Approaching Detonation Dynamics as an Ensemble of Interacting Waves

Andrew J. Higgins¹

¹McGill University Montreal, Canada

1 Introduction

The success of the Chapman-Jouguet solution to the governing conservation laws in describing detonation propagation is remarkable, and the conceptual picture of a detonation wave as a quasi-steady control volume bounded by a normal shock upstream and a sonic plane downstream continues to be the basis of almost all models of detonation propagation. In gases, the propagation speeds of detonation waves are usually within 1% of the CJ solution predicted by an equilibrium solver. Other equilibrium properties, such as the post-detonation pressure, are similarly well predicted by the CJ conditions. Even in the few exceptional cases of so-called pathological detonations, where the excursion from the equilibrium CJ velocity is not more than a few percent, the CJ equilibrium sonic condition is replaced with an analogous generalized CJ condition. [1,2] The fact that the CJ solution works so well has led it to be termed the "Rock of Gibraltar" of the detonation field by Shepherd [3], and Fay [4] has gone so far as to suggest that the success of the Chapman and Jouguet solution might have discouraged the further development of detonation theory.

The experimental agreement with the CJ solution is striking, given that all known gaseous detonations have a multidimensional and transient cellular structure that is seemingly inconsistent with the quasisteady nature of the CJ solution. Detonation cellular structure is now recognized as being the characteristic length scale that describes the dynamics of detonations, including the initiation, propagation limits, and response to changes in boundary conditions. Indeed, using the cell size as the characteristic length scale has resulted in a collection of highly practical, semi-empirical relations to predict the critical energy required for direct initiation [5], the response of detonations to propagation in small diameter channels [6, 7], the critical dimension required for transition from confined to unconfined detonation [8, 9], and transition from deflagration to detonation with confinement [10, 11]. Detailed studies of detonation cellular dynamics have revealed that most of the energy release in the detonation cell of hydrocarbon fuels in air or oxygen occurs in very concentrated pockets, often associated with the transverse shock waves and associated shear layers that define the cell boundaries. [12, 13] Indeed, kinetics calculations of a fluid element processed by the decaying shock front of a detonation cell show that the heat release zone decouples from the leading shock for the latter half of the cell cycle, meaning that the shock front is essentially an inert, decaying blast for approximately half of the cell cycle, a result that has been known since the work of Lundstrom and Oppenheim in the late 1960's [14]. The instantaneous velocity of the detonation front can vary from 50% to 200% of the average propagation speed [15], which is well predicted by the CJ solution as described above. The usual explanation provided to explain this finding is that, despite the rich dynamics of the detonation wave structure, the wave on the whole and in the average must still satisfy the conservation laws, and thus the CJ solution remains valid.

Approaching Detonation Dynamics as an Ensemble of Interacting Waves

Since the transient and multidimensional structure of detonation waves governs the dynamics of their propagation, elucidating detonation wave structure has been a unifying goal of detonation research for the last several decades, a period that has seen the rise of computational simulation join experimental and theoretical methods. Since the pioneering simulations of Taki and Fijiwara [16] and Oran, Boris, and co-workers [17, 18] in the late 1970's and early 1980's that computationally reproduced cellular structure for the first time, successive decades have seen the dynamics and structure of detonation waves illuminated in greater and greater detail. Following the progression of Moore's Law, increasing computational resolution has revealed an incredibly intricate dynamics associated with the coupling between the transverse shock complex, shear layer, and chemical energy release process that defines the cellular structure of a detonation. This progression of research has led to a situation wherein advances in understanding of detonation dynamics are tied to computational power, with simulations done only a few years ago now considered obsolete. Two-dimensional simulations in recent years by Mahmoudi, Mazaheri, and co-workers have pushed the computational resolution of simulations to as great as 10^3 to 10^4 computational cells over the length of the reaction zone of detonations with activation energies $\frac{E_a}{BT_a} = 20$. [19–21] These simulations have revealed a transverse wave structure consisting of complex shock reflections and shear layers that are able to jet forward and re-kink the leading shock front, resulting in additional shock interactions and shear layers, a mechanism first identified by Mach and Radulescu [22]. Mixture energy release is associated with intense turbulent burning occurring along the shear layers and on the edges of unburned pockets that detach from the shock front. Increasing the activation energy further (to values representative of real, detonable hydrocarbon mixtures) would necessitate even greater numerical resolution. A little-reported but often-encountered phenomenon in 2-D Euler calculations with values of activation energy representative of hydrocarbon-based mixtures is that detonations in these simulations often fail to propagate as the computational grid is further refined, suggesting that 3-D or Navier-Stokes (or both) models must be considered to correctly capture the mechanism of burning in the detonation, which would be a daunting task computationally. Indeed, a fully converged, 3-D direct numerical simulation of the Navier-Stokes equations simulating the larger scales of turbulence coupled to detailed chemistry at Reynolds numbers representative of detonations is likely to remain beyond computational capability for at least another decade. [23] This state of research presents a somber challenge to further development of detonation theory, both before and after this "exascale" computational milestone is passed.

