28th International Colloquium on the Dynamics of Explosions and Reactive Systems
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A methodology to develop simplified kinetic schemes for detonations simulations

Fernando Veiga-López, Ashwin Chinnayya and Josué Melguizo-Gavilanes

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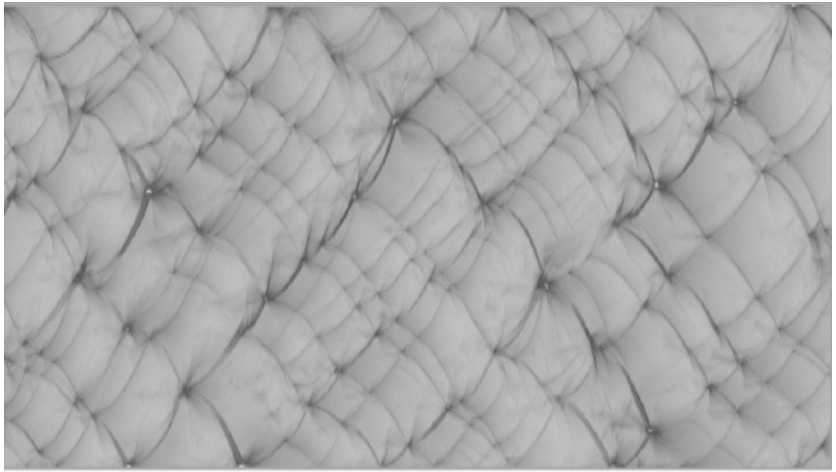
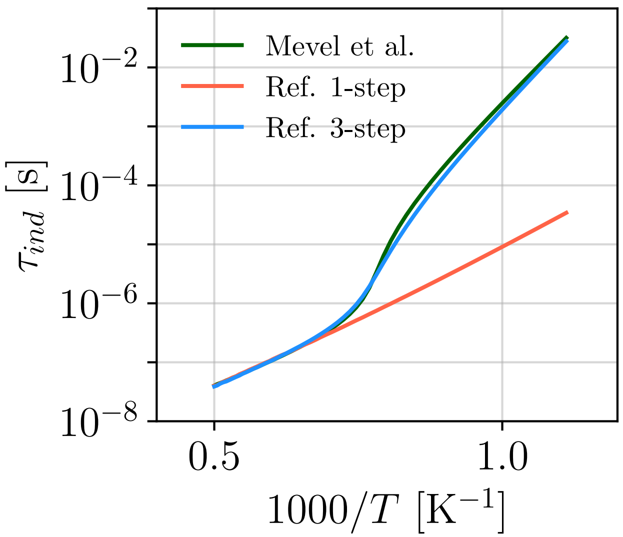


Numerical soot-foil obtained with and stoichiometric H_2-O_2 detonation

Motivation and objective

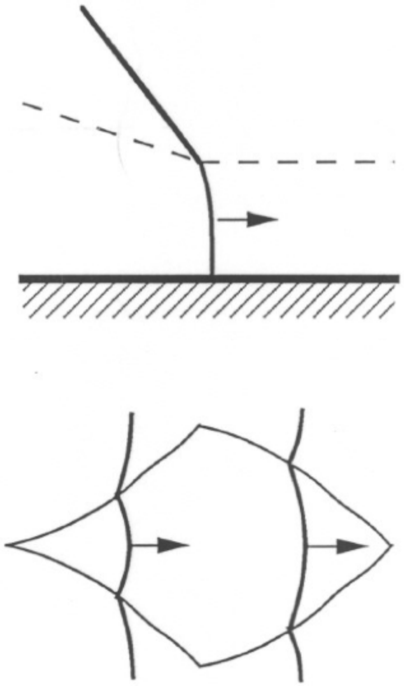
- Modeling chemistry is still a challenge
- Flames: Several approaches
  - Efforts because of industrial needs (turbulent combustion)
  - Huge detailed mechanisms for HC (~100 species; ~1000 reactions)
  - Improved reduction techniques
- Detonations: usually single-step Arrhenius
  - Fair qualitative agreement
  - Lack for quantitative predictions (initiation, quenching)
  - Conventional 0D (induction time) or 1D (ideal ZND) fitting procedures



Motivation and **objective**

- Propose a new fitting procedure for reduced chemical mechanisms for stoichiometric hydrogen-oxygen detonations
    - Steady 1D curved (κ) detonations
    - Matching the predicted critical curvatures (κ_{crit})
    - Predictive reduced chemistry

- Check the implications on multi-dimensional simulations



Pictures taken from Klein et al. report FM95-04

1D model including small curvature

Mathematical formulation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\frac{\left(\dot{\sigma} - wM^2\alpha\right)}{1 - M^2}$$

$$\frac{\mathrm{d}w}{\mathrm{d}t} = w\frac{(\dot{\sigma} - w\alpha)}{1 - M^2}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\rho w^2\frac{(\dot{\sigma} - w\alpha)}{1 - M^2}$$

$$\frac{\mathrm{d}Y_k}{\mathrm{d}t} = \frac{W_k\dot{\omega}_k}{\rho}, \quad \left(k = 1, \ldots, N\right)$$

$$\dot{\sigma} = \sum_{k=1}^{N}\left(\frac{\overline{W}}{W_k} - \frac{h_k}{c_pT}\right)\frac{\mathrm{d}Y_k}{\mathrm{d}t}$$ Thermicity

$$\alpha = \frac{1}{A}\frac{\mathrm{d}A}{\mathrm{d}x} = \kappa\left(\frac{D}{w} - 1\right)$$ Detonation curvature term

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$T_o = 300$ K ; $p_o = 100$ kPa; $2H_2 + O_2$

Single step chemistry

$$F \to P \qquad k_T = k\exp\left(-\frac{E_a}{R_uT}\right)$$

Three step chemistry

Initiation	$F \to Y$	$k_I = k_C\exp\left[-\frac{E_I}{R_u}\left(\frac{1}{T_I} - \frac{1}{T}\right)\right]$
Branching	$F + Y \to 2Y$	$k_B = k_C\exp\left[-\frac{E_B}{R_u}\left(\frac{1}{T_B} - \frac{1}{T}\right)\right]$
Termination	$Y \to P$	$k_T = k_C$

