A new single-step reaction mechanism for propane explosions covering the entire spectrum of flame acceleration, transition to detonation and detonation

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Outline

- The new single-step reaction mechanism
- Governing equations & CFD code
- Validation
  - Comparison with detailed chemistry model
  - Detonation cell size
  - Flame acceleration in a vented duct
- Exploratory study - shock and detonation propagation through a U-bend
- Concluding remarks

Limitations of existing reaction mechanisms

(1) Berkeley GRI-mechanism (53 species, 325 reactions)

computationally intensive

(2) Westbrook's mechanism (1981)

$$-\frac{d[C_3H_8]}{dt} = 8.6\times10^{11}\exp(-15000/T)[C_3H_8]^{0.1}[O_2]^{1.65}$$

under-predicting half reaction length

(3) Frolov's model (2007)

$$-\frac{d[C_3H_8]}{dt} = 7\times10^{14}\times p^{n}\times\exp(-454600/RT)[C_3H_8][O_2]$$

under-predicting half reaction length for rich gas

Our group's previous approach in detonation modelling

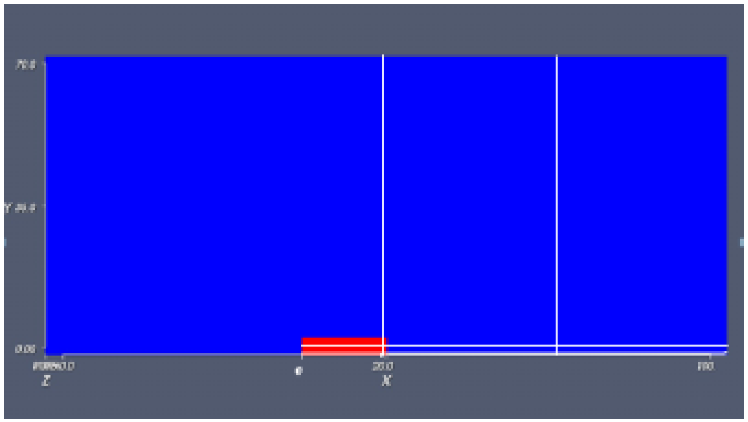
Wen, JX , Heidari, A , Ferraris, S and Tam, VHY (2011) Numerical simulation of propane detonation in medium and large scale geometries. *Journal of Loss Prevention in the Process Industries, 24(2), pp. 187-193. ISSN (print) 0950-4230.*

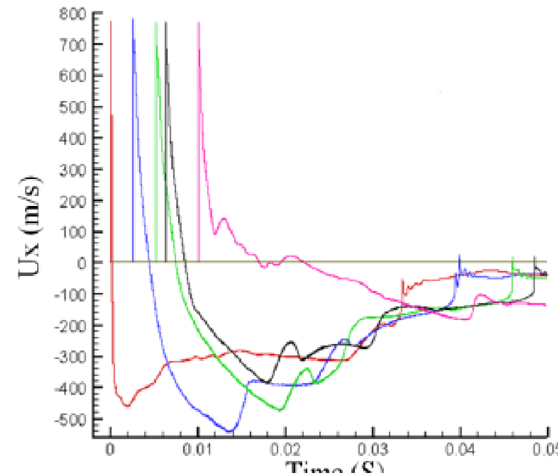
Reaction progress equation: $$\frac{\partial \rho \alpha}{\partial t} = -\nabla(\rho \alpha V) + \rho \omega \quad (4)$$

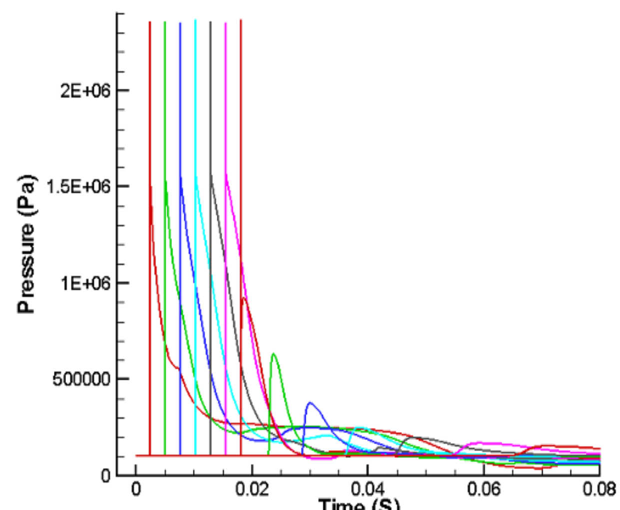
$$\omega = A(1-\alpha)EXP(-\frac{E_a}{RT})$$

The predicted overpressure and velocity *vs* time

Wen, JX , Heidari, A , Ferraris, S and Tam, VHY (2011) Numerical simulation of propane detonation in medium and large scale geometries. *Journal of Loss Prevention in the Process Industries, 24(2), pp. 187-193. ISSN (print) 0950-4230.*







The new single-step reaction mechanism

A singe-step overall reaction for propane-air combustion

$$C_3H_8 + 5O_2 + 18.8N_2 \rightarrow 3CO_2 + 4H_2O + 18.8N_2$$

The reaction rate in Arrhenius form

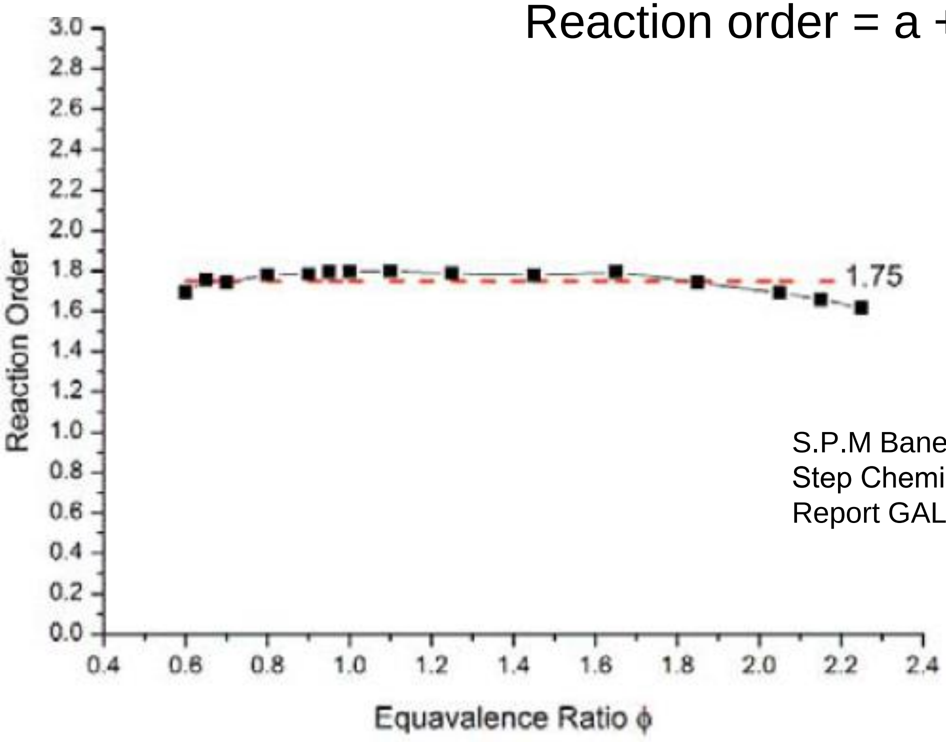
$$\omega = k[C_3H_8]^a[O_2]^b$$

where $\mathrm{k = Aexp}\left(-\frac{\mathrm{E_a}}{\mathrm{RT}}\right)$, $[\mathrm{C_3H_8}]$, $[\mathrm{O_2}]$, . a and b are the rate constant, propane and oxygen molar concentrations, propane and oxygen rate exponents respectively. A and $\mathrm{E_a}$ denote pre-exponential factor and activation energy, respectively.

