Numerical simulation of detonation wave propagation and quenching process in in-line crimped-ribbon flame arrester

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Abstract: A new numerical model for simulating the propagation and quenching of a detonation wave in in-line flame arrester was developed by using FORTRAN language. Accordingly, this study analysed the initiating process, quenching rule of a detonation wave in an arrester element and effect of arrester structural parameters on the propagation process of a detonation wave. Results showed that the quenching length of detonation wave increases with porosity, and the two parameters present a quadratic function relationship. Quenching length minimally varied with the increase in arrester thickness. The detonation wave collided with the element wall whilst porosity decreased when detonation wave propagated in the arrester element. Consequently, a pressure peak drop of the detonation wave was observed. As arrester thickness increased, the pressure peak of the detonation wave in the arrester element and the value of temperature on the position where the transmitted shock wave lies decreased, thereby cause a strong inhibition to the detonation wave. Simulation result showed that detonation pressure decreased progressively as porosity increased, and the two parameters exhibited a quadratic

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The research team focuses on the safety of petrochemical, chemical, biopharmaceutical, mining and other industrial production fields. The characteristics of typical industrial fires and explosion accidents, the industrial disaster accidents, the theoretical models of disaster processes and hazard analysis simulations, the process hazard characteristics, the equipment and safety control technologies were studied. Based on the theory of explosion mechanics, combustion, thermodynamics and kinetic theory of gases, theoretical analysis, experimental research and numerical simulation are combined to analyse the explosion process. The team has been engaged in the theoretical and simulation research of the detonation wave propagation and quenching process in in-line crimped-ribbon flame arrester. The research for detonation suppression technology and engineering in this paper is focused on the quenching mechanism of detonation wave in arrester element and effect of arrester structural parameters on the propagation process of detonation wave.

PUBLIC INTEREST STATEMENT

Modern industry is developing rapidly; thus, research on prevention and suppression of gas explosion of industrial medium has become an academic frontier project. Therefore, studying the suppression of combustion and explosion of flammable gas in pipelines is an important subject in safety technology, especially for the detonation phenomenon. However, less attention has been paid to detonation wave propagation in flame arrester to date. A flame arrester is a device permeable to gas flow that can quench both a flame and its combustion products sufficiently to prevent reignition at the arrester outlet. The present study aims to obtain further simulated data and discussion on the detonation wave propagation and quenching processes in crimped-ribbon flame arresters, such as the quenching rule of the detonation wave in the arrester element. The effect of porosity and element thickness on the propagation of detonation wave will also be investigated.
function relationship. By contrast, detonation pressure increased progressively as arrester thickness grew, and the two parameters presented a quadratic function relationship.

Subjects: Engineering & Technology; Mechanical Engineering Design; Technology

Keywords: numerical simulation; detonation wave; crimped-ribbon flame arrester; quenching length; porosity; element thickness

1. Introduction

A crimped-ribbon flame arrester is a device permeable to gas flow but impermeable to any flame. It can quench the flame and cool products sufficiently to prevent reignition at the arrester outlet (Grossel, 2002). Combustible gas explosions occur frequently in modern industry operations, thereby resulting in a significant number of casualties and amount of property losses. Therefore, studying the suppression of combustion and explosion of flammable gas in pipelines is an important subject in safety technology (Asano, Ikeda, Kagawa, & Youn, 2010; Beauvais, Mayinger, & Strube, 1994; Britton, 2000; Desai, 1996; Howard, 1982, 1988; Kawashima, Youn, & Kagawa, 2007; Lee, Knystautas, & Freiman, 1984; Lietze, 1995, 2002; Popp & Baun, 1997; Sun, Bi, Liu, & Liu, 2014; Sun et al., 2017), especially for the detonation phenomenon (Brochet, Brossard, Manson, Cheret, & Verdes, 1970; Camargo, Ng, Chao, & Lee, 2010; Carnasciali, Lee, Knystautas, & Fineschi, 1991, Eaton, Zhang, Berghorst, & Ng, 2012; Gamezo, Desbordes, & Oran, 1999; Kitano et al., 2009; Laberge, Knystautas, & Lee, 1993; Lee, Jesuthasan, & Ng, 2013; Lee & Matsui, 1977, Monwar, Ishii, & Tsuboi, 2009, Monwar, YamamotoO, Ishii, & Tsuboi, 2007).

A detonation wave is a supersonic combustion wave across which the thermodynamic states increase sharply. Scholars have conducted numerous studies on the detonation wave phenomenon, such as 2D and 3D cellular structures, development of detonation propulsion, e.g. oblique detonation engines (Teng, Jiang, & Ng, 2014; Teng, Ng, Kang, Luo, & Jiang, 2015, Yang, Ng, Teng, & Jiang, 2017), and detonation strength attenuation, through numerical methods. However, minimal attention has been accorded to detonation wave propagation in flame arrester to date.

As a result of heating the critical diameter of flame, quenching decreases and flame propagates through the porous flame-arresting element. The progress in filtration gas combustion has provided correct understanding of the reasons for flame arrester burning-through. The course of burning-through is flame propagation through the porous flame-arresting element in the low-velocity regime of filtration gas combustion (Babkin, 1993, 1999; Babkin & Laevskii, 1987; Kroshkina, 1984). On the basis of this conception, the burning-through laws of filled flame arresters were analysed in Kakutkina, Korzhavin, Namyatov, and Rychkov (2007b) by use of 1D approximation.