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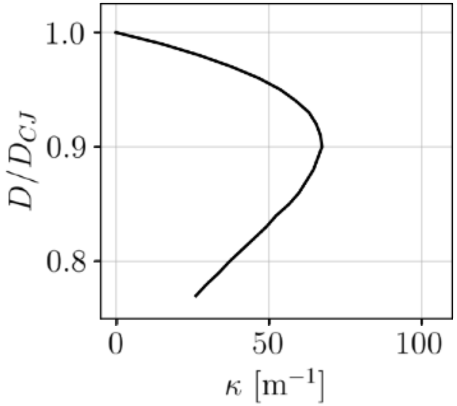

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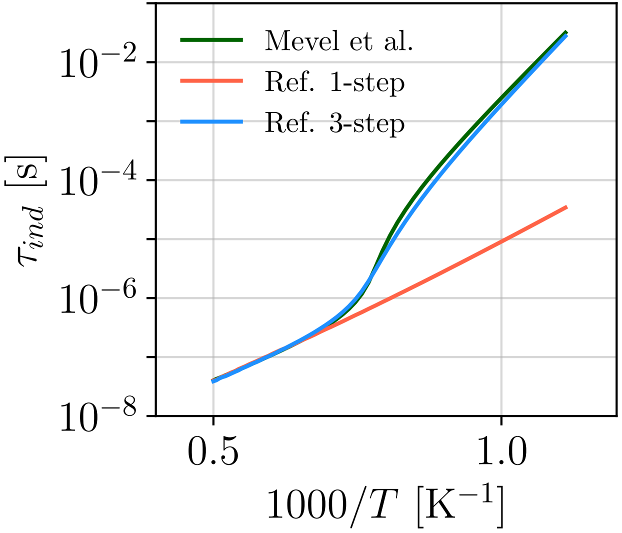
Termination	$Y \rightarrow P$	$k_T = k_C$

1D Results

Chemistry: standard 0D fitting with induction time - **D-kappa curves**

Induction time vs. 1000/T



Mevel et al. IJHE, vol. 41, no. 16, pp. 6905-6916, 2016.
Taileb et al. CNF, vol. 218, pp. 460-473, 2021.

Chemical parameters

Single step chemistry

$$k = 1.1 \times 10^9 \ \mathrm{s}^{-1}$$

$$E_a/R_u = 11277 \ \mathrm{K}$$

Three step chemistry

$$k_C = 2 \times 10^7 \ \mathrm{s}^{-1}$$

$$E_I/R_u = 25000 \ \mathrm{K}$$

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$$T_I = 2431 \ \mathrm{K}$$

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Chemistry: standard 0D fitting with induction time - **D-kappa curves**

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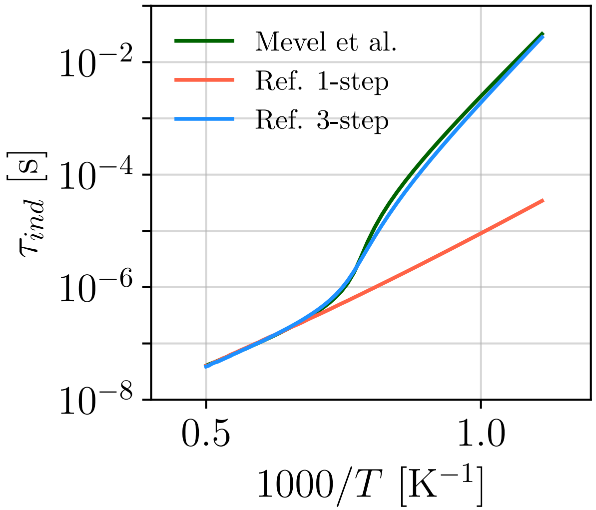

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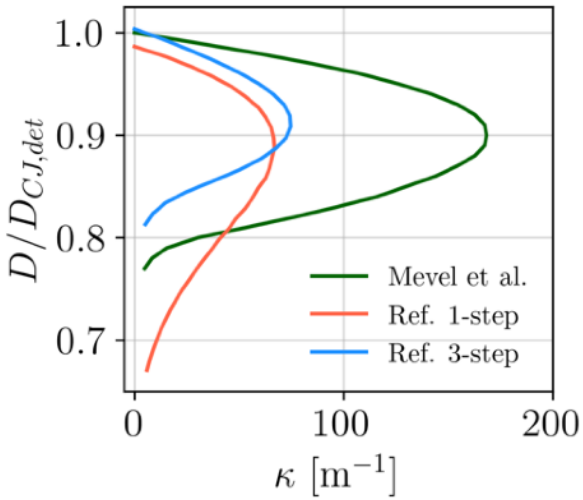
Detonation speed vs. curvature



