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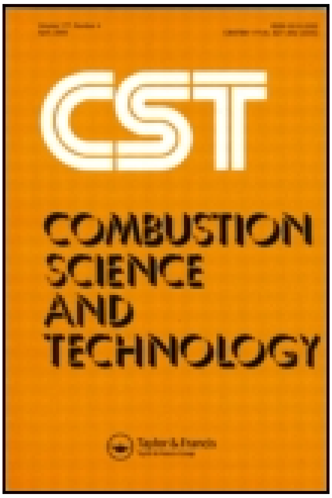

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Large-Scale Experiments and Absolute Detonability of Methane/Air Mixtures

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LARGE-SCALE EXPERIMENTS AND ABSOLUTE DETONABILITY OF METHANE/AIR MIXTURES

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The Gas Explosions Research Facility at Lake Lynn Experimental Mines was used to determine the detonability limit of methane for a 1-meter diameter tube as a function of the percent of methane in air. The measurements showed detonation limits of 5.3% (lean) and 15.6% (rich). A method for extrapolating these limits to larger systems, more relevant to coal mine tunnels, was proposed based on a simple scaling law and some empirical information on the number of cells required for a detonation to propagate in closed, open, and partially open geometries. The scaling law reproduces the measured detonation-cell sizes measured in the 1-m tube. Applying this to a tunnel the size of a coal mine produces a detonability limit less than the currently measured flammability limit for methane/air at atmospheric conditions, which raises interesting questions for detonation and combustion theory and suggests measurements in larger tubes.

Keywords: Absolute detonability; Detonation cell size; Explosion limits; Methane-air explosions; Methane detonability

INTRODUCTION

Accidental explosions in mixtures of natural gas (NG) and air can cost us greatly in human lives and property, and cause untold trauma in communities. The largest of these explosions is usually reported in the press, but there are less costly, smaller ones that are not reported or documented. Explosions occur in coal mines, where NG seeps in from walls and accumulates in sealed-off areas of tunnels. This was the source of the Sago Mine explosions in 2006. Leaks of NG were also the source of the Richmond Hill explosion in 2012, which caused massive human injury and damage. In these cases, the explosion arose because of dangerous concentrations of NG accumulating in enclosed or partially confined areas, which ignited and either directly caused or triggered events that led to a catastrophe.

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There have been many reviews and references to these types of large-scale explosions (see, for example, Bartknecht, 1961; Johnson, 2013, 2014; McMahon et al., 2007; Zipf et al. 2007), and these explicitly show the explosive dangers of NG and other fuels.

Explosions in coal mines are most dangerous when they occur in active areas of the mines, where workers might be present. These explosions can also start in sealed-off regions of coal mines that are no longer in use, and then spread to active areas. For example, in 2006, the explosion at the Sago Mine trapped 13 miners, and only one survived after the rescue two days later (MSHA, 2007). More recently, in 2010 at the Upper Big Branch Mine, an initial, relatively small explosion grew to devastating size, propagated for miles of the underground tunnel network, and killed 29 miners (MSHA, 2010).

There has been some confusion in the mining community about whether methane itself can detonate, although this does not seem to be an issue in the combustion community. In fact, the composition of NG is mostly methane, with a small percentage of higher hydrocarbons that ranges from 1−10%. The higher the percentage of higher hydrocarbons, the more easily the NG is ignited and the more easily it can detonate. In the discussion that follows, however, we focus on methane and use the terms “NG,” “methane,” and “CH_4” interchangeably.

Because of the danger of accumulating NG in the coal-mining environment, we were challenged by the Pittsburgh Research Laboratory (PRL) of the National Institute of Occupational Safety and Health (NIOSH) with this question: Given a large enough volume of a flammable mixture of NG and air, such as may exist in a coal mine, can a weak spark ignition develop into a detonation? Our task was to address this in two ways: (1) computationally, using large-scale numerical simulations of deflagrations and detonations in methane-air mixtures, and (2) experimentally, in existing and possibly new facilities.

The existing facility was the Lake Lynn Experimental Mine (LLEM) in Pennsylvania, just north of Morgantown, West Virginia. This facility, shown schematically in Figure 1, was developed from an old limestone mine and consisted of five tunnels arranged to simulate a longwall coal-mining operation. All of the tunnels measured about 6 m wide × 2 m high. Three of the tunnels were about 500 m long and connected with cross-cuts. Another

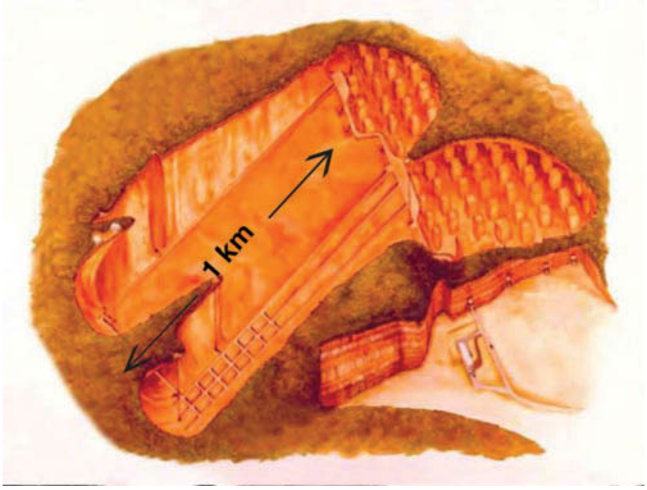

Figure 1 Schematic of Lake Lynn Experimental Mine (LLEM).

was about 500 m long with no cross-cuts, and another, which was a perpendicular tunnel at one end, was 150 m long.