The new single-step reaction mechanism

$$\omega = k[C_3H_8]^a[O_2]^b$$

Reaction order = a + b



$$n = -\frac{\rho}{\tau_i}\left(\frac{\partial \tau_i}{\partial \rho}\right)_{T_0} + 1$$

S.P.M Bane, J.L.Ziegler and J.E. Shepherd. “Development of One-Step Chemistry Model for flame and ignition simulation”. GALCIT Report GALTCITFM:2010.002, 2010

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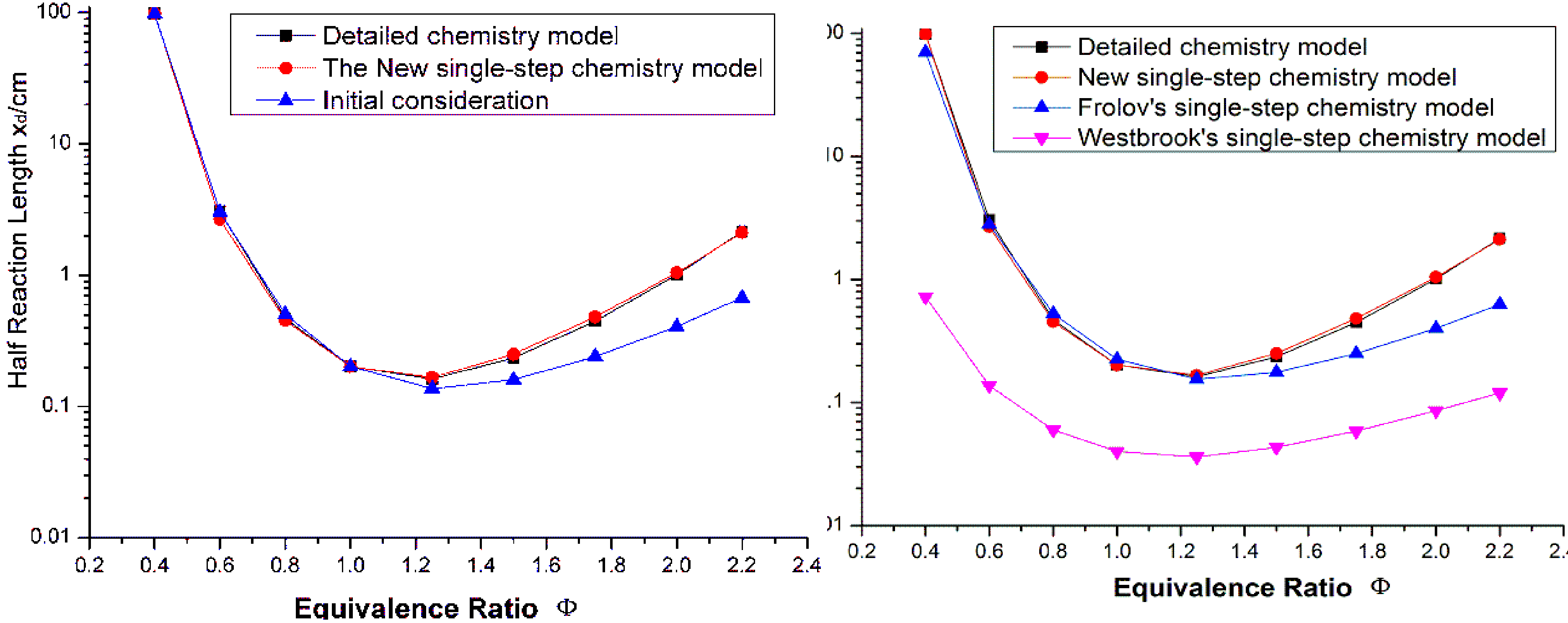
The new single-step reaction mechanism

$$-\frac{d[C_3H_8]}{dt} = 3.11 \times 10^{14} \exp\left(\frac{-55910}{RT}\right)[C_3H_8]^{0.1}[O_2]^{1.65}$$



Governing equations

$$\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_j}{\partial x_j}=0$$

$$\frac{\partial\rho u_i}{\partial t}+\frac{\partial\rho u_i u_j}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right]$$

$$\frac{\partial\rho h_s}{\partial t}+\frac{\partial\rho u_j h_s}{\partial x_j}=\frac{dp}{dt}+\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial h_s}{\partial x_j}\right)+Q$$

$$\frac{\partial\rho Y_k}{\partial t}+\frac{\partial\rho u_j Y_k}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial Y_k}{\partial x_j}\right)+\omega_k$$

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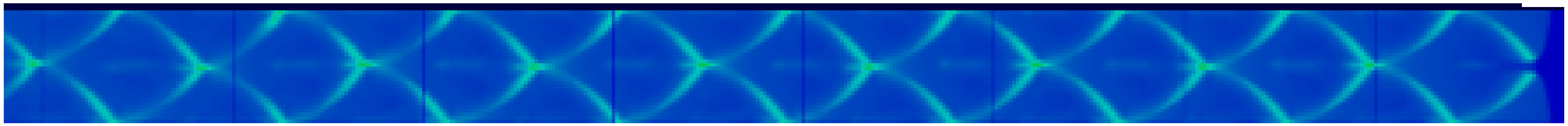
Numerical setup

Time: second-order Crank-Nicholson scheme

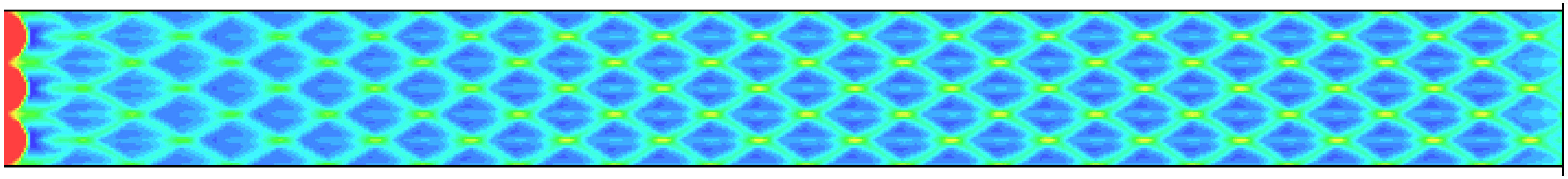
The convective terms: 2rd MUSCL scheme (TVD)

The viscous terms: second-order central differencing discretization

Validation – detonation cell size



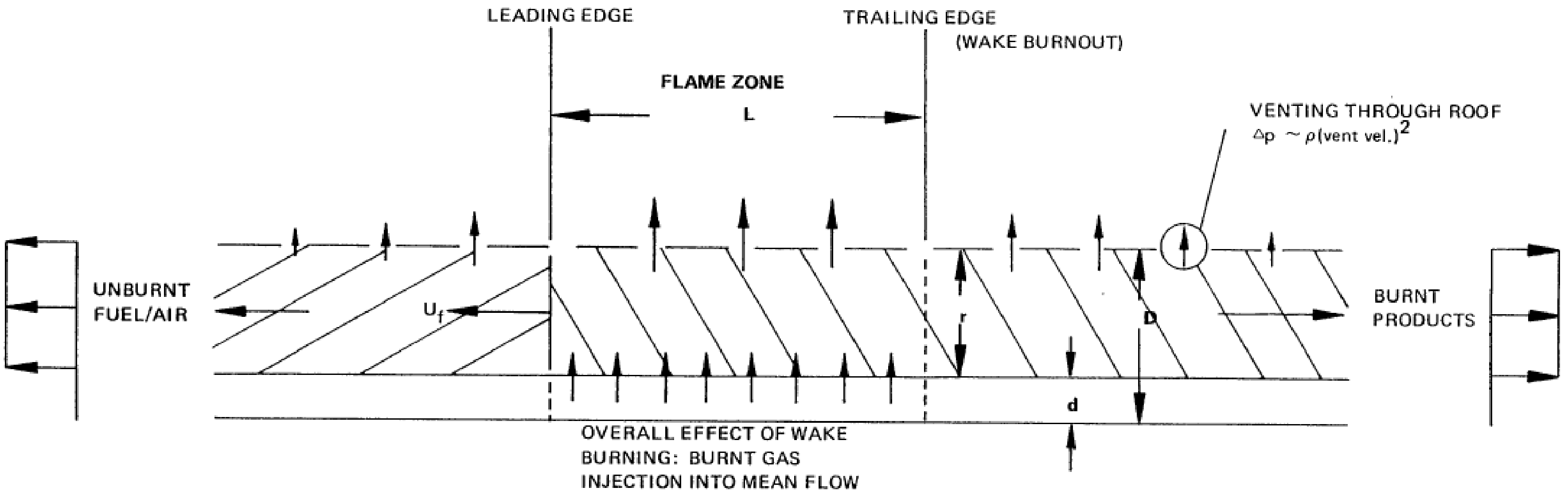
Experimental cell width: 55mm
Predicted value: 60mm

