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Simulations of flame acceleration and transition to detonation: How accurate are they?

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August 30, 2017

The 1st International Workshop on Near-Limit Flames

Deflagration-to-detonation transition (DDT) is an important research topic in reactive flows

Pulse Detonation Engine

Hydrogen Explosion in a Pipe. Norsk Hydro Ammonia Plant, Norway, 1997

Several mechanisms of DDT have been seen in reactive gas systems

- Reactivity-gradient mechanism through hot spots
  - Zeldovich et al. (1970), Lee et al. (1978), and Oran (2007, 2015)
- Direct initiation of detonation by multi-shock collision
  - Goodwin et al. (2016, 2017), and Maeda et al. (2016)
- Self-intensified turbulent flame accelerating to CJ velocity
  - This is a possible mechanism for unconfined DDT
  - Poludnenko et al. (2011, 2012)

Mechanisms of DDT are not fully understood and quantitative modeling still remains a challenge

- Very rapid, nonlinear, and complex process
  - Involves combustion instabilities, turbulence, shock-flame interactions, boundary layer effects, and detonation initiation.
- Cover an extremely broad range of spatial scale
  - 4-12 orders of magnitude in real systems, which is one of the factors making the problem computationally challenging
- Stochastic nature of DDT
  - Poses difficulties in both determining the quantitative effects of parameters and validating numerical models

There are many unanswered questions

How and where can hot spots be created in the DDT process?

What is required in a numerical model to quantitatively calculate DDT in obstructed channels?

How can we understand the effects of numerical algorithms and implementations on the accuracy of DDT calculations?

The modeling process

Start from observations of the real world

- **Define model equations**
  - Approximate the real world
- **Determine numerical schemes suitable for transforming equations into algebraic form**
  - Approximate the model equations
- **Program algorithm and implementation on computer**
  - Approximates algebraic equations
- **Analyze and present results in form of graphs, movies …**
  - Show selected interpretations of the results

The numerical simulations solve the two-dimensional, fully compressible, reactive Navier-Stokes equations

Mass: $$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$$

Momentum: $$\frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U}\mathbf{U}) + \nabla P = \nabla \cdot \hat{\tau}$$

Energy: $$\frac{\partial E}{\partial t} + \nabla \cdot ((E + P)\mathbf{U}) = \nabla \cdot (\mathbf{U} \cdot \hat{\tau}) + \nabla \cdot (K \nabla T) - \rho q \dot{w}$$

Species: $$\frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho Y \mathbf{U}) + \nabla \cdot (\rho D \nabla Y) - \rho \dot{w} = 0$$

State Equation: $$P = \frac{\rho R T}{M}$$

Stress Tensor: $$\hat{\tau} = \rho \nu ((\nabla \mathbf{U}) - (\nabla \mathbf{U})^T - \frac{2}{3}(\nabla \cdot \mathbf{U})\mathbf{I})$$

The combustion of fuel-air mixture is modeled using a single-step chemical-diffusive model

- Reaction Rate

$$\dot{\omega} = dY/dt = A\rho Y exp\left(\frac{-E_a}{RT}\right)$$

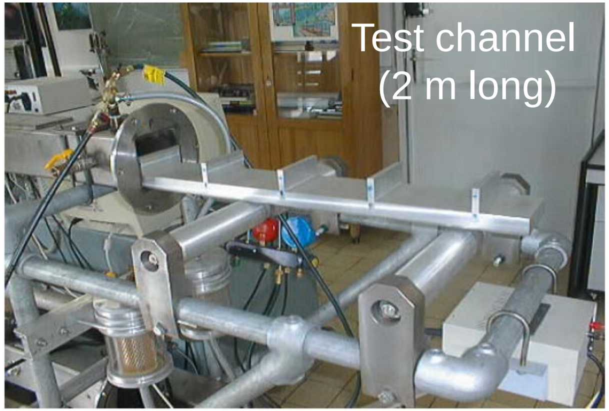
- Transport properties

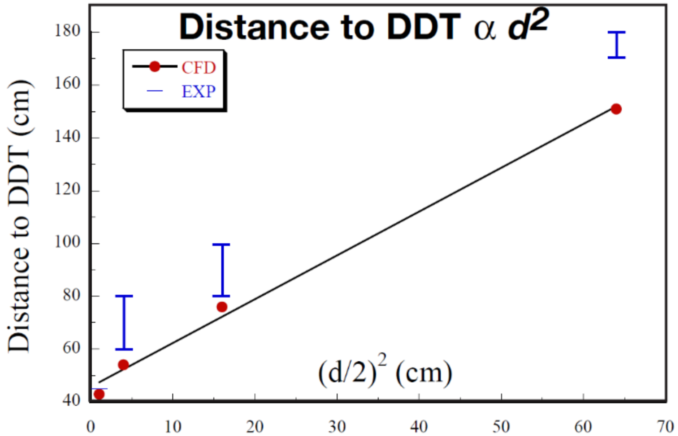
$$\mu = \mu_0 T^n,\ D = D_0 T^n,\ k = k_0 T^n \qquad (n = 0.7)$$

- The combustion model can reproduce major properties of flame, detonation, and the transitions between them for premixed combustion

Prior studies of DDT showed that the model can reproduce the major features of DDT in obstructed channels that qualitatively and quantitatively agree with experiments

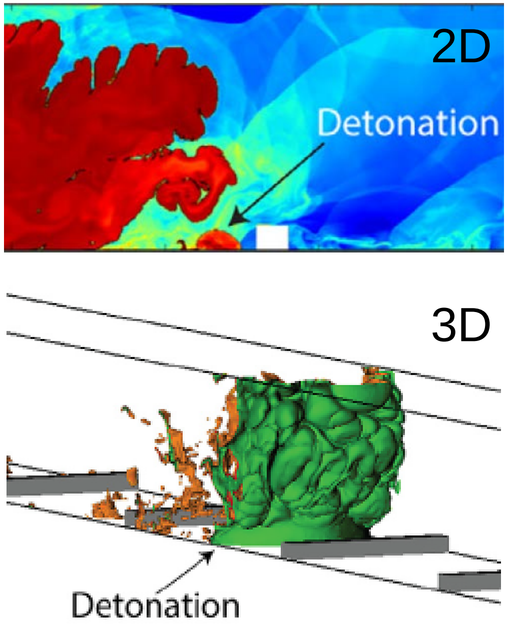
- Reproduce the main regimes observed in experiments
  - Choking flame, quasi-detonation, and detonation (Lee et al., 1984)
- Agree well with the experiments of H_2-Air DDT
  - By Teodorczyk, 2007