In most underground coal mines, NG seeps in from the coal seam and the surrounding rock strata. When mining in a particular part of the coal mine is finished, this part may be blocked off with seals made from materials such as concrete, concrete blocks, and cement foam. If enough NG accumulates in the air, it can be ignited by any spark, as might be caused by lightning or a pile of rocks dropping. If enough NG accumulates over a long enough portion of the tunnel, a combustion wave can develop into a significant explosion.

An important part of our prior research was dedicated to deciphering mechanisms for deflagration-to-detonation transition (DDT). In particular, we were interested in learning how a small ignition site or a spark could become a turbulent flame, and if so, learning how and when a flame can transition into a detonation. The original motivation of these DDT studies was to explain astrophysical explosions, which are essentially unconfined and so do not have the shocks and shock interactions that can lead to flame acceleration and even DDT. Later, however, concerns about fuel safety expanded the studies to DDT in confined or partially confined gaseous fuels. The objective then was to combine experimental studies in collaboration with other laboratories with computations using numerical methods and computational combustion models developed at the Naval Research Laboratory (NRL). Much of the earliest work on DDT is documented or referenced in Oran and Gamezo (2007).

The more recent efforts, however, focused on DDT in tubes or channels filled with an energetic gas and containing different types of obstacles. This describes a canonical geometry used to study DDT in a combustion laboratory. Obstacles promote flame acceleration and DDT by increasing the flame surface area, generating turbulence, and reflecting shocks. The results are region in the flow where local pressures and temperatures are higher than the ambient, undisturbed material, and chemical reaction times are thus shorter and can lead to local explosions. The initial computational studies of DDT in a channel laden with obstacles were used to assess dangers of accumulating hydrogen in hydrogen refueling stations (Gamezo et al., 2007, 2008; Ogawa et al., 2013). They were also applicable to assessing the extent of dangers of accumulating hydrogen in closed areas as a result of nuclear-reactor accidents.

From these studies, we learned much about the physical mechanisms leading to flame acceleration and DDT, that is, the energy release, the onset of turbulence, the effects of shocks, and hot-spot formation. For hydrogen, however, the sizes of the experimental and computational channels were 2−10 cm high and possibly many meters long. For coal mines, the relevant system size is much larger. Chemical timescales also change somewhat, but they do not change as drastically as the size of the system. Next, we asked if the same processes were dominant in much larger channels with a less energetic fuel mixture. The flames are still relatively thin, and the activation energy is high. Thus we had to deal with an even larger multiscale problem spanning 10 orders of magnitude in spatial scales.

Our first thought (and hope) was to perform experiments inside of LLEM itself. We could isolate one of the corridors to create a channel up to 500 m long. Obstacles could consist of piles of rubble, as would be found in an actual mine. Then we would fill the channel with a known amount of NG, ensure it is mixed with ambient air, and ignite the mixture at one end. As with studies of DDT in detonation tubes, we would monitor the propagation of reaction fronts and pressure waves using light and pressure sensors. We would see detonation cells formed on the wall of the tunnel, which would be the ultimate proof that a detonation occurred.* We could even observe the explosion from "inside" by using high-speed cameras in the tunnel.

These hopes for eventually using LLEM directly were dashed in late 2008 when the group from NRL arrived one morning to tour LLEM, and there was chaos everywhere! In the very early morning before we came, one section of LLEM had collapsed. The collapse had been recorded seismically, and entry to the mine was forbidden to everyone then and subsequently closed to us permanently. It would never be cleared or pronounced safe enough in time to do the experiments we required. We therefore needed another way to scale up methane DDT experiments to a size relevant to a coal mine.

That other way, which was actually conceived as a good intermediate step before the LLEM collapse, was to build a detonation tube 1 m in diameter and as long as possible, which should be larger than had been used previously for testing deflagrations and detonation in channels containing NG and air. Furthermore, the size of a computation of this problem was almost within what could be done then on current computers, so that input models useful for coal-mine studies could be tested. The actuality of this became the Gas Explosion Test Facility (GETF).

The remainder of this article describes GETF and summarizes early measurements related to direct initiation of detonations in natural gas. This leads to a discussion of absolute detonability, and so to considerations of how we can extrapolate the data we have collected to larger systems. All of this highlights the extreme importance of having access to experimental facilities such as LLEM for large-scale tests.

THE GAS EXPLOSION TEXT FACILITY (GETF)

The construction of GETF began in June 2008. The site was located in the surface quarry east of the control building and the entrances to LLEM. The quarry isolated GETF with high walls on two contiguous sides and a high hill on the other side. The fourth side was partially blocked with an earthen berm, next to which was an access road. GETF was built parallel to this road so that it fired into the quarry wall, and the ignition end of the tube was anchored into the earthen berm. A bunker located next to GETF housed instrumentation. For safety, however, experiments were controlled from the LLEM control building that was 300 m away. Pictures of the facility are shown in Figure 2, and a schematic of the tube is shown in Figure 3.

Physical parameters of GETF are summarized in Table 1 and described in detail by Gamezo et al. (2012, 2013) and Zipf et al. (2013, 2014). The main part of GETF is the 73-m long steel pipe with internal diameter 1.05 m and the wall thickness 9.5 mm. The pipe was fabricated from hot-rolled and double-submerged arc-welded (DSAW) ordinary structure steel with minimum yield strength of 248 MPa. The pipe was originally made for oil and gas production and arrived on site in lengths of about 12 m. Six pieces were welded in the field to make the body of the GETF. Because the pipe has other industrial uses, it could be purchased at a reasonable price to create the longest facility possible that could fit into the

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*One of the authors of the present paper (E.S.O.) had heard (what might have been) an apocryphal story told by Gary Schott from Los Alamos National Laboratory, 30 years earlier, who said that "meter-sized detonation cells" were observed on the walls of a coal mine in the Soviet Union after an explosion. The fact that the source of this information was Gary Schott was subsequently confirmed by Charles Mader (private communications), but it was not possible to track the rumor down to a source in Russia. No further information about the 1-m cells in Russia has been uncovered to date.

