EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Modelling strategy for the Large-Eddy Simulation of lean hydrogen-air explosions

Jean-Jacques Hok

CERFACS, Toulouse, France

ERCOFTAC Autumn Festival
20th ERCOFTAC Da Vinci Competition
Darmstadt
October, 9th 2025

www.cerfacs.fr

Hydrogen: an ambivalent energy vector

- ✓ Carbon-free fuel (at use);
- ✓ High gravimetric energy density;

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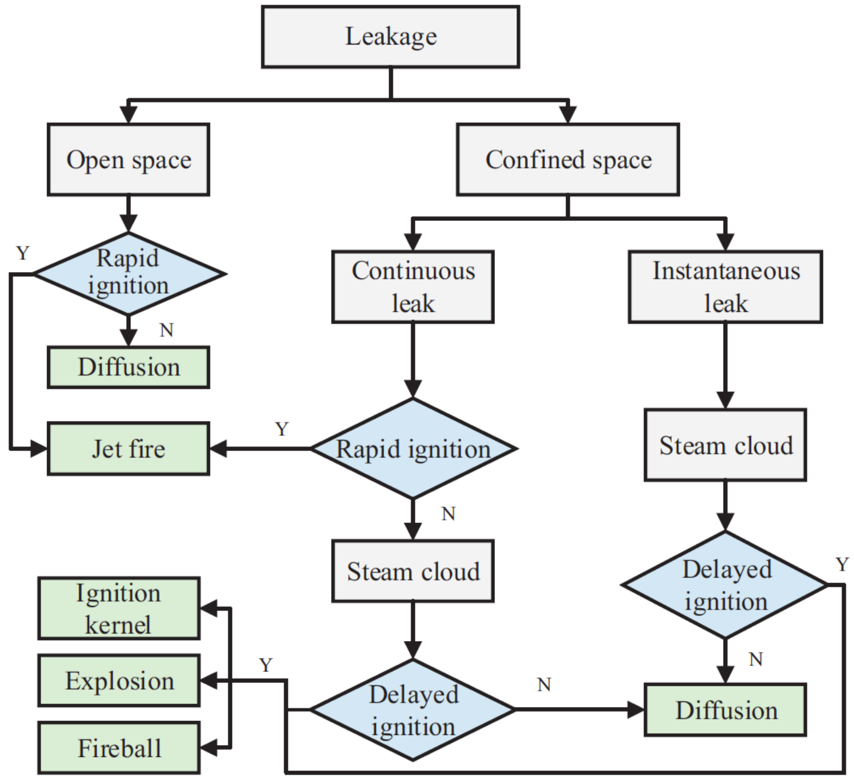
Possible hazardous events following a leakage[1].



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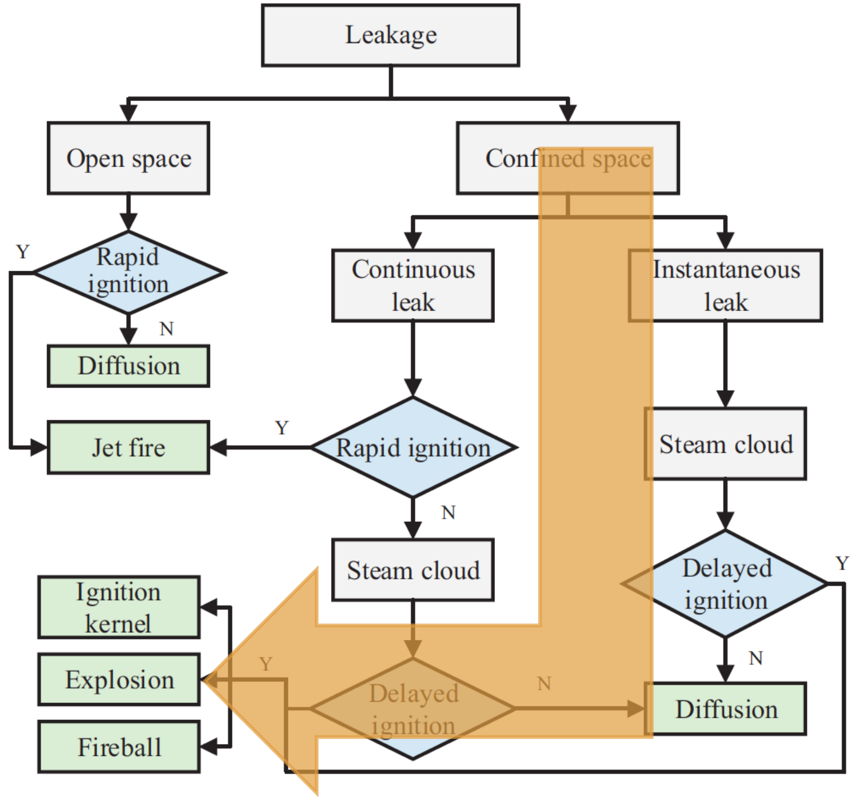