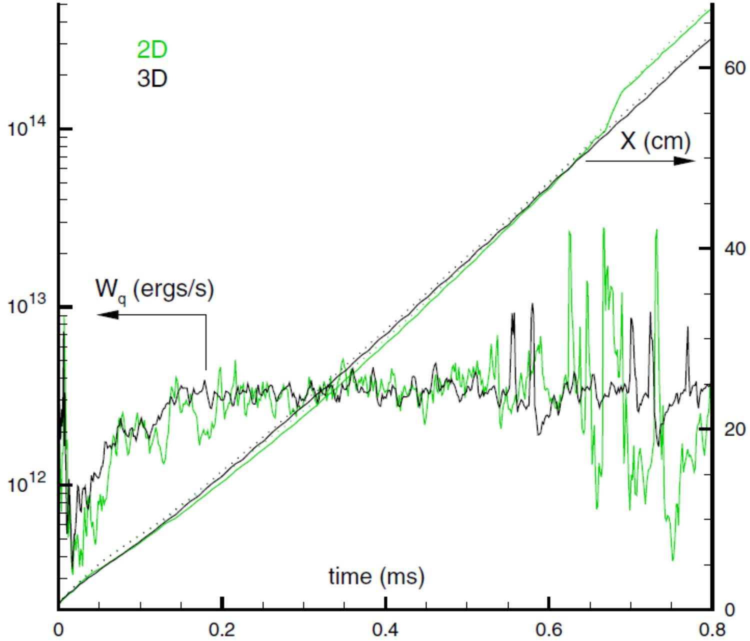




Prior studies also showed that 2D simulations agree with 3D simulations

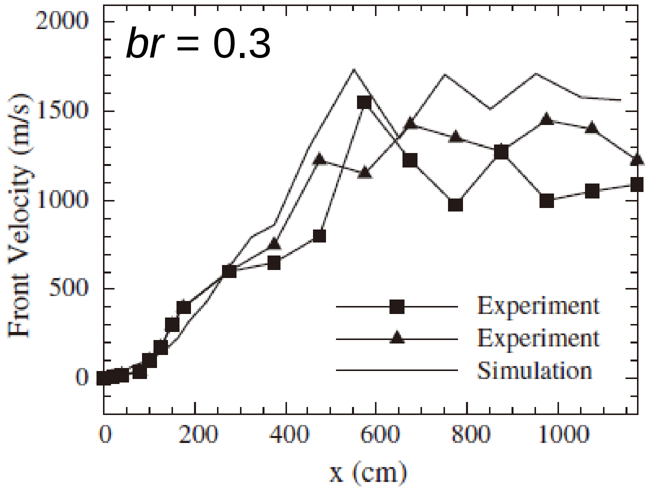
- Same flame acceleration (FA) and DDT mechanism

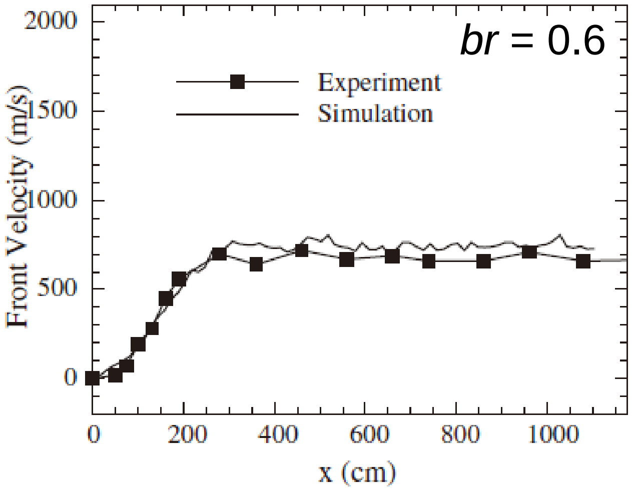




Good agreement with experiments was also shown for large-scale methane-air DDT in obstructed channels

- Experiments by Kuznetsov et al. (2002)
  - 17.4 cm in diameter, 1188 cm in length
  - 52 cm in diameter, 2130 cm in length





17.4 cm diameter channel

The modeling process

Determines the accuracy of the simulations

- **Define model equations**
  - Approximate the real world
- ***Determine numerical schemes suitable for transforming equations into algebraic form***
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Two different codes with different numerical algorithms are used to solve the same model equations

ALLA (low-order)

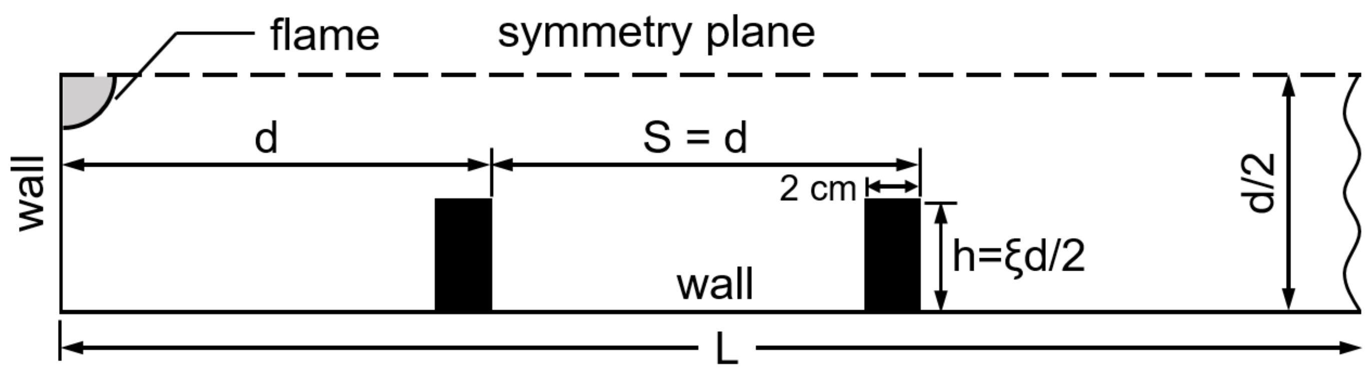
- 2nd-order Godunov method with Colella-Glaz Riemann solver
- 2nd-order direction-splitting time integration
- AMR: Fully Threaded Tree algorithm