Figure 2 Two views of LLEM.

quarry. For stoichiometric NG/air mixtures, the pressure of the quasi-static CJ detonation wave is about 1.66 MPa, which induces a hoop stress of about 91.7 MPa in the pipe wall, and therefore the safety factor against yield is about 2.7. Subsequent experiments in GETF developed short-duration pressures of about 7 MPa, which were probably localized to a few square centimeters of the pipe. Throughout all of the experiments performed, GETF never showed any evidence of deformation or damage. If a larger detonation tube could ever be fabricated from similar steel material, this experience with the GETF with a wall thickness of 9.5 mm indicates that the wall thickness required for a 2-m diameter tube is 19 mm, and so forth.

GETF was fit with pressure transducers and light sensors, the locations of which are indicated in Figure 3. Several steerable video cameras were placed at either end of the tube to view the tests. Figure 4 shows a sequence of four video frames taken about 1/30 second apart, showing the tube with a plastic diaphragm prior to rupture (top left), arrival of the detonation wave (top right), and venting of burning gases (bottom two frames). To detect detonation cells if they existed, aluminum sheets about 1-m × 1-m × 2-mm thick were

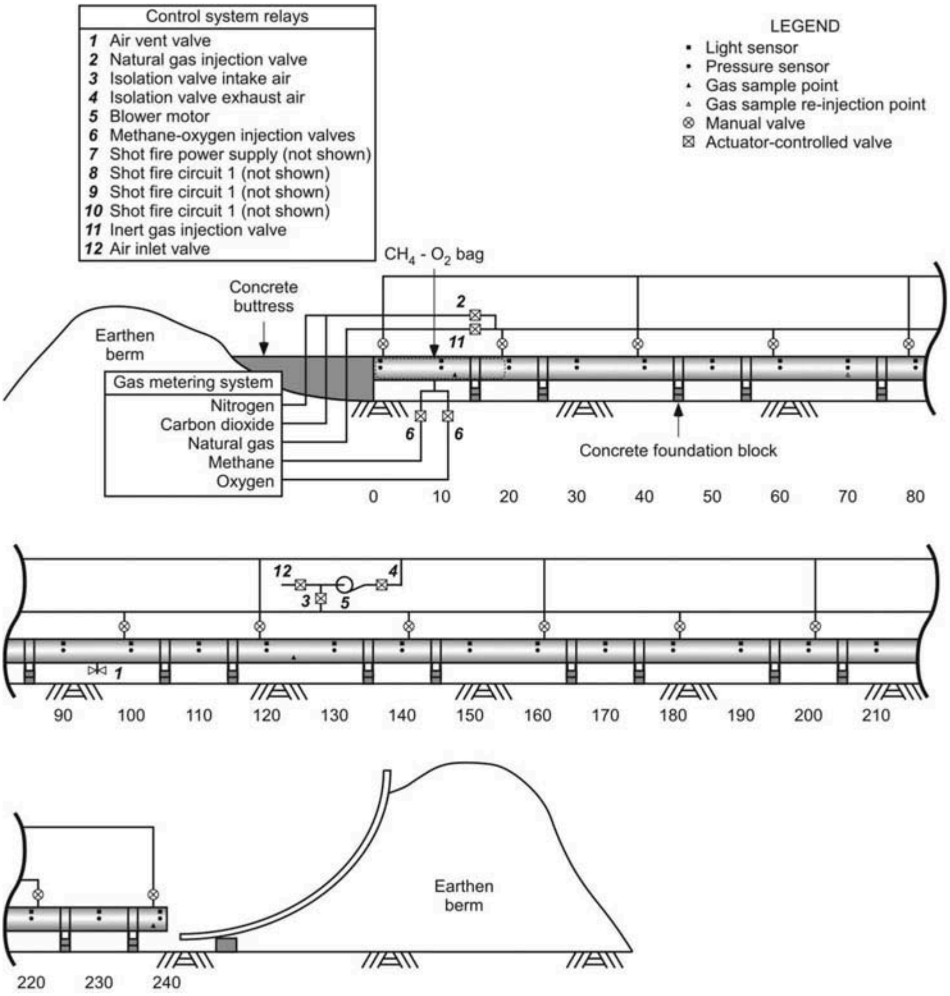

Figure 3 Schematic of the Gas Explosion Text Facility (GETF).

Table 1 GETF parameters

Property	Description
The Tube:	
Length	73.2 m
Diameter	1.05 m
Wall thickness	9.5 mm
Material	Steel - yield strength 248 MPa
The Diagnostics:	
Pressure gauges	23 quartz-piezoelectric-type 6.9 MPa with 1 μs rise time
Light sensors	23 silicon phototransistors with 2 μs rise time
Recording	2 24-channel CompactRIO with 20 μs sample rate
Smoke foils	2 aluminum sheets, 1 mm × 1 mm thick
Video	4 outside cameras, 20 fps

Figure 4 Video recording of GETF test explosion sequence with frames about 1/30 second apart. These show the tube with plastic, the diaphragm prior to rupture, the arrival of the detonation wave, and venting of burning gases.

bolted to the inner pipe wall near the end and coated with soot from the flame of a burning acetone-soaked rag.

Because GETF was outside and exposed to the local weather, which seasonally could be too cold or wet, it could only be operated for part of the year. For safety reasons, firings ceased in extreme conditions, such as thunderstorms and during winter months when the facility was covered with ice.

As the program proceeded, a number of problems and issues were discovered and fixed in turn. Here we list some of them and briefly describe or reference the remedies.