A method for numerical solution of the system was described in detail in Kakutkina, Korzhavin, and Rychkov (2009). The equation system that describes the propagation of a 1D unsteady combustion wave in a chemically inert porous flame arrester consisted of the equations of heat transfer for the gas and porous medium, mass transfer for the deficient component of the gas mixture, conservation of the total amount of materials in the flow and the equations of state for the gas. Kakutkina, Korzhavin, Namyatov, and Rychkov (2007a) used a numerical method and determined that a flame cannot propagate when the heat loss to the walls of the quenching element is significantly high and when the effective diameter of the quenching element is smaller than the critical diameter.

Systematisation and depth for the propagation theory of detonation wave in in-line flame arrester still present certain shortcomings. The relevant numerical simulation work is minimally reported given few complicated factors. For example, problems occur in the experiment and calculation considering a high nonlinearity in mathematics and multi-field coupling in physics.
The rapid development of computer fluid mechanics has required accurate numerical analysis to support and improve the detonation quenching theory of flame arresters.

Therefore, propane–air premixed gas is used in this study to develop mathematical and physical models for a detonation wave process in transient state induced by a premixed gas in the pipe flame arrester and a detonation quenching process of the arrester element. A numerical modeling research is conducted on the propagation process of the detonation inside an in-line crimped-ribbon flame arrester by using a theoretical model and numerical method.

The present study is aimed at obtaining further simulated data and discussion on the detonation wave propagation and quenching processes, such as variation rules of pressure, velocity, temperature and density during the initial stage of the detonation and quenching rule of the detonation wave in the arrester element, in crimped-ribbon flame arresters. The effect of porosity and element thickness on the propagation of detonation wave will also be investigated. This study provides theoretical references for detonation quenching and designing flame arresters.

2. Numerical model

2.1. Governing equations

2.1.1. Governing equation of gas-phase fluid

A solution to the numerical simulation for the gas-phase detonation wave is generated using the basic equation group of 2D unsteady viscous compressible flow with chemical source term (i.e. N-S equation group). Thus, the governing equation can be expressed as

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = \frac{\partial F_v}{\partial x} + \frac{\partial G_v}{\partial y} + S
\]

(1)

\[
U = \begin{bmatrix}
\rho e \\
\rho u e \\
\rho v e \\
\rho e E \\
\rho e f_1 \\
\vdots \\
\rho e f_n \\
\end{bmatrix}, \quad F = \begin{bmatrix}
\rho e u \\
\rho e u^2 + p \\
\rho e u v \\
(\rho e + p) u \\
\rho e u f_1 \\
\vdots \\
\rho e u f_n \\
\end{bmatrix}, \quad G = \begin{bmatrix}
\rho e v \\
\rho e u v \\
\rho e v^2 + p \\
(\rho e + p) v \\
\rho e v f_1 \\
\vdots \\
\rho e v f_n \\
\end{bmatrix}
\]

\[
F_v = \begin{bmatrix}
\rho e D_{f_{xx}} \\
\rho e D_{f_{xy}} \\
\rho e D_{f_{yx}} \\
\rho e D_{f_{yy}} \\
\vdots \\
\rho e D_{f_{nx}} \\
\rho e D_{f_{nx}} \\
\end{bmatrix}, \quad G_v = \begin{bmatrix}
\epsilon (\rho_{f_{xx}} + \nu_{f_{xy}} + q_{x}) \\
\epsilon (\rho_{f_{xy}} + \nu_{f_{yy}} + q_{y}) \\
\rho e D_{f_{xx}} \\
\rho e D_{f_{xy}} \\
\vdots \\
\rho e D_{f_{nx}} \\
\rho e D_{f_{nx}} \\
\end{bmatrix}, \quad S = \begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
\frac{\partial}{\partial x} \left[ \frac{0}{u^2 + v^2} \right] \\
\frac{\partial}{\partial y} \left[ \frac{0}{u^2 + v^2} \right] \\
\frac{\partial}{\partial x} \left[ \frac{0}{u^2 + v^2} \right] \\
\frac{\partial}{\partial y} \left[ \frac{0}{u^2 + v^2} \right] \\
\end{bmatrix}
\]
where \( \rho \) is the density of mixed gas; \( p \) is the pressure of the mixed gas; and \( u \) and \( v \) are the velocity in the direction of \( x \) and \( y \), respectively. \( \varepsilon \) represents the coefficient of a porous medium, \( \varepsilon = 1 \) in the pure gas-phase flow and \( \varepsilon \) is the porosity in a porous medium. \( f_i (i = 1, \ldots, i \cdots n) \) is the mass fraction of component \( i \), \( E \) is the total energy of gas mixture, \( E = \sum_{i}^{N} h_i - \frac{c_p}{2} (u^2 + v^2) \). \( \chi \) is the coefficient of heat conduction, \( \kappa = \mu \frac{C_p}{\rho} \). The heat conduction coefficient of laminar flow is \( \kappa = \kappa_L = \mu \frac{C_p}{\rho_T} \), when turbulence flow, \( \kappa = \kappa_L + \kappa_T = \mu \frac{C_p}{\rho_T} + \mu_t \frac{C_p}{\rho_T} \). Pr\(_L\) and Pr\(_T\) are the laminar and turbulent Prandtl number correspondingly. \( D \) is the diffusion coefficient, \( \nu = \frac{\lambda}{\rho} \). \( \omega \) is the Schmidt number and can be used as 1.0 in the calculation. \( S \) is the chemical source term and \( \dot{\omega} \) indicates the chemical source term for a component. \( h_s \) is the coefficient of volumetric heat transfer between gas and solid phases, \( T \) is the temperature of gas-phase medium and \( T_s \) is the temperature of solid-phase medium. \( \mu \) is the coefficient of viscosity of the gas phase, \( \alpha \) is the permeability and \( C_2 \) is the inertial resistance factor.