1D Results

Chemistry: standard 0D fitting with induction time - **ZND profiles**

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$$T_I = 2431 \ \mathrm{K}$$

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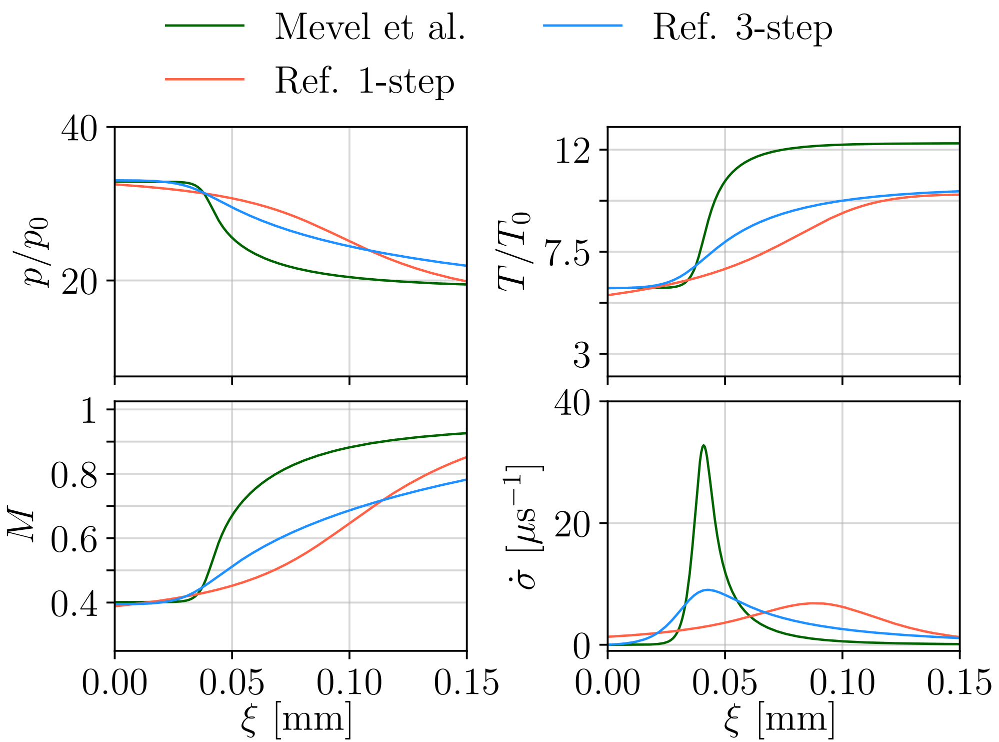
- Chapman-Jouguet conditions do not match
- Thermicity profiles are smoother with simplified mechanisms



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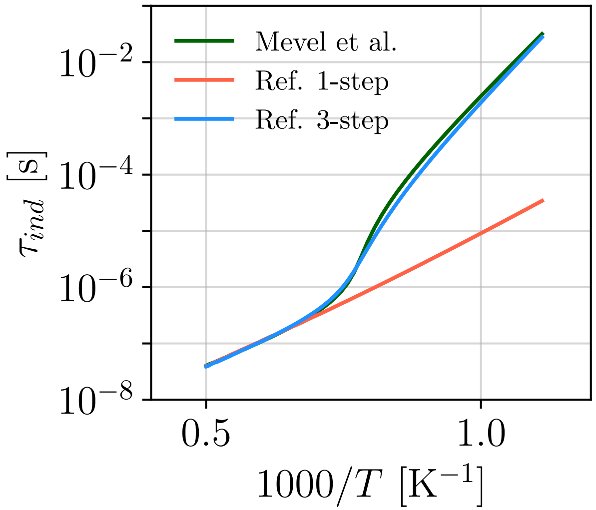
Chemistry: standard 0D fitting with induction time - **D-kappa curves**

Induction time vs. 1000/T



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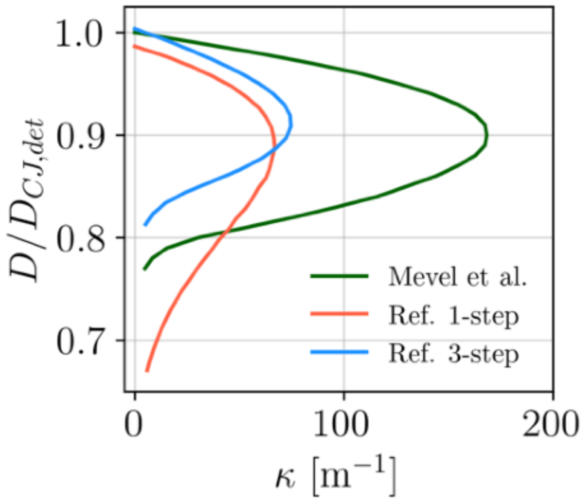
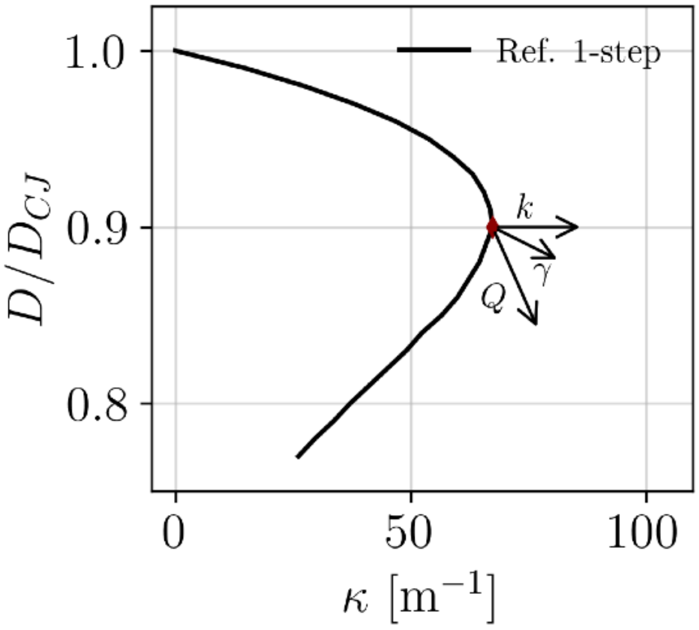


	1-step	3-step	Mevel et al.	
κ_{crit} $[\mathrm{m}^{-1}]$	67.4	74.8	168.5	This study
$1/h_{crit}$ $[\mathrm{m}^{-1}]$	41.7	50	166.7	Reference