The Mixing System

The original mixing system had one inlet at the ignition end of GETF, one outlet at the other end of the tube, and a 1-kW blower fan. This simple system did not circulate enough gas, and it took many hours of mixing to achieve a test mixture that was homogeneous enough. The redesigned mixing system was equipped with a 2.25-kW blower fan that drew gas in through six inlets and an intake manifold, and blew gas out through seven outlets and an exhaust manifold. The mixture composition was tested and controlled by (1) injecting a precalculated amount of NG into the tube; (2) analyzing the gas from three locations in the tube, in real time, during the mixing process using a remote infrared gas analyzer; and (3) extracting two samples of the gas mixture after the mixing was completed and analyzing this later, off-site, using gas chromatography. With the new design, it was possible to have the prescribed test mixture in the entire tube to within ±0.2% in about 1 hour. [See Gamezo et al. (2012) for more details.]

Reducing Vibrations

At first, the pressure sensors were screwed into threaded holes in the GETF pipe wall. Because the sound speed in steel is about 5,900 m/s, extraneous vibrations induced in the steel by NG/air combustion would arrive at the pressure sensor before the gas-explosion shock waves, and this masked the gas pressure signals we needed to detect. To remedy this noise problem, the pressure sensor was decoupled from the GETF surface by suspending it over a hole and using a special bracket equipped with double-studded silicone gel anti-vibration mounts. [See Zipf et al. (2011) and Gamezo et al. (2012) for more details.]

Baffles

In early DDT experiments using spark ignition, we tried to make concentric baffles out of thick steel plates with 1-inch diameter rods to anchor the baffles to the ignition end of the tube. Figure 5 is a picture of several of these baffles fastened inside of GETF and before a firing. The limiting factor was the weight that a man could reasonably lift and assemble inside the tube, which was about 20 kg. This system, however, did not survive the DDT environment, which made a lot of scrap steel. To solve this problem, we used horizontal steel beams (H sections W200 × 100) placed across the tube, as shown in Figure 6, and they survived all experiments. [See Zipf et al. (2014) for more details]

Noise Generated by Explosions

In later experiments, neighbors from as far as 1 km, on the other side of the hill, complained about noise from GETF. In an attempt to break up and dissipate the blast wave and so reduce noise, a deflector and baffles were placed at the exit to GETF. The deflector and baffles are shown in Figure 7 and are also visible from various angles at the end of GETF in Figures 2 and 4. Limited noise reduction was achieved.

Figure 5 Initial baffle system that failed.

Figure 6 New baffle system using 200 W × 100 H sections.

Figure 7 Silencer at the exit of GETF.

Local Wildlife

Another issue was wildlife in the vicinity of GETF. Black bears and other smaller animals roamed the area. To prevent them from setting up housekeeping inside GETF, a substantial grate was bolted over the tube exit after each test. The grate can be seen attached to the end of GETF on the top frame of Figure 2.

The initial series of experiments, performed before any obstacles were inserted, focused on direct initiation of a detonation. These were performed to test the robustness of the tube and debug operational procedures and diagnostics. Because extrapolations indicated that it might take tens of kilograms of a high explosive to ignite a methane/air mixture directly, we used a polyethylene booster bag filled with CH_4/O_2, and placed it near the closed end of the tube. CH_4/O_2 is a much more reactive mixture, which has a detonation cell size of about 2 mm (compared to approximately 20 cm in CH_4/air). The detonation in CH_4/O_2 was promptly initiated by a blasting cap containing several grams of explosive. Even though these direct initiation experiments were done primarily to set up and test diagnostics, they provided the critical information that is a theme of this article.

A second set of experiments that included the presence of obstacles in the flow was designed to study flame acceleration and DDT. These obstacles, their placement, and the test results have been described in detail by Zipf et al. (2014), and they are not the subject of this article.

ABSOLUTE DETONABILITY AND ITS IMPORTANCE TO MINING SAFETY

The first set of experiments, completed in late Fall 2009, looked at direct initiation of detonations in methane/air mixtures containing from 5% to 17% methane. We defined a standard polyethylene booster bag as one that was 3 m long and 1 m in diameter, filled with stoichiometric CH_4/O_2, which is equivalent in energy to 40 MJ/m^2. The procedure was to use one bag initially and progressively increase or decrease the stoichiometry of test mixtures from 1.0 until no detonation was formed. Then, we tried two bags for mixtures that did not detonate. Three bags were tried for a few mixtures. Approximately 30 separate experiments were performed with up to two bags. The procedures for these experiments were reported in Gamezo et al. (2012).

Detonations were detected using light and pressure sensors. They were confirmed by cell structures recorded on soot-covered plates placed inside the tube, close to the open end. A few of the foils with cells etched from a detonation are shown in Figure 8. Extremely irregular detonation cell sizes were measured on the plates, some of which were as long as 1.7 m for the leanest mixtures. There were often very complex, small cells produced inside the larger ones. Of particular interest is the detonation structure around the limit, where there is a spinning detonation in the tube. This structure is discussed in more detail by Gamezo et al. (2012).

The *absolute detonability*, which is the ability of a mixture, in a fixed geometry, to support a detonation in principle, no matter how this detonation is ignited (Gamezo et al., 2012; Oran et al., 2010). The experiments in GETF established absolute detonation limits for methane/air mixtures at 1-m scale as 5.3% through 15.6% methane. This is in contrast to *conditional detonability*, which is “the ability of a mixture to develop a detonation for a

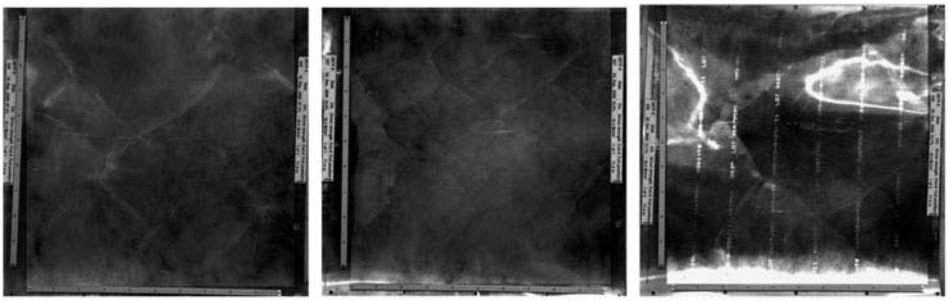

Figure 8 Detonation cells on smoke foils. The full size of the 1.2 m × 1.2 m foils is shown. Left: 2.3% NG. Middle: 10.2% NG. Right: 13.7% NG.

particular geometry and a particular ignition source." Absolute detonability can be determined by direct initiation of a detonation when enough energy can be used to initiate a strong enough shock wave.