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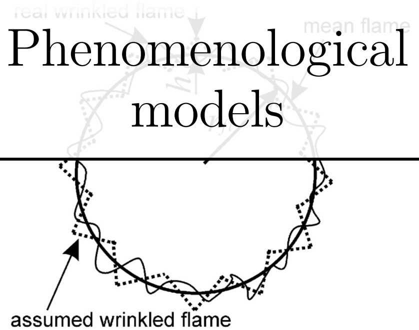
Towards reliable predictions of explosions

Experiments

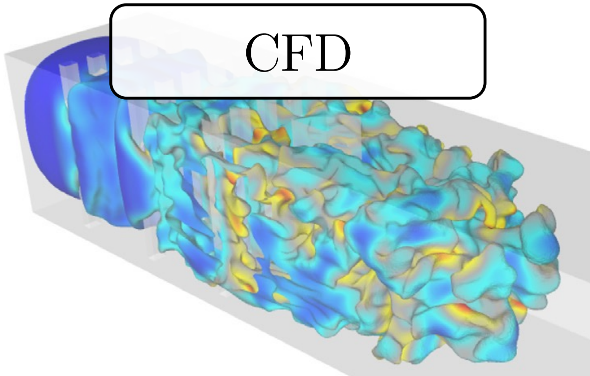
Shadowgraph image of a lean hydrogen-air flame propagating in an obstructed channel[1].

Phenomenological models



Schematic of a flame-surface-based phenomenological model for explosions[2].

CFD



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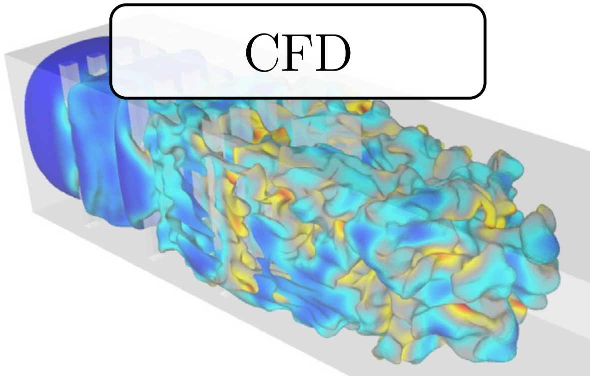

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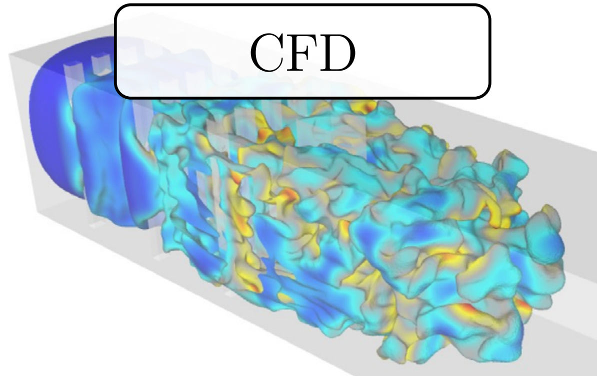

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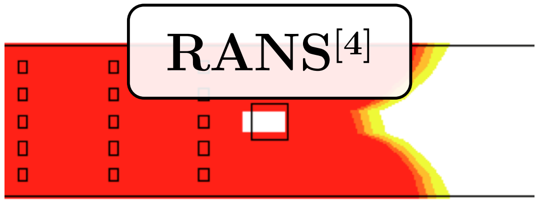