This paper will suggest some possible approaches to developing a theoretical approach to describing detonation dynamics that is largely independent of the underlying mechanism of energy release, by drawing upon ideas in statistical mechanics. The detonation will be viewed as a wave that propagates by an interacting ensemble of blast waves driven by discrete, energetic sources. As a conceptual guide, imagine a mixture of sensitive acetylene and oxygen, heavily diluted with inert nitrogen. If the acetylene and oxygen molecules were collected together into concentrated sheets, separated by layers of pure nitrogen, then this one-dimensional system would propagate as a sequence of "sympathetic detonations" that are triggered by blast waves transmitted from the previous sheet (Fig. 1(b)). This conceptual model could be extended into multidimensions if the acetylene/oxygen was concentrated into pockets embedded in nitrogen (Fig. 1(c)). If the placement of these pockets of gas is randomized in space, the picture becomes a conceptual link to multidimensional detonation propagation in mixtures with highly irregular cellular structure (Fig. 1(d)). Treatment of this problem will be done using heuristic or *ad hoc* methods in order to make the solution analytically tractable. This approach will come at the expense of working with models that do not derive rigorously from the governing conservation laws.

This concept of examining the asymptotic limit of discretized energy sources has been explored for the case of heterogeneous combustion in recent years. [24, 25] While heterogeneous combustion is a well-developed field, it usually treats the reactive medium as being spatially uniform, averaging out the effect of the discretized nature of energy sources, and the particulate nature of the sources only



Figure 1: Schematic of an explosive medium with (a) source energy uniformly distributed and with source energy collected into (b) planar sheets, (c) regular array of point-like sources, or (d) random array of point-like sources.

appears in the diffusion-limited reaction rate law. This averaging approach may not always be justified, however, and models that take into account the local, spatial diffusion of heat from source to source have identified unique behavior. An example of such a prediction is the independence of flame propagation in suspensions of fuel particles on the oxygen concentration and particle burning time for the case of a fast-burning particle in a low diffusivity oxidizer, a result that has now been verified by experiments. [26, 27] This approach is now termed "discrete combustion," and has revealed links with reactive wave propagation in other fields, such as calcium wave signaling in biological cells, a problem that has been shown to be mathematically identical to flame propagation in systems of discrete sources. [28–30] The remainder of this paper will outline a similar approach to detonation.

2 Literature Review

The consideration of discrete effects in detonation propagation has been suggested previously by a number of researchers, which will be briefly recounted here. One of the earliest attempts to develop a model of a cellular detonation is that of Vasiliev and Nikolaev [31], who recognized the similarity between the cell cycle resulting from the local explosion-like release of energy at the start of a cell, which is associated with the collision of transverse waves from neighboring cells, and blast wave propagation. Vasiliev and Nikolaev did not, however, consider the statistical aspects of ensemble interactions of these blast-like waves.

Perhaps the clearest statement of the discrete detonation approach is that of Stewart and Asay [32], who in examining the response of propellant beds comprised of explosive grains to strong shock stimuli, proposed a "theory of discrete interactions." Drawing inspiration from the bubble detonation experiments of

Higgins, A. J. Approaching Detonation Dynamics as an Ensemble of Interacting Waves

Fujiwara and others [33], they considered a chain of explosive grains that, upon being triggered by pressure waves, release their energy instantaneously as a blast wave. The subsequent interaction of sources were proposed to be described by a nonlinear recursion relation. Their preliminary exploration of this model identified a number of interesting features, including the existence of high-speed, high-pressure and low-speed, low-pressure wave regimes, depending on the model parameters.

In an unusual paper [34] and later book [35], Leiber pointed out a variety of phenomenon in detonation, such as the existence of cellular structure, irregular detonation fronts, the duality of low velocity and high velocity detonation in condensed-phase explosives, and critical diameter phenomenon, that cannot be described by classical detonation theory. He suggested that these processes can be described by treating detonation wave propagation as an assembly of monopole and dipole pressure sources. It is difficult to reconcile Leiber's approach, based on acoustic waves, with the inherent nonlinearity of the shock waves at comprise the detonation front.

A study by Morano and Shepherd [36] examined detonation propagation in a one-dimensional medium in which a spatial inhomogeneity was introduced in the form of a sinusoidal ripple in the reaction rate constant. The system they examined was tuned to match that of a solid explosive, with the inhomogeneity intended to play the role of a synthetic hot-spot. They noted a small ($\approx 2\%$) velocity decrement below the CJ speed as the amplitude of the perturbation in reaction rate approached 100%. This approach has recently been expanded upon to two-dimensional spatial inhomogeneities (perturbations in density/temperature, rather than reaction rate) in a study by Li et al. [37] Extension of this approach to two-dimensional and three-dimensional spatially randomized inhomogeneities is essentially the strategy being suggested in this paper.

3 A Sample Problem: Discrete Detonation in One-Dimension

As a demonstration of the discrete source approach, the problem of detonation propagation in a onedimensional system consisting of infinitely thin sheets of energy release separated by layers of inert gas will be considered (Fig. 1(b)). The sheets are assumed to remain fixed (as if attached to the tube wall) and do not move with the passage of the shock front or subsequent gas motion. The sheets of source energy are assumed to be triggered by the passage of the shock front and, after a fixed delay time, are triggered to release their energy. The released energy then drives a blast wave outward, both forward in the direction of propagation and backward towards previously triggered sources.