1D Results

Influence of the fitting parameters

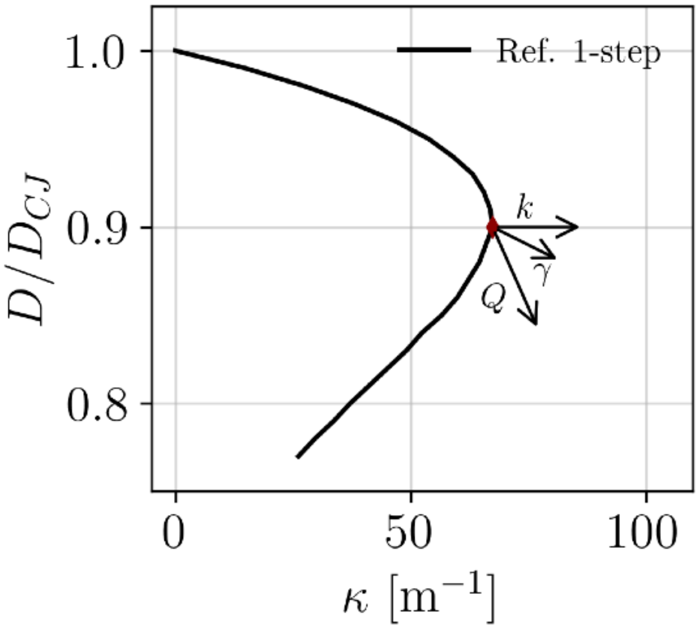
Single step chemistry



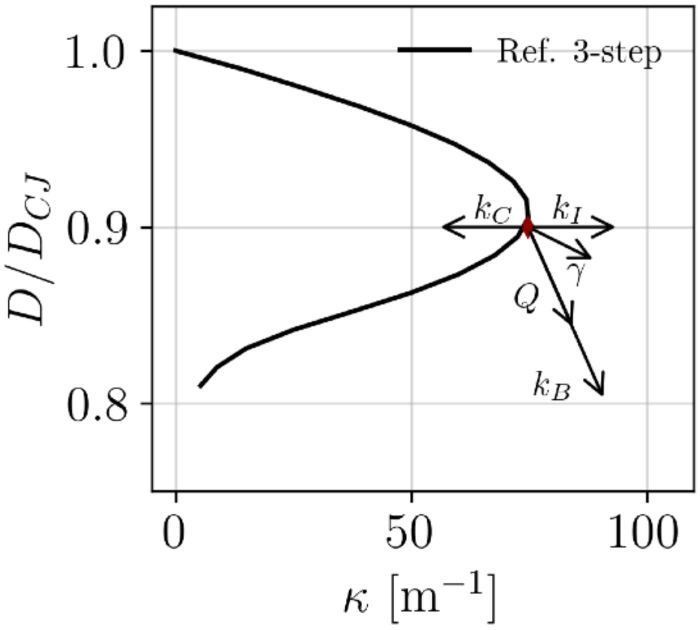
1D Results

Influence of the fitting parameters

Single step chemistry



Three step chemistry



1D Results

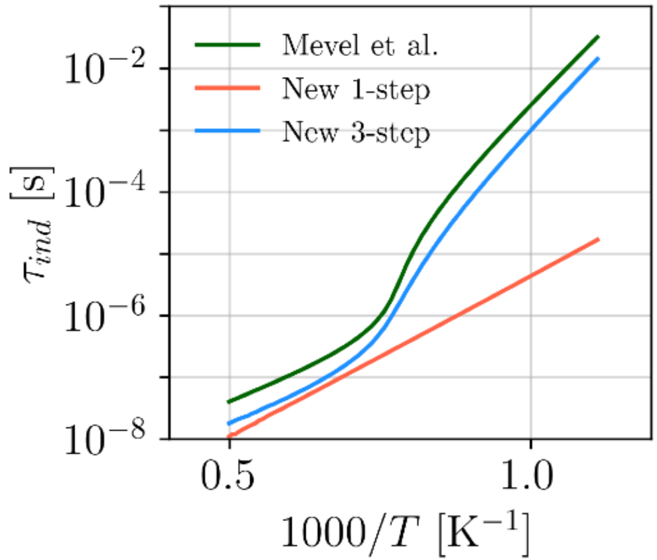
Optimal selection of the chemical parameters

	γ(0 – vN – CJ)	Q [MJ/kg]	k ; k_C [s^{-1}]	D_{CJ} [m/s]	T_{vN} [K]	l_{ind} [μm]
Mevel et al.	1.4 - 1.35 - 1.218	-	-	2839.9	1768.7	41
Ref. 1-step	1.33	4.8	6×10^9	2801.5	1674.8	87.9
New 1-step	1.35	4,606	1.08×10^{10}	2836.9	1769.5	36.2
Ref. 3-step	1.33	4.99	2×10^7	2850.4	1723.7	46.8
New 3-step	1.35	4,613	4×10^7	2836.2	1768.7	21.4

1D Results

Chemistry: 1D fitting with critical curvature - **D-kappa curves**

Induction time vs. 1000/T



Chemical parameters

Single step chemistry

$$k = 1.08 \times 10^{10}\ \mathrm{s}^{-1}$$

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Three step chemistry

$$k_C = 4 \times 10^{7}\ \mathrm{s}^{-1}$$

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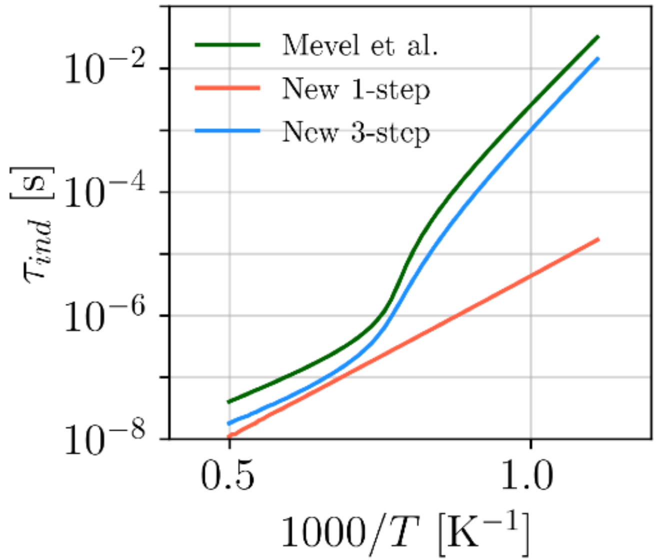