FAST (high-order)

- 3rd/5th-order WENO algorithm with HLLC Riemann solver
- 2nd-order Runge-Kutta time integration
- AMR: block-structured gridding using Boxlib

The computational domain is a channel, closed at the left end, with evenly-spaced obstacles

- No-slip, adiabatic boundary conditions are used at all the walls and obstacle surfaces
- Symmetry conditions are applied along the center line
- Non-reflecting conditions are used at the right end



Two channel diameters, 17.4 and 52 cm, are selected, corresponding to available experimental configurations*

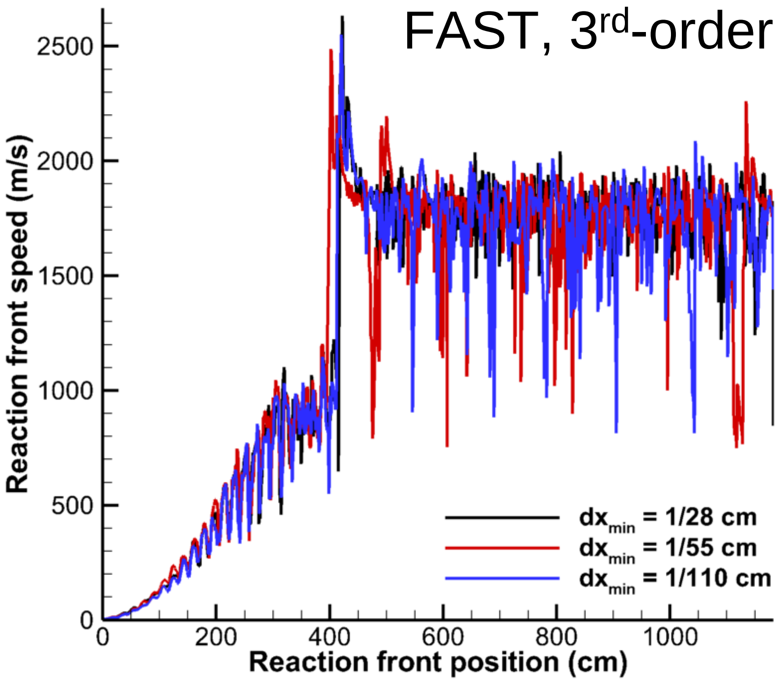
Diameter *d* (cm)	17.4	52
Length *L* (cm)	1187.8	2130
Blockage ratio *br*	0.3, 0.6	0.3, 0.6

- The computations are performed using ALLA and FAST, and the results will be compared to each other and to the existing experimental data by Kuznetsov et al.*

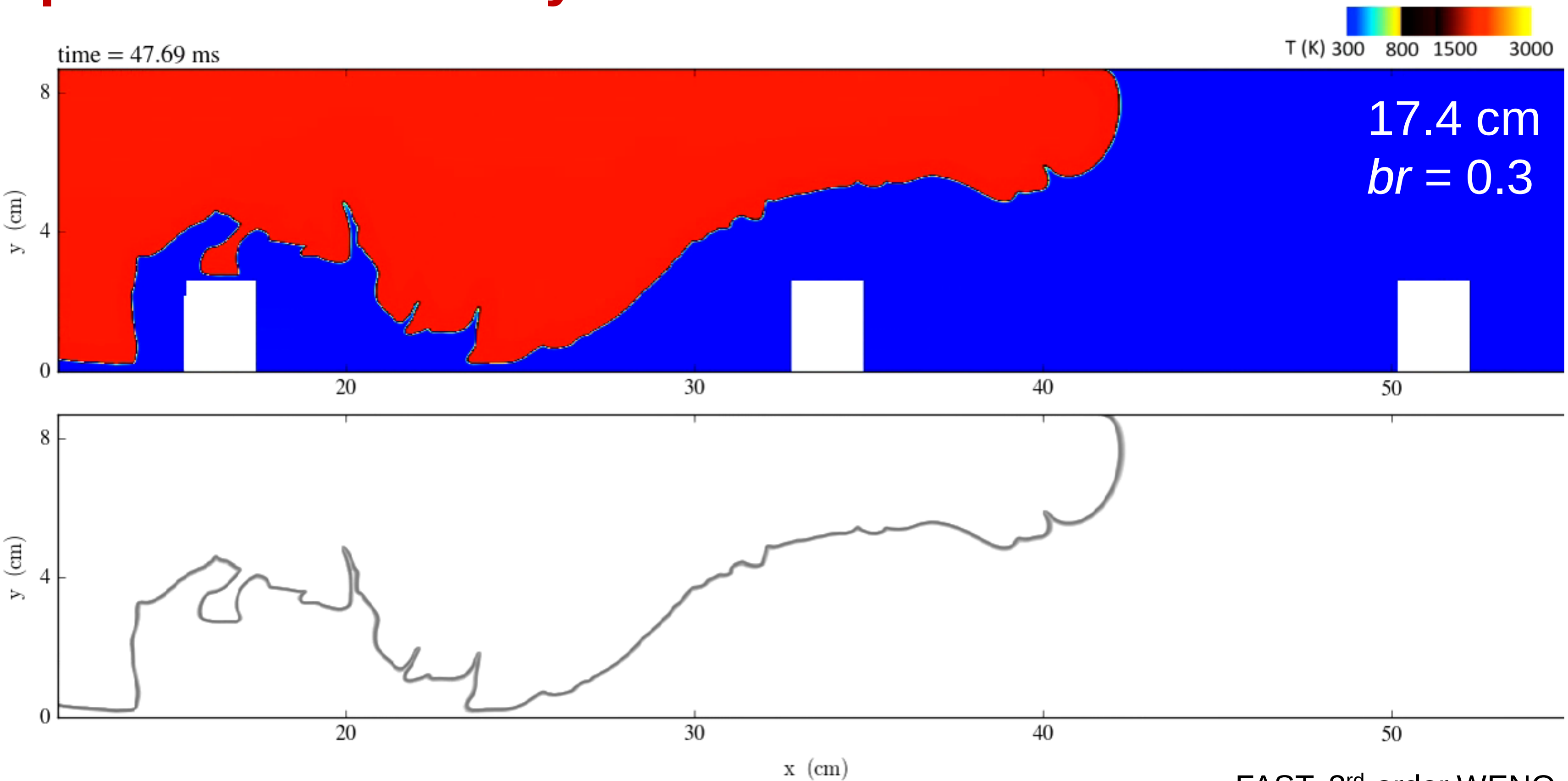
*Kuznetsov et al., Shock Waves (2002)

