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## Category

Research Article


### Abstract

In a coal mine, natural gas can leak through walls and accumulate in enclosed regions that are no longer being mined or ventilated. If there is an accidental spark in the region containing this gas, it can ignite a flame that may transition to detonation (DDT). An important problem is to assess if, when, and where DDT can occur, and thus provide information needed to design strong enough barriers to protect active mining areas. We describe results of numerical simulations of flame acceleration and DDT in obstacle-laden channels to find a scaling law for $?_{DDT}$, the distance the deflagration travels before a detonation forms as a function of channel size d. The scaling law is derived for a stoichiometric natural-gas air mixture in a channel with blockage ratio 0.3 and channel sizes ranging from 0.17 to 3.0 m.



### Keywords

Natural gas, Explosions, Detonations, Deflagration-to-detonation transition, Fast flames, Mine explosions



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# Towards scaling laws for DDT in obstructed channels

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**Abstract**

In a coal mine, natural gas can leak through walls and accumulate in enclosed regions that are no longer being mined or ventilated. If there is an accidental spark in the region containing this gas, it can ignite a flame that may transition to detonation (DDT). An important problem is to assess if, when, and where DDT can occur, and thus provide information needed to design strong enough barriers to protect active mining areas. We describe results of numerical simulations of flame acceleration and DDT in obstacle-laden channels to find a scaling law for $L_{\mathrm{DDT}}$, the distance the deflagration travels before a detonation forms as a function of channel size $d$. The scaling law is derived for a stoichiometric natural-gas air mixture in a channel with blockage ratio 0.3 and channel sizes ranging from 0.17 to 3.0 m.

*Keywords:* Natural gas; Explosions; Detonations; Deflagration-to-detonation transition; Fast flames; Mine explosions

## Introduction

A critical issue for safety in coal mines is whether a detonation can develop during an explosion of natural gas (mostly methane) that seeps naturally from the walls into confined, underground tunnels and chambers. Such explosions are possible when the methane reaches a concentration that is ignitable by accidental sparks, such as could arise from falling rocks, operating equipment, spontaneous coal ignition, or lightning strikes. For this reason, estimates of the system scales and geometrical features that could allow a detonation to develop as well as the pressures that arise from a detonation or deflagration-to-detonation event are important for design and risk management.

In the past twenty years, considerable progress has been seen in understanding the mechanism of deflagration-to-detonation transition (DDT) in gas-phase reactive systems [1, 2]. To a large extent, this knowledge has arisen through numerical simulations showing details of the transition accompanied by detailed comparisons to experimental data. Numerical models that have been used for this work include three key ingredients: (1) a chemical-diffusive model that adequately emulates the chemical transformations and energy release in the reactive mixture; (2) an adequate model for solving the fluid dynamics equations; and (3) a method for adaptive refinement of the computational mesh on which the fluid dynamics can be solved and the reaction fronts can be resolved. When properly calibrated, these numerical models allow physically acceptable simulations of DDT in fairly complex geometrical systems.

The scales that need to be resolved in computations of DDT in realistic systems range from a laminar flame thickness to the size of a system. These scales may differ by four orders of magnitude for small systems, and by up to eight orders of magnitude for large systems such as coal mine tunnels. Here, the focus is on large systems, and a generic problem of numerical modeling of multiple physical processes that occur and interact with each other in a wide range of spatial and temporal scales.

At least two approaches are possible to assess this problem. One is from t*he large spatial scale* working *downward*, and the other is *from the small spatial scale working to larger scales.*

Working from the large scale downward, the process is to resolve the largest spatial scales of a system and postulate a reasonable model, e.g. a subgrid model, for the small scale. This is typical of what has been done for modeling turbulent fluid systems, where the model of the small scales may be a “turbulence model” in which dissipation at small scales is prescribed to ensure

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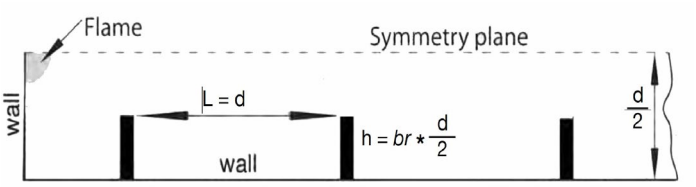


Fig. 1. Schematic of the computational domain giving relative dimensions and boundary conditions. Note that half of the system is computed and a symmetry condition is used on the upper boundary of the domain.

reasonable physical behavior. As a result, success can be obtained for some types of fluid turbulence because the behavior often scales, but it may not be as successful when unresolved, new and different physical processes are involved such as reactions and ignition, which is the case with DDT.