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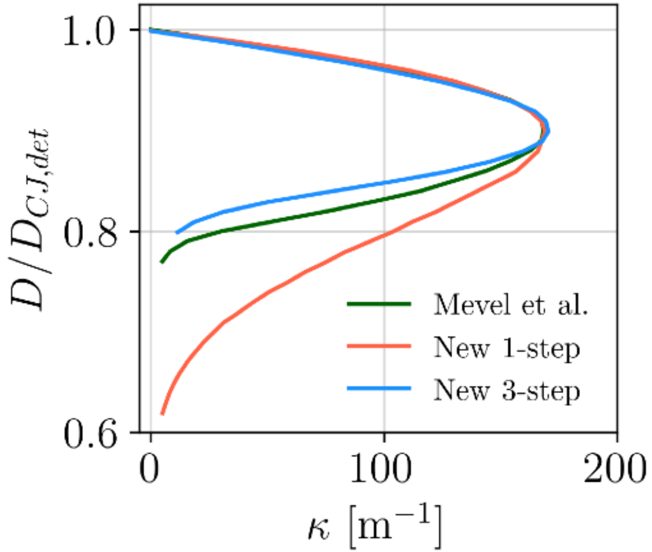

1D Results

Chemistry: 1D fitting with critical curvature - **ZND profiles**

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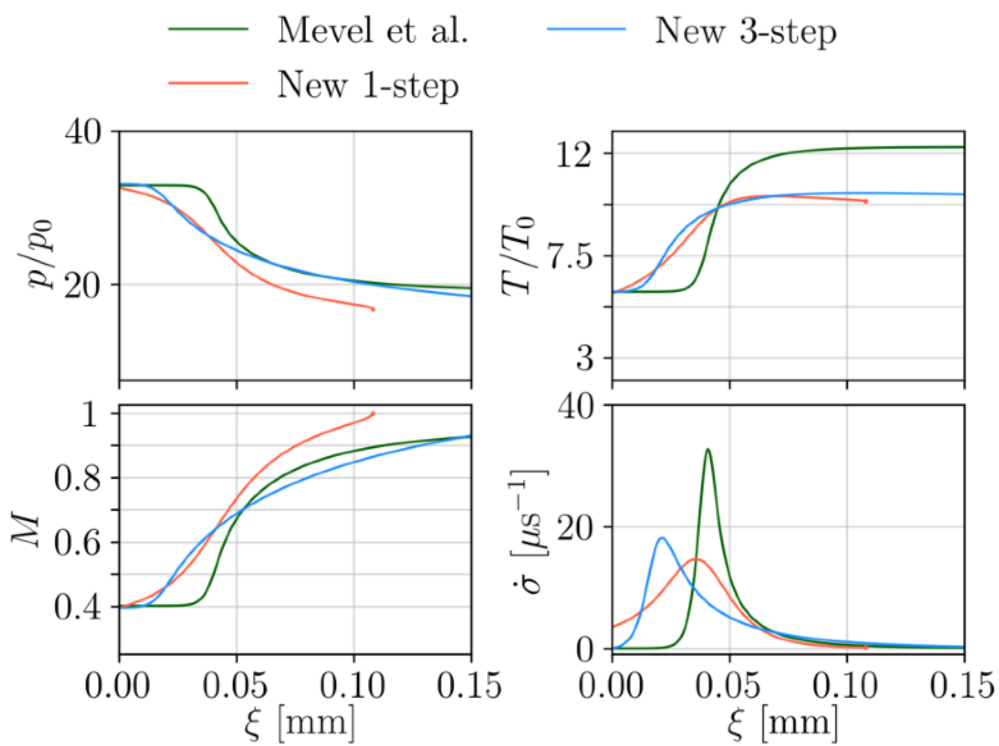
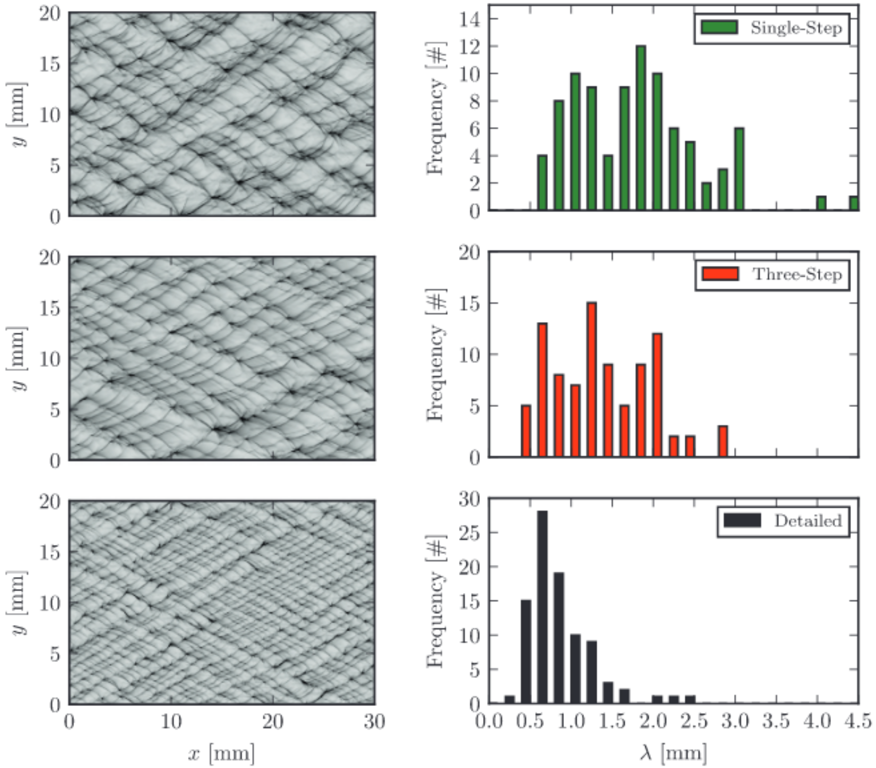
- Chapman-Jouguet conditions still do not match
- Thermicity profiles are closer to the detailed chemistry result



2D Results

Numerical soot foils cell size (single-step)



