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# Flame-turbulence interactions during the flame acceleration using solid and fluid obstacles

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#### 13 ABSTRACT

14 A combination of solid and transverse jet obstacles is proposed to trigger flame acceleration and deflagration-to-15 detonation transition (DDT). A numerical study of this approach is performed by solving the reactive Navier-Stokes equations deploying an adaptive mesh refinement technique. A detailed hydrogen-air reaction mechanism with 12 16 17 species and 42 steps is employed. The efficiency and mechanisms of the combined obstacles on the flame acceleration 18 are investigated comprehensively. The effects of multiple jets, jet start time, and jet stagnation pressure on the DDT 19 process are studied. Results show that there is a 22.26% improvement in the DDT run-up time and a 33.36% reduction 20 in the DDT run-up distance for the combined obstacles compared to that having only solid obstacles. The jet acts as 21 an obstruction by producing a suitable blockage ratio and introducing an intense turbulent region due to the Kelvin-22 Helmholtz instability. This leads to dramatic flame-turbulence interactions, increasing the flame surface area 23 dramatically. The dual jet produces mushroom-like vortices, leading to a significantly stretched flame front and 24 intensive Kelvin-Helmholtz instabilities, and therefore these features produce a high flame acceleration. As the jet 25 operation time decreases, the jet obstacle almost changes its role from both physical blockage ratio as well as 26 turbulence and vorticity generator to a physical blockage ratio. There is a moderate jet stagnation pressure that reduces 27 the run-up time to detonation and run-up distance to detonation in the obstacle-laden chamber. While further increasing 28 the jet stagnation pressure, it does not have a positive effect on shortening the DDT run-up time and DDT run-up 29 distance. 30

31 KEY WORDS: Flame acceleration, deflagration-to-detonation transition (DDT), flame-turbulence interaction,

32 Kelvin-Helmholtz (K-H) instability, transverse jet

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Abbreviations				
AMR	adaptive mesh refinement	Pts	grid points	
AMROC	Adaptive Mesh Refinement in Object-	R-T	Rayleigh-Taylor	
	oriented C++	Roe-HLL	Roe-Harten-Lax-Van Leer	
Br	blockage ratio	SW	shock wave	
CJ	Chapman–Jouguet	SWACER	Shock Wave Amplification by Coherent	
DDT	deflagration-to-detonation transition		Energy Release	
jet	jet obstacle	$T_{DDT}$	DDT run-up time	
K-H	Kelvin-Helmholtz	VN	von Neumann	
L <sub>DDT</sub>	DDT run-up distance	ZND	Zel'dovich-Neumann-Do"ring	
MUSCL	Monotone Upwind Scheme for	2D	two-dimensional	
	Conservation Laws	3D	three-dimensional	
PDE	pulse detonation engine			

#### 37 I. INTRODUCTION

Detonation combustion is considered as thermodynamically particularly efficient because of its constant volume combustion behavior, which would result in high thermal cycle efficiency <sup>1-3</sup>. The detonation combustion mode can be utilized in different engineering applications, including the pulse detonation engine (PDE) and rotating detonation engine, which have a high potential to augment the aerospace thrust performance for the future advanced propulsion system. Such system should be capable to operate within a confined combustion duct, resulting in a lower weight and cost <sup>4</sup>. Although detonation combustors have a higher thermodynamic performance than traditional deflagration systems, employing detonation combustion is still a challenge as a result of its unstable behavior <sup>5-8</sup>.

45 One of the key obstacles to the detonation combustion engine is how to obtain a robust and stable detonation initiation <sup>6</sup>. Tremendous efforts have been made to ignite detonation combustion, such as direct ignition <sup>9, 10</sup>, pre-46 detonator ignition underlying within a small-scale tube <sup>11-13</sup>, and deflagration-to-detonation transition (DDT) 47 approaches <sup>13-16</sup>. Manipulating detonation combustion through a direct ignition will require significant transient 48 49 deposition of energy for the mixture. Therefore, it is still difficult and impractical to carry out a detonation initiation 50 in a practical environment using the high and transient energy release from an external device. The pre-detonator 51 ignition approach can be easily operated for a typical combustion chamber. However, it still encounters some 52 drawbacks including the requirement for an extra gas mixture supply system, which increases the complexity of the 53 device and the possibility of failure in transition to detonation in the combustor compared to other typical ignition methods <sup>17, 18</sup>. Generally, a detonation wave achieved by the DDT process is considered a more reliable and efficient 54 55 method in combustors because of their lower requirement of ignition energy and easy operation within the chamber <sup>2</sup>. 56 <sup>6</sup>. There are still some fundamental drawbacks with the DDT approach, including a long start time and large combustor length required for a successful DDT <sup>19</sup>. As such, obtaining a rapid onset of detonation is a major issue that requires
further investigation.

59 Past studies have demonstrated that maintaining a highly turbulent flow within the combustion chamber is crucial 60 to accelerate the flame propagation speed. The traditional method of turbulence generation consists mainly of multiple 61 fixed objects that are placed into the combustion tube, e.g., rings, orifice plates, wedges, and Shchelkin spirals <sup>20-24</sup>. Hence, a large number of investigations were carried out to study the effect of physically fixed solid obstacles for 62 turbulence induction and consequently promoting the flame acceleration and DDT process 14, 25-29. These solid 63 64 obstructions act as a blockage for the flame and fluid flow, resulting in a high flame propagation velocity as well as 65 triggering the Kelvin-Helmholtz (K-H) instabilities shedded from the tips of the obstacles. Such an instability leads to the generation of large turbulent eddies that interact with the flame front, which, in turn, increase the flame surface 66 67 area and flame acceleration accordingly, owing to the high energy release rate <sup>30</sup>. After these series of flame accelerations, a compression wave is formed as a response of the rate of the specific volume of mixture across the 68 69 flame. A subsequent shock wave is generated within the chamber when the compression waves coalesce together, which further preheats the unburned material <sup>30-32</sup>. At the subsequent stage, the fixed obstructions provide shock 70 71 reflection and shock focusing, which leads to the generation of hot spots around the obstacles <sup>30</sup>. The energy released by the autoignition of these localized hot spots can enhance the DDT process <sup>30, 33</sup>. Subsequently, the detonation occurs 72 73 when a hot spot is generated in the space region between the leading shock and the flame front due to the shock wave, 74 amplified by the coherent energy release (SWACER) mechanism associated with the gradients within the mixture, such as temperature, density and pressure <sup>30, 34, 35</sup>. However, when operating a particular detonation engine such as 75 76 PDE, these obstacles, which are fixed within the chamber, result in pressure losses and introduce thermal reservoirs <sup>16, 17, 36, 37</sup>. This leads to ~25% engine thrust loss as confirmed by previous research  $^{2, 38}$ . 77

To overcome the above shortcoming of the obstacle-loaden chamber in the DDT process, the fluidic transverse jet approach is introduced, which provides a similar function as the solid obstacle and has lower pressure loss <sup>17, 39</sup>. These fluidic crossflow jets have an advantage to be adjusted easily to form different turbulent flows and eddies by changing the jet width and stagnation pressure, which can efficiently control the DDT process <sup>40</sup>. Prior work on the effects of a transverse jet in crossflow on the DDT process was successfully produced by Knox et. al <sup>17, 41</sup>. They demonstrated that the transverse jet acts as a physical obstruction and introduces a high level of turbulence within the chamber. Their result showed that jet compositions of air and mixture do not have a significant influence on the DDT run-up time 85  $(T_{DDT})$  and DDT run-up length  $(L_{DDT})$ . The transverse jet composed of kerosene-air, however, has a dramatically positive influence on flame acceleration and detonation initiation <sup>42</sup>. Subsequently, several experimental studies were 86 87 carried out to evaluate the effect of a single transverse jet on the flame acceleration at an early stage of the DDT process <sup>43-45</sup>. It was found that in comparison to the solid obstacle's case, the transverse jet is more effective in 88 introducing a transition from a laminar flame to a turbulent flame <sup>43-45</sup>. In addition, a transverse jet with a supersonic 89 90 flow was injected into the combustion chamber, resulting in a successful DDT process with significantly shorter  $T_{DDT}$ 91 and  $L_{DDT}$ <sup>46</sup>. In the recent experiment and numerical research by Peng et al. <sup>16</sup> on flame acceleration and DDT, the 92 detonation wave was triggered by a single or two crosswise transverse jets composed of a methane-oxygen mixture in 93 smooth tubes. The result revealed that the transverse jet could reduce the required length of the detonation tube and 94 shorten the start time of DDT occurrence<sup>16</sup>. Moreover, other jet parameters (including the composition, temperature 95 and pressure, as well as the exit width of the jet) influencing the flame acceleration and the DDT process in smooth combustion tubes were comprehensively investigated <sup>47</sup>. Most recently, the non-reactive transverse jets, composed of 96 97 carbon dioxide, helium, or nitrogen, were also injected into the smooth chamber to investigate the acceleration of a 98 methane-oxygen flame. The obtained results demonstrated that the non-reactive jet promotes a rapid flame 99 acceleration, resulting in a shorter distance of the DDT formation <sup>48, 49</sup>.