### 2.1.2. Governing equation of solid-phase heat transfer in a porous medium

Heat transfer effect is the major indicator of the flame suppression mechanism for the arrester element. Heat will dissipate quickly, and quenching will occur whilst the flame constantly makes contact with the wall face of the arrester element. A certain pressure drop will be observed before and after the arrester element when the medium passes through the arrester element. Notably, the size of pressure drop depends on its structure and flow rate. Therefore, the area of the arrester element inside the pipe can be unified as the area of the porous medium during the numerical modelling in this study.

Owing to the heat transfer in the solid medium and the direct heat transfer in the gas and solid phases, the governing equation in the solid phase of the porous medium is

\[
\frac{\partial T_s}{\partial t} - k_{eff} \left( \frac{\partial^2 T_s}{\partial x^2} + \frac{\partial^2 T_s}{\partial y^2} \right) = h_s (T - T_s),
\]

where \( k_{eff} \) is the coefficient of equivalent heat transfer for the solid phase in a porous medium and is calculated using the following formula:

\[
k_{eff} = \varepsilon k_f + (1 - \varepsilon) k_s,
\]

where \( k_f \) is the heat transfer coefficient of the gas phase in a porous medium and \( k_s \) is the heat transfer coefficient of the solid phase in a porous medium.

### 2.2. Chemical reaction model

The elementary reaction model is widely used for deflagrating and detonating hydrocarbon and hydrogen fuels because this model can describe the chemical reaction process in detail. The propane–air chemical reaction is used in this study. A total of 30 components and 85 reaction equations are involved. \( \dot{\omega}_i \) is calculated using the elementary reaction kinetic model as follows:

\[
\dot{\omega}_i = W_i \sum_{j=1}^{\nu} \left( \nu_{ji}^+ - \nu_{ji}^- \right) (k_{f,j} \prod_{l=1}^{N} [n_{lj}]^{\nu_{lj}} - k_{b,j} \prod_{l=1}^{N} [n_{lj}]^{\nu_{lj}^-}) \quad (i = 1, 2, \cdots, ns)
\]

where \( W_i \) is the molar mass of component; \( \nu^+ \) is the forward reaction stoichiometry coefficient matrix; \( \nu^- \) is the backward and forward reaction stoichiometry coefficient matrix; \( n_i \) is the molar
concentration of a component and \( k_f \) and \( k_b \) are the forward and backward reaction rate coefficients, correspondingly, and are provided by the following Arrhenius equation:

\[
k = A_k \cdot T^n \cdot e^{\left(-\frac{E_a}{R_u T}\right)},
\]

where \( A_k \) is the frequency factor, \( n \) is the exponential term related to temperature \( T \), \( E_a \) is the activation energy of the chemical reaction and \( R_u \) is the universal gas constant. The parameter dimensions are mole, s, cm, K and cal. The dimension of \( E_a \) is cal/mole.

The propane–air premixed gas is used in the numerical simulation of detonation. Jachimowski (1984) proposed and applied a detailed reaction kinetic mechanism, including the primary, secondary and tertiary molecular reactions. The chemical reaction rate is expressed by the Arrhenius equation. The detailed reaction process for combustion of propane is described in this reaction mechanism. The specific parameters are presented in the Appendix.

### 2.3. Discretisation of governing equation

The convection term is discretised using a non-oscillatory and non-free-parameter dissipation (NND) difference scheme to capture shock waves efficiently.

Several discretisation methods of convection term, being a strong non-linearity, are available in the governing equation group of fluid mechanics. The discretisation is performed before and after the interruption of the shock wave in the NND with the nature of Total Variation Diminishing (TVD) derived by Zhang (1988) with a favourable capturing capability of the shock wave. The difference scheme is simple with second-order accuracy, easy programming, minimal calculation work and physical solution.

### 2.4. Mesh generation

The computation domain is a 2D axis-symmetrical domain, and half of the computation domain is numerically computed. The computation mesh uses a 2D uniformed structural mesh. The mesh nodes are \( 8001 \times 41 \) in the \( x \) and \( y \) directions. The minimal grid sizes are 0.275 and 1 mm in the \( x \) and \( y \) directions, correspondingly.

Such mesh resolution cannot simulate the detailed feature in the reaction zone of detonation front but is sufficient for simulating the macro properties of gaseous detonation, including detonation speed, interaction of detonation and fluid interface and interaction of detonation and porous media. Numerical validations of mesh independence with current and refined mesh resolution indicate that the numerical simulation results and experimental data deviation increase when the grid is significantly large. Moreover, the grid size and number and the computational workload must be constantly increased, and the maximum accuracy of detonation pressure and speed slightly changes. The current mesh resolution does not influence the macro parameters of detonation, such as detonation and transmitting shock speeds. The main mechanism of detonation blocking with porous media can be simulated accurately.
2.5. Initial and boundary conditions
The geometry of the computational domain is depicted in Figure 1. The propane–air mixture is filled in the straight pipe (DN80) which is closed at both ends. The flame arrester is located in the middle and back parts of the pipe (shaded area in Figure 1), and an initiating source is applied to the left end. Detailed parameters of the propane flame arrester element are listed in Table 1.