The grid resolution test shows that different resolutions give similar flame acceleration and length to DDT

- In the following calculations
  - First compare the 2^{nd} (ALLA) to the 3^{rd} (FAST), then to the 5^{th}-order scheme (FAST)
  - dx_{min} = 0.18125 (~1/55) mm

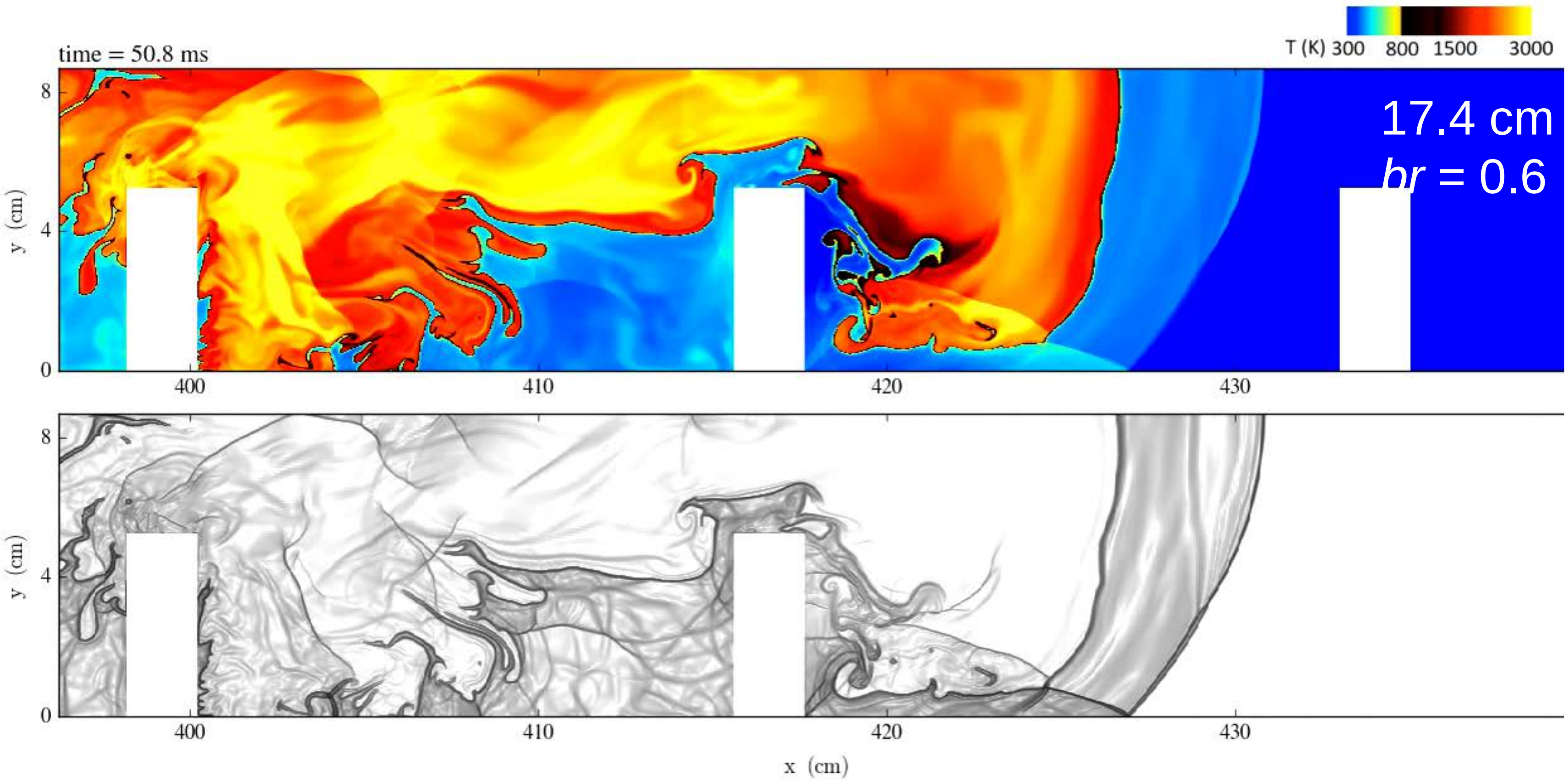


Flame acceleration involves thermal expansion, fluid instabilities, vortices, and turbulence. DDT occurs as hot spots are created by Mach stem reflection



FAST, 3rd-order WENO

Overall, flame propagates in a “choking” regime at high blockage ratio *br* = 0.6.