100 In current literature, there is no consideration of the combined effect of fluid and solid obstacles on the flame 101 acceleration and DDT. The combination approach would couple the different advantages from two kinds of obstacles 102 to shorten  $T_{DDT}$  and  $L_{DDT}$ . In addition, only few studies have evaluated the start time and the required length of 103 detonation initiation by transverse jets. Furthermore, the effect of the start time of the jet stream after ignition on the 104 DDT process has not been studied. Hence, this work aims at closing the above-mentioned gaps through a detailed 105 numerical analysis of combined solid and transverse jet obstructions in a combustion tube. The results obtained for 106 the combined configuration are compared against those obtained for a solid obstacle configuration. Additionally, the 107 effect of the dual jet stream and the start time of the transverse jet on the flame acceleration and DDT processes were 108 further investigated. The current research is an extension of our previous study <sup>50</sup>. The numerical simulations were 109 performed by solving the reactive Naiver-Stokes equations together with a detailed hydrogen-air reactive kinetics 110 model consisting of 12 species and 42 reaction steps. The structured adaptive mesh refinement (AMR) technique was 111 employed in the calculating framework <sup>51</sup> to enable high-resolution simulations.

#### 113 II. COMPUTATIONAL MODEL AND NUMERICAL METHODS

#### 114 A. Computational configuration

115 A two-dimensional (2D) computational domain was employed in the current study to investigate the entire flame 116 acceleration and DDT process. The 2D configuration enables us to reduce the computational cost while resolving the prominent features influencing the DDT processes, as demonstrated in previous studies <sup>30, 40</sup>. The computational 117 domain (Fig. 1) is a rectangular tube of  $L_{x \times Ly} = 700 \times 20$  mm<sup>2</sup>. Three configurations termed A, B and C were 118 119 considered. Configuration A incorporates multiple solid obstructions to accelerate the flame. As presented in Fig. 1, 120 the pipe is confined on the left, upper, and lower sides, while it allows free outflow on the right side of the domain. 121 The upper and lower sides of the tube are arranged with several typical rectangular solid obstacles with a size of  $d \times h$ . 122 The interval between the solid obstacles is S, and the distance between the left boundary to the first obstacle L is set 123 to be 48 mm. To prompt the occurrence of DDT, a high spacing of S=50 mm is considered between the solid obstacles for the formation of Mach stems, as reported in previous studies  $^{32}$ . With the obstacle's height of h=3 mm the blockage 124 ratio (Br) is 0.3, which is within the recommended range for flame acceleration <sup>52</sup>. Hence a slight lower Br is 125 126 considered to balance the flame acceleration ratio and lower the pressure loss, as discussed in the previous section. 127 The width of the obstacle is d=2 mm. Ten pairs of solid plates were employed on the upper and lower side of the computational domain. For configuration B (see Fig. 1(b)), the arrangement for configuration A was modified such 128 129 that one of the solid obstructions is replaced by a single crosswise transverse jet located at the bottom wall, and the 130 combined solid and transverse jet obstacles were adopted to stimulate the flame acceleration. The width of the jet is 131 also the same as the solid, in order to control the extra influence on the flame acceleration and DDT. Configuration C (see Fig. 1(c)) incorporates multiple jets to detect the effect of multiple jets on the flame acceleration. Adiabatic and 132 133 no-slip wall boundary conditions were specified on all walls, including the upper and lower walls as well as solid obstacles. It is noted that the width of the current research is close to the critical limit <sup>6</sup> with respect to the detonation 134 cell size (1-1.6 cm) of the initial mixture, and also Gamezo et al.'s <sup>14</sup> have revealed that the combustion wave 135 136 experiences a chocking flame regime propagating about half of CJ speed. In our previous study <sup>50</sup> on the same 137 configuration as Fig. 1(b), it is demonstrated that the chocking flame regime is formed when there is an early flame 138 turbulent interaction when the jet position is located at X=50cm. But in the current jet position, no chocking flame 139 region is observed.

140 Several cases were considered, as shown in Table II. Cases 1 and 2 were employed to study the influence of the 141 combined fluid/solid obstacles compared to the solid obstacle only. The composition of the transverse jet is a premixed 142 stoichiometric H<sub>2</sub>/air with temperature  $T_{iet}$ =298 K, whereas it has a slightly high stagnation pressure of  $P_{iet}$ =0.35 MPa. 143 Furthermore, dual impact jet obstacles arranged at Lx=100 mm, as used in configuration C in Fig. 1, were also utilized 144 to study the effect of multiple jets on the flame acceleration and DDT processes, corresponding to Case 3. The start time of the transverse jet was set to t=0.001 ms in Cases 2 and 3. Additionally, Cases 4 and 5 were considered to study 145 146 the effect of jet start time after the ignition of the premixed mixture on the flame acceleration, which was set as t=0.25 147 ms and t=0.5ms, respectively, with a motivation to detect the perturbance time of turbulence generation. To detect the 148 stagnation pressure of the transverse jet on the DDT process, Case 6, 7 and 8 employed lower as well as higher 149 stagnation pressure compared to Case 2, corresponding to Case 6  $Br_i=2.0$ , Case 7  $Br_i=5.0$  and Case 8  $Br_i=6.5$ , where 150  $Br_i$  represents the Br generated by the transverse jet, where the relation is assumed as  $Br_i = P_{iet}/P_0$ . These three cases 151 are aimed at studying the effect of the strength of perturbation caused by the jet on the DDT process. The width of the 152 transverse jet was kept the same as the solid obstruction to control the external influence on the flame acceleration 153 and DDT.

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FIG. 1. Schematic illustration of the computational domain for the flame acceleration and DDT. (a) Configuration A:
only the solid obstacles are adopted; (b) Configuration B: a single jet and solid obstacles are employed for flame
acceleration; (c) Configuration C: the dual impact jet and solid obstacles are applied.

The combustion chamber was filled with a premixed stoichiometric H<sub>2</sub>-Air mixture under standard atmospheric 160 pressure and temperature with P=0.1 MPa and T=298 K. A semi-sphere hot spot with a radius of r=4 mm on the left 161 162 boundary with T=2500 K and P=0.1 MPa is employed to ignite the perfectly stirred mixture. A similar approach has been considered in the previous literature <sup>14, 16, 32, 53</sup>. A low-pressure source prevents a high propagation velocity of the 163 164 flame front and the formation of the shock wave at the early stage of the flame propagation, enabling us to analyze 165 the effect of the obstacle only. The detailed parameters of the initial premixed mixture are given in Table I. The theoretical parameters of the Chapman-Jouguet (CJ) condition and laminar flame properties for the current mixture 166 167 in Table I are obtained from Cantera <sup>54</sup>. Note that the detonation cell size is calculated by an empirical correlation model provided by Ng et al.<sup>55</sup> that considers the ZND reaction zone as well as the reaction structure. 168

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TABLE I. The thermodynamic properties of hydrogen-air mixture and the corresponding CJ parameters.

Quantity	Value	Definition
$P_0$	0.1 MPa	Initial pressure
$T_{O}$	298 K	Initial temperature
M	21 g/mol	Molecular weight
$P_{VN}$	27.7 <i>P</i> <sup>0</sup> MPa	Pressure at von Neumann state
$T_{VN}$	5.14 <i>T</i> <sup>0</sup> K	Temperature at von Neumann state
$ ho_{_{\!V\!N}}$	2.109 kg/m <sup>3</sup>	Density at von Neumann state
$S_I$	≈ 2.98 m/s	Laminar flame speed
$L_{l}$	≈ 0.35 mm	Laminar flame thickness
$P_{CJ}$	15.58P <sub>0</sub> MPa	CJ pressure
$T_{CJ}$	9.875 <i>T</i> <sup>0</sup> K	CJ temperature
$ ho_{\scriptscriptstyle CJ}$	1.5205 kg/m <sup>3</sup>	CJ density
V <sub>CJ</sub>	1965 m/s	CJ speed
$X_d$	1-1.6 cm	Detonation cell width

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#### 172 **B.** Governing equations and numerical methods

173 The above-mentioned DDT process was modeled by solving the 2D unsteady reactive Navier-Stokes equations,

174 which are given by the following equations in conversation form  $^{56}$ :