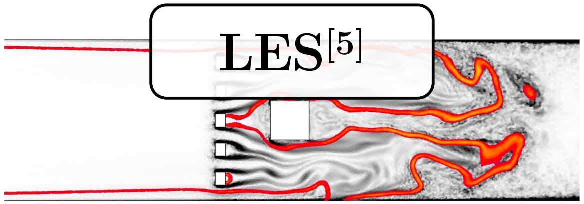

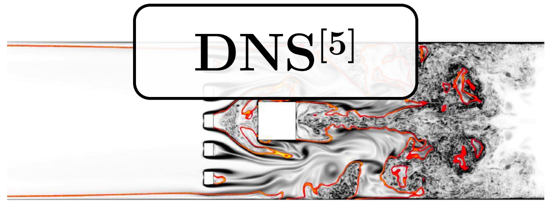

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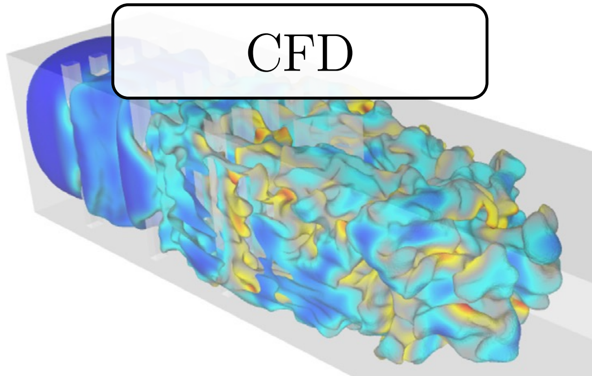

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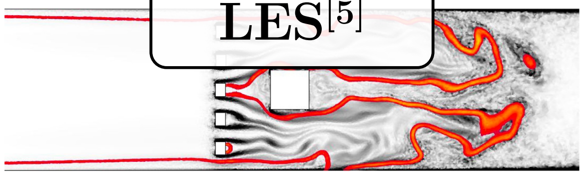

Best cost/accuracy trade-off

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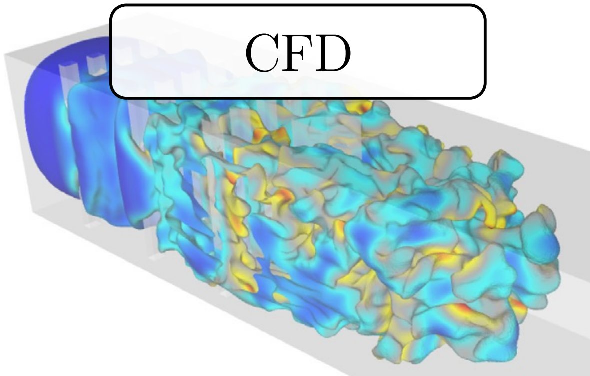

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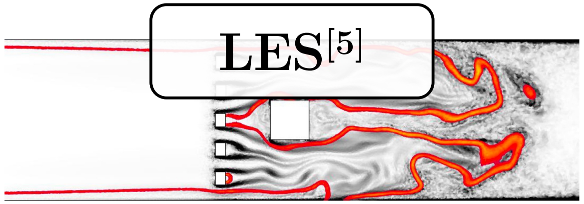

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LEFEX project
(Large-Eddy simulation For EXplosions)

TotalEnergies natran (ex-GRTGaz) Air Liquide

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7.65 m

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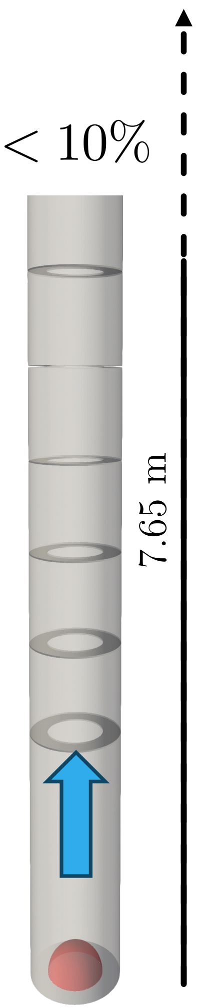

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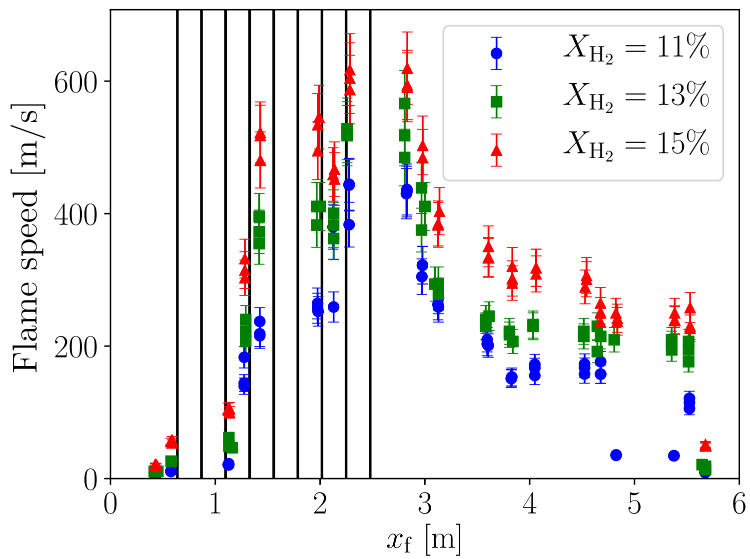