The quenching effect of the arrester element on the detonation wave is mainly considered. Therefore, the initial stage of the numerical simulation can be simplified whilst the mixed flammable gas is directly ignited in the high-temperature and high-pressure ignition zone. Then, the Deflagration-to-Detonation Transition (DDT) process is completed in a short period to form a steadily propagating plane detonation wave.

The dimension marked in the figure is in mm, and only half of the domain is calculated in the numerical simulation in consideration of a symmetry to the computational domain. In the initial conditions, the flammable gas and porous medium areas are filled with the $C_3H_8/air$ mixture at a mixed equivalent ratio of ER = 1, an initial temperature of 300 K and an initial pressure of 1 atm. The high-temperature initiating zone is filled with high-temperature and high-pressure flammable gas at an equivalent ratio of $C_3H_8/air$ of 1:1, an initiating temperature of 1800 K and a pressure of 20 atm. In setting the boundary conditions, the gliding non-penetrable plane is used on the solid wall at the inlet and on the side solid wall. In particular, the velocity of the vertical plane is zero. Other parameters are obtained by extrapolation from the inner flow field. The symmetric boundary conditions are used on the symmetry plane. Specifically, the velocity of a vertical centre plane is zero. The rest of the parameters ensure that both sides of the symmetry plane are symmetrical and equal.

3. Results and discussion
3.1. Model validation
The experiment of propane–air (4.3 vol.% propane mixture in air initially at 23 Pisa) detonation in a horizontal pipe closed at both ends in CCPS (1993) is simulated in the current study. The run-up distance in a straight 3-inch-diameter pipe is 24 ft. The run-up distance is the distance in the direction of the flame propagation from the point of ignition to any point in the pipe system. Deflagration flames accelerate over this distance given turbulence and pre-compression effects. This distance may be sufficient for the occurrence of DDT depending on the pipe diameter, the surface roughness and the presence of turbulence-producing obstacles (e.g. elbows and valves). In this case, initiation is at the closed end of the pipe with an arrester plus bursting disk at the other end. The propagation speed value from the experiment is 2243.3 m/s when the flame approaches the arrester. The result is 2128.8 m/s in the simulation, and the pressure value from the experiment is 14.09 MPa. The result is 12.1 MPa in the simulation. The model result is close to the experimental result and can reveal the gaseous detonation in the long-closed pipe with an in-line flame arrester. Furthermore, the Mach reflection phenomenon for a wedge angle of 30° obtained with $2H_2+O_2+Ar$ in the initial pressure of 20.0 kPa is simulated based on the governing equations and calculation method. The comparison results between the proposed model and the Spark Schlieren photographs (Thomas & Williams, 2002) are displayed in Figure 2.
Figure 2 demonstrates that the simulated detonation wave reflection structure and the three-wave point trajectory agree well with the experimental results. The reliability of the simulated detonation wave phenomenon is verified. The numerical validation of a detonation wave is difficult. Notably, the comparison above can be used as a rough validation of calculation.

3.2. Initiating process of detonation wave

The variation in the flow field parameters, including pressure, density, velocity and temperature, along the pipe is illustrated in Figures 3–6. The figures present that the combustion induced by the high-temperature flame accelerates continuously. The DDT process from deflagration to detonation is completed in a short period, and the steady detonation is formed in the upstream region.

Figure 3. Distribution of pressure at different time during detonation setup process in the pipe \( D = 80 \text{ mm} \).
The above-mentioned figures illustrate the process in which the flame accelerates to result in an explosion and further grows to the detonation wave in a steady propagation. The variation rules of all the inner flow field parameters in the pipe are also demonstrated with time lapse, where the pressure amplitude is up to 4.12 MPa during the steady propagation.

Figure 3 depicts the pressure distribution in the initial process from 0 s to 0.10234167E-03 s. In the initial condition, a shock wave and a high-temperature and high-pressure zone after the wave are formed. In this zone, the mixed gas is ignited immediately, thereby resulting in a high pressure to overcome the rarefaction wave effect from the walls and gradually form the detonation. The build-up of pressure in the reaction area causes the rapid change in the pressure gradient after the
shock wave because the detonation is formed in the area after the shock wave. This condition accelerates the shock wave to the overdriven detonation. The reaction energy released before the wave will gradually influence its propagation whilst the detonation wave diffuses. Therefore, the detonation that is initially formed is the overpressure detonation. The detonation speed of the overpressure detonation is faster than the normal speed. Thus, the detonation wave front will rapidly run over the shock wave front, and the detonation pressure will drop, thereby resulting in a steady detonation whilst its strength attenuates gradually.

At \( t = 0.10234167 \times 10^{-3} \) s, the flow field velocity and the pressure distribution (Figures 3 and 5) indicate that the leading shock constitutes the detonation wave front with the reaction zone which comes after the wave. The wave front is strongly interrupted by thermodynamic parameters (e.g. pressure and temperature). Taylor rarefaction wave follows the wave front. The particle velocity in the flow field slows down in the rarefaction wave area, becomes 0 m/s at a distance approximately one-half to detonation and is 0 m/s whilst traversing to the stable area. The detonation pressure remains unchanged. This result agrees well with the self-similar solution of the C-J model. The main difference is that the structure of the detonation wave is indicated (i.e. the state distribution of leading shock and reaction zone) but cannot be described by the C-J model.