175 
$$\frac{\partial U}{\partial t} + \frac{\partial (F_x - G_x)}{\partial x} + \frac{\partial (F_y - G_y)}{\partial y} = S_{chem}, \qquad (1)$$

176 in which U denotes the vector of state.  $F_x$  and  $F_y$  represent the convection fluxes, and  $S_{chem}$  denotes the source

177 term that gives by the mixture's chemical reaction <sup>56</sup>. These vector-valued quantities read

178 
$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \\ \rho Y_i \end{bmatrix}, F_x = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(\rho e + p) \\ \rho uY_i \end{bmatrix}, F_y = \begin{bmatrix} \rho v \\ \rho uv \\ \rho uv \\ \rho v^2 + p \\ v(\rho e + p) \\ \rho vY_i \end{bmatrix}, S_{chem} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_i \end{bmatrix},$$
(2)

where u, v, e are the horizontal velocity, the normal velocity and total energy, respectively <sup>56</sup>.  $\dot{\alpha}$  are the mass generation rates of the species, which can be obtained from a specific chemical reaction mechanism of J as

181 
$$\dot{\omega}_{i} = \sum_{j=1}^{J} (v_{ji}^{r} - v_{ji}^{f}) \left[ k_{j}^{f} \prod_{n=1}^{N_{sp}} (\frac{\rho_{n}}{W_{n}})^{v_{jn}^{f}} - k_{j}^{r} \prod_{n=1}^{N_{sp}} (\frac{\rho_{n}}{W_{n}})^{v_{jn}^{f}} \right], \ i = 1, \dots, N_{sp} . \tag{3}$$

In the current simulation, only elementary chemical reactions were adopted. Therefore, the Arrhenius equation was
 employed to evaluate the reaction rates, which has widely been used in detonation simulations in previous work <sup>32, 33,</sup>
 <sup>57</sup> and reads

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$$k_{j}^{f/r} = A_{j}^{f/r} T^{\beta_{j}^{f/r}} \exp\left(-\frac{E_{j}^{f/r}}{RT}\right).$$
(4)

The chemical kinetics package CHEMKIN is employed to evaluate Equations (3) and (4) based on the specific chemical reactive mechanism.  $\rho$  in Equation (2) denotes the total density, where *i* equals to 1, 2, 3 ...,  $N_{sp}$ , with  $N_{sp}$ denoting the total number of species. The total energy *e* is determined by

189 
$$e = h - \frac{p}{\rho} + \frac{1}{2}(u^2 + v^2), \qquad (5)$$

<sup>190</sup> where Y and h denote the mass fraction and the enthalpy of species. The quantities  $G_x$  and  $G_y$  in Equation (1)

## 191 represent the diffusion fluxes obtained as

192 
$$G_x = (0, \tau_{xx}, \tau_{xy}, u\tau_{xx} + v\tau_{xy} - q_x, \rho_i D_i \partial Y_i / \partial x), \qquad (6)$$

193 
$$G_{y} = (0, \tau_{yx}, \tau_{yy}, u\tau_{yx} + v\tau_{yy} - q_{y}, \rho_{i}D_{i}\partial Y_{i} / \partial y)$$
(7)

194 The shear stress terms in Equations (6) and (7) are determined by

195 
$$\tau_{xx} = \mu(\frac{4}{3}\frac{\partial u}{\partial x} - \frac{2}{3}\frac{\partial v}{\partial y}), \tau_{yx} = \tau_{xy} = \mu(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}), \tau_{yy} = \mu(\frac{4}{3}\frac{\partial v}{\partial y} - \frac{2}{3}\frac{\partial u}{\partial x}), \tag{8}$$

196 where  $\mu$  represents the mixture viscosity. The heat fluxes in equations (6) and (7) are given by

197 
$$q_x = -k\partial T/\partial x - \rho \sum_{i=1}^n h_i D_i \partial Y_i / \partial x$$
(9)

198 
$$q_{y} = -k\partial T / \partial y - \rho \sum_{i=1}^{n} h_{i} D_{i} \partial Y_{i} / \partial y, \qquad (10)$$

199 where k and  $D_i$  are mixture-averaged thermal conductivity and mass diffusivities, respectively. The mixture dynamic viscosity  $\mu$  and the thermal conductivity k coefficients are modeled by the formulas of Wilke <sup>58</sup> and Mathur 200 201 <sup>59</sup>, while the mass diffusion coefficients for averaged molecular species are modeled by a simplified equation that is 202 inversely proportional to pressure. The thermodynamic and transport properties are calculated by the CHEMKIN-II 203 package. Finally, Equation (1) is closed by employing the perfect gas equation of state for each species. The above-204 mentioned equations were solved via AMROC (Adaptive Mesh Refinement in Object-oriented C++) <sup>51</sup>, which has been extensively utilized for multi-dimensional detonation simulations <sup>50, 56, 57, 60-64</sup>. The solver has also been 205 successfully adopted for analyzing flame acceleration and DDT processes in previous research <sup>16, 47, 62</sup>. 206

207 A first-order dimensional splitting was adopted to solve the governing equations. In addition, a first-order Godunov 208 splitting was used for solving the reaction equations because of the significant difference in time scales for the fluid 209 flow and the source term of the chemical reaction <sup>51</sup>. A hybrid Roe-HLL (Roe-Harten-Lax-Van Leer) Riemann solver 210 <sup>51</sup> was employed for discretizing the upwind fluxes to potentially avoid unphysical total density and internal energy 211 near vacuum due to the Roe linearization. The Minmod limiter with MUSCL (Monotone Upwind Scheme for 212 Conservation Laws) reconstruction was adopted to obtain second-order accuracy in space. A central difference scheme 213 was utilized to handle the diffusion terms of the Naiver-Stokes equations in Equation (1). A semi-implicit generalized 214 Runge-Kutta scheme with fourth-order accuracy was utilized for integration of the chemical kinetics. For the chemical 215 reaction source, the Godunov splitting with first-order accuracy was employed, and it has a enough accuracy compared 216 to Strang splitting as reported by former study <sup>51</sup>. The level-set technique with ghost fluid approach <sup>65</sup> was introduced 217 to implement the embedded solid wall boundaries when introducing the solid obstructions in the upper and lower 218 walls, as highlighted by the yellow objects in Fig. 1.

Case number	Study purpose	Jet position (mm)	Jet start time (ms)	Jet pressure (MPa)	Configuration
1	Comparisons of both	-	-	-	А
2	obstacles	100	0.001	0.35	В
3	Effect of dual jet	100	0.001	0.35	С
4	Effect of jet start time	100	0.25	0.35	В
5		100	0.5	0.35	В
6	Effect of jet pressure	100	0.001	0.2	В
7		100	0.001	0.5	В
8		100	0.001	0.65	В

In particular, a detailed chemical kinetic model of hydrogen-air <sup>66</sup> with 12 species and 42 elementary reactions was 222 employed for modeling the chemical reaction for the flame acceleration and DDT processes. A comparison of 223 224 Westbrook's and Burke's mechanisms <sup>67</sup> for the flame acceleration and DDT in Case 1 was also conducted. The results 225 demonstrate that the  $T_{DDT}$  for Burke's and Westbrook's mechanisms are t=1.41543 ms and t=1.37514 ms, respectively, 226 which corresponds to just a 2.8% difference. The required  $L_{DDT}$  for the Burke and Westbrook reactive mechanism are 227 L=462 mm and L=505 mm so that the difference is 9.3%. The influence of the specific reaction mechanism on the 228 current research appears to be small, and therefore the Westbrook mechanism was primarily employed to simulate the 229 DDT process throughout this study. It has also been employed in the previous study <sup>47</sup>.

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### 231 C. Mesh resolution test

An initial grid of  $Lx \times Ly = 1750 \times 50$  was employed as basic resolution with a maximum mesh size of  $4.0 \times 10^{-4}$  m in both x- and y-directions. The AMR approach <sup>16, 51, 68</sup> was employed during the simulation of the entire DDT process. Three different refinements were taken into consideration to verify the effect of grid resolution on the flame acceleration. Consequently, the refined mesh size was reduced to  $1.0 \times 10^{-4}$  m,  $5.0 \times 10^{-5}$  m and  $2.5 \times 10^{-5}$  m for the three meshes A, B and C, respectively. The laminar flame thickness for the present mixture given in Table I is L<sub>1</sub>=

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 $3.5 \times 10^{-4}$  m. As a result, three different refined levels were considered with 3.5, 7, and 14 grid points (Pts) in the laminar flame thickness (Pts/L<sub>1</sub>).