An approximate, heuristic solution to this problem for the case where the delay time is taken to the limit of zero delay can be found based on the similarity solution for the planar version of the well-known point-blast solution of Taylor and Sedov. [38] The motion of the shock front x_s is given by

$$\frac{dx_{\rm s}}{dt} = \sqrt{\frac{E_0}{\rho_0 B}} x_{\rm s}^{-\frac{1}{2}} \tag{1}$$

where E_0 is the energy of a given source, ρ_0 the initial density of the medium, B is a dimensionless energy parameter depending on the specific heat capacity ratio γ .

Since the source releases its energy at the shock front originating from the previous source, the partitioning of blast energy into forward and backward propagating blast waves can be estimated as follows. If the mechanism of source energy deposition is assumed to be two massless pistons, one that pushes outward into the undisturbed gas ahead of the blast and the other the pushes into the gas behind the blast from the prior source, the pressure on both piston faces must be equal (since, being massless, they can exert no net force on the flow). This condition permits the ratio of piston velocities to be solved for and, Approaching Detonation Dynamics as an Ensemble of Interacting Waves

Higgins, A. J.

since the pistons must act for the same duration of time to conserve momentum, this ratio also determines the ratio of work done. In the limit of strong shock relations, the equal pressure condition permits the partitioning of energy into forward and backward propagating blasts to be expressed analytically as a function of γ

$$\eta = \frac{E_{\text{forward}}}{E_0} = \frac{1}{\sqrt{\frac{\gamma - 1}{\gamma + 1}} + 1} \tag{2}$$

Since only ηE_0 contributes to the forward propagating blast, the equation describing the motion of the leading shock front needs to be modified

$$\frac{dx_{\rm s}}{dt} = \sqrt{\frac{\eta E_0}{\rho_0 B}} x_{\rm s}^{-\frac{1}{2}} \tag{3}$$

Interestingly, this is the same partition of blast energy found by Sakuri [39] in examining blast wave energy release at a stationary density interface (as opposed to energy release at a moving shock front in the current problem).



Figure 2: The one-dimensional discrete-source detonation propagation problem, as an x-t (space-time) diagram. In the inset, the energy deposition at each source is assumed to occur via the impulsive motion of two outward-facing pistons. Equal pressure is required on both piston faces (by momentum conservation), permitting the partitioning of energy into forward and backward directed blast waves to be determined.

Following the release of source energy, the subsequent blast wave motion is additionally influenced by the particle velocity that was imposed by the blast wave from the previous source. This problem (in position-time space) is analogous via hypersonic similarity to the two-dimensional hypersonic flow past a blunted wedge, a problem previously treated by Chernyi [40]. The blunt leading edge of the wedge represents the instantaneous energy release of the source under the hypersonic blast wave analogy, and the surface of the wedge represents the particle motion imposed by the previous blast wave (as determined by the blast strength from the previous source as it reached the new source). Considering the energy partitioned into the forward propagating blast and the particle motion imposed by the previous

source, the motion of the blast wave propagation from one source to the next (x_s from 0 to L, where L is the spacing between two adjacent discrete sources) is given by:

$$\frac{dx_{\rm s}}{dt} = \sqrt{\frac{\eta E_0}{\rho_0 B} x_{\rm s}^{-\frac{1}{2}} + u_{\rm p}(x_{\rm s})} \tag{4}$$

where u_p is the particle velocity carried forward from the previous source. When the blast wave generated by the previous source just reaches the current source, i.e., $x_s = 0$, u_p can be approximated as the piston velocity required to sustain the shock front moving at its instantaneous velocity,

$$u_{\mathrm{p},0} = \frac{2}{\gamma+1} \sqrt{\frac{\eta E_0}{\rho_0 BL}} \tag{5}$$

As the blast wave propagates to the next source, the influence of the previous source on the particle motion should diminish. In order to consider this effect, u_p is modeled to be inversely proportional to x_s ,

$$u_{\rm p}(x_{\rm s}) = \frac{L}{x_{\rm s} + L} u_{p,0} \tag{6}$$

This simple approximation can be justified by the fact that the particle velocity profile of a blast wave is approximately linear. Thus, the approximate, analytic solution of the leading shock wave propagation from one discrete source to the next can be obtained by integrating (4) with (5) and (6).



Figure 3: The propagation of detonation in the discrete source system, showing (a) the evolution of the shock pressure of the front for the case of $\gamma = 1.666$ and $\frac{\Delta q}{RT_0} = 50$ and (b) the average velocity obtained after the source has propagated through a sufficient number of sources to reach a steady average velocity. The dashed curve is the heuristic model with zero delay of the source triggering, based upon the similarity solution with blast propagation and blast energy partitioning. The solid curve in (a) and solid curve with data points in (b) are results of a computational simulation of the Euler equations where energy is added via a pressure boost in a small (5%) region of the computational domain. Calculations performed by Xiaocheng Mi.