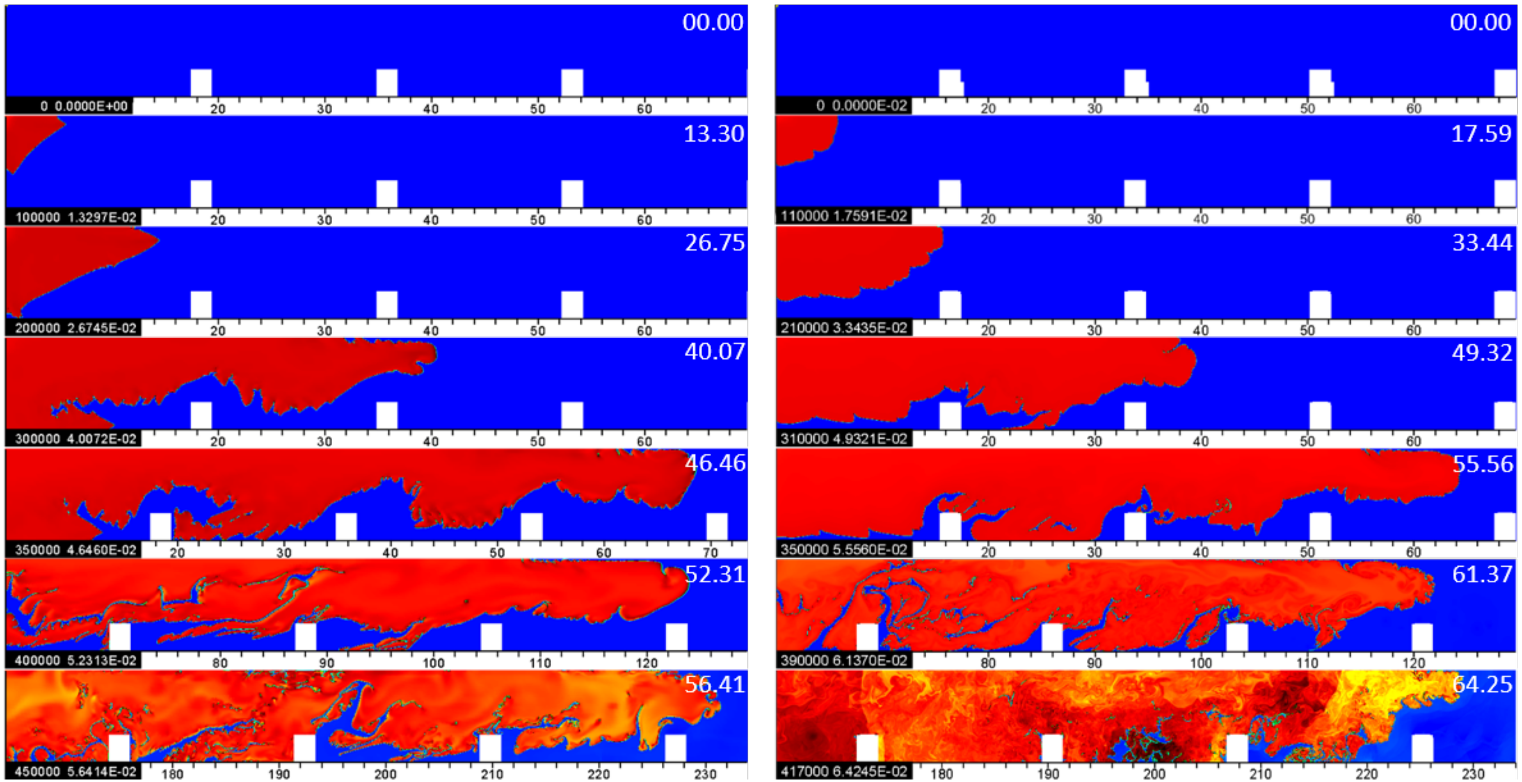


FAST, 3rd-order WENO

ALLA and FAST show the same mechanism of flame acceleration and DDT

17.4 cm, *br* = 0.3

ALLA FAST