239 Case 1 in Table II was chosen as a physical model for the mesh resolution test. To reduce the computational cost, a 240 limited computation time was considered to simulate the initial stage of the DDT process, and a higher initial pressure 241 with P=0.6 MPa in the hot spot with a radius of 10 mm was employed to trigger the flame acceleration. The obtained 242 results of the flame propagation for the flame tip from three meshes are illustrated in Fig. 2, where the vertical ordinate 243 is scaled logarithmically. The simulations converge as the mesh resolution increases during the flame acceleration. As 244 the mesh resolution increases, the locations of the flame front are almost collapsed into one as shown in Mesh B and 245 Mesh C. As such, the mesh resolution in Mesh B is accurate to resolve the flame acceleration process properly, corresponding to 7  $Pts/L_1$ . This result is in accordance with the literature where it was found that a mesh resolution 246 from 5-10 Pts/L<sub>1</sub> has little effect on the flame acceleration in the DDT simulation  $^{14, 16, 32, 40}$ . See especially Kessler et 247 al.'s report  $^{40}$  where the flame surface area has only a tiny difference between 5 and 10 Pts/L<sub>1</sub> resolution. 248

249 It is found that the computing time  $(cpu \times h)$  for Mesh C almost requires four times that for Mesh A. Hence, it would 250 take high computational resources for the high resolution in Mesh C when the flame propagates through the entire 251 tube combustor. Consequently, since the current study does not emphasize the detonation wave propagation, the mesh 252 resolution B corresponding to the level 4 refinement is adopted in the following flame acceleration and DDT studies, 253 in order to balance the computing requirements with accuracy in the current engineering simulations. The highest 254 refinement factor is also applied on the upper and lower boundary walls. Adaptive results of AMROC for detonations 255 <sup>7, 56, 57, 68</sup> and DDT processes <sup>16</sup> were also validated in previous works. Hence, the AMR criteria is effective and robust in the current model to deal with the flame acceleration and DDT. The computations were carried out on the Tianhe-256 257 1 supercomputer located in the Changsha Computer Center, where 18 nodes with 216 cores were employed for 258 simulating a single DDT process.



# 261

FIG. 2. Propagation of the flame front in the combustion tube for different mesh resolutions.

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### 263 III. RESULTS AND DISCUSSION

#### 264 A. Comparisons of flame acceleration and DDT

The flame front and temperature contours over time for the solid obstacles only (Case 1 in Table I) are shown in 265 Fig. 3. The mixture is ignited by a hot spot from the semi-circle (Fig. 3(a). The leading flame front propagates slowly 266 267 at the initial stage but accelerates rapidly when it passes through the first solid obstacles with a velocity of 282 m/s at 268 0.47 ms (Fig. 3(c)). The surface area of the propagating flame is dramatically wrinkled at t=0.538 ms (Fig. 3(d)), caused by the flow instability generated by the flow acceleration <sup>30, 32</sup>. This results in an elevated surface area and 269 270 instability of the flame front, which is mainly due to the high interactions between the turbulent flow and flame because of a series of instabilities including Rayleigh-Taylor (R-T) and K-H<sup>14, 33, 40, 53</sup>. These further increase the energy release 271 ratio as confirmed by previous research <sup>32</sup>. Simultaneously, the continuously increasing combustion flame introduces 272 273 the compression wave, and the leading shock wave is subsequently generated when the compression waves focus 274 together. The flame surface area is increasing dramatically when the flame front propagates into the recirculation zone and passes through the solid obstacles owing to the K-H and R-T instabilities, inducing two larger parallel eddies as 275 276 marked in rectangles A1 and A2.

The flame goes into a deflagration stage, and the propagating velocity continues to be augmented to a magnitude of a half CJ velocity from t=1.0082 ms (Figs. 3(k) and 3(n)). Consequently, the deflagration combustion produces a large number of complex shock waves that also induce a Richtmyer-Meshkov instability. The leading shock wave heats the unburnt mixture before the leading flame front approaches, as seen in previous research  $^{69, 70}$ . The complicated interactions of the shock-shock, shock-turbulence, and shock-flame occur, leading to intense turbulent flow and pressure rise when there is a shock wave focusing  $^{71}$ . Such features further lead to the occurrence of a local detonation starting at t=1.37514 ms (Fig. 3(p)); hence, the DDT takes place successfully because of pressure gain combustion.

285 The occurrence of DDT requires ten pairs of solid obstacles. There is no doubt that it would be difficult to induce 286 detonation combustion in an engineering application of a PDE when the ignition is started from the low-energy ignition. 287 However, the requirement of detonation combustion triggered by a high-energy ignition is difficult for a discontinuous 288 detonation engine because many solid obstacles placed in the combustion chamber also produce considerable 289 propulsion loss, as discussed in the introduction. Therefore, the fluid obstacle is introduced into the combustion 290 chamber. The obtained flow and temperature evolution as a function of time for Case 2 are presented in Fig. 4. The 291 initial stage of combustion is similar to Case 1 from t=0.0 ms (Fig. 4(a)) to t=0.64 ms (Fig. 5(e)), where there is a large 292 blockage of turbulent flow generated by the jet, as highlighted with lower temperature regions in Fig. 4(b). The 293 crossflow deflection forms in the chamber because of the influence of the mainstream flow. Subsequently, the 294 interaction between the flame and turbulence flow is formed clearly as marked by a black dashed rectangle at t=0.793 295 ms. The flame surface area increases significantly, enhancing the flame propagation velocity accordingly. Due to the 296 intense flame acceleration, a shock wave and a preheated zone of the mixture between this shock wave and the flame 297 front are also generated (see Figs. 4(k) and 4(m)). Meanwhile, the intense leading shock wave is reflected from the bottom wall, forming a remarkable Mach stem at t=1.04882 ms, promoting the detonation initiation. 298



FIG. 3. Snapshots of temperature contours with time evolution for the entire DDT process that occurred in the
 combustion chamber with only solid obstacles (Case 1).

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304 The distance between the leading shock wave and the flame front is almost constant throughout this regime. These characteristics are called a pattern of "shock-flame" complex <sup>25, 30</sup>, meaning that the flame velocity is almost the same 305 306 as the leading shock wave. This stage also suggests that the detonation will be generated automatically in the region 307 between the leading shock and the flame front. In particular, a localized explosion spot is formed, as denoted by a 308 black dashed circle in Fig. 4(n), where a higher temperature area is generated. This localized explosion further 309 propagates downstream through the chamber, generating an overdriven detonation. Meanwhile, the flame front is 310 mostly spherical. This is due to the onset of detonation in DDT scenarios being overdriven, which is less cellularly 311 unstable as the ratio of the overall activation temperature to the leading post-shock temperature is reduced. The 312 subsequent Mach stem is generated, enhancing the detonation combustion (see Fig. 4(p)).



FIG. 4. DDT characteristics rendered by temperature in the combustion tube using the combined obstacles of thetransverse jet and solid in Case 2.

The detailed variations of the temperature and pressure contours before and after the detonation initiation are 318 319 illustrated in Fig. 5. As the two reflected shock waves (see arrow SW1 and arrow SW2 in Fig. 5(a1)) collide together, 320 a hot spot with increasing pressure, as highlighted by the red dashed circles B1 and B2, is formed (Figs. 5(a2) and 321 5(b2)). The maximum pressure value of the spot reaches 9.20 MPa, which is almost six times that of the theoretical 322 CJ pressure. Therefore, the mixture in this spot is preheated due to the intense reflected shock wave focusing. Meanwhile, the reaction front of the flame also interacts with the high-pressure spot region as denoted by the black 323 dashed circle in Fig. 5(b1). Consequently, a localization explosion region induced by these factors is formed (see Fig. 324 5(c1)), resulting in a detonation transition. This DDT mechanism contributs to rapid energy deposition in a small 325 326 localized region on a quite small timescale. Such onset of detonation is also observed in the numerical result of 327 Goodwin et al.'s study 53. This detonation transition is a typical DDT mechanism in a low Br configuration, which is

often formed by a spot that has high pressure and high temperature before direct initiation generated by the shock wave focusing. The current ignition mechanism always takes place in a condition where there is a slightly large spatial interval (*S* in Fig. 1) between the solid obstructions. It is also consistent with direction initiation theory <sup>72</sup>, as reported in experimental research for a low Br <sup>73</sup>. After that, the overdriven detonation wave expands to the downstream chamber as shown at t=1.07108 ms.

333 The pressure records along the central line of the chamber varying with time for Case 2 are further superimposed 334 on Fig. 6. As shown, the pressure gain is produced by the gas expansion in the left side region of the tube at t=0.31333 335 ms. Note how two parallel regions, that are lower than the initial charge pressure, are formed, which is attributed to 336 the transverse jet that produces lower pressure regions. The pressure in the left side of the tube continues to be 337 augmented as the mixture burns out with a higher energy release ratio, which can be proved by the red arrow A in Fig. 338 6(a). Therefore, the combustion mode within the tube is a pressure gain combustion. Subsequently, the compression 339 wave is generated in the combustor as a result of the response of the thermomechanical energy caused by the elevated 340 energy release ratio  $^{74}$ , and it further propagates along the tube (see t=0.8015 ms and t=0.9035 ms). In addition, there 341 is a high fluctuating pressure due to the reflected shock wave propagating from the upper and lower walls, or the solid 342 obstacles.