Figure 3(a) shows the pressure history of the shock front predicted by this model for the particular case of $\gamma = 1.666$ and source energy equivalent to a homogeneous energy release of $\frac{\Delta q}{RT_0} = 50$. Note that each successive blast wave is stronger than the previous one (most easily seen by examining the minimum in shock pressure immediately prior to the triggering of new sources), exhibiting the recursive build-up resulting from successive blast wave interactions. The final average propagation velocity after

propagating through a large number of sources is plotted in Fig. 3(b) as a function of the ratio of specific heats and normalized by the initial sound speed. Also plotted is the CJ detonation solution for the equivalent homogenized energy release, given by

$$M_{\rm CJ} = \sqrt{\left(\frac{\gamma^2 - 1}{\gamma}\right)\frac{E_0}{Lp_0} + \sqrt{\left[\left(\frac{\gamma^2 - 1}{\gamma}\right)\frac{E_0}{Lp_0} + 1\right]^2 - 1} + 1}$$
(7)

where p_0 is the initial pressure of the medium.

The velocity of the wave is seen to be qualitatively similar to the Chapman Jouguet velocity, but always greater than the CJ speed. The deviation of the results of this model away from the CJ solution decreases as the value of γ increases.

In order to compare this heuristic model to a fully unsteady solution of the governing Euler equations, computational fluid dynamics (CFD) is employed. The code used a second-order accurate total variation diminishing scheme and MUSCL-Hancock approach based on Godunov's flux-difference splitting with van Leer non-smooth slope limiter. Computational simulation of this problem necessitates that the sources be spatially discretized and, as a result, must be spread out over a minimum of 50 computational cells (about 5% of the domain from the start of one source to the next). The source energy in these simulations is added by increasing the pressure to result in an energy addition according to:

$$\Delta p = \frac{(\gamma - 1)E_0}{w} \tag{8}$$

where w is the volume occupied by each discrete source.

Simulations can also be extended to examine sources with finite widths between 5% discrete up to sources that are spatially continuous. While the CFD simulations do not exhibit as large of a deviation from the CJ solution as the heuristic model discussed above, the observed trend to decreasing super-CJ velocities as the value of γ increases is qualitatively the same as that in the heuristic model.

Further simulations have shown that if the sources are spread out to occupy more than about 30% of the domain, the deviation away from CJ becomes less than 2% for values of $1.2 < \gamma < 1.666$. This result may provide some explanation of the success of the Chapman Jouguet condition for cellular detonations, which concentrate the energy release within approximately the first one third of the cell cycle, and thus we would not expect a significant deviation from the CJ value for this amount of discreteness. If the source energy release in the simulations is made spatially continuous (i.e., no longer concentrated in pockets separated by inert gas), then the average wave velocity converges to the CJ velocity exactly.

An earlier examination of the discrete source detonation problem using an analog system based on the Burgers equation did not find any deviation from the analogous CJ solution for the equivalent homogenous system. [41] In the Burgers equation system, taking the limit to zero delay time and δ -function-like sources, the resulting quasi-steady propagation speed can be shown to be identical to that of the analogous CJ solution of the homogenized medium. Exact solutions considering both fixed and random delays also showed that the wave average propagation speed converged to within 1% of the analogous CJ solution of the homogenized medium. [41] The fact that a fundamentally different qualitative solution was obtained in the Burgers equation-based analog system (which agree with the CJ solution) compare to the Euler-equation based system (which exhibit super-CJ velocities, as discussed above) should serve as a caveat to analog studies, namely, that results obtained in analog systems may not always carry over to the actual system of interest.

4 Toward Multidimensional Problems

The extension of the ansatz proposed in the previous section to multidimensions is only in its nascent development, but this approach can draw upon previously established formalisms from statistical mechanics, such as percolation theory. In multidimensional models, more interesting problems beyond just quantifying the average propagation velocity can be examined, such as how the detonation responds to area change (the critical diameter problem of gaseous detonation) or yielding confinement (the critical diameter problem for condensed-phase explosives). Even in these cases, however, average propagation velocity continues to be a convenient parameter to quantify the detonation, simply because it is easy and unambiguous to measure.

A preliminary exploration of detonation propagation through a three-dimensional random array of pointlike energy sources was performed by the author in 2009. [42] In this study, each source was assumed to generate a spherical blast wave described by the Taylor-Sedov similarity solution, and linear superposition of these blast waves was used, with new sources being triggered upon reaching a designated pressure activation value. This model was used to examine the dimensional scaling between propagation in cylindrical clouds and slab-shaped clouds comprised of point-like sources.

The dimensional scaling problem has received attention in recent years in both gaseous [43–45] and condensed-phase detonations [46–49]. In the presence of losses at the perimeter of the detonable media, for example due to boundary layer growth or yielding confinement, a detonation wave exhibits an increasing velocity deficit as the transverse dimension (diameter or thickness) of the charge is reduced. If a detonation wave is governed by global front curvature, such as in the classical model of Wood and Kirkwood [50], then the scaling between these two geometries should be approximately 2:1, meaning the same detonation velocity observed in a tube of diameter d would be observed in a wide aspect ratio channel of thickness t = d/2, since the detonation in a channel only experiences curvature on one axis, while within the tube it is equally curved on both orthogonal axes. [51] Experiments in heavily argondiluted mixtures in porous walled channels have shown a scaling that is indeed about 2:1, reinforcing the hypothesis that detonation in these mixtures is a laminar, shock-induced-combustion-like mechanism. [43, 44] Mixtures with highly irregular structure do not obey this scaling, however, suggesting their propagation mechanism is dominated by local interaction of transverse waves. A related problem is the critical diameter problem in gases, wherein a detonation emerges from a tube (or channel) into an unconfined environment, either to fail (if below a critical dimension) or continues to propagate (if supercritical). [52] Although this is a highly unsteady problem (as opposed to quasi-steady propagation in a channel), the scaling between the axisymmetric (critical diameter) and two-dimensional (critical slot) problems might be expected to take on a value of 2:1 if the front is controlled by its global curvature. [52, 53] Indeed, studies examining mixtures with heavy argon dilution have recovered a scaling of approximately 2:1, while mixtures characterized by an irregular cellular structure consistently exhibit a scaling of approximately 4:1. [45]