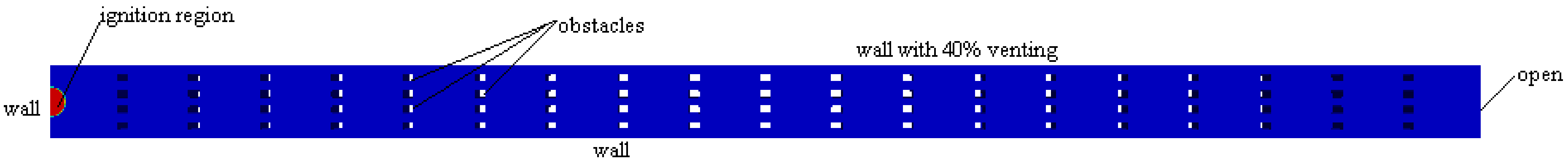


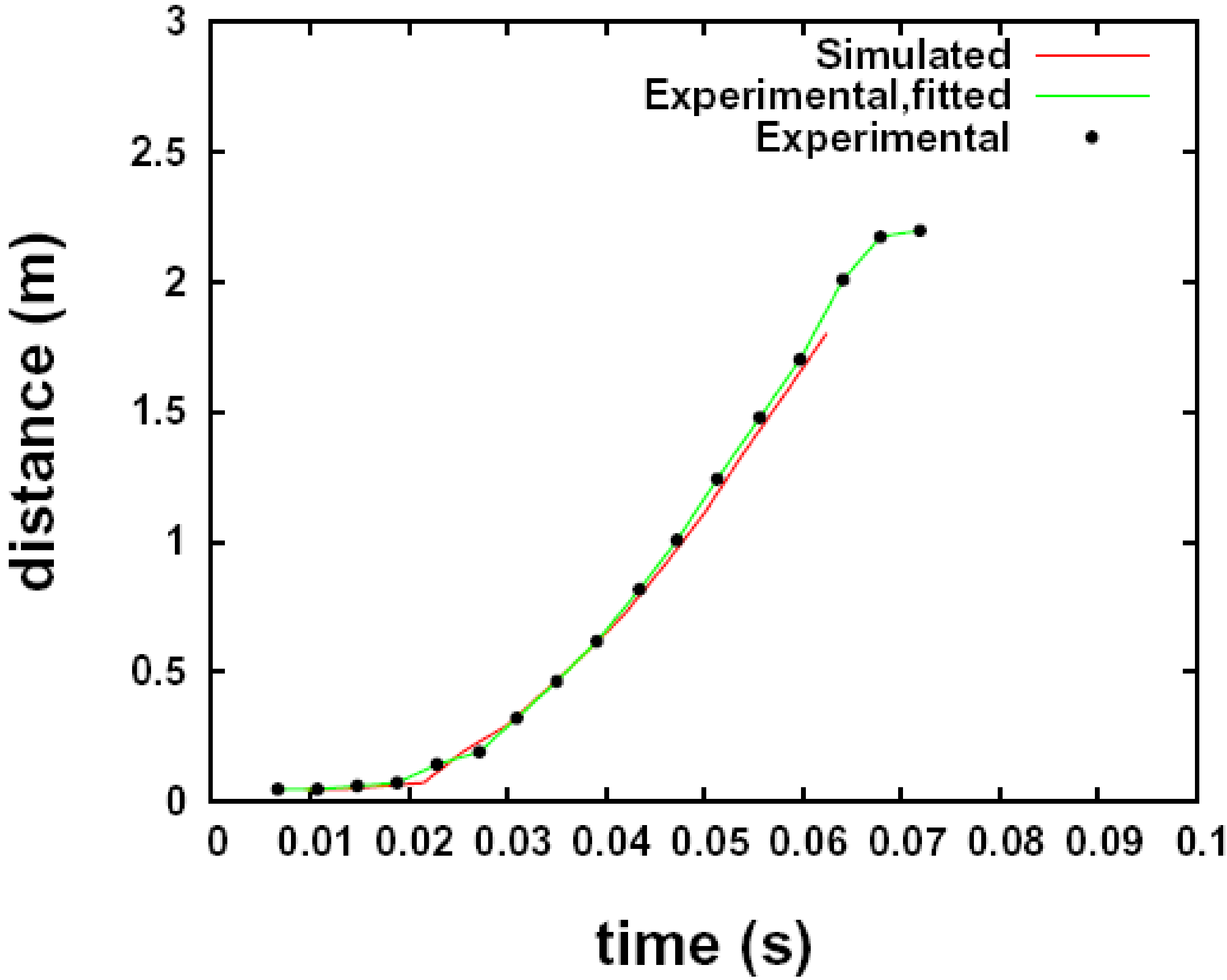
Westbrook's model (cell size: ~20mm)

Validation - Flame acceleration in a vented duct

(P. H. Taylor and S. J. Bimson, "Flame propagation along a vented duct containing grids .," 22nd International Symposium on Combustion, August 1988, pp. 1355–1362, 1989.)

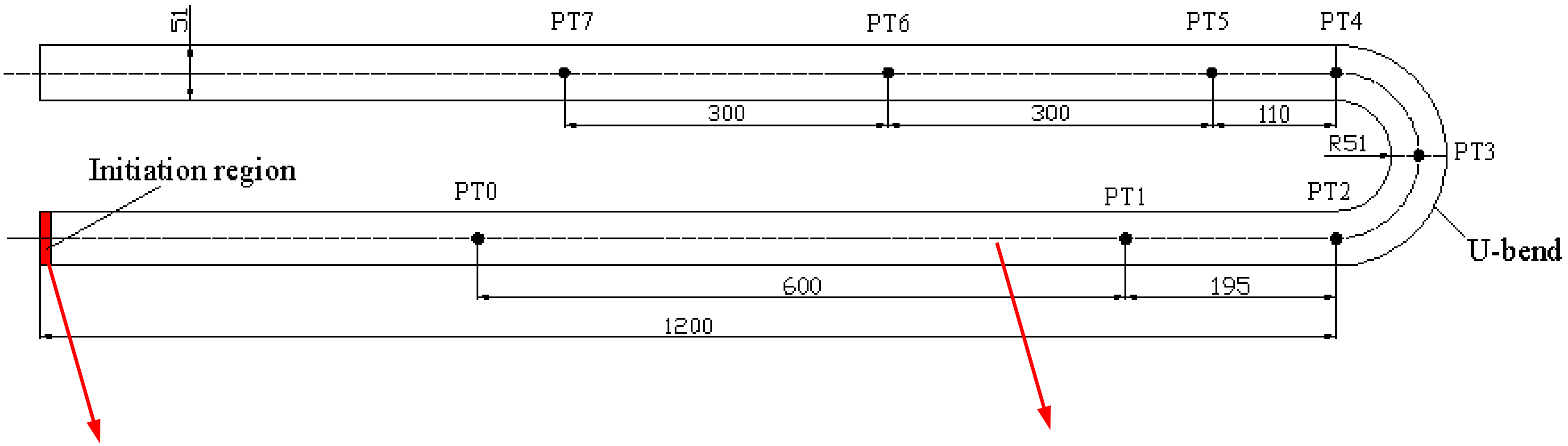





Simulated
Experimental,fitted
Experimental
distance (m)
time (s)
0
0.5
1
1.5
2
2.5
3
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1

Exploratory study - shock and detonation propagation through a U-bend

S. M. Frolov, V. S. Aksenov, and I. O. Shamshin, "Shock wave and detonation propagation through U-bend tubes," Proceedings of the Combustion Institute, vol. 31, no. 2, pp. 2421–2428, Jan. 2007.



