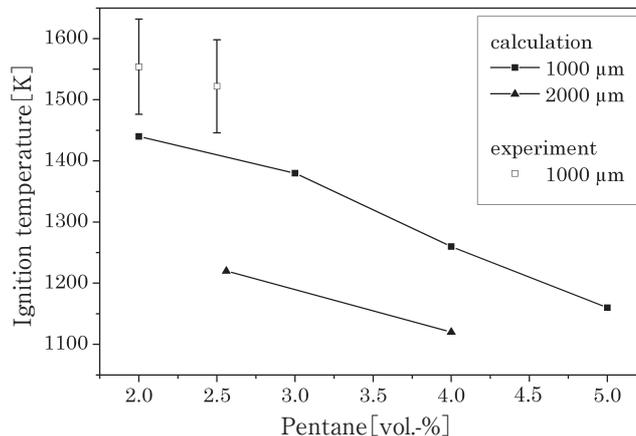


Fig. 7 Ignition of pentane/air atmosphere by particles of different diameters.

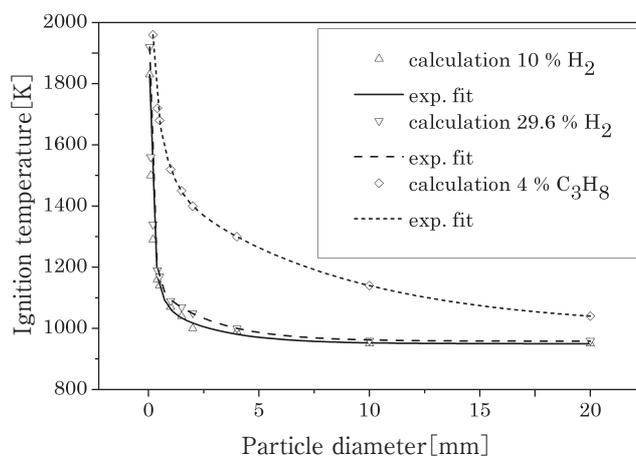


Fig. 8 Particle ignition temperature in dependence on particle diameter.

between the two combustibles whereas the influence of the mixture composition for hydrogen is relatively weak. This is in line with Fig. 4 and Fig. 6. For large particles an asymptote exists which is related to the AIT (see Table 1). It is obvious that this threshold value is higher than the AIT, because spherical particles are an inefficient heating source for the explosive atmosphere compared with the AIT experiment. For small particles the ignition temperature of propane is several hundred K higher than the particle ignition temperature of hydrogen. This difference is much larger than could be expected from the safety characteristic data (Table 1). Furthermore, Fig. 8 shows that the expression "small particle" has a different meaning for different combustibles. The difference of the ignition temperatures of hydrogen/air mixtures between 1 mm and 20 mm particles is approx. 120 K, whereas this difference is about 500 K for propane. As can be seen from Fig. 8, the asymptotic value for hydrogen has been nearly reached for particles with a 1 mm diameter while for propane it needs even more than a 20 mm diameter.

## 5. Discussion

Firstly, how the measured temperature is correlated with the relevant ignition temperature for the different mixtures is discussed. The measuring spot in the focus of the pyrometer has a diameter of 1 mm. That fits best for

the 1000  $\mu\text{m}$  particles. Therefore, for particles larger than 1 mm the temperature may be underestimated because the temperature distribution on the particles' surface differs and the hot test parts of the particle (see Fig. 2) are not inside the measuring spot. For particles smaller than 1 mm the particle temperature measured may be overestimated. Even though this error is small compared to the dependency of the ignition temperature from the particle diameter, the measuring technique has to be improved to measure a representative average particle temperature.

A particle moving upwards with the velocity of the convective flow would be the worst-case condition with respect to the ignition event as the superimposed flow due to buoyancy influences the heat transport into the gas phase. If the ignition delay time is longer than the residence time, the hot gas phase is transported away from the particle surface due to convection before ignition can take place resulting in higher temperatures necessary for ignition. Even though we cannot determine the ignition delay time in experiments, the numerical results indicate ignition delay times in the range of a few seconds (see Fig. 3). However, calculations are carried out only one-dimensionally, i.e. buoyancy effects are not taken into account by the simulation results, which can explain that the experimentally determined ignition temperatures are higher in general.

Weak dependencies such as for mixture composition cannot be evaluated from experimental results as they are overlaid by measurement uncertainties and statistical influences of the ignition itself according to different convective flows depending on temperature, different particle diameters and the temperature gradient of the particle surface temperature. Hence, the lowest ignition temperatures were measured nearly always with particle diameters above the nominal diameter; the highest temperatures without ignition in contrast with particles smaller than the nominal diameter. The surprisingly modest impact of the mixture composition is affected by thermal diffusion causing hydrogen enrichment near the surface of the particles under the different conditions<sup>7)</sup>.

The ignition temperature of small spheres is not correlated to the AIT. Larger hot surfaces cause a higher energy density in the mixture around the particle. This explains the particle diameter affecting the ignition temperature. Nevertheless, a minimum volume is required for ignition. The comparison of the particle diameter necessary for ignition with a dimension typical for the ignition limit (e.g. the quenching distance or as a substitute the MESH, see Table 1) illustrates that experimental ignition in the case of propane or pentane cannot be expected for particle diameters much smaller than 1 mm and also that the whole particle surface has to contribute to the ignition. For hydrogen, in fact, a hot spot on the surface of a 1000  $\mu\text{m}$  particle, as is caused by the laser radiation (see Fig. 2), may be sufficient to ignite the gas mixture.

The ignition temperatures for 1000  $\mu\text{m}$  particles are, even for hydrogen, above the onset temperature for

mechanical sparks (approx. 400°C for mild steel<sup>8)</sup> and approx. 650°C for stainless steel<sup>9)</sup>. Thus, it can be concluded that it is highly improbable that single non-burning particles separated during mechanical wear processes are capable of igniting explosive gas and vapour atmospheres.

## 6. Conclusion

The particle ignition temperature shows low dependence on mixture composition but is highly dependent on the combustible gas or vapour. As a result of thermal diffusion, the most ignitable mixture composition for small molecules of the burnable component is in the lean mixture near LEL; for large burnable molecules it is in the rich mixture.

The particle ignition temperature shows strong dependence on particle diameter. Particle diameters up to a few mm, i.e. smaller particles, need higher temperatures to ignite the explosive mixture.

The ignition temperatures for 1000  $\mu\text{m}$  particles are, even for hydrogen, above the onset temperature for mechanical sparks. Therefore, it is highly improbable that single non-burning particles separated during mechanical wear processes are capable of igniting explosive and vapour atmospheres.

The experimental and numerical results show good agreement for 1000  $\mu\text{m}$  particles confirming the critical temperature values determined. This may build a basis for further experimental investigations into ignition by more than one hot particle and for numerical calculations regarding several small hot particles influencing each other.

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