The study of Higgins [42] examining the propagation of detonation as an ensemble of interacting blast waves originating from point-like energy sources in random arrays of the two different geometries (cylindrical and slab) found that a 4:1 scaling was obtained if the sources were sensitive to initiation, meaning that a new source could be triggered from a single blast wave from a previously initiated source. This problem is essentially that of *continuum percolation* (see an introduction by Torquato [54]), wherein overlapping spheres from each source with a radius corresponding to the critical shock strength necessary to initiate a new source form a cluster of connected spheres that span the explosive domain. As the shock strength necessary to initiate a new source was increased (beyond that which can be generated by a single blast), then multiple shock interactions are necessary to trigger a new source. Propagation in this case becomes more of a collective or global phenomenon, and the simulations in this case appeared

Approaching Detonation Dynamics as an Ensemble of Interacting Waves

to converge to a scaling between cylindrical and slab geometries of 2:1, recovering the expected scaling of classical, front curvature-governed detonations.

The original study of Higgins [42] considered a simple pressure "switch" criterion to activate new sources and used simple linear superposition of the blast waves. Use of linear superposition for the strong shock waves that comprise blast fronts is a gross oversimplification. This fact motivated Higgins and Mehrjoo [55] to repeat these calculations using the so-called Low Altitute Multiple Blast (LAMB) approximation, which asserts to be an analytic method for nonlinear superposition of blast waves. [56,57] The inclusion of the LAMB superposition method did not qualitatively affect the results: in the case of a highly discrete mode of propagation, a 4:1 scaling was obtained between cylindrical and slab-like clouds of sources, while a 2:1 scaling was recovered as the sources were made insensitive, resulting a global, front-curvature-governed mode of propagation. The fact that this result was obtained independent of the method of treating the interacting blast waves (linear superposition *vs.* LAMB non-linear superposition) suggests that this result may be insensitive to the particular details of the shock interactions and source initiation criterion.

Ultimately, the problem of detonation propagation in discrete media needs to be simulated using the full, multidimensional Euler equations. A first step in this direction was recently reported by Li et al. [37] In this study, a spatial inhomogeneity was introduced via a sinusoidal ripple in density and temperature, and detonation propagation in layers of explosive gas bounded by inert gas was examined near the critical thickness of the layer. The use of a sinusoidal inhomogeneity is a computationally easier problem than that of having to resolve point-like discrete sources. A pressure-dependent reaction rate model was used so as to avoid the extreme state sensitivity of the Arrhenius reaction rate. Although pressure-depended reaction rates ($r \sim p^n$) with a pressure exponent sufficiently large to exhibit critical behavior ($n \gtrsim 2$) are unstable [58], these instabilities only appear at very high computational resolution, enabling a laminar-like wave structure to be realized. This study showed that shock interactions resulting from inhomogeneous explosive. Extensions of this study to three dimensions with both spatially regular and irregular (random) inhomogenities would be of great interest to see if percolation-like behavior is observed.

5 Concluding Remarks

If advances in understanding of detonation dynamics continue to originate in simulations of the governing conservation laws coupled with detailed chemistry conducted with ever increasing computational resolution, riding along the curve of Moore's Law, then there is likely little ability for theory to make a contribution in the coming decade. Following the epoch of fully resolved simulations of compressible, reactive turbulence, expected to occur after the next decade, there may simply be no need for detonation theory at all. To date, the successful applications of theory to detonation wave propagation has mainly been in the area of normal mode stability analysis, originating with Erpenbeck [59], which can predict the onset of instability and subsequent early dynamics, when the instability is in the linear regime. For fully developed unstable detonations, the formalism of nonlinear dynamics (e.g., phase-space trajectories, limit cycles, Lyapunov exponents, bifurcation diagrams, etc.) has found some application in describing the dynamics of detonations propagating in one-dimension. [60–63] The nonlinear dynamics paradigm, however, is limited to low-dimensional systems, and thus it is unclear how to extend these results to multidimensional transient systems. Another approach that might be profitably explored in understanding detonation dynamics is fractal analysis, which is well-suited to describing the inherent cascading scales of turbulence. [63–65] The approach suggested in this paper and accompanying talk follows from ideas in percolation theory, wherein the detonation is viewed as discrete pockets of energy release randomly distributed in space that must connect in order for the wave to propagate. For

detonations in a gaseous medium with an irregular cellular structure (e.g., hydrocarbon fuels in air), this spatial randomness arises from the instability of the wave itself, even though the gaseous mixture is perfectly uniform. This approach might also be able to explain features of detonation in heterogeneous explosives, which have an intrinsic spatially discrete and random structure, as suggested by the author in [66]. Percolation theory has found application in modeling of diffusion flames [67] and heterogeneous propellants [68, 69], and it is possible that these approaches might illuminate the problem of detonation dynamics in gaseous and heterogeneous explosives as well.