The temperature distribution curve (Figure 6) demonstrates that the reaction zone initially recedes from the leading shock whilst the pressure wave attenuates after the overdriven detonation. Thereafter, the receding trend of the reaction zone gradually shrinks. The fixed induction distance remains when the shock and combustion waves are close to the C-J state and reaches the final position that corresponds to the C-J detonation state of the mixture.

3.3. Quenching rule of a detonation wave in the in-line flame arrester

The quenching rule of a detonation wave in the different porosities and thicknesses of the arrester in the in-line flame arrester system with \( D = 80 \) mm is investigated.

The quenching length of detonation wave can be determined by the position where decoupling occurs (i.e. the position where the flame front separates from the precursor shock wave). The calculation result of quenching length with arrester porosities of 0.2, 0.3, 0.5, 0.7, 0.8 and 0.9 and arrester thicknesses of 60, 80, 100, 120, 160 and 200 mm is exhibited in Figures 7 and 8.
Figure 7. Quenching length and approximation curve with different porosities in the pipe $D = 80$ mm.

Figure 8. Quenching length with different element thickness in the pipe $D = 80$ mm.

Table 2. Formulas of quenching length and porosity

| Mixed gas | Fitting formula | Max. relative error |
|-----------|-----------------|---------------------|
| C$_3$H$_8$-Air | $L = 6.18176 - 2.68135\gamma + 18.05845\gamma^2$ | 10.2% |

Note: $L$ is quenching length and $\gamma$ is porosity.

Figure 7 illustrates that the quenching length of detonation wave increases with porosity; the quenching length rapidly increases when the porosity is also increased. Therefore, quenching length and porosity present an approximate quadratic function relationship. The fitting formulas for the data and maximum relative error are displayed in Table 2. These formulas denote that a decrease in porosity can reduce the quenching length, although the flame speed tends to increase...
progressively, and the arrester performance improves (Sun et al., 2017). This result is due to that the pressure wave will be reflected and scattered relatively fully in its internal interstice whilst the porosity decreases. The energy dissipation is increased, the heat transfer performance is enhanced and quenching becomes significantly effective.

Figure 8 depicts that the quenching length varies minimally with the increase in the thickness of the arrester. This rule is mainly due to the precondition for the simulation (i.e. a stable detonation is formed at the initial stage). Therefore, arrester thickness slightly influences the quenching of detonation wave in this condition.

3.4. Effect of porosity on the propagation process of the detonation wave

3.4.1. Effect of porosity on the inhibition mechanism of detonation wave
The effect of porosity on the propagation and attenuation of detonation wave is examined. In particular, the effect of porosities of 0.3 and 0.7 on inhibition to the detonation wave is explored.

The variation curves of pressure and temperature along the pipe at different moments with the porosity of 0.3 when the detonation wave passes through the arrester element are demonstrated in Figures 9 and 10, correspondingly. The variation curves of pressure and temperature along the pipe at different moments with the porosity of 0.5 when the detonation wave passes through the arrester element are exhibited in Figures 11 and 12, respectively.

The pressure value of detonation wave is reduced from 6.8595E+06 Pa to 0.12717E+06 Pa when the detonation wave enters the arrester element until the transmitted shock wave leaves the end of the arrester element (t = 0.1362E-02 s - t = 0.1506E-02 s) when the porosity is 0.3. The pressure value of detonation wave is reduced from 3.6981E+06 Pa to 0.12152E+06 Pa from t = 0.1366E-02 s to t = 0.1527E-02 s when the porosity is 0.5. A pressure peak drop of a detonation wave in the arrester element is observed whilst the porosity decreases. Therefore, the decrease in porosity increases the specific surface area of the element. This increase also increases the probability of detonation wave to collide with the element wall (thereby causing a high-pressure peak), the resistance on the detonation wave when it moves inside the arrester element and the attenuation amplitude of detonation wave pressure. Moreover, the convective heat exchange of gas and solid in the element is strengthened, the heat transfer between the gas and solid is significant and the
temperature difference between the gas and solid is decreased whilst the volume of the arrester element becomes dense. The element under the action of the two mechanisms exhibits a robust inhibition of the detonation wave whilst the porosity becomes small.

The temperatures on the position where the transmitted shock wave lies at the end of the arrester element are approximately 328.31 and 540.17 K when porosity increases from 0.3 to 0.7. In other words, the arrester element can effectively lower the flame temperature and reduce the porosity appropriately, which are favourable for the heat transfer inside the arrester element.

3.4.2. Variation rule of detonation pressure
The detonation pressure at the front end of the arrester with porosities of 0.2, 0.3, 0.5, 0.7, 0.8 and 0.9 is calculated. The optimal square approximation is conducted by using least squares. The simulated data and fitting curve are illustrated in Figure 13.
The above-mentioned figure demonstrates that detonation pressure decreases progressively whilst porosity increases. The decrease in porosity causes the detonation wave to be fully reflected in its internal interstice, thereby significantly increasing the detonation pressure at the front end of the arrester. The fitting formula for the simulated data and the relative error is displayed in Table 3.