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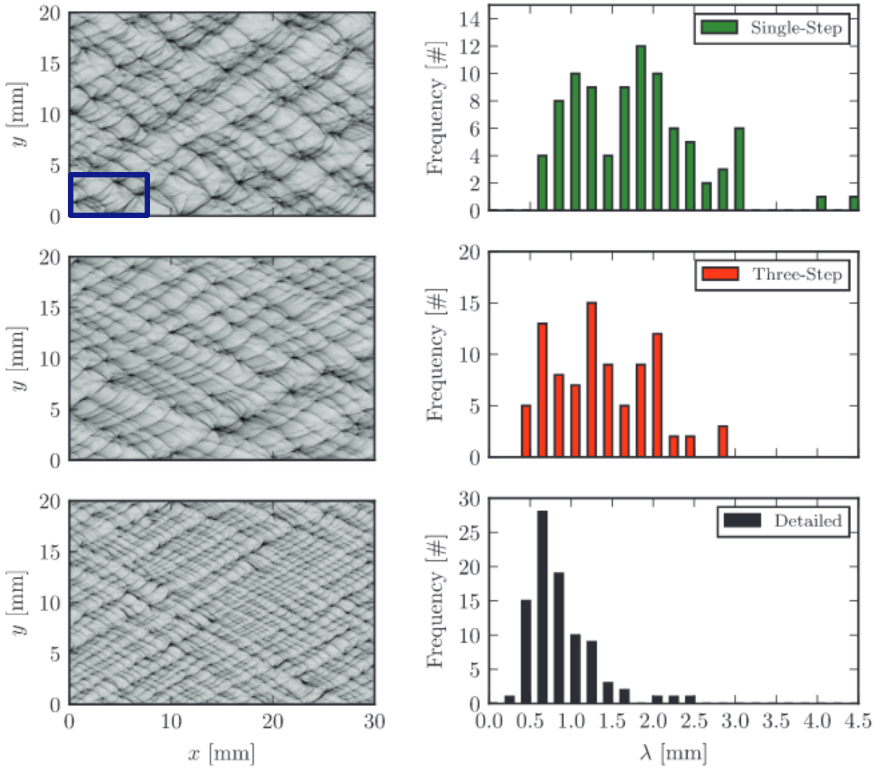

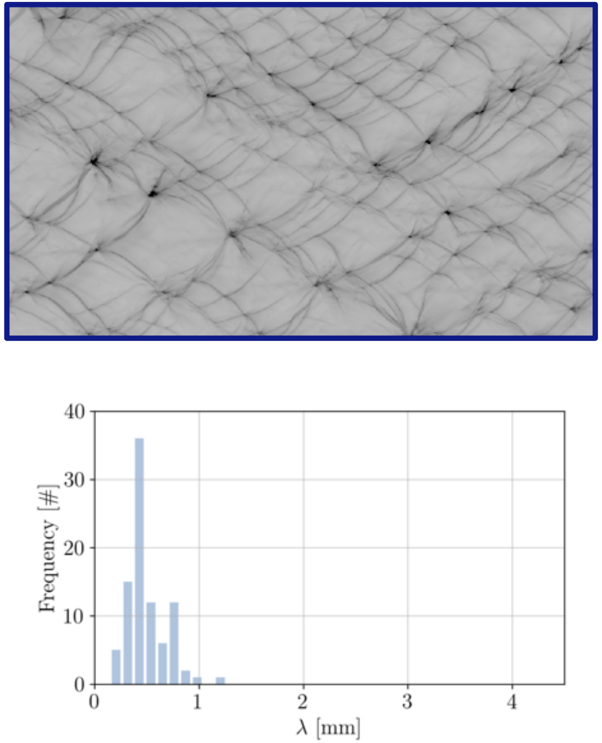

2D Results

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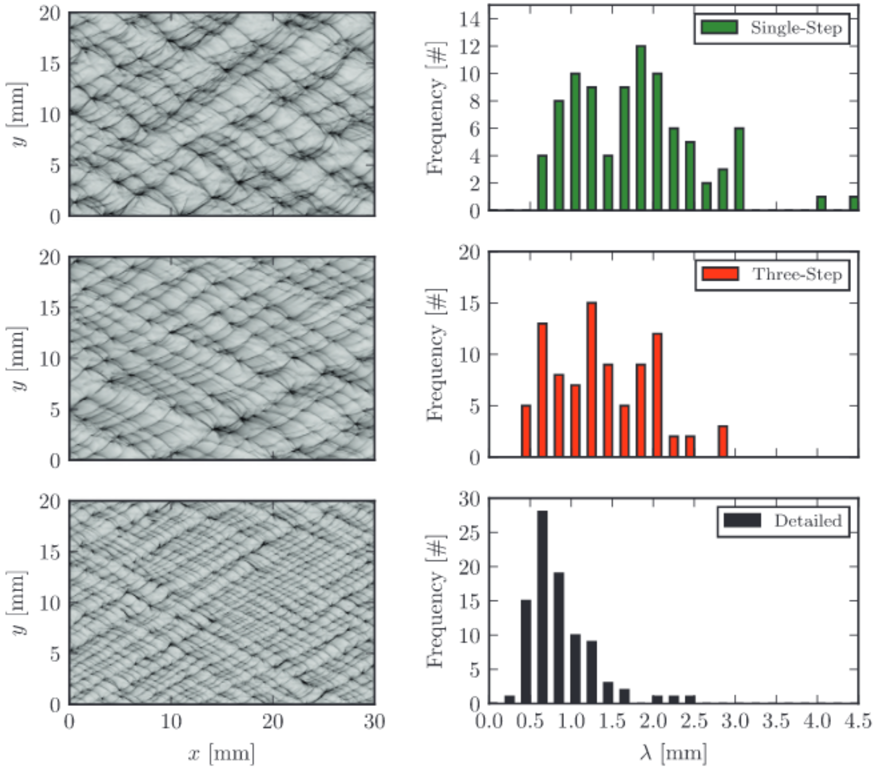