For weak ignition sources that do not initially involve strong shocks and detonations, conditional detonability is defined by the ability of a system to undergo a deflagration-to-detonation transition (DDT). It is important to know the absolute detonability limits in a system because they define whether it is even possible for DDT to occur by *any* mechanism at all (e.g., Oran and Gamezo, 2007). Detailed results of experiments to determine absolute detonability of methane/air mixtures in GETF are reported elsewhere (Gamezo et al., 2012). Cell sizes and velocities were measured as a function of stoichiometry, as discussed below.

Figure 9 places the detonation limits measured in GETF on the same graph as prior experiments in smaller channels. This shows that as the size of the system increases, the minimum percentage of CH_4 that can sustain a detonation decreases. This means that in large channels, even relatively lean mixtures ignited by a weak spark can develop detonations. In real-world environments, such as coal mines, explosive mixtures are usually nonuniform.

From Figure 9, we can be fairly confident of the absolute detonability for system sizes between the points of this curve. It is less certain how to extrapolate to systems considerably larger than 1 m in diameter. Note that the detonability limit is shown here as a function of the percentage of natural gas as a function of $1/d$, the inverse of the tube diameter d.

Figure 10 shows detonation velocities derived from the pressure transducer measurements in GETF. The black line is a fit through the separate experimental results. Note that the data points used to construct the velocity curve are larger than the uncertainty in the particular measurements taken from the raw data. In all of the direct initiation experiments

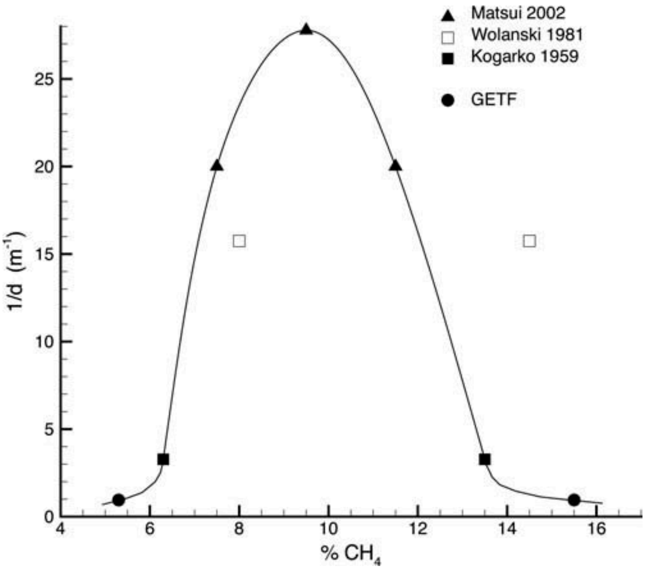

Figure 9 Measured GETF limits and prior experiments in smaller channels. Note that the vertical scale is $1/d$, where d is the scale of the experimental apparatus, here the tube diameter. Experimental data are by Matsui (2002), Wolanski et al. (1981), and Kogarko (1959).

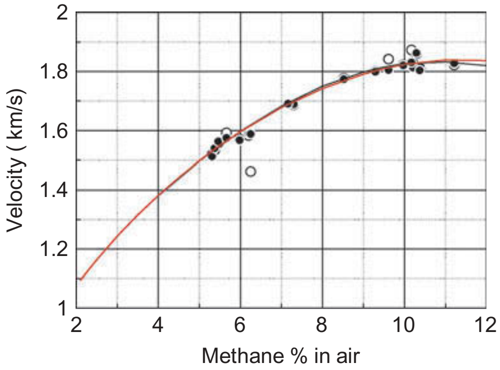

Figure 10 Average shock and flame velocities (black and white points, respectively) measured in direct initiation experiments (Gamezo et al., 2012) for methane/air mixtures at 1 atm as a function of mixture composition. Black and red lines show CJ detonation velocity computed using two codes: Fried et al. (2000) and Caltech (2000), respectively.

in which detonations were successfully initiated, the detonation velocity reached D_{CJ} very quickly, within the first 10 m or less of the tube. This is true even in the limiting case at 5.3%. (See, for example, figure 7b in Gamezo et al., 2012.) If the detonation failed, the front velocity quickly dipped below D_{CJ} and continued to fall.