A complementary approach is to model the systems from smaller spatial scales upwards, which means performing the simulations first at small scales where the phenomena are resolved and then systematically increase the system size. This approach allows the scales of the problem (here, DDT) to be defined, and it may be possible to extend the computations to larger and larger scales. Alternatively, it may be possible to develop subgrid models that would include the effects of other physical processes besides fluid dynamics. For example, for the DDT problem where it is necessary to resolve the scales from the laminar flame thickness to the size of the system, smaller-scale simulations could be used to find basic mechanisms for the transition. Then, larger-scale simulations could describe the total environment which leads up to the types of conditions in which the transition mechanism is able to arise.

In this paper, a series of DDT simulations are described for obstacle-laden channels filled with a stoichiometric, premixed methane-air gas. In these simulations, the channel height *d* was varied between 0.174 m and 3 m, while the blockage ratio and the ratio of obstacle spacing to system size were held constant. These simulations were tested extensively for resolution and consistency and then compared with pre-existing experimental data. The results provided the distance to DDT, $L_{\mathrm{DDT}}$, as a function of channel height *d* for a range of scales including the sizes typical of coal-mine tunnels.

**Overview of flame acceleration and DDT**

Recent results have been reported from simulations that used a computational model based on the reactive Navier-Stokes equations coupled to the ideal gas equation of state and one-step Arrhenius kinetics of energy release. This model and results obtained from it have been discussed extensively in the literature [3]. The solution procedure was based on a second-order numerical method in space and was second-order in time, with AMR implemented by the Fully Threaded Tree (FTT) algorithm [4]. The FTT is an extremely efficient approach based on a tree structure, and it refines the grid on a cell-by-cell basis as needed. The grid was structured and characterized by a range of cell sizes between $dx_{\mathrm{min}}$ and $dx_{\mathrm{max}}$.

The energy release was controlled by a chemical-diffusive model that was developed and optimized for methane-air flames and detonations [5]. The laminar flame thickness computed with this model was 0.0439 cm, and the half-reaction thickness of a steady-state Chapman-Jouguet detonation was 0.229 cm. The minimum computational cell size, $dx_{\mathrm{min}}$, in the simulations was varied between 0.01625 cm and 0.065 cm. The maximum computational cell size, $dx_{\mathrm{max}}$, was kept constant at 0.26 cm. A schematic of the computational domain is shown in Fig. 1.

Fig. 2 shows computed temperature fields at selected times for a 17.4 cm case with $br$ = 0.3 and $dx_{\mathrm{min}}$ = 0.1625 cm. Each frame shows only part of the computational domain. The evolution of the flame to a detonation after repeated interactions with obstacles has been discussed extensively in prior papers [3, 5]; this simulation followed essentially the same patterns. The flame was ignited by a small spark in the upper left-hand corner of the domain. Initially, this flame grew slowly as it spread at essentially a laminar flame speed of the methane-air mixture. The speed was 38 cm/s relative to the unburned material, but the flame spread faster in the laboratory frame of reference because the burning material expanded and pushed the unburned material away from the ignition point.

Then, due to acoustic interactions with the walls and laminar flame instabilities, the flame began to wrinkle. As it wrinkled, the surface area increased and the flame speed began to accelerate as it moved down the channel. The flow ahead of the flame became nonuniform as it interacted with obstacles. This nonuniform flow stretched the flame surface and contributed to an increased flame surface area that then caused further flame acceleration. The flame also interacted with turbulence generated in the wakes of obstacles, and this turbulence contributed to further burning rate increases. These effects dominated up to about 53 ms, as shown in the figure.