### 3.5. Effect of element thickness on the propagation process of the detonation wave

#### 3.5.1. Effect of element thickness on the inhibition mechanism of detonation wave

The effect of element thickness on the propagation and attenuation of a detonation wave is explored. Specifically, the effect of element thicknesses of 50 and 200 mm on the inhibition of the detonation wave is examined.

The variation in the curves of pressure and temperature along the pipe at different times when the detonation wave propagates to the arrester element with element thickness of 50 mm is depicted in
Figures 14 and 15, respectively. In these figures, the leading shock propagates only to the arrester element when $t = 0.1369E-02$ s. The transmitted shock wave leaves the element when $t = 0.1432E-02$ s. In this period, the pressure of the detonation wave drops from $3.5081E+06$ Pa to $0.32715E+06$ Pa. The temperature on the position where the transmitted shock wave lies is $577.63^\circ$C.

The variation in the curves of pressure and temperature along the pipe at different times when the detonation wave propagates to the arrester element with element thickness of 200 mm is plotted in Table 3. Formulas of detonation pressure and porosity

| Mixed gas   | Fitting formula                                                                 | Max. relative error |
|-------------|---------------------------------------------------------------------------------|---------------------|
| C3H8–Air    | $P = 9.5777e^6 - 1.38758e^7y + 7.75274e^6y^2$                                  | 18.5%               |

Note: $P$ is detonation pressure and $y$ is porosity.

Figure 14. Distribution of pressure at different time in the pipe $D = 80$ mm and element thickness = 50 mm.

Figure 15. Distribution of temperature at different time in the pipe $D = 80$ mm and element thickness = 50 mm.
Figures 16 and 17, correspondingly. The figures indicate that the leading shock propagates only to the arrester element when $t = 0.1368E-02$ s. The transmitted shock wave leaves the element when $t = 0.1625E-02$ s. In this period, the pressure of the detonation wave drops from $3.1666E+06$ Pa to $0.6031E+06$ Pa. The temperature on the position where the transmitted shock wave lies is 311.41°C. The difference in the pressure drops for the detonation wave is smaller than the simulation condition with a thickness of 50 mm. However, the peak value of the detonation wave in the arrester element and the temperature value on the position where the transmitted shock wave lies are significantly lesser than those values under the simulation condition of 50 mm. Therefore, the length of the narrow channel increases whilst the arrester element thickens, and the inhibition of the detonation wave remarkably strengthens.
3.5.2. Variation rule of detonation pressure

The detonation pressure at the front end of the arrester with thicknesses of 60, 80, 100, 120, 160 and 200 mm is calculated. The optimal square approximation is performed by using the least squares. The data and fitting curve are presented in Figure 18.

Figure 18 illustrates that the value of detonation pressure increases whilst the arrester also thickens; that is, the detonation pressure rapidly rises when the arrester thickens. In particular, detonation pressure and arrester thickness present an approximate quadratic function relationship. The fitting formula for the data and the maximum relative error are summarised in Table 4.

4. Conclusion

A numerical model was developed in this study for the propagation and quenching of detonation wave in in-line flame arrester. The discretisation was performed in an NND difference scheme with second-order accuracy, and the numerical analysis results were as follows:

(i) In the initial condition at the initial stage, the mixed gas was ignited immediately in the high-temperature and high-pressure zone, thereby resulting in a high pressure. This pressure overcame the rarefaction waves on the wall surface and gradually formed the steady detonation.

(ii) The quenching length of detonation wave increased whilst porosity became large; the increase in quenching length is rapid when the porosity is large. In particular, quenching length and porosity exhibited an approximate quadratic function relationship. The precondition for simulation was to build up a stable detonation. Thus, quenching length varied minimally with the increase in arrester thickness.

(iii) The probability for the detonation wave to collide with the element wall increased with the decrease in porosity. Accordingly, a pressure peak drop of detonation wave in the arrester element was observed. The propagation rules of a detonation wave under different porosities were investigated. The result showed that the detonation pressure at the front end of the

![Figure 18. Detonation pressure with different element thickness in the pipe D = 80 mm.](image)

![Table 4. Formulas of detonation pressure and element thickness](table)

| Mixed gas   | Fitting formula                                                                 | Max. relative error |
|-------------|---------------------------------------------------------------------------------|---------------------|
| C\textsubscript{3}H\textsubscript{8}–Air | $P = 1.9174e^6 - 1495.0376l + 19.73697l^2$ | 12.4%               |

Note: $P$ is detonation pressure and $l$ is element thickness.
arrester decreased progressively with the increase in porosity, and the two parameters presented a quadratic function relationship. The corresponding empirical formulas were summarised.

(iv) The increase in arrester thickness decreased the pressure peak of the detonation wave in the element and the temperature value on the position where the transmitted shock wave lies, thereby exerting an inhibition effect on the detonation wave. The propagation rules of detonation wave under different arrester thicknesses were explored. The result showed that the detonation pressure at the front end of the arrester increased with the increase in the arrester thickness, and the two parameters exhibited a quadratic function relationship. The related empirical formulas were summarised.

**Funding**

This work was supported by the General Administration of Quality Supervision, Inspection and Quarantine of the People’s Republic of China Scientific Project [T2017-LNQTS-0005] and the National Key Research and Development Program of China [2017YFC0805600].