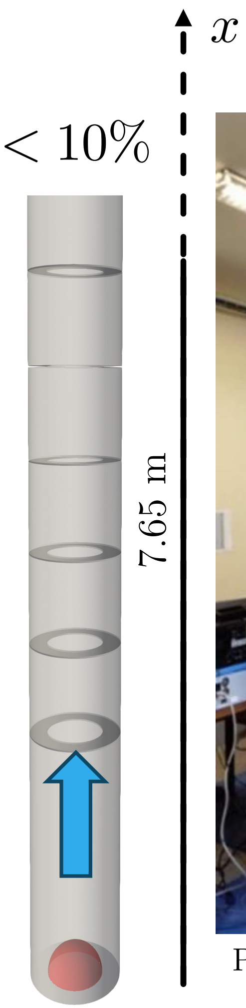

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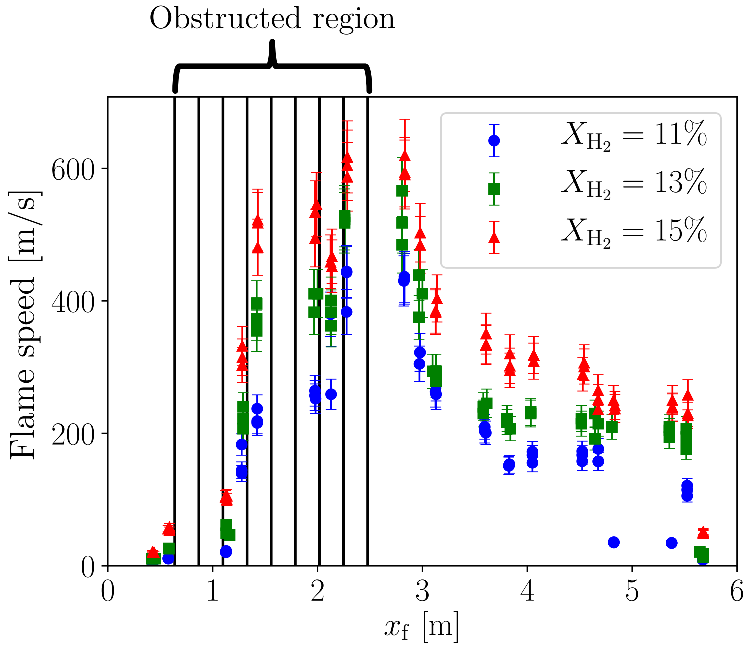

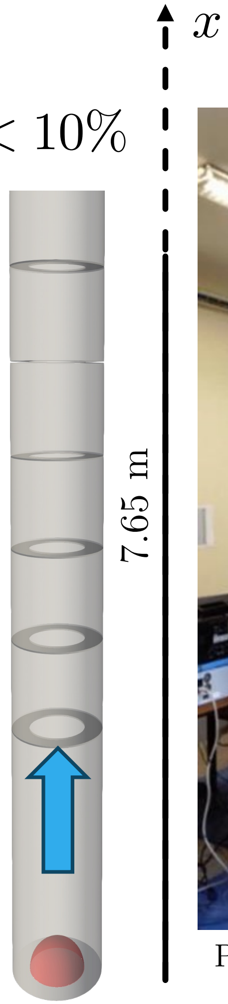

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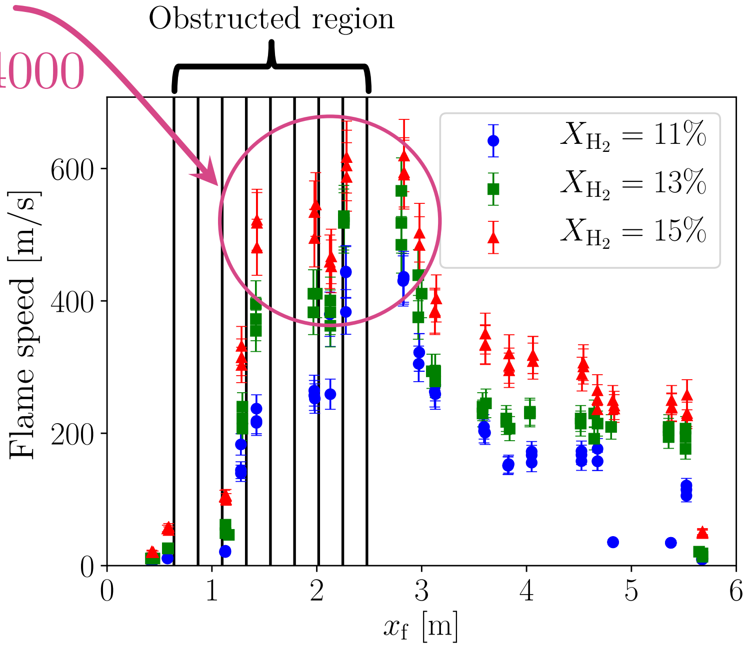