Subsequently, the acoustic waves generated by the accelerating flame began to coalesce and form shockwaves, as seen, for example, in the frame at 59.52 ms. Shocks reflected from obstacles and interacted with the flame surface causing additional turbulence

generation through RT instabilities. Overall, a "fast flame" or a "shock-flame complex" was generated in which a leading shock was followed at some distance by a turbulent flame. An important point is that the region between the leading shock and the turbulent flame was heated, compressed, and constantly being shocked and re-shocked.

Eventually, as seen at 59.56 ms, a small ignition kernel formed at the left side of the obstacle (at 470 cm). This kernel formed in a "hot spot" which also contained temperature gradients. It has been shown that, depending on the size and structure of a hot spot, ignition can produce a flame and a shock, or a detonation. In the case shown, there is a direct transition to a detonation that propagated upstream through shocked, compressed material diffracted over the obstacle, overtook the leading shock, and created a detonation in the unreacted material. The last four frames depict the detonation initiation and propagation.

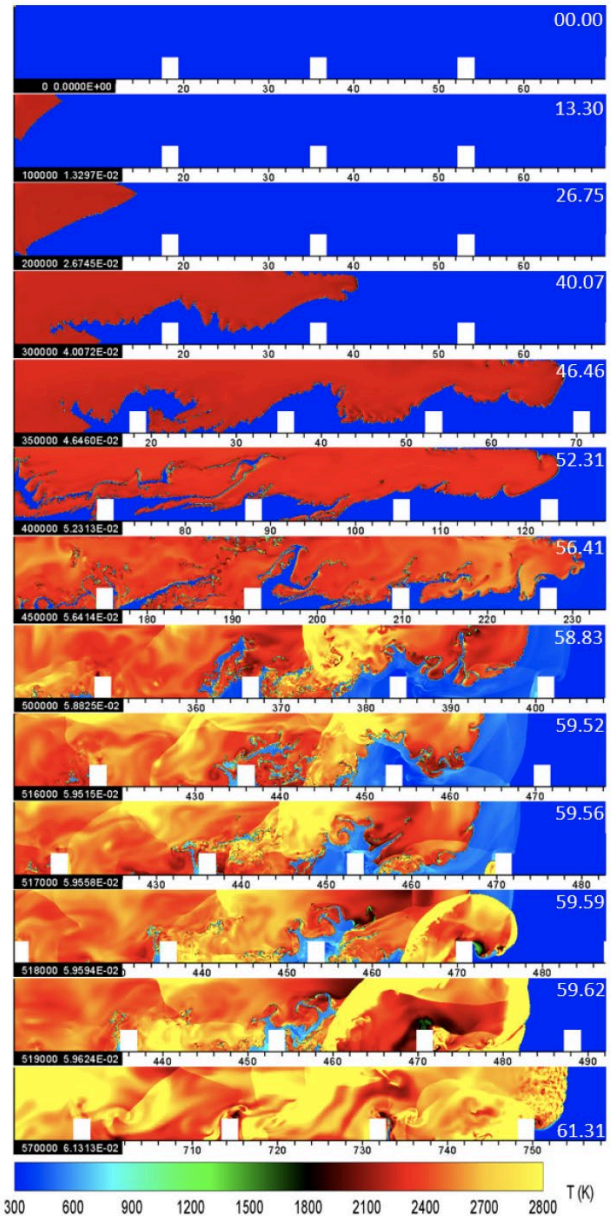


Fig. 2. Temperature maps for 17.4 cm channel, $br$ = 0.3. Locations (cm) on the $x$-axis increase in time. Time in milliseconds is noted in the bottom right corner of each frame.

Fig. 3 shows the speed of the reaction front as a function flame position, and the flame position as a function of time.

As shown in Fig. 2, the reaction front began as a relatively slow laminar flame (from about 0 s to 0.02 s), evolved into a turbulent deflagration, and finally underwent transition to a detonation (0.05956 s). Before DDT, a shock-flame complex was formed (also called a "fast flame"), as is indicated in Fig. 3 where the flame speed leveled as a function of position just before DDT.