Figure 11 shows detonation cell sizes taken by directly measuring the cells that appeared on the smoked aluminum plates attached inside GETF. It was harder to determine a consistent, measured size for a detonation cell than it was to find a reliable detonation velocity. Detonation cells are irregular, and sometimes a large cell is filled with a few or sometimes many smaller cells. This uncertainty and even confusion increases toward the limits, where the values must be affected by the size of the tube itself. Nonetheless, even in

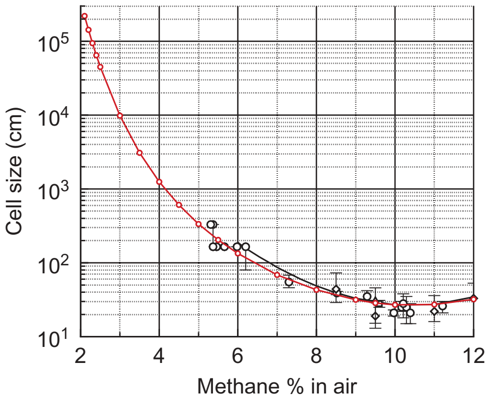

Figure 11 Detonation cell sizes λ measured for methane/air mixtures at 1 atm in GETF experiments (circles) and reported by other researchers [see Gamezo et al. (2012) for more details]. The black line shows computed cell size based on a model by Gavrikov et al. (2000). The red line is computed using the detailed chemical kinetics scheme (San Diego, 2014) and the ZND structure code Caltech (2000). The reaction zone length X_{ZND} is defined as the distance from the shock to the maximum temperature gradient. $\lambda/_{ZND} = 14.5$.

cases near limits, we could often pick out large, clear cells that repeated themselves in the expected detonation cell pattern.

CAN WE COMPUTE ABSOLUTE DETONABILITY?

As shown above, experiments are difficult and expensive, but not impossible, although scaling up to the physical size of a structure of interest is not always practical. (Recall the collapse in LLEM.) Reactive-flow simulations to determine absolute detonability are also difficult and would require substantial computational resources. Even with the large, fast computers and well-tuned numerical models that now exist, such computations are not likely to produce accurate results, given our limited knowledge of chemical and other physical processes involved at very high temperatures and pressures.

For these reasons, it is important to find some way to use the information we already have to estimate absolute detonability for larger systems. We often rely on scaling rules, power laws, or simply useful empirical relations to make predictions. Scaling laws can be found in a number of ways. One is a result of direct analysis of the governing equations to produce dimensionless numbers and simple relationships that can be used over a range of time and space scales. Another way is to find useful empirical relations for extending the range of scales.

Here we give a simple prescription for extending the range in Figure 9. The approach is based on an extensive history of attempts to relate X_{ZND}, the one-dimensional reaction-zone length for a ZND detonation, to the detonation cell size λ. This approach was originally proposed by Schelkin and Troshin (1965), and subsequently there was extensive work to refine the idea and to explain why and how it should work. A good recent history and an examination of the underlying principles are given in Gavrikov et al. (2000). As shown below, this gives rather reasonable and somewhat thought-provoking results.

First, we computed values of X_{ZND}, the one-dimensional reaction-zone length for a ZND detonation as a function of the percent of methane dilution (% CH_4) for methane/air mixtures initially at 1 atm and 300 K. The San Diego chemical kinetics mechanism (San Diego, 2014) was used as the chemical model in the ZND structure code, Caltech (2000). The third column shows the detonation velocities, D_{CJ}, computed using both Caltech 2000 and the CHEETAH code (Fried, 2000) for the other dilutions. These two codes gave essentially identical results, so just one value is shown in Table 2. In Figure 10, computed values of D_{CJ} are compared to the values derived from GETF measurements.

Then using *only one of the measured values of detonation cell size*, here selected to be the value at 10% CH_4 from the GETF experiments (see point on Figure 11), and the value of $X_{ZND}(10\%CH_4)$ in Table 2, we define a ratio, α, such that

Table 2 Input for estimation of detonate cell size for lean mixtures

CH_4 (%)	ZND zone (cm)	D_{CJ} (m/s)	Cell size (m)
10	2	1810	0.25 – Experiment
4	82	1380	10 – Equation (1)
3	590	1252	74 – ”
2.5	2515	1174	314 – ”
2.2	7746	1122	968 – ”
2.1	11622	1105	1453 – ”

$$\alpha = \frac{\lambda}{X_{ZND}\,(10\%CH_4)} = 14.5. \tag{1}$$

In principle, we could have chosen any of the measured values of λ from the series of GETF experiments. Here we show what happens if we select the value close to stoichiometric conditions, where measurements are easiest to interpret.

By assuming, for simplicity, that α is a constant independent of %CH_4, we can compute λ for a series of dilutions from Eq. (1), and these are shown in the fourth column of Table 2. In Table 2, D_{CJ} is a computed value, which is quite close to a measured value. The size of the ZND zone is also computed from a full detailed chemical reaction mechanism. The detonation cell sizes listed in Table 2 are computed from Eq. (1), except for the one value selected from the measured ones and used to derive the (hopefully) constant α. The computed λ shown here can be compared to the measured values of λ by comparing the red and black lines in Figure 11.

To date, detonation cells in methane and air have not been computed reliably with a full, detailed chemical reaction mechanism. The only computations performed have used reduced or simple calibrated couple-step models that attempt to reproduce the features of chemical reaction and energy release inherent in detailed chemical models. One example of this is the work of Kessler et al. (2011), which computed detonation cell sizes for stoichiometric methane in air that were too small by factors of 3–5, as well as a qualitatively wrong type of detonation cell structure. This was the same type of result, both qualitatively and quantitatively, found for computations of hydrogen detonation cells that compared detonation cell sizes computed by a number of different chemical mechanisms (Taylor et al., 2012).

Figure 11 tests the consistency of the values of λ computed from Eq. (1) and the values measured in GETF (compare red and black lines) down to the experimentally measured detonability limit of 5.3% CH_4 in the 1 m diameter tube. Using this approach, the curves have been arbitrarily extended to 2.1% CH_4 [which is well below the methane *flammability* limit determined by Cashdollar et al. (2000) to be 5% CH_4].

Now the question is how to relate computed λ's to the size of the system *d*. This is done based on empirical knowledge and is quite approximate. Detonations in channels are supported by shock reflections from channel walls and can propagate in channels larger than $0.2\lambda - 0.3\lambda$. Experiments show that detonations in unconfined gas require at least 13 cells to propagate in cylindrical geometry, and at least 10 cells for a flat layer. If the reactive layer is adjacent to a smooth solid surface, this surface can be considered as a reflecting (symmetry) plane, and the layer thickness required for the detonation propagation is reduced to about 5λ.