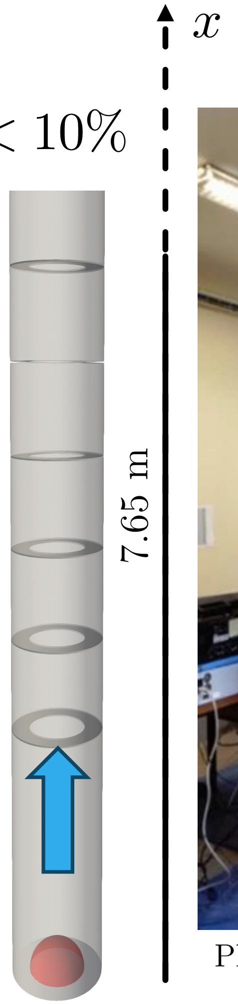

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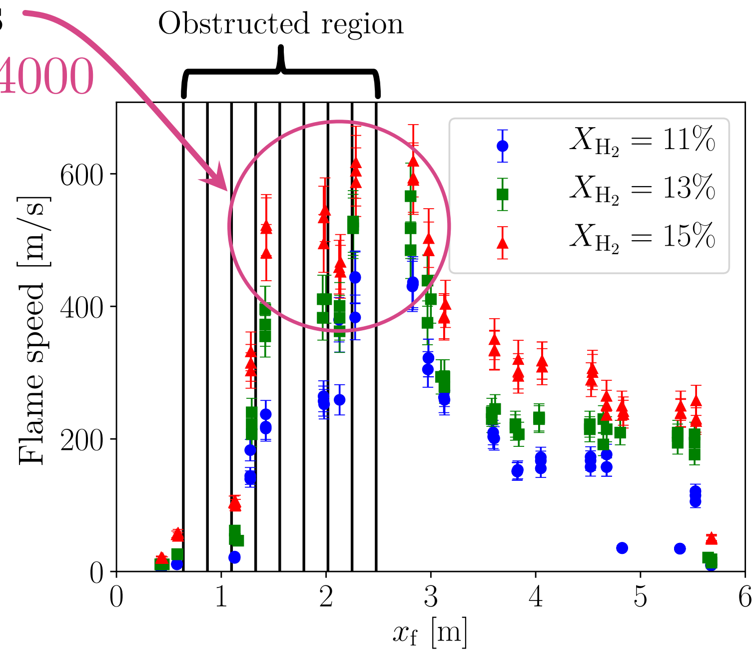