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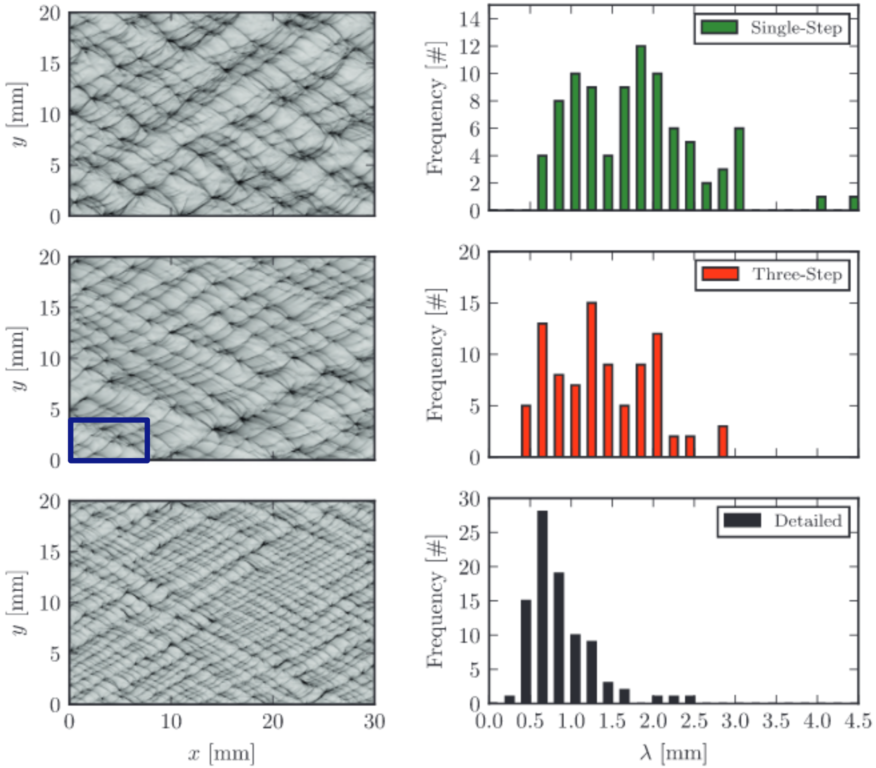
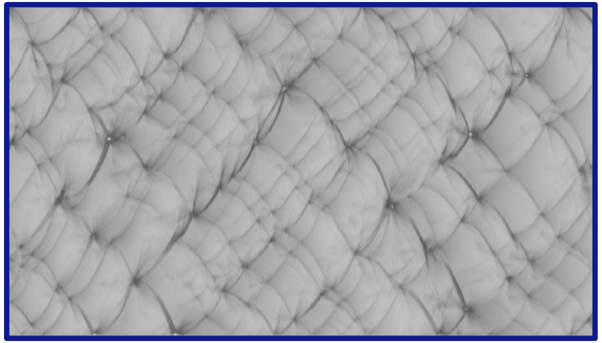
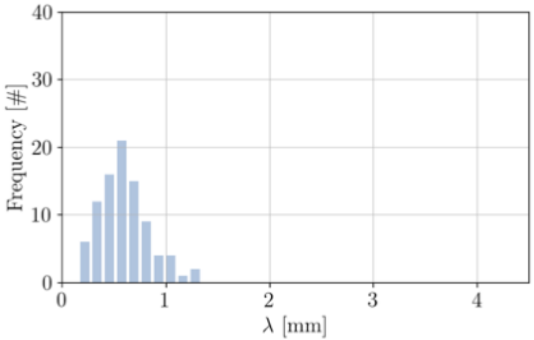
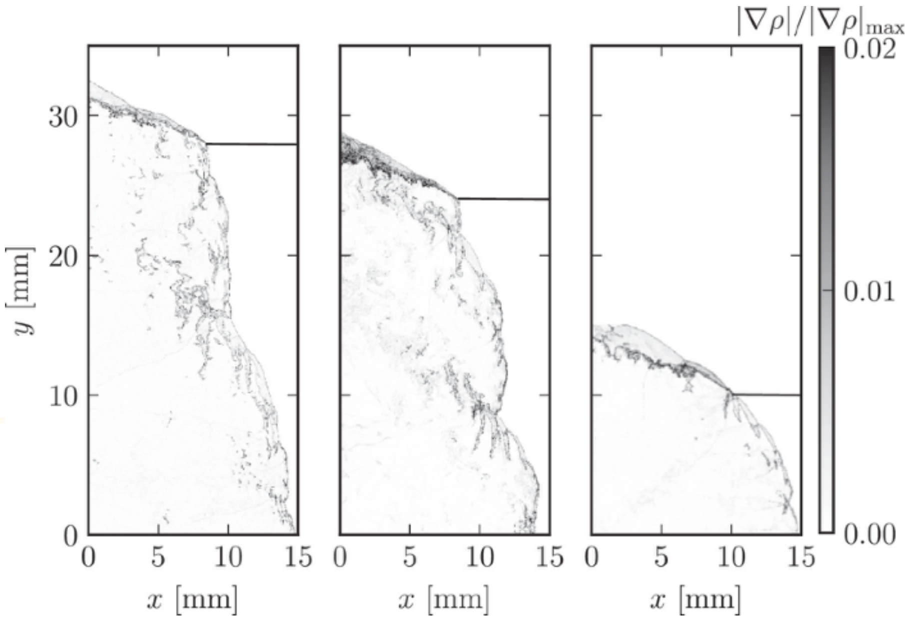






2D Results

Interaction with an inert layer - previous results

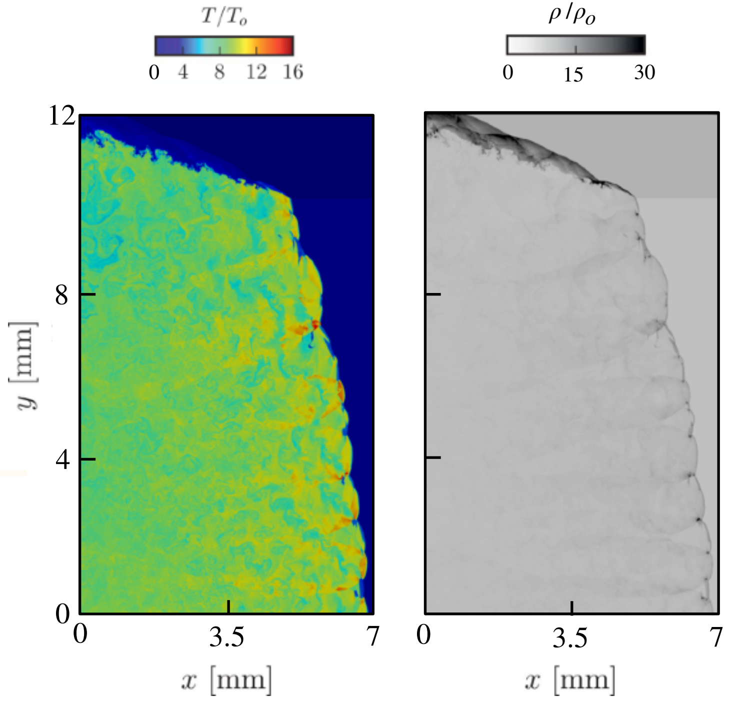


	h_{crit} [mm]
Experimental	4.6
Mevel et al.	6
Ref. 1-step	24
New 1-step	
Ref. 3-step	20
New 3-step	

Taileb et al. CNF, vol. 218, pp. 460-473, 2021.