## Large-channel simulations and a scaling law

Simulations such as those shown in Fig. 2 were performed for a series of channel heights $d$ ranging from 17.4 cm to 300 cm. The blockage ratio $br$ = 0.3 and the ratio $L/d$ = 1 of obstacle spacing $L$ to channel height $d$ were fixed. The results for the smaller channels of size 17.4 and 52 cm could be compared to experiments by Kuznetsov et al. [6], and the simulations for 104 cm could be compared to the large detonation tube experiments performed at Lake Lynn Laboratory [7].

Results from all of the simulations and experiments are shown in Fig. 4. Simulations for the smaller channels that were accomplished for several numerical resolutions have shown that the distance to DDT is practically independent of $dx_{\min}$. This independence made the computations for larger channels easier by the fact that lower grid resolutions could be used. One of the large channels, $d$ = 2.08 m, was computed with

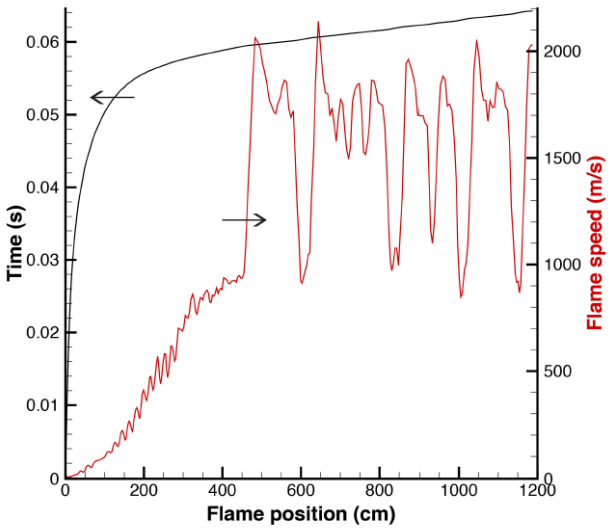


Fig. 3. Flame position (actually, the front of the reaction front (flame or detonation) and speed as a function of time for simulation shown in Fig. 2.

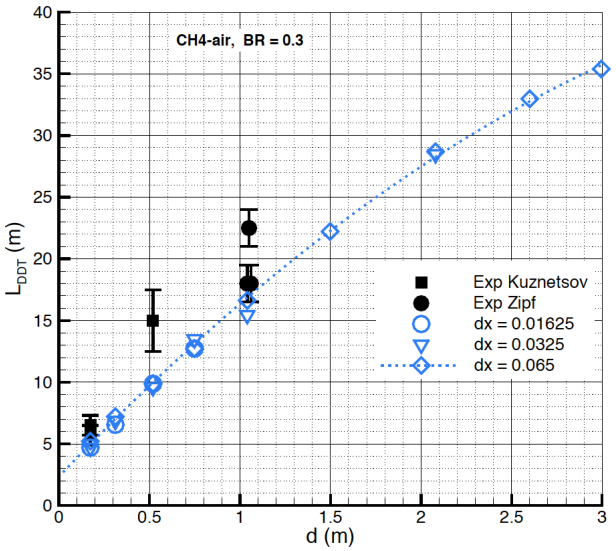


Fig. 4. Compilation of computed and experimental distances to detonation, $L_{\mathrm{DDT}}$, as a function of channel height $d$ for channels filled with a stoichiometric methane-air mixture. All computations have the same coarse mesh size, $dx_{\max}$ = 0.26 cm. Three fine mesh sizes are tested: blue circles: $dx_{\min}$ = 0.01625 cm; blue triangles: $dx_{\min}$ = 0.0325 cm; blue diamonds: $dx_{\min}$ = 0.065 cm. Black circles correspond to experiments [6,7] in 105 cm tube with $br$ = 0.25 and methane concentrations 8.0% ($L_{\mathrm{DDT}}$ = 22.5 m), 8.8% ($L_{\mathrm{DDT}}$ = 18 m), and 10.1% ($L_{\mathrm{DDT}}$ = 18 m). All other points correspond to $br$ = 0.3 and 9.5% $CH_4$.

two resolutions, and both produced the same $L_{\mathrm{DDT}}$. Hence, confidence was built that the large-channel simulations were accurate enough to simulate DDT. An important result here is that for the stoichiometric mixture of natural gas and air, the distance to DDT was about 35 m for the 3 m channel.