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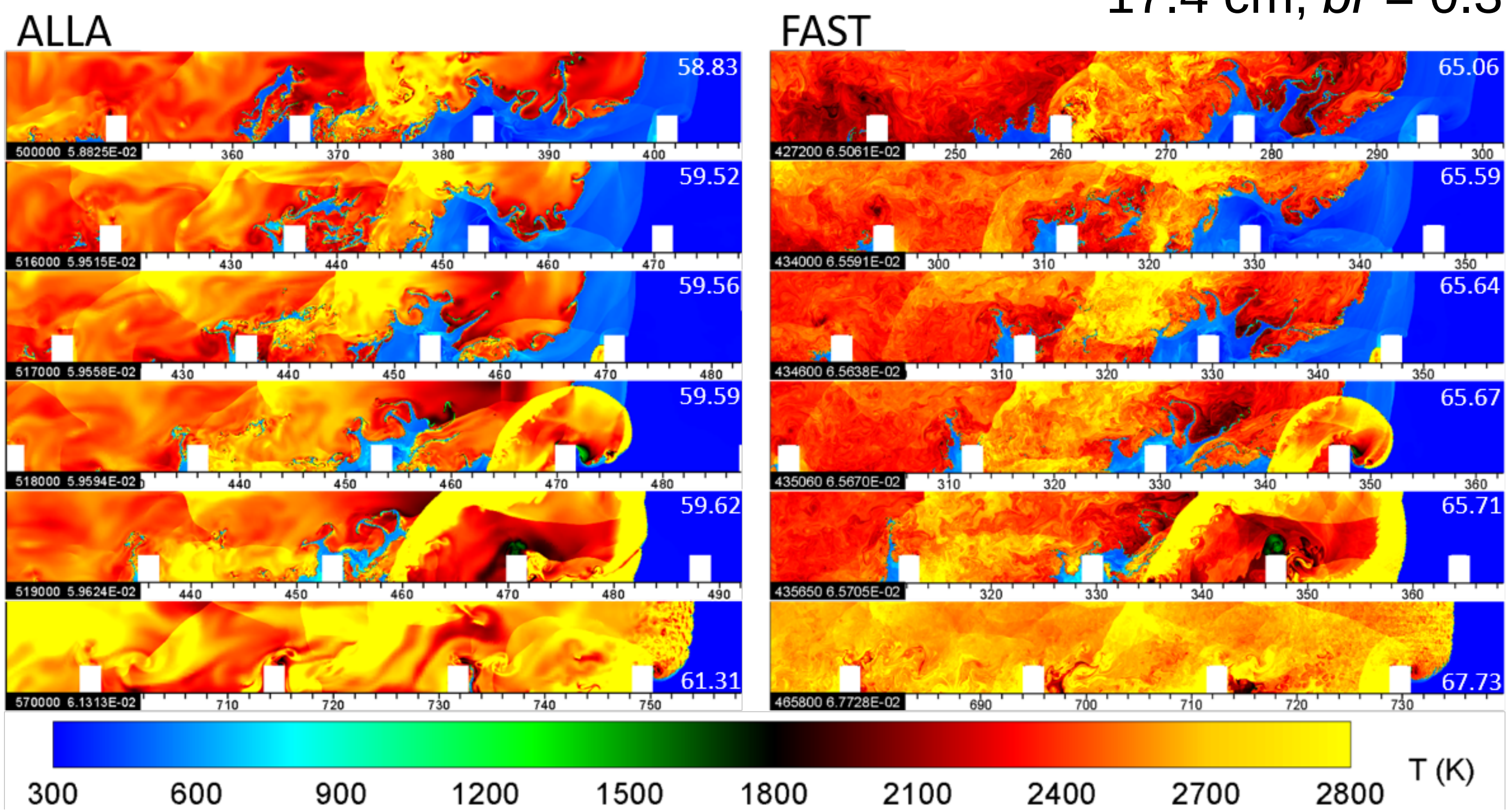
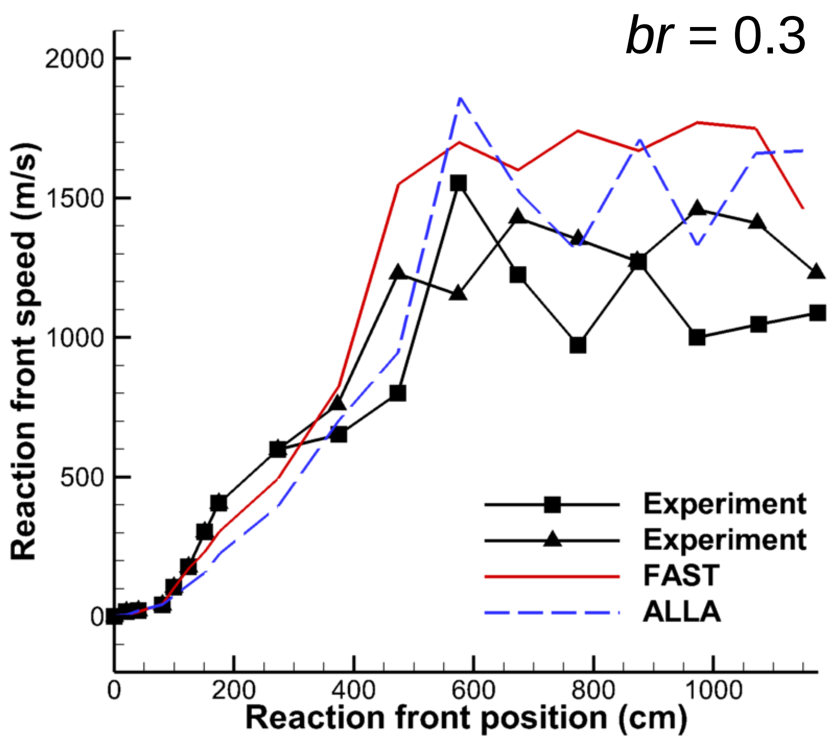
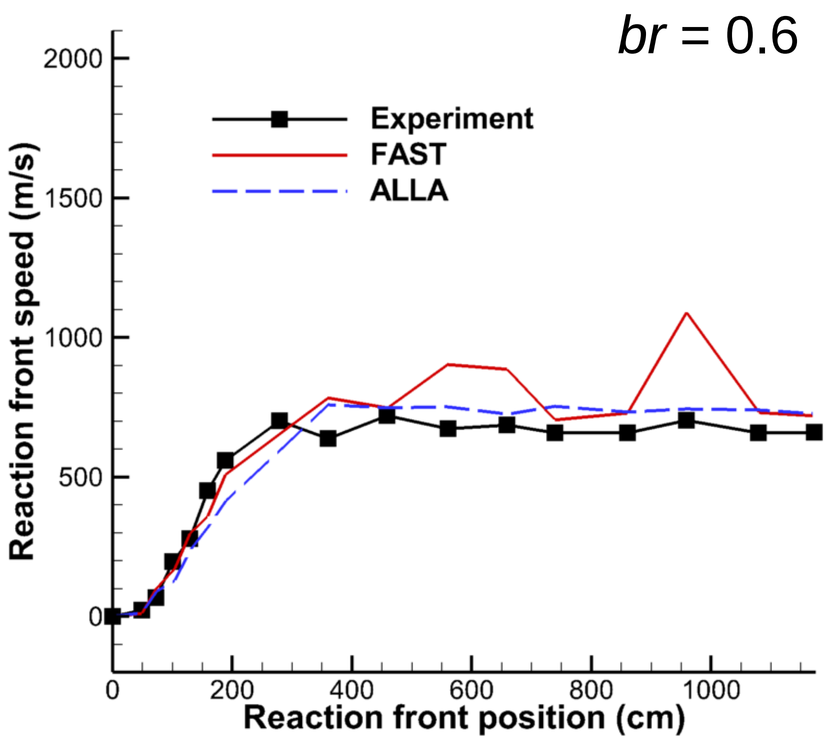
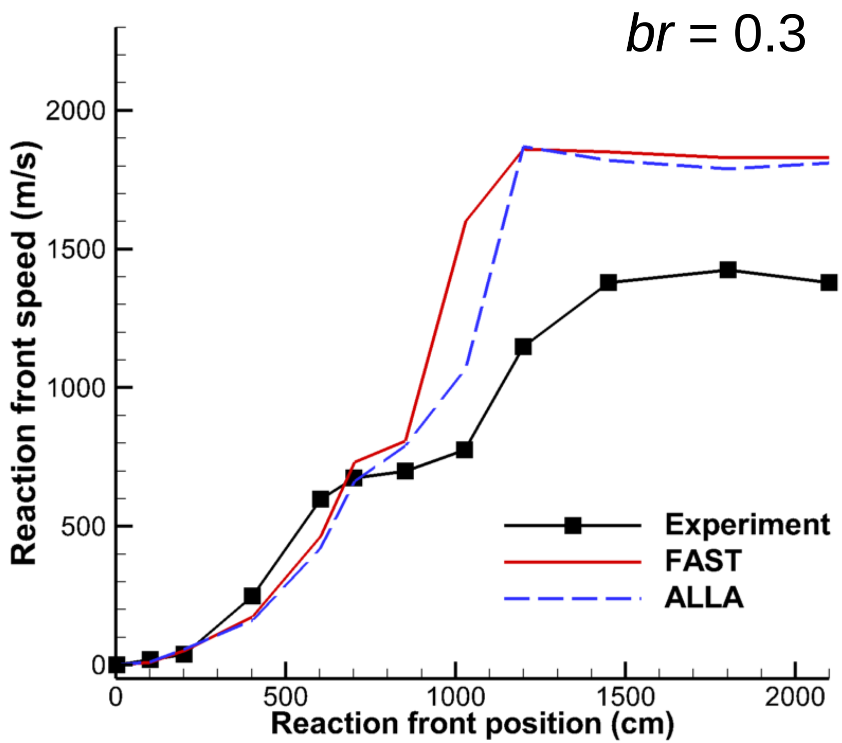