The pressure continues to be increased from P=1.2 MPa to P=2.0 MPa, as shown by the maximum point at t=1.0343 344 ms and t=1.041ms, feeding back to heat the unburned material and creating a condition that induces the detonation 345 initiation. Hence, the leading shock wave incorporated in the flame front evolves into a detonation wave, resulting in a high-pressure difference between the induced reaction zone and fresh mixture, as illustrated at t=1.091 ms and 346 t=1.144 ms. The detonation combustion is still in a stage of overdrive. Hence, its pressure is higher than the CJ value 347 <sup>75, 76</sup>. It is worth mentioning that the pressure ratio in the current tube combustor is still close to the range of 15-20 348 349 across the detonation wave, as confirmed by previous research. It is around two times of that produced in the 350 deflagration combustion under the almost constant volume conditions <sup>2, 6</sup>.



FIG. 5. Temperature (left) and pressure (right) color plots for different times before and after the occurrence ofdetonation. SW-shock wave.

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356 To clearly picture the variations of the flame tip in both cases, comparisons of the flame front and the corresponding flame front propagation velocity with time evolution for Cases 1 and 2 are plotted in Figs. 7(a) and 7(b), respectively. 357 358 At the initial stage, the flame tip that takes place in Case 1 is slightly higher than that in Case2, indicating that the 359 flame propagation velocity in Case 1 is larger than that in Case 2, which is confirmed by the incipient stage of velocity variation in Fig. 7(b). This is caused by the later transverse jet that introduces a high Br around t=0.53800-0.64000 360 ms, which generates a high-pressure region and blocks the initial propagation of the flame slightly before the flame 361 tip approaches the jet exit, whereas the axial position of the flame front in Case 2 catches up with Case 1 after around 362 363 t=0.9 ms, as demonstrated in the zoomed view of Fig. 7(a). The latter is attributed to the flame-turbulence interactions during the state from t=0.759 ms (Fig. 4(f)) to t=0.9035 ms (Fig. 4(i)), leading to an increasing flame surface area that 364 365 increases the flame propagation velocity, as identified by the blue dash circle in Fig. 7(b). Such an increased flame 366 surface area produced by the flame-turbulence interactions was also observed in previous numerical simulations in a

367 smooth chamber and experimental investigations at the early stage of the transaction from the laminar flame to 368 turbulent flame <sup>43, 44</sup>. After t=0.9 ms, the axial flame position in Case 2 is gradually higher than that in Case 1. 369



FIG. 6. Pressure records along the central line of the chamber for Case 2, (a) initial stage of combustion; (b) stage
around the detonation occurrence.

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374 Figure 7(b) presents a typical flame front velocity variation during the flame acceleration and DDT processes. The 375 flame propagation velocity increasingly fluctuates from almost zero to a velocity that is higher than the theoretical CJ 376 value, implying that the transition from deflagration to detonation has occurred. The initial detonation is almost an overdriven detonation during the incipient DDT process <sup>6,30</sup>. Subsequently, the flame velocity decreases gradually for 377 378 both cases and approaches the theoretical CJ value, suggesting that the detonation enters a stable state. There is an 379 apparent velocity difference after the occurrence of detonation, and the magnitude of the deflagration velocity is almost 380 half the CJ value. Hence a propagating flame speed of about half the theoretical CJ value is required before the 381 occurrence of detonation. This is because there is no continuous transition from the deflagration combustion in the 382 lower branch to the detonation model in the upper branch associated with the Hugoniot curve <sup>31</sup>, derived from the 383 theoretical solution. This observation is also consistent with recent experimental and numerical research on the DDT 384 process <sup>33, 49, 53, 76</sup>. But this rule is a rough criterion only, and the onset of detonation also depends on the obstruction and lower values (40% CJ speed) can be sufficient <sup>76</sup>. In terms of the stage before the detonation, there is a high 385

fluctuating velocity for the propagating flame, which contributes to the influence of the solid obstruction. A more detailed discussion associated with these deflagration mechanisms in both cases will be given in section III.B.

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FIG. 7. (a) Axial position of the flame front and (b) the flame front velocity versus time for the chamber with solid
obstacles only Case 1, and the case with combined fluid and solid obstacles (Case 2).

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The above-obtained results of the  $T_{DDT}$  and  $L_{DDT}$  or Cases 1 and 2 are listed in Table III, which can be obtained from Fig. 7(a) as marked by Points A and B. The  $T_{DDT}$  is shortened from t=1.37514 ms to t=1.06906 ms when employing a single transverse jet; hence there is a 22.26% improvement in the  $T_{DDT}$ . Besides, the  $L_{DDT}$  is also shorted from L=505 mm to L=336.55 mm so that the improvement reaches 33.36% compared to the chamber only having solid objects, meaning that the required number of solid obstacles can be reduced from 10 pairs to 7 pairs. Furthermore, the reduced time and length of the DDT process further suggest that the performance of a PDE would be elevated due to its high operating frequency.

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- 401

TABLE III. The obtained  $T_{DDT}$  and  $L_{DDT}$  for the onset of detonation for Cases 1 and 2.

	Case 1	Case2	Enhanced efficiency
DDT run-up time (ms)	1.37514	1.06906	22.26%
DDT run-up distance (mm)	505	336.55	33.36%

#### 403 B. The mechanisms of flame acceleration in combined obstacles

404 For revealing the mechanisms of the combined obstacles on the flame acceleration, further detailed information 405 involved in the combustion evolution and flame-turbulence interactions for Cases 1 and 2 are given in Fig. 8 before 406 t=0.9 ms. These snapshots are rendered from the density, where the black regions represent the combustion product 407 due to the lower density while the much higher density denotes the mixture downstream of the transverse jet. At t=0.64 408 ms (Fig. 8(a1)), the flame fronts of both cases are almost the same. The flame penetration is formed in Case 1 in Fig. 409 8(b1). Next, the surface area of the flame continues to increase, resulting in a high-energy release ratio from the 410 mixture that further augments the propagation velocity in Case 1. As a consequence, the baseline A in Case 1, 411 constructed from the flame tip at different times, has a large slope compared to that in Case 2 at the incipient stage. 412 However, the surface area with no conspicuous distortion decreases within the chamber in the range of 5 cm<X<10 413 cm in Fig. 8(e1) due to the increasing volume of the chamber when there is no obstruction. Yet, it undergoes the next 414 acceleration due to the decrease of flow area caused by the paired solid obstructions at X=15 cm. The reflected 415 compression wave is formed as denoted by arrow C. Meanwhile, the small vortices shedding from the tip of the solid 416 obstruction is generated in the red dashed box D.

417 In terms of combined obstacles in Case 2, the flame penetration occurs later, and it persistently continues from 418 t=0.7335 ms to t=0.81 ms. This is due to the gradual decrease of the free flow area of the flame, which is partially 419 occupied by the transverse jet, as shown in Fig. 8(d2), leading to the flame acceleration. Besides, the flame front is far 420 away from the tip of the solid and the outer boundary of the transverse jet and almost has a symmetry structure along 421 the central line of the chamber, as shown in Fig. 8(c2). This is attributed to the accumulation of a high-pressure region ahead of the combined obstructions from the solid plate and transverse jet. It indicates that the transverse jet obstacle 422 423 can play the same role as a solid obstruction. The large turbulent eddies stemming from the exit of the transverse jet 424 are formed by the influence of the mainstream fluid flow. Next, the outer shear layer introduced from the jet stream interacts with the lower flame front, yielding a conspicuous deformation, deflection, and recirculation flow of the 425 flame tip, as indicated by the rectangles F1, F2, and F3, which further augments the flame surface area, producing a 426 427 persistent flame acceleration.





FIG. 8. Snapshots of density distribution in the downstream chamber during the initial time and before the occurrence
of DDT (the left column is the chamber only having solid obstacles in Case 1, while the right column is the combined
fluid and solid obstacles in Case 2).