Width=10mm
P_0=(60-200)atm
T_0=2500K

stoichiometric propane-air mixture
P_0=1atm
T_0=300K

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Numerical setup

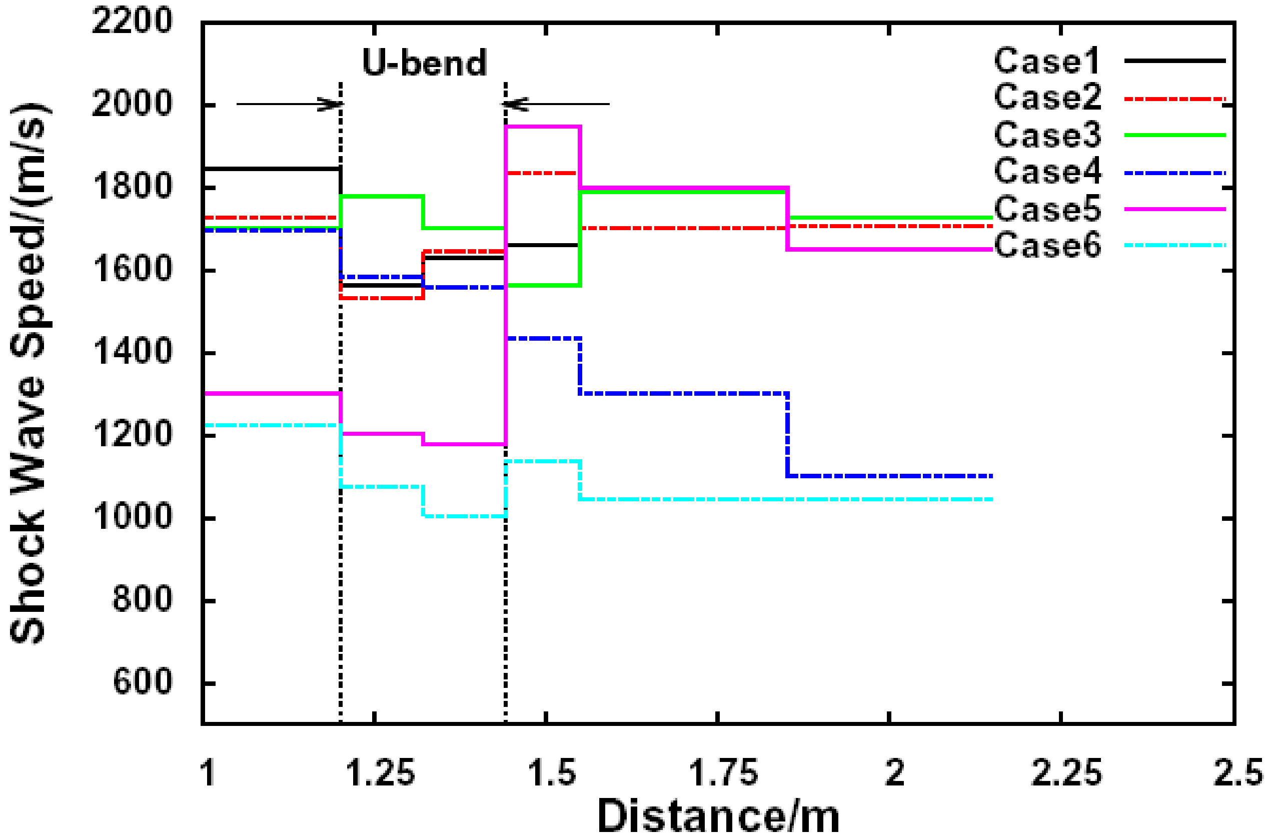
- The geometry and set up mimics that of Frolov et al.'s experiments.
- The grid size is 0.25mm (8 grids in half reaction length) total grid number is 2.15M (10562×204)
- Six cases as listed below

Cases	Initial Pressure	Initial Tempreature
1	150 atm	2500K
2	100 atm	2500K
3	85 atm	2500K
4	75 atm	2500K
5	65 atm	2500K
6	60 atm	2500K

Results

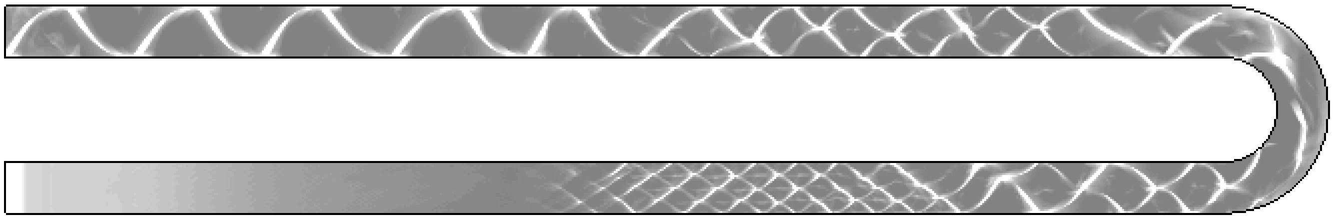
The effects of the U-Bend:

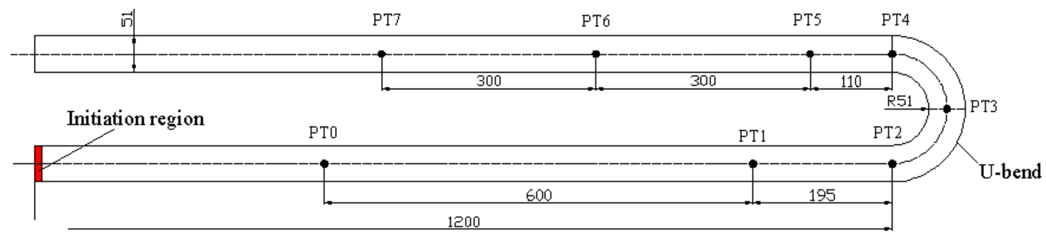
(1) First decelerating and then accelerating (Cases1 and 2)
(2) First accelerating and then decelerating (Case 3)
(3) Continuously decelerating (Case 4)
(4) Decelerating shock wave followed separately by a flame (Cases 5 and 6)