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**Citation information**

Cite this article as: Numerical simulation of detonation wave propagation and quenching process in in-line crimped-ribbon flame arrester, ShaoChen Sun, Yuan Shu, Yu Feng, DaChao Sun, HaiTao Long & MingShu Bi, Cogent Engineering (2018), 5: 1469377.

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Appendix

Table A1. Detailed chemical reaction model of propane-air mixture

| No. | Reaction equation | Log A | n | E   |
|-----|-------------------|-------|---|-----|
| 1   | C3H8=C2H6+CH4     | 16.6  | 0 | 84,800 |
| 2   | C3H8+O2=N2+2OH    | 13.0  | 0 | 52,000 |
| 3   | C3H8+O2=CO+2H2O   | 12.5  | 0 | 52,000 |
| 4   | CH3+CH4=N2+CH4    | 12.5  | 0 | 11,400 |
| 5   | CH4+CH4=2H2+CH4   | 11.9  | 0 | 8600  |
| 6   | H+H2=C2H2+H2      | 13.7  | 0 | 9100  |
| 7   | H+CH4=CH3+H2      | 13.1  | 0 | 6400  |
| 8   | O+CH3=CH2+OH      | 13.6  | 0 | 11,100 |
| 9   | O+CH3=CH2+OH      | 13.0  | 0 | 8400  |
| 10  | OH+CH3=CH2+H2O    | 4.7   | 2.7 | 100  |
| 11  | OH+CH3=CH2+H2O    | 3.7   | 2.8 | -1700 |
| 12  | HO2+CH3=CH2+H2O2  | 11.8  | 0 | 10,500 |

(Continued)
| No. | Reaction equation | Log A | n   | E   |
|-----|-------------------|-------|-----|-----|
| 13  | HO$_2$+C$_2$H$_6$=I·C$_2$H$_5$+H$_2$O$_2$ | 11.3  | 0   | 10,500 |
| 14  | N·C$_2$H$_5$=C$_2$H$_6$+CH$_3$ | 13.6  | 0   | 33,200 |
| 15  | I-C$_2$H$_5$=CH$_2$+CH$_3$ | 12.0  | 0   | 34,500 |
| 16  | N·C$_2$H$_5$=C$_2$H$_6$+H | 13.8  | 0   | 38,000 |
| 17  | I-C$_2$H$_5$=C$_2$H$_6$+H | 14.3  | 0   | 41,300 |
| 18  | N·C$_2$H$_5$+O$_2$=C$_2$H$_6$+HO$_2$ | 12.0  | 0   | 5000 |
| 19  | I-C$_2$H$_5$+O$_2$=C$_2$H$_6$+HO$_2$ | 12.0  | 0   | 5000 |
| 20  | CH$_3$+C$_2$H$_5$=C$_2$H$_6$+CH$_4$ | 12.4  | 0   | 5400 |
| 21  | H+CH$_2$=C$_2$H$_5$+CH$_3$ | 12.6  | 0   | 0   |
| 22  | H+CH$_2$=C$_2$H$_5$+H | 13.7  | 0   | 5000 |
| 23  | OH+CH$_2$=C$_2$H$_5$+H | 13.0  | 0   | 0   |
| 24  | O+CH$_2$=C$_2$H$_5$+HCO | 13.4  | 0   | 2700 |
| 25  | OH+CH$_2$=C$_2$H$_5$+H | 13.0  | 0   | 0   |
| 26  | C$_2$H$_5$=C$_2$H$_6$+H | 13.5  | 0   | 40,700 |
| 27  | M+CH$_4$=CH$_3$+H+M | 17.1  | 0   | 88,400 |
| 28  | H+CH$_2$=CH$_3$+H | 14.8  | 0   | 15,100 |
| 29  | O+CH$_2$=CH$_3$+OH | 14.6  | 0   | 14,000 |
| 30  | OH+CH$_2$=CH$_3$+H | 13.5  | 0   | 6000 |
| 31  | CH$_3$+O=CH$_2$+O | 14.1  | 0   | 2000 |
| 32  | CH$_3$+O=CH$_2$O+H | 13.4  | 0   | 29,000 |
| 33  | CH$_3$+HO=OH+CH | 13.2  | 0   | 0 |
| 34  | CH$_3$+OH=CH$_2$O+H | 12.6  | 0   | 0 |
| 35  | M+CH=CH$_2$+H | 13.7  | 0   | 21,000 |
| 36  | CH$_2$O+O=CH$_3$+HO$_2$ | 12.0  | 0   | 6000 |
| 37  | CH$_3$+CH$_3$=C$_2$H$_5$ | 12.8  | 0   | 1000 |
| 38  | CH$_3$+CH$_3$=C$_2$H$_5$+CH$_4$ | -0.3  | 4.0 | 8300 |
| 39  | H+CH$_2$=C$_2$H$_5$+H | 7.5   | 2.0 | 6900 |
| 40  | O+CH$_2$=CH$_3$+OH | 13.2  | 0   | 6100 |
| 41  | OH+CH$_2$=C$_2$H$_5$+H | 13.8  | 0   | 3600 |
| 42  | HO$_2$+C$_2$H$_5$=C$_2$H$_6$+HO$_2$ | 12.0  | 0   | 10,000 |
| 43  | C$_2$H$_5$=C$_2$H$_6$+H | 12.0  | 0   | 5000 |
| 44  | H+CH$_2$=CH$_3$+H | 13.0  | 0   | 0 |
| 45  | H+CH$_2$=CH$_3$+H | 13.7  | 0   | 0 |
| 46  | H+CH$_2$=CH$_3$+H | 14.0  | 0   | 8500 |
| 47  | O+CH$_2$=CH$_3$+HCO | 13.4  | 0   | 2700 |
| 48  | OH+CH$_2$=C$_2$H$_5$+H | 14.0  | 0   | 3500 |
| 49  | M+CH$_2$=CH$_3$+H+M | 14.9  | 0   | 31,500 |
| 50  | H+C$_2$H$_5$=C$_2$H$_6$+H | 14.3  | 0   | 19,000 |
| 51  | O+CH$_2$=CH$_3$+CO | 13.7  | 0   | 3700 |
| 52  | OH+CH$_2$=C$_2$H$_6$+H | 12.8  | 0   | 7000 |
| 53  | CH$_2$O=HCO+CO | 13.0  | 0   | 7000 |
| 54  | CH$_2$O=HCO+OH | 14.0  | 0   | 3700 |
| 55  | H+CH$_2$O=HCO+H | 14.5  | 0   | 10,500 |
| 56  | CH$_2$O=HCO+CD | 13.3  | 0   | 3100 |
| 57  | OH+CH$_2$O=HCO+H | 12.9  | 0   | 200 |