Further inspecting the downstream flame front in the same region, as denoted by a red dashed box B, it can be found 434 435 that there is a dramatic difference. No prominent turbulent flow forms in Case 1; conversely, remarkable turbulent flow penetration and eddies are observed, and these turbulent flows interact with the fixed solid obstructions, 436 437 producing a large block of K-H instabilities from the tip of the solids, which gradually propagate downstream the channel. It also expands the influential regions with time evolution, as indicated by the blue dashed boxes G1 and H1 438 to G2 and H2. A lot of K-H instabilities are generated at an early stage as shown by the blue dashed box I in Case 2. 439 440 These flow characteristics will influence the upcoming flame front (see Fig. 8(g2)). Recent works <sup>16,77</sup> have conducted 441 detailed research of the transverse jet on the DDT process in a smooth channel, and the results demonstrated that there 442 are a lot of mushroom vortices in the jet exit downstream, but no significant K-H instabilities can be formed in the 443 downstream tube.

## To compare the flame propagation differences in Cases 1 and 2, Fig. 9 provides the variations of velocity, vorticity, and pressure contours, where the black line within these contours represents the flame front, which was extracted from

446 the OH elementary contour. A high-velocity region appears in the penetration flame front in the red rectangles A1 and 447 A3 in Case 1 and the red box A4 in Case 2. However, the flame propagation velocity decreases when the flame tip 448 propagates into the separated interval between the obstructions in Case 2 (see Fig. 9(a2-2)). Moreover, there is almost 449 a symmetric distribution of velocity along the central line of the tube as shown by box A2, while a more non-uniform 450 distribution of velocity contour is generated because of the transverse jet influence (see box A5 in Case 2). Note that 451 this region has a higher velocity than that in Case 1 at the same time. Hence, it can be concluded that the transverse 452 jet stream can significantly influence the downstream flow field. A high magnitude of fluid flow with non-uniform 453 distribution can be formed early ahead of the upstream flame front.

The flame-turbulence interactions can be further evidenced by the vorticity contours. The jet in crossflow mainly forms a large part of clockwise (negative) vorticities under the influence of the mainstream flow, which prompts the turbulent reactant transport when the flame front approaches the outside boundary layer of the transverse jet (see Fig. 9(b2-2)). A large part of anti-clockwise (positive) vorticities is generated and it is growing from the tip of solid obstruction from boxes B2 to B3 in Case 2. These vorticities evolve into large turbulent vortexes at the next time and enhance the turbulent reactant transport when the flame front propagates in those regions <sup>43, 44</sup>. By contrast, just a few vorticities with lower magnitude are gradually forming due to the K-H instability (see box B1).

461 The lower pressure regions are formed behind the solid objects, as shown by box A1 associated with Case 1. The pressure increase is formed as marked by box C1 in Case 1 due to the Br<sup>14, 32</sup>. As such the flame front is wrinkled and 462 463 stretched. Regarding Case 2, the non-uniform distribution of pressure contour in box C3 is generated because of the 464 large turbulent flow and eddies, as proved by Figs. 9(b). The high asymmetry pressure spots are generated in the red dashed box C4, deflecting the flame front later. Moreover, there is a high-pressure region in the unconfined space 465 between 10 cm< X <15 cm (boxes C4 and C5) in the same regions, resulting in a higher flame acceleration in Case 2. 466 467 The next flame propagation rendering from temperature for both cases after t=0.9 ms are shown in Fig. 10. The baseline A established from the flame front in Case 1, has a lower slope from Fig. 17(a1)) to Fig. 17(d1). In contrast, 468 there is a high slope of line B in Case 2 due to the different flame acceleration ratios. A flat flame front is formed 469 470 before the solid obstruction at X=20 cm thanks to the Richtmyer-Meshkov instability <sup>78</sup> caused by the reflected wave. 471 On the other hand, a penetration flame front is generated as shown by the black dashed box A caused by the flame-472 turbulence interactions. The flame front is further wrinkled and stretched by the turbulent vortices generated by the

- 473 transverse jet at the last stage visualized by Fig. 9(b). These characteristics stimulate the increase of the flame surface
- 474 area, hence an abrupt energy release ratio introduces a high flame acceleration <sup>32, 33, 53</sup>.
- 475



477 FIG. 9. Time evolution of (a) velocity, (b) vorticity, and (c) pressure contours during the flame propagation for two

<sup>478</sup> cases; the left side is Case 1, while the right side is Case 2.



480 FIG. 10. Time record of temperature contours with the flame propagation for Cases 1 (left column) and 2 (right481 column).

To further reveal the flame propagating mechanisms in Case 2, Fig. 11 presents the evolution of pressure, vorticity, 483 and velocity vector at the same time with Fig. 11(b). An increasing pressure region appears in the top boundary ahead 484 of the solid object (see boxes A1 and A2) due to the flame deflection, which contributes to the negative vorticity 485 influence, as shown by the boxes B1 and B2. These vorticities further deflect the flame front and form remarkable 486 487 flame-turbulence vortexes, as demonstrated by the rectangles B3 and B5. Subsequently, the high-pressure region 488 appears in the box A2 and the low-pressure region shown in the box A3 is further deflecting the flame tip, as shown 489 in box B4, yielding a stretched flame front, then increasing the flame surface area. These combined influences act on 490 the flame front result in continuously increased velocity when the flame tip crosses a confined area, as confirmed by 491 the high magnitude of the velocity vector marked by the boxes C1-C4.



FIG. 11. Variation of the flame propagation downstream of the transverse jet in Case 2 (the upper row is the pressure
contour; the middle rows are the vorticity contours; while the lower row is the corresponding velocity vector; and the
background is the density contour).

498 For the purpose of quantitatively revealing the mechanisms of flame acceleration, Fig. 12 presents the temporal flame tip propagation velocity and the corresponding acceleration of flame spreading along with the axial position of 499 500 the channel at the incipient stage for Cases 1 and 2. The variations for both variables can be categorized into three 501 stages. In stage I, the profiles in both cases have almost the same trend ahead of X<100 mm because the configuration 502 at the front tube is the same and there is yet no noticable influence from the downstream transverse jet in Case 2. In stage II, the flame velocity for case 2 is higher, then lower than that in Case 1. This is due to the jet influence, which 503 initially provides a high Br that has a negative effect on the flame front propagation, then produces an intense flame-504 505 turbulence interaction that increases the surface area. These interactions can also be observed in Fig. 8(F1-F3). As a

506 result, an initial increase, then a sudden decrease in the flame acceleration is observed at stage II in Fig. 12(b). Then, 507 the flame front experiences the next acceleration under the paired solid obstructions at X=150 mm. Both cases have 508 an abrupt increase of flame speed around the barrier, resulting in a sharp increase in the flame acceleration. However, 509 a quick decrease of the flame velocity in Case 1 occurs in box B because of the increase of flow area as discussed 510 above. Conversely, a preserved increase with no obvious decrease in the flame velocity in Case 2 is observed as 511 denoted by frame A. This is because of the turbulent vortices' influence in the current stage as discussed in Fig. 11. 512 After these complicated flame accelerations, the speed is further accelerated to a scale of half CJ value (1000 m/s) in 513 the next acceleration stage III in Case 2 as demonstrated in Fig. 12(a). Consequently, the combined obstacles in Case 514 2 result in a shorter run-up time and less run-up distance of the occurrence of the DDT. Almost the same value of 515 flame propagating velocity (700 m/s) is generated in the next accelerating stage associated with Case 1, which will 516 require more run-up time and run-up distance to accelerate the flame speed into a magnitude of one-half of the CJ 517 speed.











524 In summary, the main results demonstrate that the jet obstacle plays a similar role for the Br as the solid obstacle 525 when the flame front passes the upper jet position. Besides, the early flame-turbulence interactions ahead of the jet

526 exit presented in Fig. 8 result in the flame deflection and a significant augment of the flame surface area, forming a 527 remarkable pressure gain combustion as proved by the pressure contour in Figs. 9(c2-2) and 9(c2-3). Furthermore, the 528 early transverse jet under the effect of mainstream flow introduces more intense turbulent flow and eddies that interact 529 with the fixed obstacles, producing a lot of K-H instabilities shedding from the solid plates compared to that with only solid obstacles in Case 1, as demonstrated by the vorticity contours in Figs. 9(b2-1) and 9(b2-2). Subsequently, these 530 531 characteristics introduce further flame-turbulence interactions that curve and stretch the flame tip as shown in Fig. 532 9(a2-c2); therefore, a persisted flame acceleration without conspicuous decrease is formed, as confirmed by the record 533 of flame velocity in Fig. 12(a). These main outcomes lead to the propagating velocity of the flame front in Case 2 534 reach about half of the theoretical CJ velocity, promoting the onset of detonation.