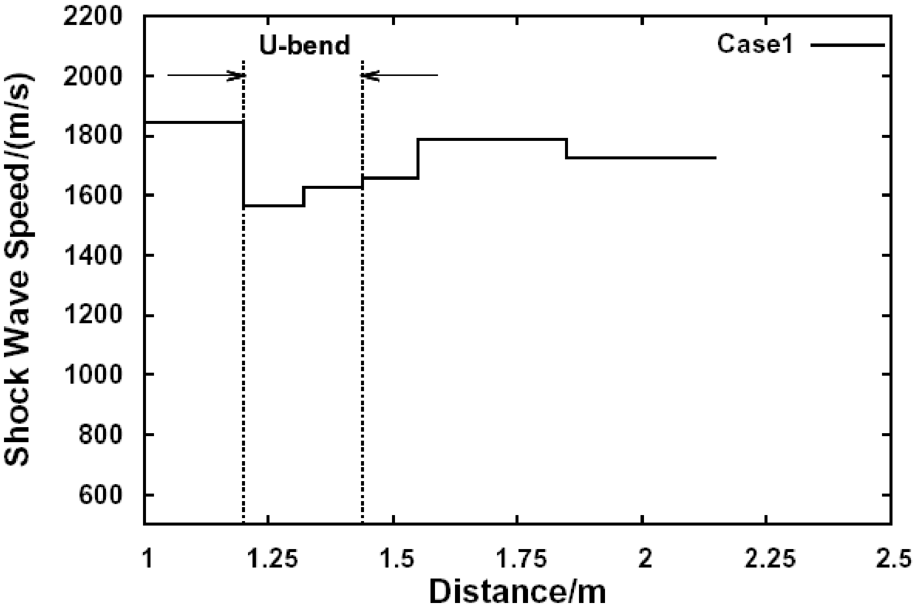


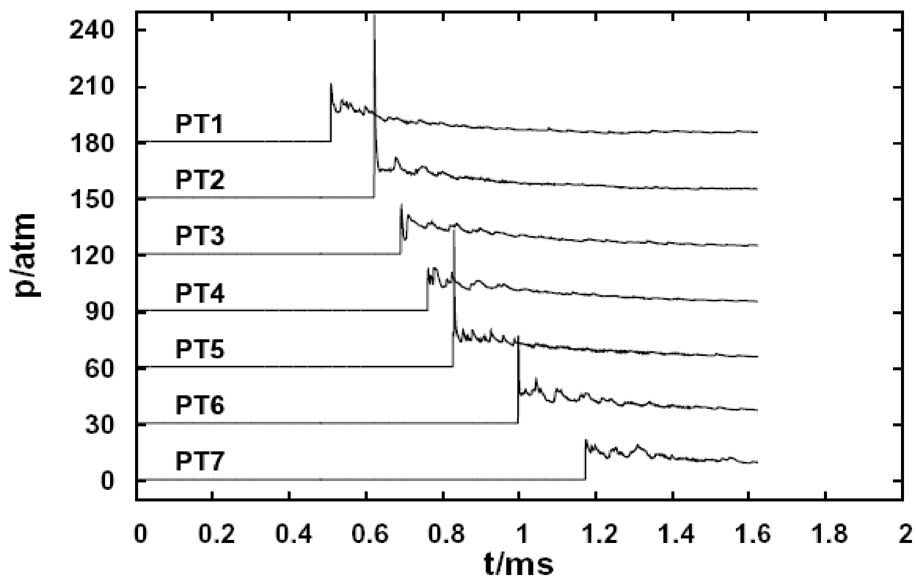
Case-1: First decelerating and then accelerating