## Discussion and conclusion

A scaling law was determined that can be used to estimate the run-up distance to detonation, $L_{\mathrm{DDT}}$, using multidimensional numerical simulations of the deflagration-to-detonation process in an obstacle-laden channel filled with stoichiometric methane-air. This scaling law was established for a wide range of channel heights from 0.174 m to 3 m, sizes of which are typical of coal mine tunnels. The blockage ratio $br$ = 0.3 and the equivalence ratio 1 used in the simulations corresponded to a worst-case scenario for an accidental methane explosion in a coal mine. Interesting questions that could now be explored are how this curve changes with equivalence ratios, blockage ratios, and other system parameters.

For all of the channel sizes studied, the mechanism of DDT was essentially the same: the formation of a turbulent flame, a shock-flame complex, and then a Mach stem reflection from an obstacle that ignited a detonation. Although the details of ignition were not examined for all computed cases, all of the simulations produced a characteristic "kink" on flame position-vs-time curve that appeared when a detonation was ignited ahead of the main flame by a shock colliding with the bottom of an obstacle, then propagating to the top of the obstacle, spreading past the obstacle and catching up with the leading shock.

The simulations tended to predict DDT slightly sooner than the experiments, although the simulations were still reasonably close. The blockage ratio in experiments [7] with the 105 cm tube was slightly lower ($br$ = 0.25) than in other experiments and simulations ($br$ = 0.3), and the methane-air ratio was slightly off the stoichiometric (see details in the caption for Fig. 4), so the black points in Fig. 4 are probably a little higher than they would be for stoichiometric composition and $br$ = 0.3.

The derived $L_{\mathrm{DDT}}$ vs $d$ curve looks rather like a straight line for small $d$, but then tends to bend slightly as $d$ increases. In fact, some curvature existed even for small systems where data were available, e.g. at 17.4 to 104 cm, but it was only noticeable when looking at the entire range. This curvature appeared because DDT in larger systems required fewer obstacles, meaning that the flame accelerated more while moving from one obstacle to another in the larger system. This may be related to the increasing range of scales between the laminar flame thickness and the system size that allowed more flame folding scales that increased the burning rate of a turbulent flame.

One fair question is: *How good is the prediction of $L_{\mathrm{DDT}}$ for large-scale methane-air systems?* Unfortunately, it is not easy to answer given the model approximations and a very limited amount of experimental data available for model validation. To-date, $L_{\mathrm{DDT}}$ in methane-air systems was measured only for 17.4, 52, and 105 cm round tubes whereas the obstacle geometry in 105 cm tube was quite different from the smaller-scale experiments. By comparing all these data to 2D simulations it was conjectured that the blockage ratio was more important for $L_{\mathrm{DDT}}$ than the actual geometry. Two-dimensional simulations also ignored effects of 3D turbulence that may become more important for larger systems. Any heat losses to the walls that remained unmeasured in experimental systems were also ignored by the adiabatic model. Although a one-step chemistry model was used that had been calibrated with experimental data for both flames and detonations, the model was obviously too simple to ensure the calibration would be ideal. Finally, the intrinsic stochasticity of the DDT process resulted in uncertainties of $L_{\mathrm{DDT}}$. For the type of geometries considered here, the stochastic variation of $L_{\mathrm{DDT}}$ in simulations was about three obstacle spacings but was still not systematically measured in experiments.

Despite all these approximations, limitations, and uncertainties, comparisons between existing experimental data and the simulations showed that the models were good enough to reproduce key experimental observations. Since experimental data on DDT in methane-air systems are currently available only up to a 1 m scale, the computed scaling law remains the only way to predict DDT distances in methane-air mixtures on larger scales.

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