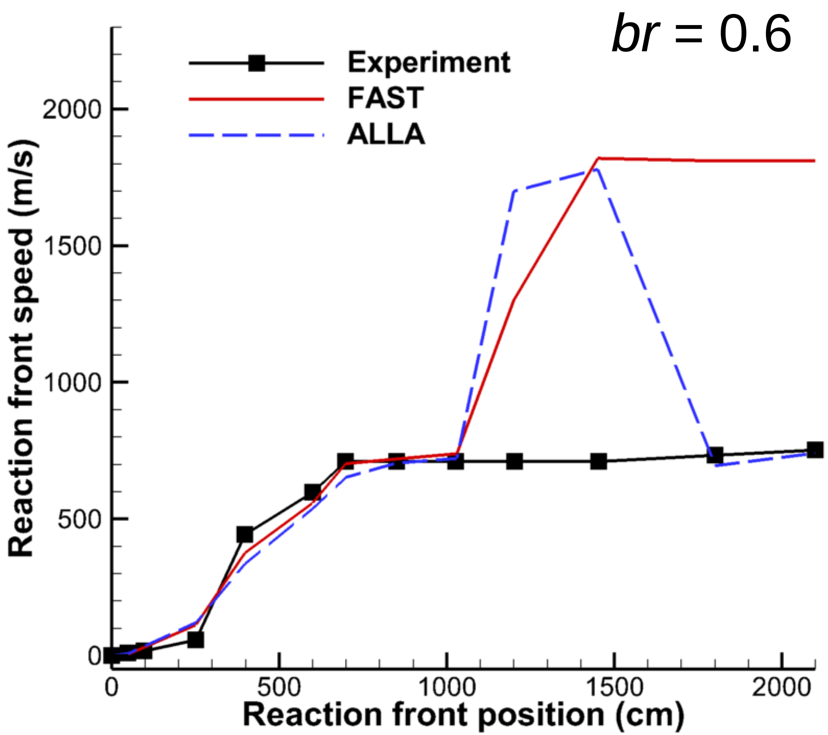
The computational results are in quantitative agreement with experiment for the channel with diameter 17.4 cm





The computations show a difference in the occurrence of DDT for the 52 cm channel with large blockage 0.6





Why can there be a difference in the occurrence of DDT for the 52 cm channel with large blockage ratio 0.6

- DDT criteria from experiments

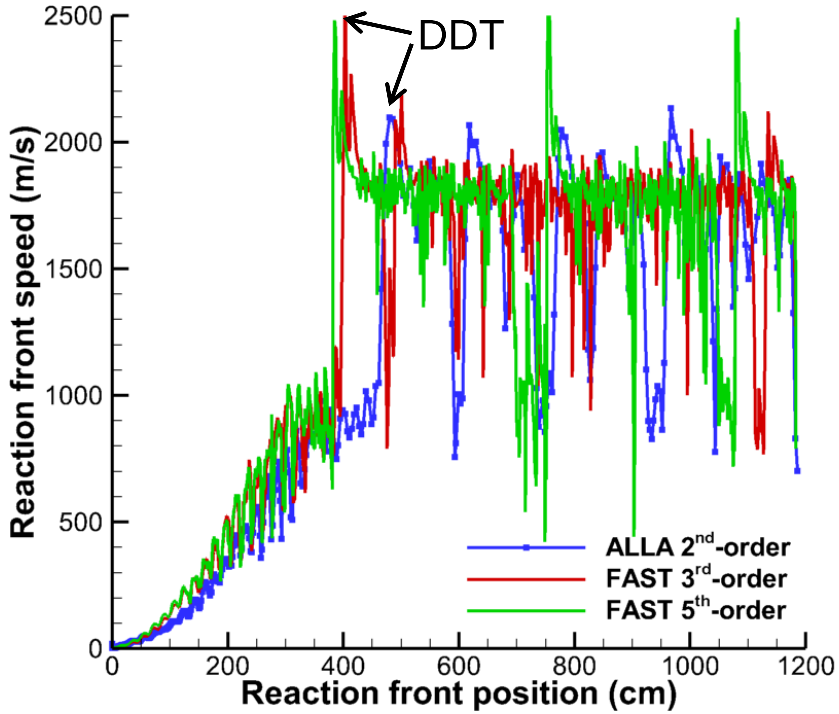
$d^* > \lambda$ *(Peraldi et al., Proc Combust Inst, 1986)*

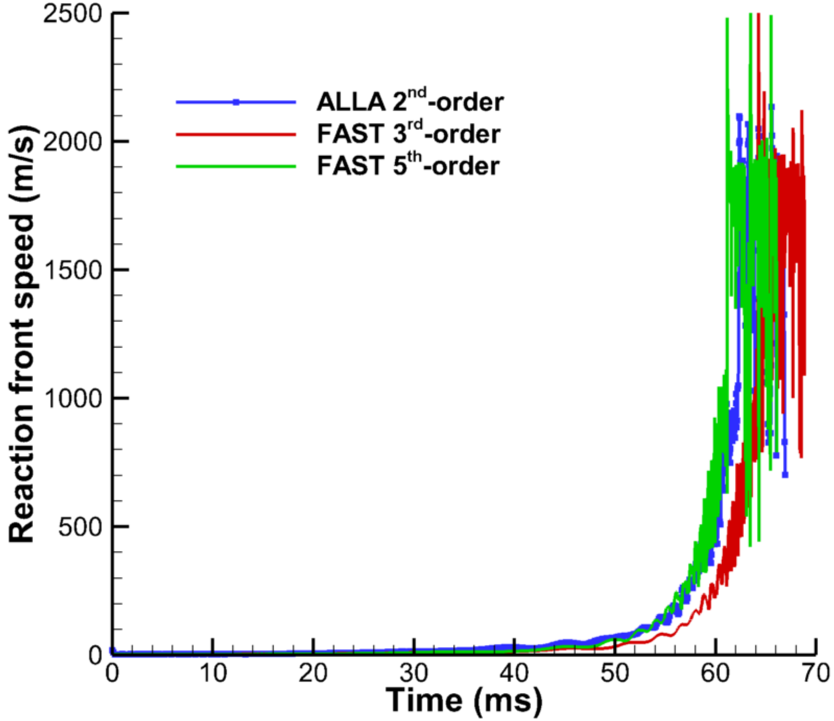
$L^* = (S+d)/(2(1-d^*/d) > 7\lambda$ *(Dorofeev et al., Shock Waves, 2002)*