2D Results

Interaction with an inert layer - promising improvement on quenching prediction (three-step)



	h_{crit} [mm]
Experimental	4.6
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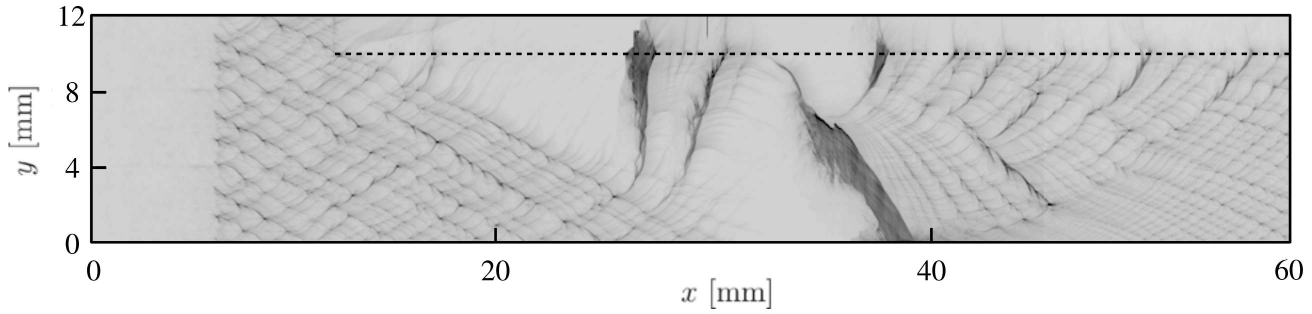
Ref. 1-step	24
New 1-step	TBD
Ref. 3-step	20
New 3-step	< 10

2D Results

Interaction with an inert layer - promising improvement on quenching prediction (three-step)



Propagated for almost 5 cm interacting with and inert gas through a 10-mm height layer

	h_{crit} [mm]
Experimental	4.6
Mevel et al.	6
Ref. 1-step	24
New 1-step	TBD
Ref. 3-step	20
New 3-step	< 10

Conclusions and future efforts

- We propose a new fitting procedure for simplified chemical kinetics
- κ_{crit} as fitting target ($D - \kappa$ curves)
- Promising preliminary results in 2D
  - Cell size histogram better agreement with the detailed scheme
  - Critical height reduction with three-step

$$h_{crit} = 20\,\text{mm} \rightarrow h_{crit} < 10\,\text{mm}$$

Conclusions and **future efforts**

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- Promising preliminary results in 2D
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    $h_{crit} = 20\,\mathrm{mm} \rightarrow h_{crit} < 10\,\mathrm{mm}$

- Finish the 2D analysis for quenching limits
- Variable thermodynamics
- Check our procedure for different fuels
- Extend for friction and heat losses, problem dependent

Thank you for your attention!

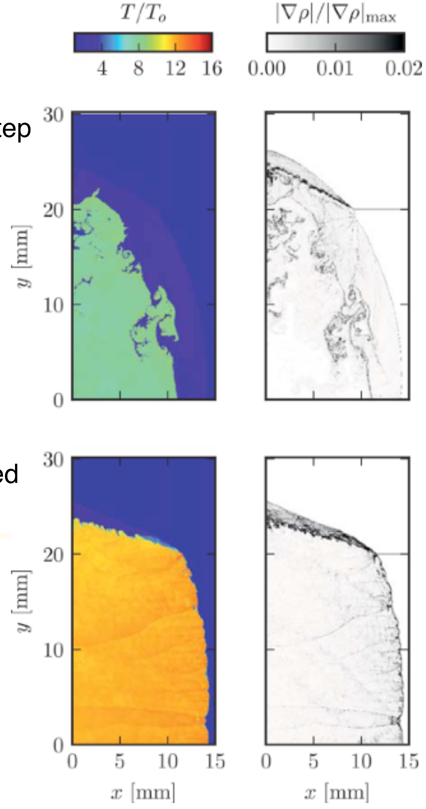
2D Results

Interaction with an inert layer - improve on quenching prediction (three-step)

$h = 20\,\mathrm{mm}$

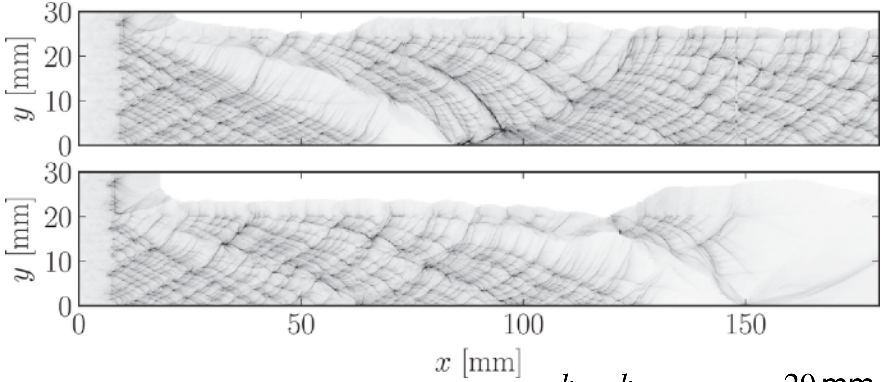
Old 3-step

Detailed



Old 3-step

$h = 24\,\mathrm{mm}$



$h = h_{crit,\,3-step} = 20\,\mathrm{mm}$