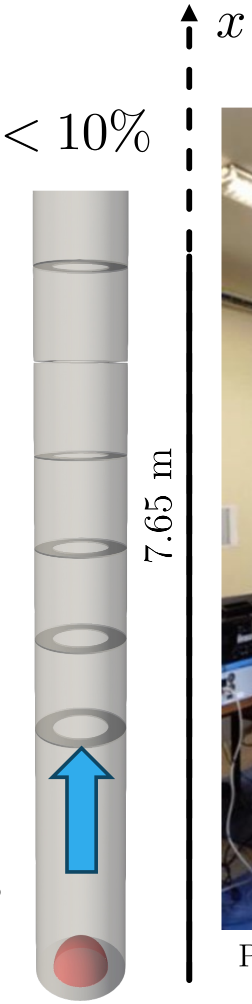

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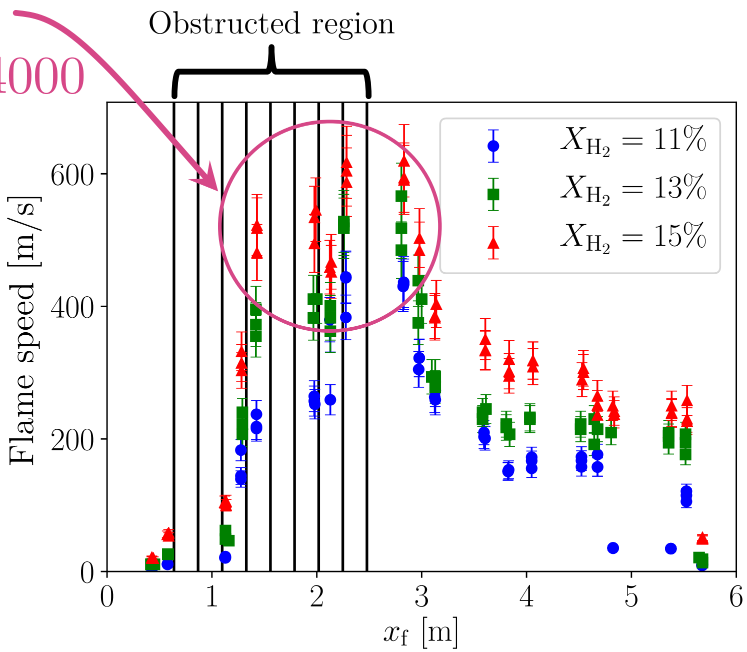
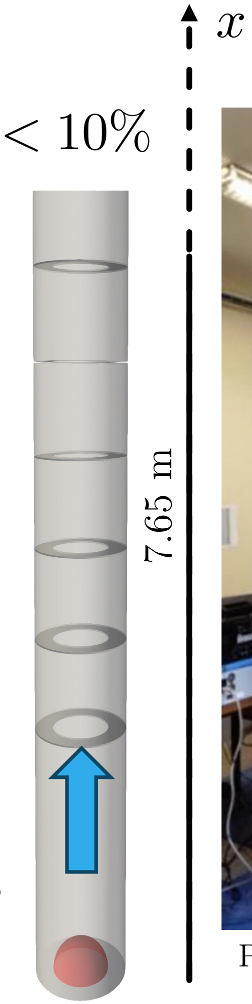
Lean H_2-air explosions are dangerous, we must study them!





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What are the acceleration mechanisms behind the severity of lean H_2-air explosions?

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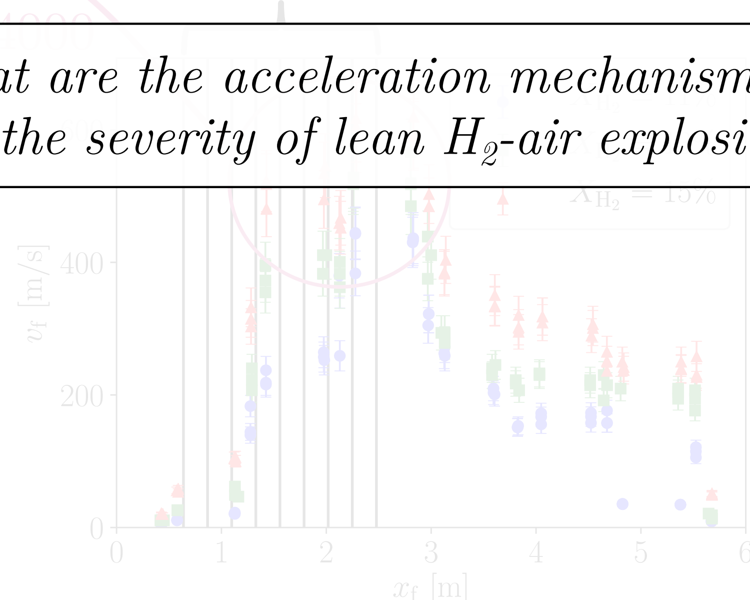

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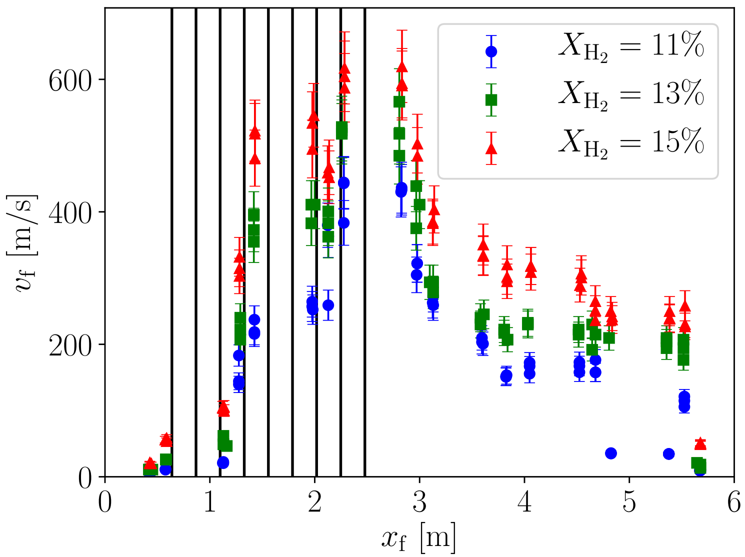
Flame acceleration mechanisms in obstructed channels