(Continued)
| No. | Reaction equation | Log $A$ | $n$ | $E$  |
|-----|------------------|---------|-----|-----|
| 58  | $\text{HO}_2^+\text{CH}_2=\text{HCO}+\text{H}_2\text{O}_2$ | 12.1    | 0   | 8000|
| 59  | $\text{M}^+\text{HCO}=\text{CO}+\text{H}+\text{M}$ | 14.7    | 0   | 19,000|
| 60  | $\text{H}^+\text{HCO}=\text{CO}+\text{H}_2$ | 14.3    | 0   | 0   |
| 61  | $\text{O}^+\text{HCO}=\text{CO}+\text{OH}$ | 14.0    | 0   | 0   |
| 62  | $\text{OH}^+\text{HCO}=\text{CO}+\text{H}_2\text{O}$ | 14.0    | 0   | 0   |
| 63  | $\text{HCO}+\text{O}_2=\text{CO}+\text{HO}_2$ | 12.5    | 0   | 7000|
| 64  | $\text{OH}^+\text{CO}=\text{CO}+\text{H}$ | 7.2     | 1.3 | $-700$|
| 65  | $\text{HO}_2+\text{CO}=\text{CO}_2+\text{OH}$ | 14.2    | 0   | 23,600|
| 66  | $\text{CO}+\text{O}+\text{M}+\text{CO}_2+\text{M}$ | 15.4    | 0   | 4400|
| 67  | $\text{H}^+\text{O}_2=\text{OH}+\text{O}$ | 17.1    | $-0.9$ | 16,600|
| 68  | $\text{OH}^+\text{H}_2\text{O}+\text{H}$ | 7.5     | 1.8 | 3000|
| 69  | $\text{O}^+\text{H}_2=\text{OH}+\text{H}$ | 14.3    | 0   | 13,800|
| 70  | $\text{OH}^+\text{H}_2\text{O}+\text{O}$ | 13.7    | 0   | 7000|
| 71  | $\text{H}^+\text{OH}+\text{M}+\text{H}_2\text{O}+\text{M}$ | 22.3    | $-2.0$ | 0   |
| 72  | $\text{H}^+\text{H}+\text{M}^+\text{H}_2\text{O}+\text{M}$ | 17.8    | $-1.0$ | 0   |
| 73  | $\text{H}^+\text{O}_2+\text{M}=\text{HO}_2+\text{M}$ | 18.5    | $-1.0$ | 0   |
| 74  | $\text{OH}^+\text{HO}_2=\text{H}_2\text{O}+\text{O}_2$ | 13.7    | 0   | 1000|
| 75  | $\text{H}^+\text{HO}_2=\text{H}_2+\text{O}_2$ | 13.4    | 0   | 700|
| 76  | $\text{H}^+\text{HO}_2=2\text{OH}$ | 14.7    | 0   | 1800|
| 77  | $\text{OH}^+\text{HO}_2=\text{OH}+\text{O}_2$ | 13.7    | 0   | 1000|
| 78  | $\text{HO}_2^+\text{H}_2\text{O}_2+\text{O}_2$ | 12.3    | 0   | 0   |
| 79  | $\text{HO}_2^+\text{H}_2\text{O}_2+\text{H}$ | 11.5    | 0   | 18,700|
| 80  | $\text{OH}^+\text{H}_2\text{O}_2=\text{HO}_2+\text{H}_2\text{O}$ | 13.0    | 0   | 1900|
| 81  | $\text{OH}^+\text{HO}_2=\text{2OH}+\text{M}$ | 17.1    | 0   | 45,500|
| 82  | $\text{H}^+\text{H}_2\text{O}_2=\text{H}_2\text{O}+\text{OH}$ | 12.7    | 0   | 9900|
| 83  | $\text{O}^+\text{H}_2\text{O}_2=\text{HO}_2+\text{OH}$ | 13.3    | 0   | 5900|
| 84  | $\text{N}^+\text{O}=\text{N}^+\text{NO}$ | 14.3    | 0   | 76,100|
| 85  | $\text{N}^+\text{O}_2=\text{NO}+\text{O}$ | 9.95    | 0   | 6500|