535

#### 536 C. The effect of head-on jets on the flame acceleration and DDT

537 For further revealing the flame-turbulence interactions that have a positive effect on shortening the  $T_{DDT}$  and  $L_{DDT}$ . 538 the dual jets in crossflow placed in the chamber are investigated here, as demonstrated by configuration C in Fig. 1(c). 539 The evolution of the head-on jet stream and the flame acceleration rendering from density and the subsequent DDT 540 process are presented in Figs. 13(A) and 13(B), respectively, corresponding to Case 3 in Table II. As shown in Fig. 541 8(A), two mushroom vortices are generated and propagate upstream and downstream along the axial direction, due to 542 the head-on impact of the jet. Then, the leading mushroom eddies propagate anti-clockwise and clockwise along with 543 the chamber. Under the effect of the mainstream, the jet stream is perturbed, then the disordered and intense vortexes 544 are formed accordingly (Fig. 13(A-c)). More turbulent flows and eddies are generated in the downstream chamber 545 compared to Case 2 at the same time of t=0.64 ms. Meanwhile, the leading mushroom vortex in the upstream tube interacts with the leading flame front, as denoted by arrows A and B. This flame-turbulence interaction further 546 547 propagates, forming a slim and stretched flame front as denoted by boxes B1-B4 in Fig. 13(a). This interaction enlarges 548 the flame surface area dramatically, resulting in a high propagation velocity of the flame. The turbulent flow interacts 549 with solid obstacles, resulting in triggering the K-H instabilities. As such, as shown in box C, more regions of turbulent 550 flow in the downstream tube are observed. These outcomes further result in a high flame propagation velocity. 551 Subsequently, a shock-flame complex feature is generated as shown in Figs. 13(B-m), 13(B-n), and 13(B-o). As a 552 result, a localized explosion is activated at the bottom wall boundary, and it further expands to the downstream 553 chamber, leading to a significant detonation wave and Mach stem with a shorter  $T_{DDT}$ .

The propagation of the flame front and the corresponding velocity for Cases 1, 2 and 3 are compared in Figs. 14(a) and 14(b), respectively. The flame front in these three cases almost collapses into one. However, as more transverse jets are injected into the chamber, the velocity of the flame front increase abruptly (see circle A). The  $T_{DDT}$  in Case 3 is shortened by about 28.72% compared to that in Case 1 with solid obstacles (Fig. 1(a)). The  $L_{DDT}$  in Cases 2 and 3 is almost the same, but an 8.15% decrease of the  $T_{DDT}$  in the head-on jet stream is obtained compared to that in the single jet and solid obstacles (Case 2).

560



562 FIG. 13. The density contour and the subsequent flame front versus with time for Case 3 (the upper row is (A) density

<sup>563</sup> contour, and the lower row is (B) temperature contour).



FIG. 14. (a) Axial position of the flame front and (b) velocity versus time for different flame acceleration methods
(Case 1: solid obstacles; Case 2: single jet and solid obstacles; Case 3: dual head-on jets and solid obstacles).

#### 568 D. The effect of initial time of jet on the flame acceleration and DDT

569 The start time of the transverse jet after the ignition of the mixture is studied. Cases 4 and 5 are employed here, 570 corresponding to t=0.25 ms and t=0.5 ms to detect the downstream turbulent flow effect on the DDT process. The 571 evolution of the flame front and transverse jet penetration at the initial stage and the subsequent flame acceleration 572 are presented in Fig. 15 for Case 4. A conspicuous deflection is formed in the chamber after the jet is injected into the 573 channel due to the mainstream flow influence and the delayed start time of the transverse jet; as such no visible 574 turbulent flow is formed ahead of the exit of the jet. However, there is still enough distance between the jet exit and 575 the current flame front. Consequently, the intense turbulent vortexes are gradually formed at the downstream tube 576 before the flame front reaches the transverse jet exit. The fluid is only propagating along the lower boundary wall 577 owing to the increasing mainstream flow, and the K-H instability is occurring and shedding from the tip of solid objects at t=0.691 ms (Fig. 15(c)). Nevertheless, the influence region generated by turbulent flow is less than that in 578 579 Case 2 due to the less jet flowing into the chamber. Next time, similar outcomes of flame-turbulence interactions with Case 2 also appear in Fig. 15(d), introducing a stark increase in the flame surface area. After experiencing a series of 580 flame acceleration, a strong leading shock wave is generated, forming a Mach stem within the obstruction interval in 581 582 Fig. 15(g). Hence, overdriven detonation combustion with a higher temperature occurs in this preheated zone ahead 583 of the solid objects at t=1.2218 ms.



FIG. 15. The propagation of density contour at the initial stage and the subsequent flame front evolution for Case 4(the left column is density contour, while the right column is temperature contour).

589 Figure 16 also presents the snapshots of flame propagation and flame-turbulence interactions rendered from density 590 at the early stage and temperature contours at the next stage, respectively, for Case 5. Just a tiny jet is injected into the 591 chamber, and the transverse jet is directly deflected by the mainstream flow. Consequently, a small influence region 592 that disturbs by the transverse jet is introduced. The transverse jet stream is stretched along the bottom wall as shown 593 in Fig. 16(b). No obvious curved flame front is generated as shown in Figs. 16(c) and 16(d). The transverse jet with a delayed start time has just the same function as a fixed solid obstruction. Subsequently, the flame propagation nearly 594 595 experiences the same processes as in Case 1, including the wrinkled flame and enlarging of the surface area caused 596 by the recirculation flow and shock-flame interaction as presented by the series of snapshots in Fig. 16(e-g). The DDT 597 is activated by the same preheated region between the leading shock wave and flame front.

Variations of flame front position and flame front propagating velocity with time for Cases 2, 4, and 5 are plotted in Figs. 17(a) and 17(b), respectively. The detonation combustion is formed in all cases successfully in a limited length of the tube, as denoted by the corner point by points A, B, and C in Fig. 17(a). The  $T_{DDT}$  for Cases 2, 4, and 5 are t=1.067 ms, t=1.218 ms, and t=1.347 ms, respectively. Hence, there is an improvement of 20.79% of  $T_{DDT}$  in Case 2 compared to that in Case 5, whereas for Cases 4 and 5, although the detonation initiation in Case 4 is faster than that in Case 5, the  $L_{DDT}$  in both cases are almost the same. The strength of flame-turbulence interaction in Case 4 is more

intense than that in Case 5, caused by the additional jet stream injection into the chamber in Case 4, resulting in a



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FIG. 16. The time evolution of the density contour and the subsequent temperature contour for Case 5 (the left columnis density contour, while the right column is temperature contour).

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As shown in Fig. 17(b), the propagation velocity of the flame front for Cases 4 and 5 are almost similar to Case 2 611 at the initial stage time, while with more fluids injected into the chamber,  $T_{DDT}$  is reduced. Additionally, the flame 612 613 velocity variations gradually decrease to the theoretical CJ value after the occurrence of the DDT. Such feature is 614 attributed to the fact that the overdriven detonation generated at the initial time gradually falls into a stable detonation, which is in accordance with the previous experimental and numerical research  $^{16, 32, 76}$ . Furthermore,  $T_{DDT}$  in Cases 1 615 and 5 is almost the same, corresponding to t=1.3745 ms and t=1.347 ms, respectively. Hence, the transverse jet in 616 Case 5 almost plays a single role as a solid obstacle. In general, it can be concluded that the start time of a transverse 617 jet with an early operation is conducive to flame acceleration. With the increase of the delay time of jet operation after 618 619 the mixture ignition, the transverse jet is changed from two functions that form a suitable Br and produce a lot of 620 turbulent flow and vortices to the single function of providing the required Br.



FIG. 17. (a) Axial position of the flame tip and (b) flame front velocity with time for different start time of the transverse jet after ignition (Case 2: t=0.001 ms; Case 4: t=0.25 ms; Case 5: t=0.5 ms).

#### 626 E. The effect of jet stagnation pressure on flame acceleration and DDT

Figure 18 exhibits the variations of  $T_{DDT}$  and  $L_{DDT}$  with the increasing stagnation pressure of the transverse jet obstacle. When  $Br_j$  is increased from 2 to 3.5,  $T_{DDT}$  and  $L_{DDT}$  are reduced by 24.46% and 37.75%, respectively. However, when  $Br_j$  is raised to 5, it has a negative effect on the onset of detonation. Further increasing its pressure has a slight positive effect on the detonation transition, but the stagnation pressure of the jet has no significant effect on the  $T_{DDT}$  when its pressure increases from  $Br_j=3.5$  to  $Br_j=6.5$ . Therefore, just increasing the stagnation pressure does not have a positive influence on shortening  $L_{DDT}$  and  $T_{DDT}$  in the obstacle-laden combustion tube, and it even has a negative effect.