Case 1: First decelerating and then accelerating

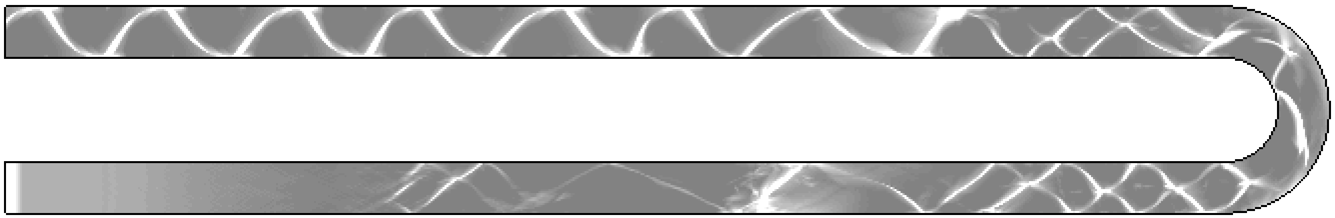


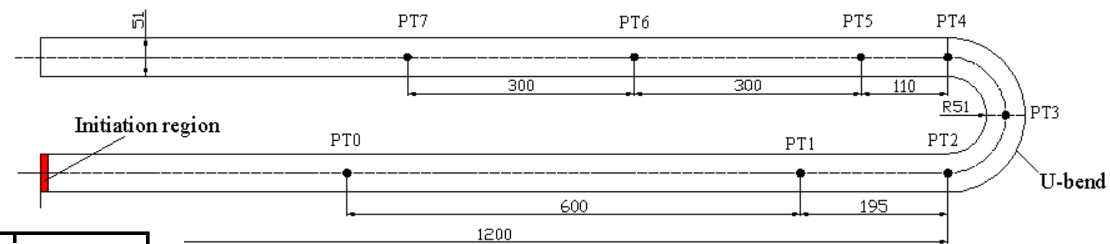


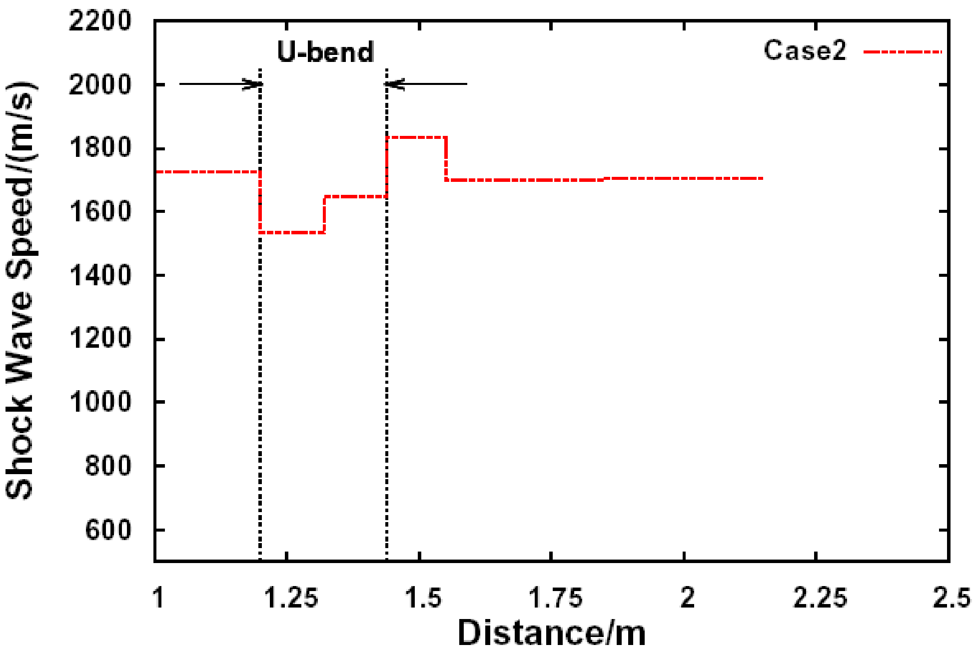


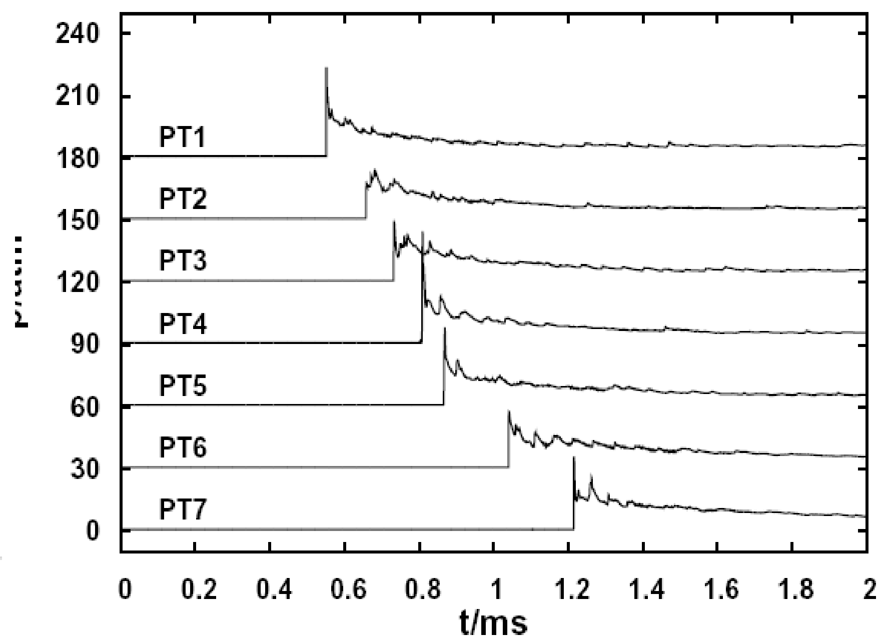


Case 2: First decelerating and then accelerating

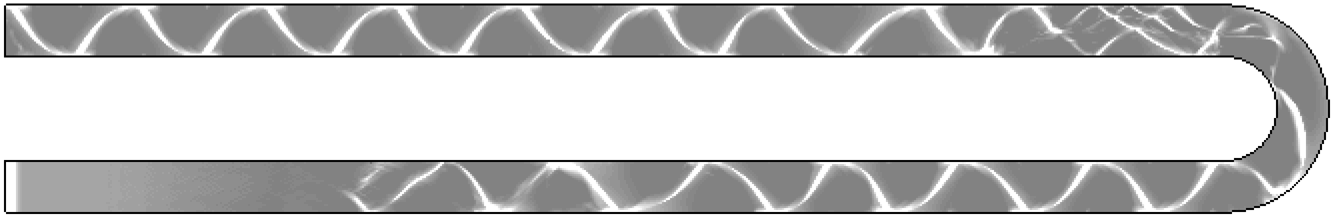


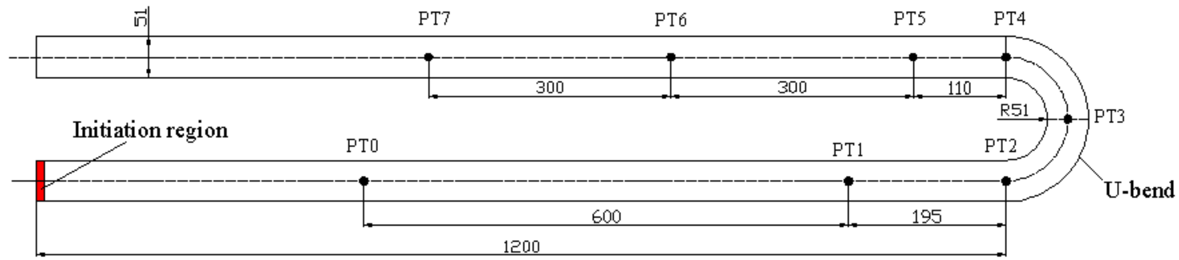


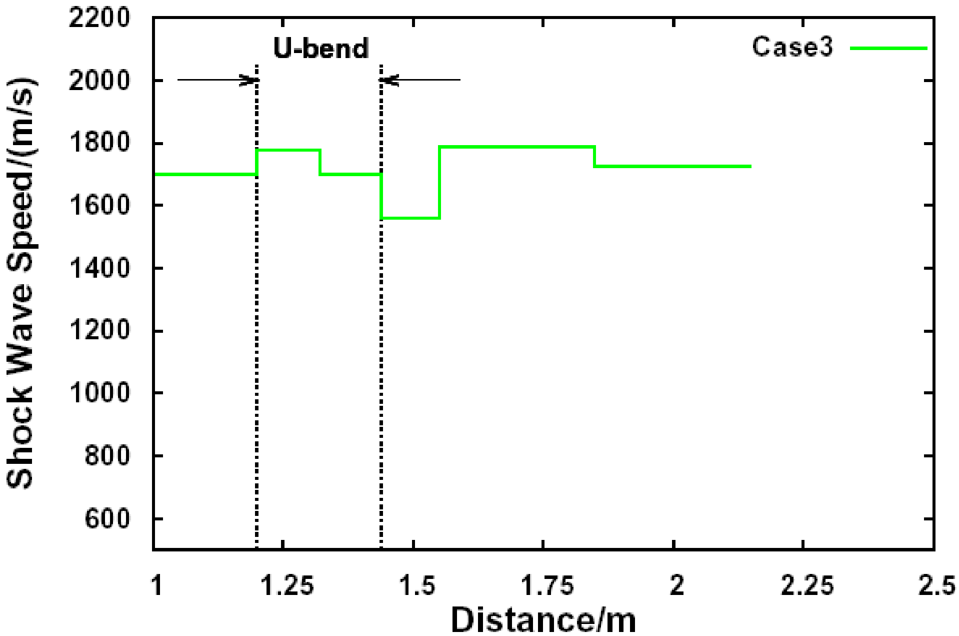


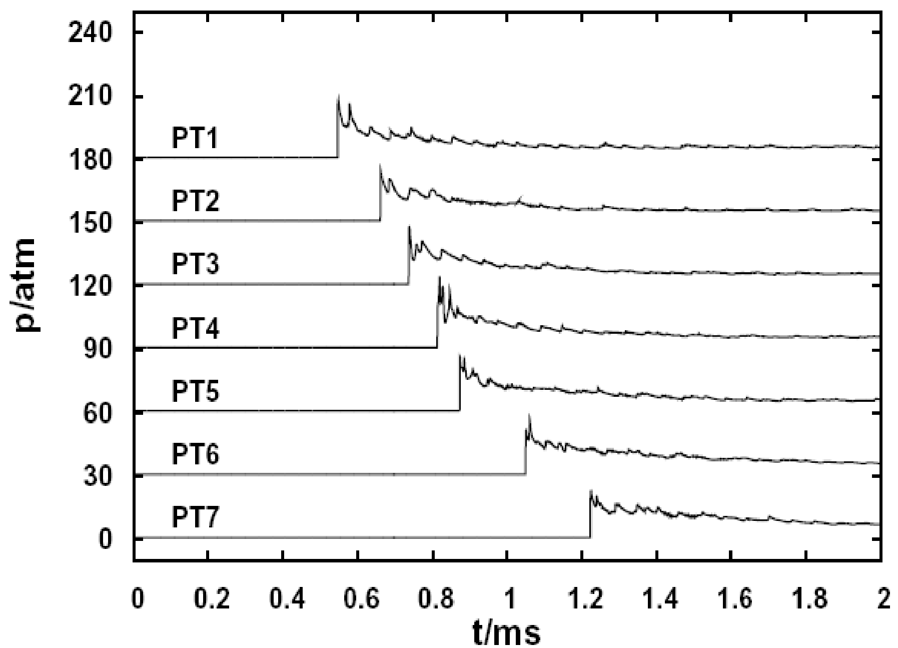


Case 3: First accelerating and then decelerating

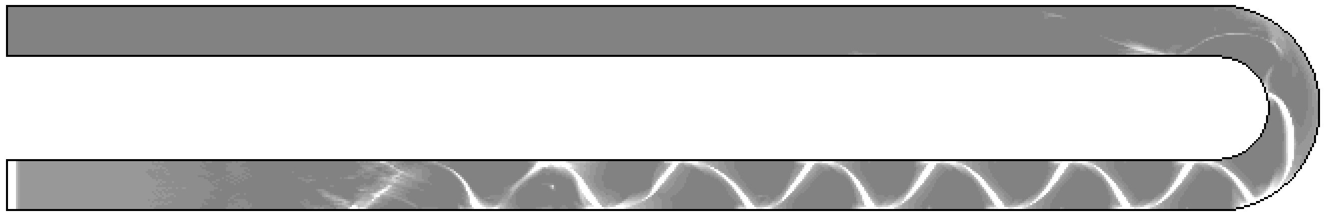


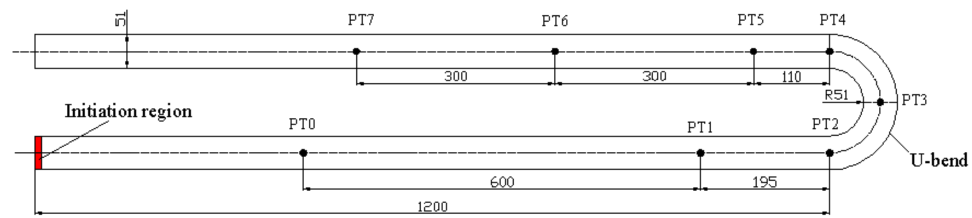


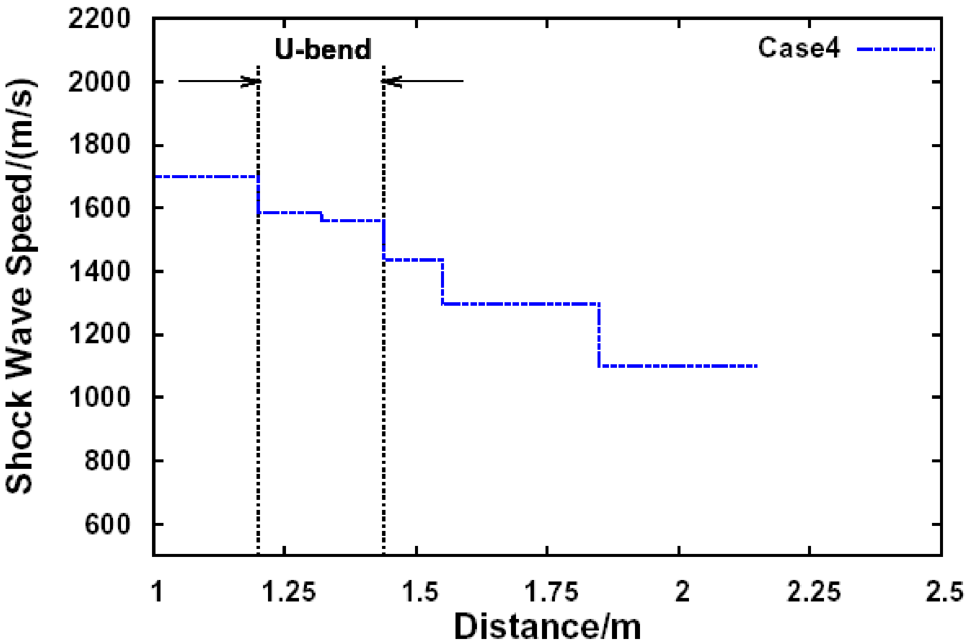