Acknowledgements

The author would like to acknowledge the seminal role of Samuel Goroshin, who has long championed recognition of the role of discrete effects in heterogeneous combustion. Sam challenged the author to consider a discrete approach to detonation more than 15 years ago and has maintained a continuous, coercive pressure ever since. A number of extended discussions with John Lee, Matei Radulescu, Vincent Tanguay, and Charles Kiyanda provided impetus along the way. Oren Petel's Masters thesis at McGill generated earlier experimental stimulation for us to consider discrete effects in heterogeneous explosives, and many of Oren's ideas are reflected here. My sabbatical leave with Vitali Nesterenko at UC San Diego in 2010-2011 gave me the opportunity to explore these ideas from a materials science perspective. Computational and analytical simulations done by Evgeny Timofeev, Mehshan Javaid, and Navid Mehrjoo contributed to these studies. Finally, Xiaocheng Mi has taken up the torch on this problem and carried it much farther than I could have hope for or imagined. I look to him for many exciting advances yet to come.

References

- [1] J. Dionne, R. Duquette, A. Yoshinaka, and J. Lee, "Pathological detonations in H₂-Cl₂," *Combustion Science and Technology*, vol. 158, no. 1, pp. 5–14, 2000.
- [2] A. Higgins, "Steady one-dimensional detonations," in *Shock Waves Science and Technology Library*. Springer Berlin Heidelberg, 2012, vol. 6, pp. 33–105.
- [3] J. Shepherd, "Detonation in gases," 2008, presented at the Thirty-Second International Symposium on Combustion, Montreal, Canada.
- [4] J. Fay, "The structure of gaseous detonation waves," *Symposium (International) on Combustion*, vol. 8, no. 1, pp. 30–40, 1961.
- [5] J. Lee, "Initiation of gaseous detonation," *Annual Review of Physical Chemistry*, vol. 28, no. 1, pp. 75–104, 1977.
- [6] O. Peraldi, R. Knystautas, and J. Lee, "Criteria for transition to detonation in tubes," *Symposium* (*International*) on Combustion, vol. 21, no. 1, pp. 1629 1637, 1988.
- [7] Y. Gao, H. Ng, and J. Lee, "Minimum tube diameters for steady propagation of gaseous detonations," *Shock Waves*, vol. 24, no. 4, pp. 447–454, 2014.
- [8] J. Lee, "Dynamic parameters of gaseous detonations," Annual review of fluid mechanics, vol. 16, no. 1, pp. 311–336, 1984.

- [9] —, "On the critical diameter problem," in *Dynamics of Exothermicity*, J. Bowen, Ed. Gordon and Breech Publishers, Netherlands, 1996, pp. 321–336.
- [10] S. Dorofeev, V. Sidorov, M. Kuznetsov, I. Matsukov, and V. Alekseev, "Effect of scale on the onset of detonations," *Shock Waves*, vol. 10, no. 2, pp. 137–149, 2000.
- [11] G. Ciccarelli and G. Dorofeev, "Flame acceleration and transition to detonation in ducts," *Progress in Energy and Combustion Science*, vol. 34, no. 4, pp. 499 550, 2008.
- [12] M. Radulescu, G. Sharpe, J. Lee, C. Kiyanda, A. Higgins, and R. Hanson, "The ignition mechanism in irregular structure gaseous detonations," *Proceedings of the Combustion Institute*, vol. 30, no. 2, pp. 1859 – 1867, 2005.
- [13] C. Kiyanda and A. Higgins, "Photographic investigation into the mechanism of combustion in irregular detonation waves," *Shock Waves*, vol. 23, no. 2, pp. 115–130, 2013.
- [14] E. A. Lundstrom and A. K. Oppenheim, "On the influence of non-steadiness on the thickness of the detonation wave," *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, vol. 310, no. 1503, pp. 463–478, 1969.
- [15] R. Strehlow and A. Crooker, "The structure of marginal detonation waves," Acta Astronautica, vol. 1, no. 3-4, pp. 303 – 315, 1974.
- [16] S. Taki and T. Fujiwara, "Numerical analysis of two-dimensional nonsteady detonations," AIAA Journal, vol. 16, no. 1, pp. 73–77, 1978.
- [17] E. Oran, J. Boris, T. Young, M. Flanigan, T. Burks, and M. Picone, "Numerical simulations of detonations in hydrogen-air and methane-air mixtures," *Symposium (International) on Combustion*, vol. 18, no. 1, pp. 1641 – 1649, 1981.
- [18] K. Kailasanath, E. Oran, J. Boris, and T. Young, "Determination of detonation cell size and the role of transverse waves in two-dimensional detonations," *Combustion and Flame*, vol. 61, no. 3, pp. 199–209, 1985.
- [19] Y. Mahmoudi and K. Mazaheri, "High resolution numerical simulation of the structure of 2-D gaseous detonations," *Proceedings of the Combustion Institute*, vol. 33, no. 2, pp. 2187 2194, 2011.
- [20] K. Mazaheri, Y. Mahmoudi, and M. Radulescu, "Diffusion and hydrodynamic instabilities in gaseous detonations," *Combustion and Flame*, vol. 159, no. 6, pp. 2138 – 2154, 2012.
- [21] Y. Mahmoudi, K. Mazaheri, and S. Parvar, "Hydrodynamic instabilities and transverse waves in propagation mechanism of gaseous detonations," *Acta Astronautica*, vol. 91, pp. 263 – 282, 2013.
- [22] P. Mach and M. Radulescu, "Mach reflection bifurcations as a mechanism of cell multiplication in gaseous detonations," *Proceedings of the Combustion Institute*, vol. 33, no. 2, pp. 2279 – 2285, 2011.
- [23] J. Slotnick, K. A., J. Alonso, D. Darmofal, W. Gropp, E. Lurie, and D. Mavriplis, "CFD vision 2030 study: a path to revolutionary computational aerosciences," Tech. Rep. NASA/CR-2014-218178, 2013.
- [24] S. Goroshin, J. Lee, and Y. Shoshin, "Effect of the discrete nature of heat sources on flame propagation in particulate suspensions," *Proceedings of the Combustion Institute*, vol. 27, no. 1, pp. 743–749, 1998.