Coal mine tunnels are one example of large practical systems that can be affected by methane/air detonations. A typical tunnel is 6 m wide and ranges from 1 m to 4 m high, depending on the coal seam geology. We can now estimate the lean limit for this scale using the information in Figure 11. For the average diameter $d \sim 3$ m for a typical tunnel, and the ratio $d/\lambda = 0.2 - 0.3$, the detonation cell size at the limit should be 10–15 m, which corresponds to $\sim 4\%CH_4$ on the red curve in Figure 11 (which is below the reported flammability limit).

Another case to consider is a large cloud of lean methane that may form near the earth's surface as a result, for example, of a natural release or an industrial accident. Assuming the cloud thickness of $h \simeq 1$ km in the vertical direction, and the ratio $d/\lambda = 10$, the detonation cell size at the limit is $\simeq 100\ m$, which corresponds to $\sim$3% CH_4 on the red curve in Figure 11.

This extrapolation of detonation properties to extremely lean mixtures is possible (but maybe not realizable) because detonation theory does not impose any detonability limits for system size, even for infinitely large systems. There are limits for real systems of finite size, since away from the stoichiometric conditions, the reaction scales (e.g., X_{ZND}) increase sharply.

SUMMARY AND CONCLUSIONS

In this article, we have considered absolute detonability of a gaseous fuel, defined here as the ability of a mixture, in a fixed geometry, to support a detonation in principle, no matter how this detonation is ignited. Tests made in the Gas Explosion Tube Facility (GETF), formerly in Lake Lynn, Pennsylvania, provided measurement in a 1-m channel. GETF experimental data include detonation velocities and cell sizes as a function of the percentage of methane in the system.

Prior experiments, performed in various locations around the world, provided data in smaller channels. Combined with the GETF results, these data show that the lower detonability limit decreases as a function of system size, and that the limit decreases as the system size increases. The questions then arose: What is the absolutely detonability for a 2-m channel? A 10-m channel? And so forth? Can we extrapolate to larger systems? In fact, exactly how low can a detonability limit go?

We attempted to address these question by relating the reaction zone length X_{ZND} for an idealized one-dimensional detonation to the cell size, λ. The experimental quantity used to pin the model was the measured detonation cell size for 10% methane in air at atmospheric conditions, which is $\simeq$25 cm. In principle, the value used to determine α could have been any of the other measured values of λ taken from Figure 11. From this single value and the computed values of X_{ZND}, we were able to reproduce the measured cell sizes as a function of mixture composition down to 5.3% CH_4. Then extending this curve, we were able to "predict" cell sizes for leaner systems. The predicted and measured values agreed surprisingly well for those values we could measure (Figure 11).

There is a simple empirical estimate of whether a detonation can propagate in a system of a certain size d based on the detonation cell size λ. For enclosed tubes, we estimate $d/\lambda = 0.2 - 0.3$. Using all of this information, we can predict the lean limit for a methane/air mixture in a 10-m channel as $\simeq 4.0\%$.

First, it is surprising that the simple scaling algorithm proposed above works well enough to replicate the measured values of detonation cell size based on a single constant, measured at stoichiometric conditions, a chemical reaction mechanism, and ZND theory. Therefore, it might provide a reasonable way to obtain an estimate of the absolute detonability limit for a coal mine tunnel or a large vapor cloud, for example.

Another issue is that the estimated value for the absolute detonation limit for a coal mine tunnel is lower than the measured flammability limit for methane/air. Extrapolating a detonation limit to a value lower than a flammability is, to some extent, like comparing apples and oranges. Flammability limits are measured for certain conditions, detonation limits are measured in other conditions, and these might not be the same. Scale, for example, could have an effect on flammability, too.

But it is interesting to consider the consequences of this analysis: How would it be possible to ignite a detonation when the mixture is below the flammability limit and so does not support a laminar flame? The amount of energy required by direct ignition would be enormous. The detonation could not be formed by DDT in a homogeneous mixture at a low dilution of CH_4, because that mixture would not support a deflagration. Perhaps if the detonation started in a richer mixture and propagated into the lean mixture, it would continue to propagate? Or if the original lean mixture were shocked enough, and its temperature and pressures were therefore raised high enough, it would move the gas into a regime where a flame could exist? If this detonation were to be ignited, what would it look like when it extinguished? These are just a few questions of both practical and theoretical concern.

In summary, we have argued the importance of GETF data and the general need for experiments in progressively larger systems. It would have been extremely valuable to have the GETF to do these same experiments for other compositions of natural gas, which are more easily detonated than pure methane, and for systems containing other impurities, such as CO_2, coal dust, or inert rock dust.

Unfortunately, and for reasons many of us do not understand, GETF was totally dismantled and NIOSH was forced to abandon LLEM in September 2013. These were important facilities that held the possibility of extending our knowledge into the limiting regimes of combustion as well as providing important practical limits for regulations. The loss of GETF, and all of the Lake Lynn Experimental Mine, is a serious loss to the entire mining, combustion, and safety communities.

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REFERENCES

Bartknecht, W. 1981. *Explosion*. Springer-Verlag, Berlin.

Caltech. 2000. ZND Structure Computation: Detonation Structure Computation Tools. Explosion Dynamics Laboratory, California Institute of Technology. Available at: http://www2.galcit.caltech.edu/EDL/public/codes.html.

Cashdollar, K.L., Zlochower, I.A, Green, G.M., Thomas, R.A., and Hertzberg, M. 2000. Flammability of methane, propane, and hydrogen gases. *J. Loss Prev. Process Ind.*, **13**, 327.