For further insight into these results, Fig. 19 presents the axial position of the flame front and the corresponding flame front propagation velocity as a function of time when varying the stagnation pressure. The flame tip in Case 8 (P=0.65 MPa) is left behind compared to Cases 2, 6, 7 and 8 before the onset of detonation, and this is also confirmed by the propagation velocity of the flame at the time range of t=0.6-0.8 ms in circle B in Fig. 19(b). The flame acceleration rate in the next stage in Case 8 is much higher as confirmed by Fig. 19(b). Next, the transition of detonation has occurred in Cases 2, 8, and 7 consecutively as demonstrated by circles A, B, and C in the zoomed figure; however, it needs more time to activate the DDT in Case 6 as shown in circle D. The corresponding transition can also be observed in Fig. 19 as the curve of propagation velocity increases sharply, and then the velocity decreases

as the overdriven detonation is approaching the CJ detonation.

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FIG. 18. The required DDT run-up time and DDT run-up distance as a function of the blockage ratio generated by the

646 transverse jet.



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FIG. 19. (a) The axial position of the flame tip and (b) flame front propagating velocity with time evolution for different stagnation pressure of the transverse jet after mixture ignition (Case 6:  $Br_j=2$ ; Case 2:  $Br_j=3.5$ ; Case 7:  $Br_j=5$ ; Case 7:  $Br_j=6.5$ ).

652 In general, as the stagnation pressure increases, the mass flow rate and flow momentum generated by the transverse 653 jet increase, and the flow turbulence and vortices are enlarged accordingly. In other words, the extra energy generated 654 by the flow perturbation region is enlarged. Such a feature can be confirmed by box A of the density contours for four 655 cases at the same time of t=0.68250 ms in Fig. 20. As the jet stagnation pressure increases, the disturbance length in the chamber increases from 6.76 cm to 9.17 cm, as listed in Table VI. Yet, the increase rate of the disturbance area is 656 not obvious when jet stagnation pressure is greater than 0.35 MPa. Those features have a positive effect on the flame 657 658 acceleration when the flame tip approaches in these turbulent regions thanks to the flame-turbulent interactions that 659 increase the flame surface areas dramatically, as discussed in section III.A.

As shown in the pressure contours in the middle column of Fig. 20, with further augmentation of the jet pressure, 660 661 the high-pressure regions are formed in the front of the flame tip (see series snapshots box B) and within the interval between obstacles. These results can be confirmed by the pressure distributions along the Y-axial direction at Y=9.5 662 cm in Fig. 21(a), where much higher-pressure regions are formed in Case 8, whereas the high-pressure regions are 663 just located in the upper and lower tube in Case 2. The static pressure within the tube is also increased with the increase 664 665 of the jet stagnation pressure, as listed in Table VI. These high-pressure regions located in the middle area of the tube restrain the flame acceleration when the flame tip approaches these areas, as confirmed by the snapshots of the flame 666 667 front in the density contours of Fig. 20 at the same time of t=0.68250 ms so that the flame propagation velocity is 668 reduced sharply, especially in Case 8 as confirmed by circle J in Fig. 14(b).

On the other hand, the intensity of compression wave and vorticity generated by the jet is increased with the augmentation of jet pressure in Case 8 (see Fig. 22(b-d)). The vorticity variations along the central line are given in Fig. 21(b) for four cases at the same time of t=0.68250 ms, where a higher vorticity amplitude is generated with the increase of jet pressure, and the maximum vorticity within the tube is also enhanced when increasing the jet pressure as listed in Table IV. These features have a positive effect on the flame acceleration when the flame front approaches the jet downstream; therefore, the flame acceleration rate increase in the next stage.

Furthermore, owing to the intense compression wave and high flame acceleration ratio, a strong leading shock wave is formed in the combustion tube. When the leading shock wave impacts a solid obstacle, the hot spot with high pressure and temperature in the corner of the solid object is generated ahead of the flame tip, then the onset of detonation is activated (see Fig. 22(g)). This DDT can be explained as a classical hot spot-based initiation <sup>30, 69</sup> through the gradient mechanism when the Mach stem is reflected from the solid wall. The evolution of DDT scenarios is demonstrated by the sequence of temperature contours in Fig. 22(g) and 22(h). Therefore, in terms of the case with high jet pressure, the flame acceleration generates a strong leading shock wave and Mach stem, which is sufficient to activate detonation after it reflects from a solid wall. The current DDT mechanism is consistent with the result obtained in Goodwin's study <sup>53</sup>.

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FIG. 20. Comparisons of density (left column), pressure (middle column), and vorticity (right column) contours at the same time of t=0.68250 ms for four cases with different jet stagnation pressure (the first row (a) is from Case 6, the second row (b) is from Case 2, the third row (c) is from Case 7, and the lower row (d) is from Case 8).





FIG. 21. Variations of the (a) pressure distributions along Y-direction at Y=9.5 cm and (b) vorticity along the central
line of the tube for Cases 6, 2, 7 and 8 at the same time of t=0.68250 ms.

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TABLE IV. The influence parameters generated by different jet stagnation pressure at t=0.68250 ms.

Case number	Stagnation pressure (MPa)	Disturbance length (cm)	Static pressure (MPa)	Maximum Vorticity (1/s)
6	0.2	6.76	0.2075	22810
2	0.35	8.24	0.2507	25740
7	0.5	8.76	0.2489	25770
8	0.65	9.17	0.2706	28400

In summary, the transverse jet introduces flow disturbance, vortices, local high static pressure, and compression waves. With the increase of the jet stagnation pressure, the flow disturbance and vortices are not the main reasons to affect the flame acceleration in the obstacle-laden combustion tube. On the contrary, the local static pressure and compression wave have a more dominant effect on the flame acceleration, but the high local static pressure does not have a position influence on the flame acceleration before the flame front passes these high-pressure regions. Therefore, having a moderate stagnation pressure of the jet that generates appropriate flow disturbance, vortices and compression waves in the obstacle-laden configuration is beneficial for shortening  $T_{DDT}$  and  $L_{DDT}$ .

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### 708 IV. CONCLUSIONS

The unsteady reactive Naiver-Stokes equations with a detailed chemistry reaction mechanism and an adaptive mesh refinement technique were employed to numerically simulate the flame acceleration and deflagration-to-detonation transition (DDT) processes in the current study. The turbulent flow and eddies were produced using a combination of transverse jet and solid obstacles. The effects of the start time of the transverse jet, the dual jet and solid obstacles, and jet stagnation pressure on the flame acceleration and DDT process were investigated to evaluate the efficiency of the flame acceleration. The main conclusions of the current study are:

1. The combined fluid and solid obstacles arranged in a chamber significantly shorten the DDT run-up time and DDT run-up distance. The results for the combined case showed a 22.26% improvement in the DDT run-up time and a 33.36% reduction in the DDT run-up distance compared to that in the chamber with only solid obstructions. While just one width of domain size is considered in the current study, the scale effect should be further investigated, especially for a large widths.

2. The mechanism of the flame acceleration in the combined obstacles is that the transverse jet stream can act as a solid obstruction that provides an appropriate blockage ratio. It also introduces large-scale turbulent flow and eddies in the downstream chamber. This further leads to more intense Kelvin-Helmholtz instabilities shedding from the tip of solid obstacles compared to the transverse jet injected into the smooth chamber in previous studies. The highly turbulent flame interactions and a subsequently stretched flame front are presented, resulting in a sharp augmentation of the propagation velocity with no conspicuous decrease when the flame front propagates to the unconfined space.

3. The dual jets injecting into the chamber produce a lot of mushroom vortices and turbulent flow, which interact
with the flame front and the fixed solid obstacle, resulting in a significantly stretched flame front and a lot of KelvinHelmholtz instabilities stemming from the solid tips. These outcomes result in a high flame propagation velocity
and a shortened DDT run-up time.

4. A transverse jet with an early start time can act as a solid obstruction and in addition generates significant
turbulent features and eddies downstream. With a more delayed start time it only plays a role comparable to a solid
obstruction.

5. A much higher jet stagnation pressure has a negative effect on shortening the run-up time to detonation in the obstacle-laden combustion tube. With the continuous increase of jet pressure, it is found that the DDT run-up

- 736 distance cannot be further decreased, and it is even increased so that there is a moderate jet pressure value that 737 results in the shortest DDT run-up time and DDT run-up distance.
- Gamezo et al.<sup>14</sup> and Goodwin et al.<sup>53</sup> revealed that the flame acceleration and DDT mechanism in the two-738
- dimensional and three-dimensional simulations are similar. The flame acceleration is dominated by the shock wave 739
- 740 reflection. There is some difference in the leading shock wave that always decouples with the flame front. But the
- 741 current flame-turbulent interaction occurs in the initial stage of flame acceleration so that there is still no formation of
- 742 the shock wave. Hence, the jet obstacle has no significant effect in the next stage of flame acceleration. The jet
- 743 diffusion and jet blockage ratio between 2D and 3D are still different; hence 3D simulations of the combination of the
- 744 transverse jet and solid obstacles on the flame acceleration rate should be further investigated.
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