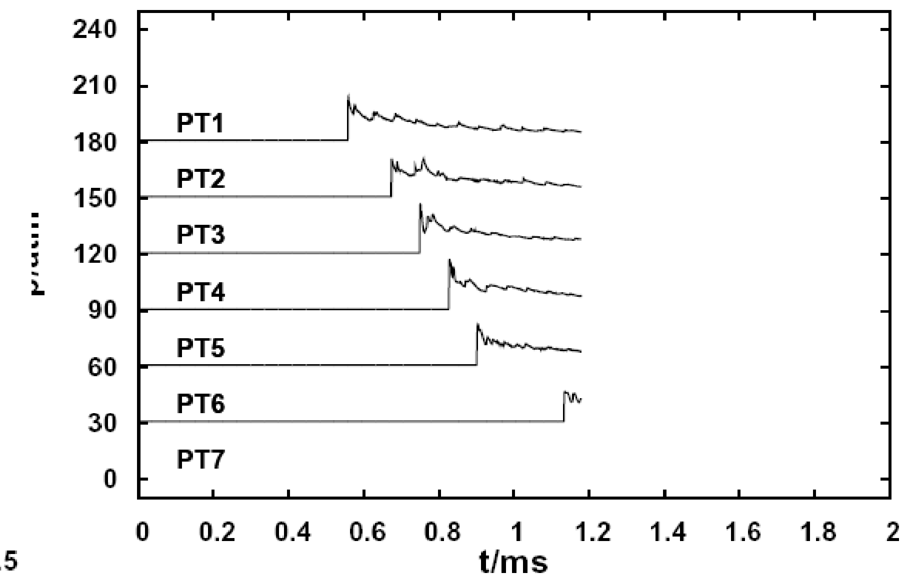


Case 4: Decelerating

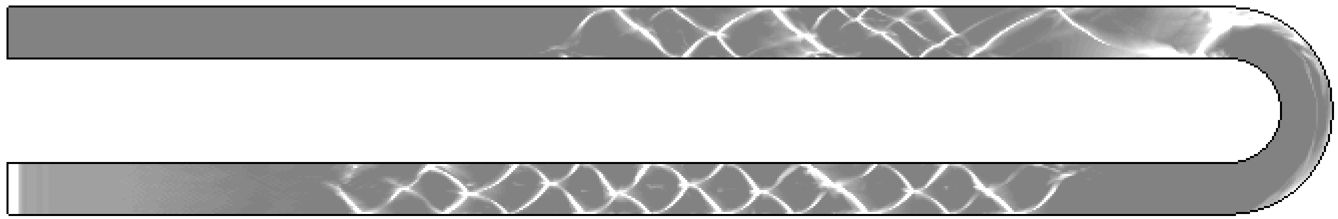


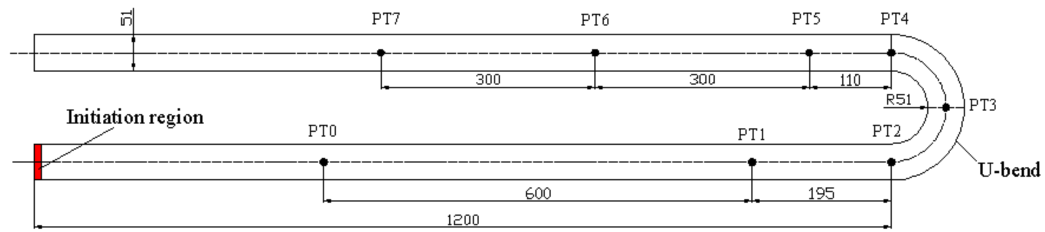


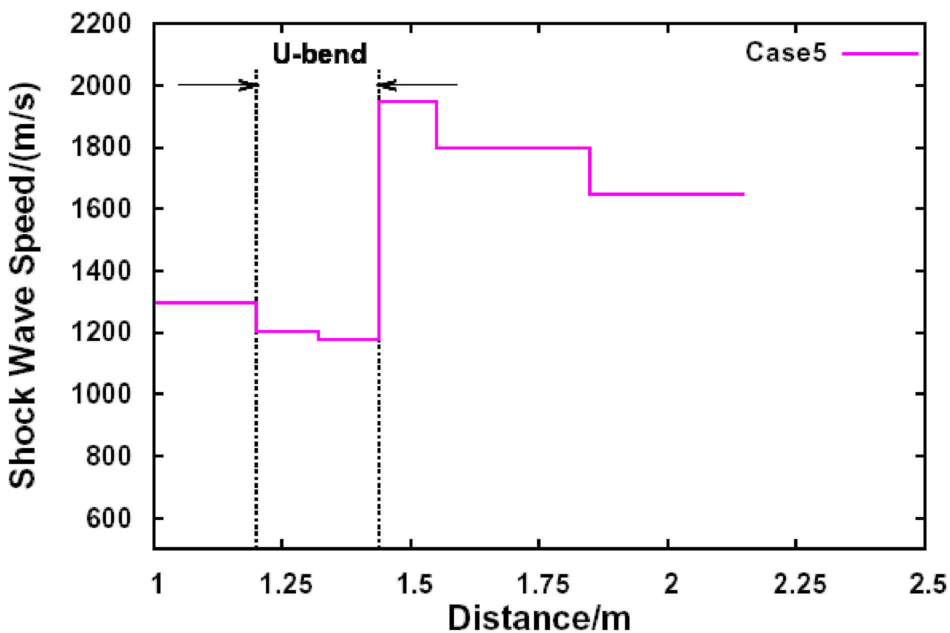


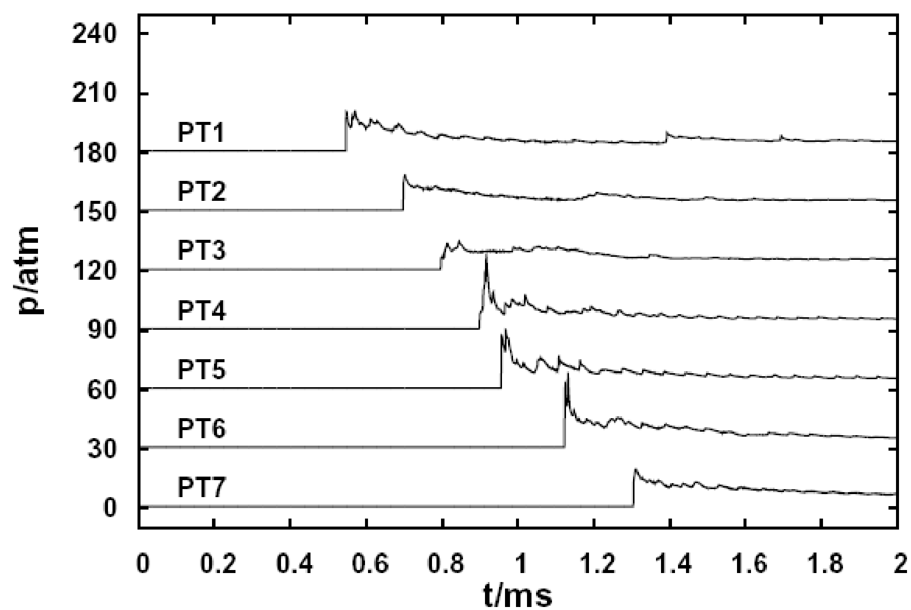


Case 5: Decelerating shock wave followed separately by a flame

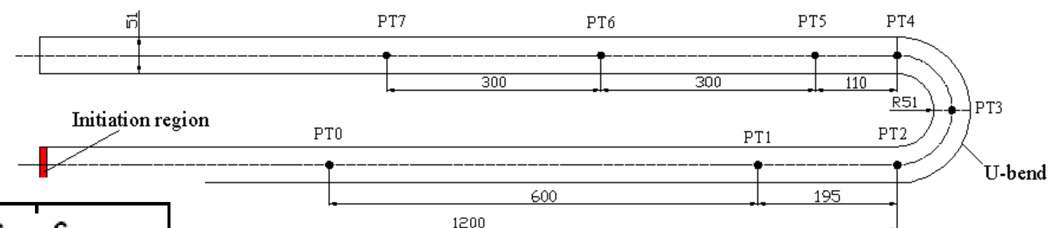


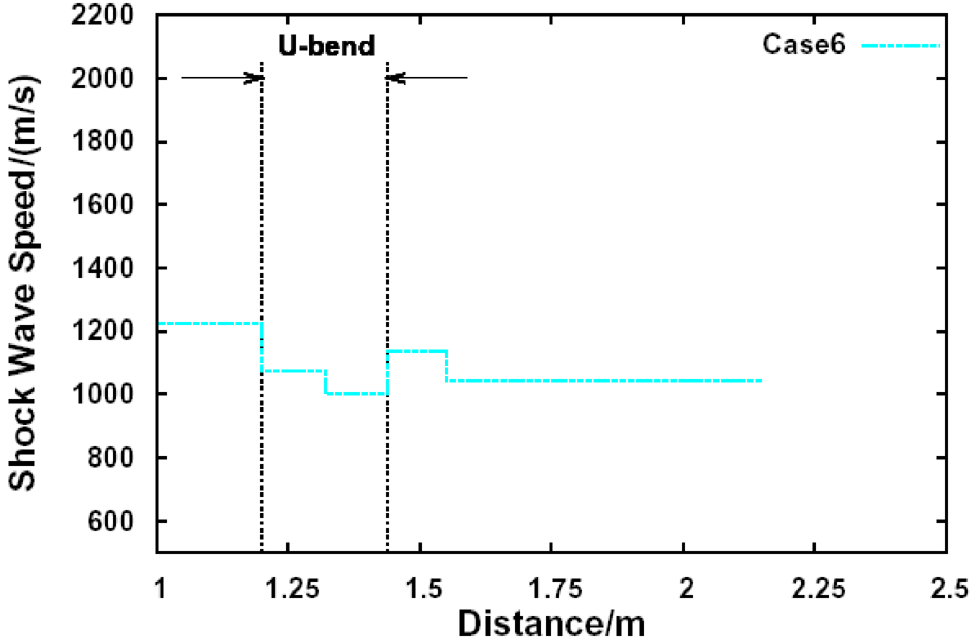


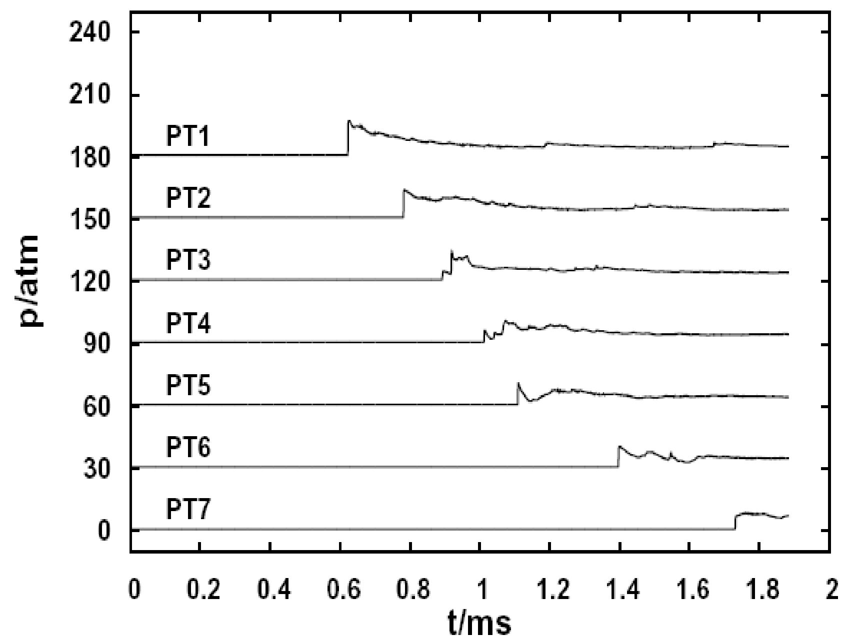




Case 6: Decelerating shock wave followed separately by a flame







Conclusions

- A new single-step reaction mechanism has been developed for propane-air mixture, covering the entire spectrum covering flame acceleration, transition to detonation and detonation.

- For the vented duct case, the predicted flame front is in good agreement with the measurements.

- For the six cases in the U-tube, the effects of the bend depend on the initial pressure. For the pressure range considered from 60 to 140 bar, four modes are predicted:
  - First decelerating and then accelerating
  - First accelerating and then decelerating
  - Continuously decelerating
  - Decelerating shock wave followed separately by a flame

Acknowledgement

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Many thanks to Geoff Chamberlain for pointing us to the vented duct flame data.