- [25] A. Mukasyan and A. Rogachev, "Discrete reaction waves: Gasless combustion of solid powder mixtures," *Progress in Energy and Combustion Science*, vol. 34, no. 3, pp. 377–416, 2008.
- [26] S. Goroshin, F. Tang, and A. Higgins, "Reaction-diffusion fronts in media with spatially discrete sources," *Physical Review E*, vol. 84, no. 2, p. 027301, 2011.
- [27] A. Wright, S. Goroshin, and A. Higgins, "An attempt to observe the discrete flame propagation regime in aluminum dust clouds," in 25th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2015.
- [28] J. Keizer, G. Smith, S. Ponce-Dawson, and J. Pearson, "Saltatory propagation of Ca²⁺ waves by Ca²⁺ sparks," *Biophysical Journal*, vol. 75, no. 2, pp. 595–600, 1998.
- [29] I. Mitkov, "One-and two-dimensional wave fronts in diffusive systems with discrete sets of nonlinear sources," *Physica D: Nonlinear Phenomena*, vol. 133, no. 1, pp. 398–403, 1999.
- [30] F. Tang, A. Higgins, and S. Goroshin, "Propagation limits and velocity of reaction-diffusion fronts in a system of discrete random sources," *Physical Review E*, vol. 85, p. 036311, Mar 2012.
- [31] A. Vasiliev and Y. Nikolaev, "Closed theoretical model of a detonation cell," Acta Astronautica, vol. 5, no. 11-12, pp. 983–996, 1978.
- [32] D. Stewart and B. Asay, "Discrete modeling of beds of propellant explosed to strong stimulus," in *Dynamical issues in combustion theory*, ser. IMA volumes in mathematics and its applications, P. Fife, A. Liñán, and F. Forman, Eds. Springer, 1991, vol. 35.
- [33] T. Hasegawa and T. Fujiwara, "Detonation in oxyhydrogen bubbled liquids," Symposium (International) on Combustion, vol. 19, no. 1, pp. 675 – 683, 1982, nineteenth Symposium (International) on Combustion.
- [34] C.-O. Leiber, "Physical model of explosion phenomena physical substantiation of kamlet's complaint," *Propellants, Explosives, Pyrotechnics*, vol. 26, no. 6, pp. 302–310, 2001.
- [35] C. Leiber, Assessment of safety and risk with a microscopic model of detonation. Elsevier, 2003.
- [36] E. Morano and J. Shepherd, "Effect of reaction rate periodicity on detonation propagation," AIP Conference Proceedings, vol. 620, no. 1, pp. 446–449, 2002.
- [37] J. Li, X. Mi, and A. Higgins, "Effect of spatial heterogeneity on near-limit propagation of a pressure-dependent detonation," *Proceedings of the Combustion Institute*, vol. 35, no. 2, pp. 2025– 2032, 2015.
- [38] D. Jones, "Strong blast waves in spherical, cylindrical, and plane shocks," *Physics of Fluids*, vol. 4, no. 9, pp. 1183–1184, 1961.
- [39] A. Sakurai, "Blast wave from a plane source at an interface," *Journal of the Physical Society of Japan*, vol. 36, no. 2, pp. 610–610, 1974.
- [40] G. Chernyi, Introduction to hypersonic flow. Academic Press, 1961.
- [41] X. Mi and A. Higgins, "Influence of discrete sources on detonation propagation in a burgers equation analog system," *Phys. Rev. E*, vol. 91, p. 053014, May 2015.
- [42] A. Higgins, "Detonation propagation as a system of randomized discrete energy sources," in 22nd International Colloquium on the Dynamics of Explosions and Reactive Systems, 2009.