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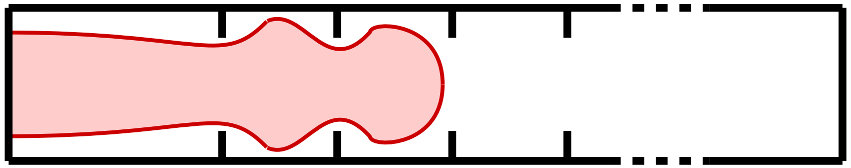
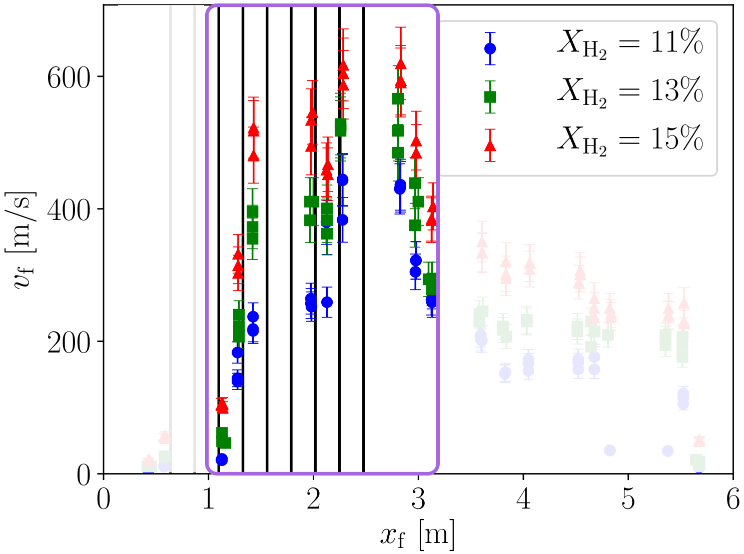


- Flow contraction
- Turbulence-flame interactions



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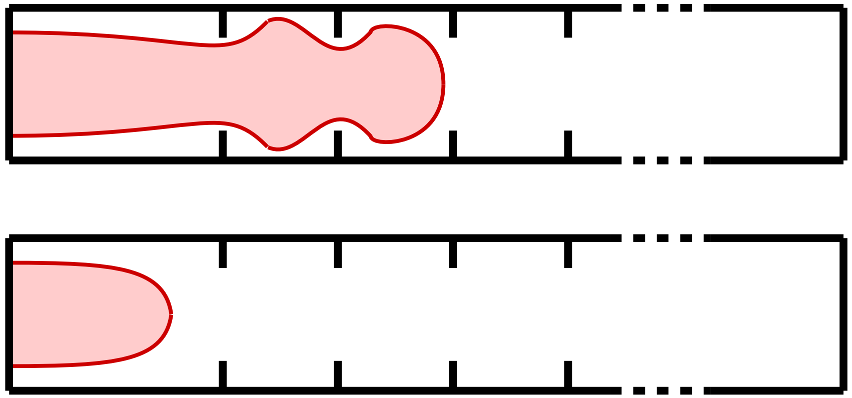