Fried, L., Glaesemann, K., Souers, P.C., Howard, W.M., and Vitello, P. 2000. A thermochemical-kinetics code CHEETAH 3.0. Livermore, CA: Lawrence Livermore National Laboratory.

Gamezo, V.N., Ogawa, T., and Oran, E.S. 2007. Numerical simulations of flame propagation and DDT in obstructed channels filled with hydrogen–air mixture. *Proc. Combust. Inst.*, **31**, 24–63.

Gamezo, V.N., Ogawa, T., and Oran, E.S. 2008. Flame acceleration and DDT in channels with obstacles: Effect of obstacle spacing. *Combust. Flame*, **155**, 302.

Gamezo, V.N., Zipf, R.K., Mohamed, K.M., Oran, E.S., and Kessler, D.A. 2013. DDT experiments with natural gas-air mixtures. In *Fire and Explosion Hazards, Proceedings of 7th International Seminar on Fire and Explosion Hazards (ISFEH7)*, D. Bradley, G. Makhviladze, V. Molkov, P. Sunderland, and F. Tamanini (Eds.), Research Publishing, Singapore, pp. 729–738.

Gamezo, V.N., Zipf, R.K., Sapko, M.J., Marchewka, W.P., Mohamed, K.M., Oran, E.S., Kessler, D.A., Weiss, E.S., Addis, J.D., Karnack, F.A, and Sellers, D.D. 2012. Detonability of natural gas-air mixtures. *Combust. Flame*, **159**, 870.

Gavrikov, A.I., Efimenko, A.A., and Dorofeev, S.B. 2000. A model for detonation cell size prediction from chemical kinetics. *Combust. Flame*, **120**, 19.

Johnson, D.M. 2010. The potential for vapour cloud explosions | Lessons from the Buncefield accident. *J. Loss Prev. Process Ind.*, **23**, 921.

Kessler, D.A., Gamezo, V.N., and Oran, E.S. 2011. Multilevel detonation cell structures in methane-air mixtures. *Proc. Combust. Inst.*, **33**, 2211.

Kogarko, S.M. 1959. Detonation of methane-air mixtures and the detonation limits of hydrocarbon-air mixtures in a large-diameter pipe. *Soviet Physics - Technical Physics*, **3**, 1904.

Matsui, H. 2002. Detonation propagation limits in homogeneous and heterogeneous systems. *J. Phys. France IV*, **12**, 7.

McMahon, G.W., Britt, J.R., and O'Daniel, J.L. 2007. CFD study and structural analysis of the Sago Mine Accident. Technical Report. U.S. Army Corps of Engineers, Engineer Research and Development Center, Geotechnical and Structures Laboratory, Vicksburg, MS.

Mine Safety and Health Administration (MSHA). 2006. Report of investigation, fatal underground coal mine explosion, January 2, 2006, Sago Mine, Wolf Run Mining Company, Tallmansville, Upshur County, West Virginia, ID No. 46–08791. U.S. Department of Labor, Mine Safety and Health Administration, Coal Mine Safety and Health, Arlington, VA. Available at: http://www.msha.gov/FATALS/2006/Sagosagoreport.asp.

Mine Safety and Health Administration (MSHA). 2010. Report of investigation, fatal underground mine explosion, April 5, 2010, Upper Big Branch Mine South, Performance Coal Company, Montcoal, Raleigh County, West Virginia, ID No. 46–08436. U.S. Department of Labor, Mine Safety and Health Administration, Coal Mine Safety and Health, Arlington, VA. Available at: http://www.msha.gov/Fatals/2010/UBB/FTL10c0331noappx.pdf.

Ogawa, T., Gamezo, V.N., and Oran, E.S. 2013. Numerical study on ame acceleration and DDT in an inclined array of cylinders using an AMR technique. *Comput. Fluids*, **85**, 63.

Oran, E.S., and Gamezo, V.N. 2007. Origins of the deflagration-to-detonation transition in gas-phase combustion. *Combust. Flame*, **48**, 4.

Oran, E.S., Gamezo, V.N., and Kessler, D.A. 2010. Deflagrations, detonations, and the deflagration-to-detonation transition in methane-air mixtures. NRL Technical Memorandum Report, NRL/MR/6400{11–9332, 2911, 9278.

San Diego Mechanism. 2014. Chemical-kinetic mechanisms for combustion applications. Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego. Available at: http://combustion.ucsd.edu.

Shchelkin, K.I., and Troshin, Y.K. 1965. *Gas Dynamics of Detonations*, Mono Book Corp., Baltimore, MD.

Taylor, B.D., Kessler, D.A., Gamezo, V.N., and Oran, E.S. 2012. Numerical simulations of hydrogen detonations with detailed chemical kinetics. *Proc. Combust. Inst.*, **34**, 2009.

Wolanski, P., Kauffman, C.W., Sichel, M., and Nicholls, J.A. 1981. Detonation of methane-air mixtures. *Proc. Combust. Inst.*, **18**, 1651.

Zipf, R.K., Gamezo, V.N., Mohamed, K.M., Oran, E.S., and Kessler, D.A. 2014. Deflagration-to-detonation transition in natural gas–air mixtures. *Combust. Flame*, **161**, 2165.

Zipf, R.K., Gamezo, V.N., Sapko, M.J., Marchewka, W.P., Mohamed, K.M., Oran, E.S., Kessler, D.A., Weiss, E.S., Addis, J.D., Karnack, F.A., and Sellers, D.D. 2013. Methane-air detonation experiments at NIOSH Lake Lynn Laboratory. *J. Loss Prev. Process Ind.*, **26**, 295.

Zipf, R.K., Sapko, M.J., and Brune, J.F. 2007. Explosion pressure design criteria for new seals in U.S. coal mines. Report IC-9500, National Institute for Occupational Safety and Health (NIOSH).