- [43] M. Radulescu and J. Lee, "The failure mechanism of gaseous detonations: experiments in porous wall tubes," *Combustion and Flame*, vol. 131, no. 12, pp. 29 – 46, 2002.
- [44] M. Radulescu, "The propagation and failure mechanism of gaseous detonations : experiments in porous-walled tubes," Ph.D. dissertation, McGill University, 2003.
- [45] J. Meredith, H. Ng, and J. Lee, "Detonation diffraction from an annular channel," *Shock Waves*, vol. 20, no. 6, pp. 449 – 455, 2010.
- [46] O. Petel, D. Mack, A. Higgins, R. Turcotte, and S. Chan, "Minimum propagation diameter and thickness of high explosives," *Journal of Loss Prevention in the Process Industries*, vol. 20, no. 4–6, pp. 578 – 583, 2007.
- [47] V. Sil'vestrov, A. Plastinin, S. Karakhanov, and V. Zykov, "Critical diameter and critical thickness of an emulsion explosive," *Combustion, Explosion, and Shock Waves*, vol. 44, no. 3, pp. 354–359, 2008.
- [48] A. Higgins, "Measurement of detonation velocity for a nonideal heterogeneous explosive in axisymmetric and two-dimensional geometries," *AIP Conference Proceedings*, vol. 1195, no. 1, pp. 193–196, 2009.
- [49] S. Jackson and M. Short, "Scaling of detonation velocity in cylinder and slab geometries for ideal, insensitive and non-ideal explosives," *Journal of Fluid Mechanics*, vol. 773, pp. 224–266, 2015.
- [50] W. Wood and J. Kirkwood, "Diameter effect in condensed explosives. the relation between velocity and radius of curvature of the detonation wave," *The Journal of Chemical Physics*, vol. 22, no. 11, pp. 1920–1924, 1954.
- [51] J. Li, X. Mi, and A. J. Higgins, "Geometric scaling for a detonation wave governed by a pressuredependent reaction rate and yielding confinement," *Physics of Fluids*, vol. 27, no. 2, 2015.
- [52] W. Benedick, R. Knystautas, and J. Lee, "Large-scale experiments on the transmission of fuel-air detonations from two-dimensional channels," in *Progress in Astronautics and Aeronautics*, vol. 94, 1984, pp. 546–555.
- [53] J. Lee, *The Detonation Phenomenon*. Cambridge University Press, 2008.
- [54] S. Torquato, *Random Heterogeneous Materials: Microstructure and Macroscopic Properties*, ser. Interdisciplinary applied mathematics. Springer Science & Business Media, 2002, vol. 16.
- [55] A. Higgins and N. Mehrjoo, "Multidimensional detonation propagation modeled via nonlinear shock wave superposition," in *APS Division of Fluid Dynamics Meeting Abstracts*, vol. 1, 2010.
- [56] H. Brode, "Quick estimates of peak overpressure from two simultaneous blast waves," Tech. Rep. DNA 4503T, 2013.
- [57] C. Needham, "Modeling blast waves," in *Blast Waves*, ser. Shock Wave and High Pressure Phenomena. Springer Berlin Heidelberg, 2010, pp. 313–331.
- [58] M. Short, I. Anguelova, T. Aslam, J. Bdzil, A. Henrick, and G. Sharpe, "Stability of detonations for an idealized condensed-phase model," *Journal of Fluid Mechanics*, vol. 595, pp. 45–82, 2008.
- [59] J. Erpenbeck, "Stability of idealized onereaction detonations," *Physics of Fluids*, vol. 7, no. 5, pp. 684–696, 1964.

- [60] H. Ng, A. Higgins, C. Kiyanda, M. Radulescu, J. Lee, K. Bates, and N. Nikiforakis, "Nonlinear dynamics and chaos analysis of one-dimensional pulsating detonations," *Combustion Theory and Modelling*, vol. 9, no. 1, pp. 159–170, 2005.
- [61] H. Ng, M. Radulescu, A. Higgins, N. Nikiforakis, and J. Lee, "Numerical investigation of the instability for one-dimensional Chapman-Jouguet detonations with chain-branching kinetics," *Combustion Theory and Modelling*, vol. 9, no. 3, pp. 385–401, 2005.
- [62] A. Henrick, T. Aslam, and J. Powers, "Simulations of pulsating one-dimensional detonations with true fifth order accuracy," *Journal of Computational Physics*, vol. 213, no. 1, pp. 311 – 329, 2006.
- [63] H. Ng and F. Zhang, "Detonation instability," in *Shock Waves Science and Technology Library*. Springer Berlin Heidelberg, 2012, vol. 6, pp. 107–212.
- [64] F. Pintgen and J. Shepherd, "Quantitative analysis of reaction front geometry in detonation," in *International colloquium on application of detonation for propulsion*, 2004, pp. 23–28.
- [65] H. Ng, H. Ait Abderrahmane, K. Bates, and N. Nikiforakis, "Geometrical characterization of cellular irregularity of gaseous detonation front using a fractal approach," in 23rd International Colloquium on the Dynamics of Explosions and Reactive Systems, 2011.
- [66] A. Higgins, "Discrete effects in energetic materials," in *Journal of Physics: Conference Series*, vol. 500, no. 5. IOP Publishing, 2014, p. 052016.
- [67] N. Peters, "Laminar diffusion flamelet models in non-premixed turbulent combustion," *Progress in Energy and Combustion Science*, vol. 10, no. 3, pp. 319 339, 1984.
- [68] A. Kerstein, "Percolation model of polydisperse composite solid propellant combustion," *Combustion and Flame*, vol. 69, no. 1, pp. 95–112, 1987.
- [69] S. Gallier and J. Guery, "Regression fronts in random sphere packs: Application to composite solid propellant burning rate," *Proceedings of the Combustion Institute*, vol. 32, no. 2, pp. 2115 – 2122, 2009.