  - For the 52 cm channel at *br* = 0.6, we have $d^* = 1.7\,\lambda$, $L^* = 7\,\lambda$

- DDT is a stochastic phenomenon in nature
  - When comparing deterministic simulations of a stochastic system to a limited set of available experiments, differences may be expected

The results for low and high-order schemes are close

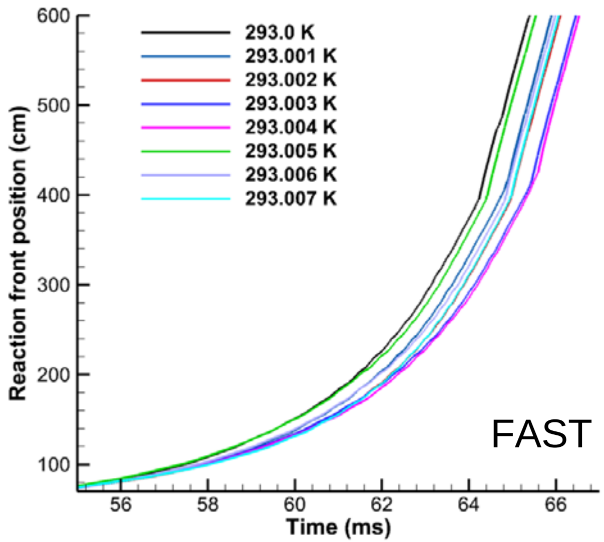


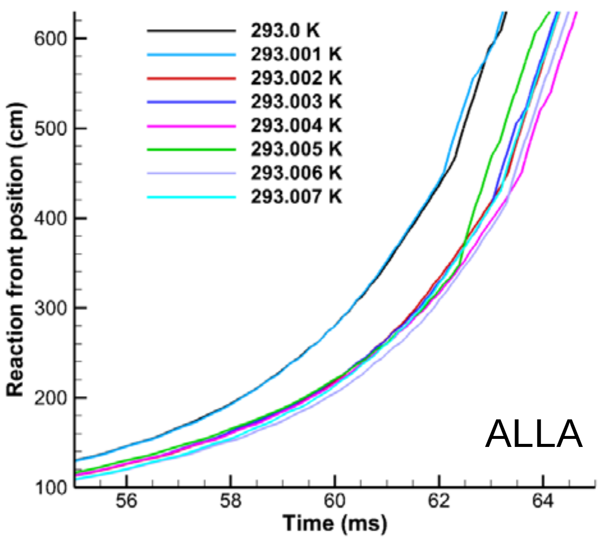


17.4 cm channel, *br* = 0.3

Stochasticity test show that the difference in DDT distance between ALLA and FAST is within the stochasticity range

- Impose random tiny perturbation in the background initial conditions corresponding to ∇T = 0.001 K
- DDT occurrence distances
  - FAST: *415–467 cm*
  - ALLA: *347–467 cm*





Zoomin plots

Conclusions

- ALLA and FAST methods with different schemes and implementations predict similar flame speeds and lengths to DDT that quantitatively agree with experiments
- The numerical model works for coarse and fine grids, high- and low-order schemes with different implementations
- The major difference between ALLA and FAST lies in the detonation failure at high blockage ratio
- Same DDT mechanism is observed, i.e., the hot-spot mechanism with Mach-stem reflection
- This work further supports the validity and reliability of the numerical model for simulating DDT in obstructed channels

Thank You !

Do you have any questions?

Example: model for stoichiometric hydrogen-air

	Quantity	Value	Definition
Input	T_0	293 K	Initial temperature
	P_0	1 atm	Initial pressure
	ρ_0	8.7345×10^{-4} g/cm^3	Initial density
	γ	1.17	Adiabatic index
	M	21 g/mol	Molecular weight
	A	6.85×10^{12} cm^3/g-s	Pre-exponential factor
	$E_a(=Q)$	$46.37\, RT_0$	Activation energy
	q	$43.28\, RT_0/M$	Chemical energy release
	$\nu_0 = \kappa_0 = D_0$	2.9×10^{-5} g/s-cm-K$^{0.7}$	Transport constants
Output	S_l	298 cm/s	Laminar flame speed
	T_b	$7.289\ T_0$	Post-flame temperature
	ρ_b	$0.1372\ \rho_0$	Post-flame density
	x_l	0.035 cm	Laminar flame thickness
	D_{CJ}	1.993×10^5 cm/s	CJ detonation velocity
	P_{ZND}	$31.47\ P_0$	Post-shock pressure
	P_{CJ}	$16.24\ P_0$	Pressure at CJ point
	T_{ZND}	$3.457\ T_0$	Post-shock temperature
	T_{CJ}	$9.010\ T_0$	Temperature at CJ point
	ρ_{ZND}	$9.104\ \rho_0$	Post-shock density
	ρ_{CJ}	$1.802\ \rho_0$	Density at CJ point
	x_d	0.01927 cm	1D half-reaction thickness
	λ	1–2 cm	Detonation cell size

Example: model for stoichiometric methane-air

Input		
P_0	1 atm	
T_0	298 K	
M	27 g/mol	
γ	1.197	
A	1.64×10^{13} cm^3/g s	
E_a	$67.55RT_0$	
q	$39.0RT_0/M$	
ν_0	3.6×10^{-6} g/s cm K$^{0.7}$	
$\kappa_0 = D_0$	6.25×10^{-6} g/s cm K$^{0.7}$	
Output		
	Calculated values	Target values
S_l	38.02 cm/s	34–45 cm/s [26,27]
T_b	2210 K	2200–2230 K [28]
x_f	0.0439 cm	
D_{CJ}	1820 m/s	~1815 m/s [42]
x_d (λ)	0.229 cm (16–23 cm)*	0.13–0.62 cm * (13–31 cm) [19]