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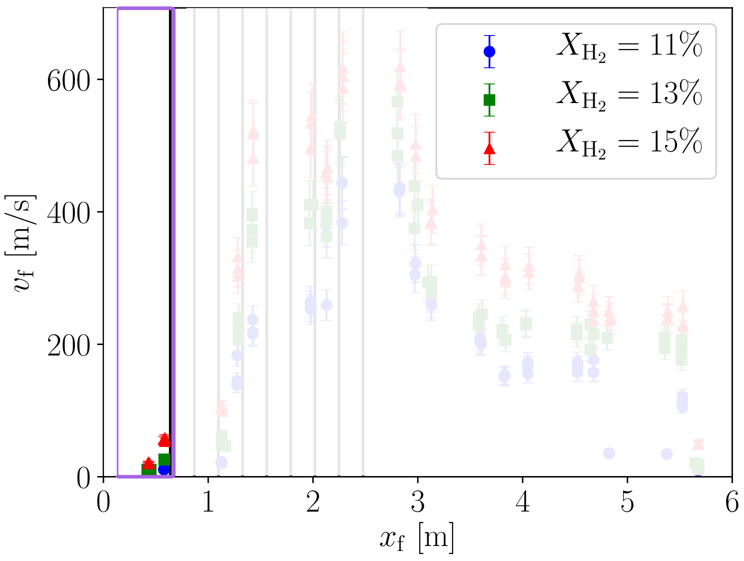
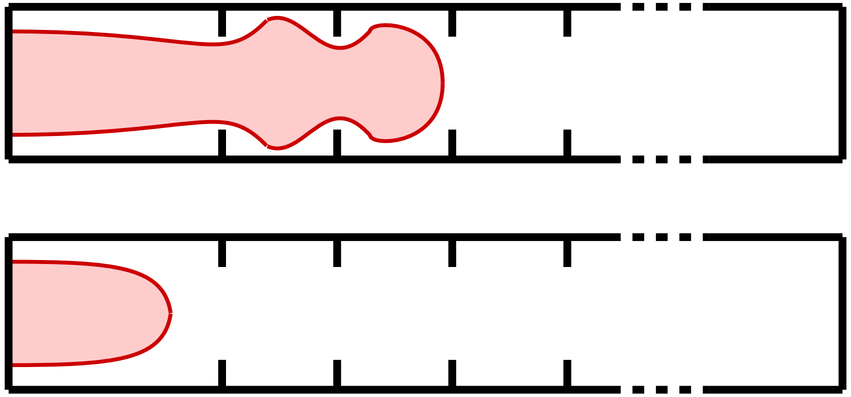


Flame acceleration mechanisms in obstructed channels

Mechanisms common to all fuels



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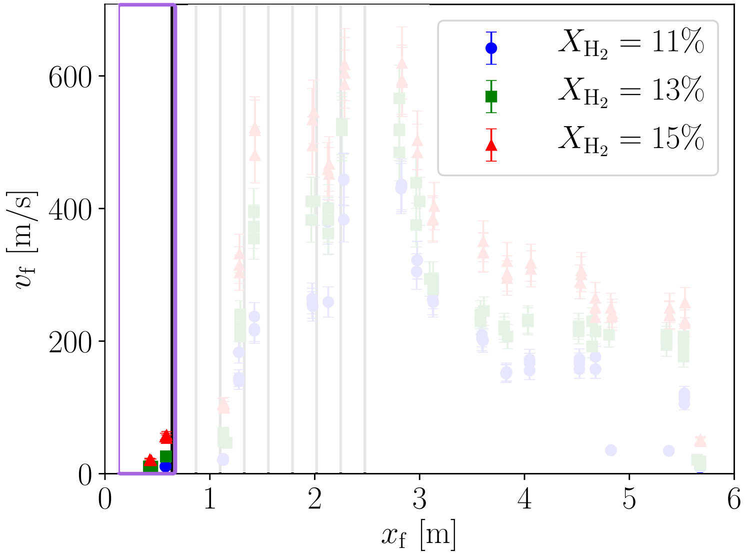

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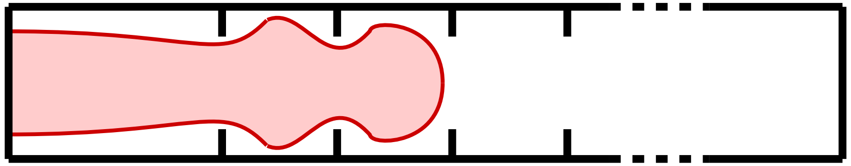

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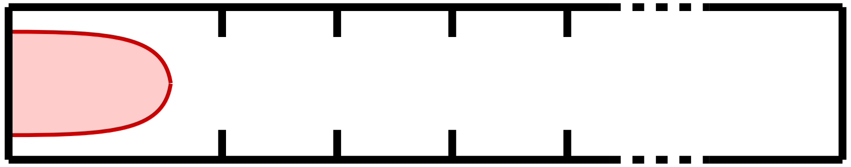

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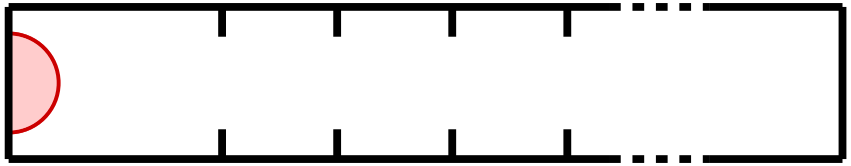
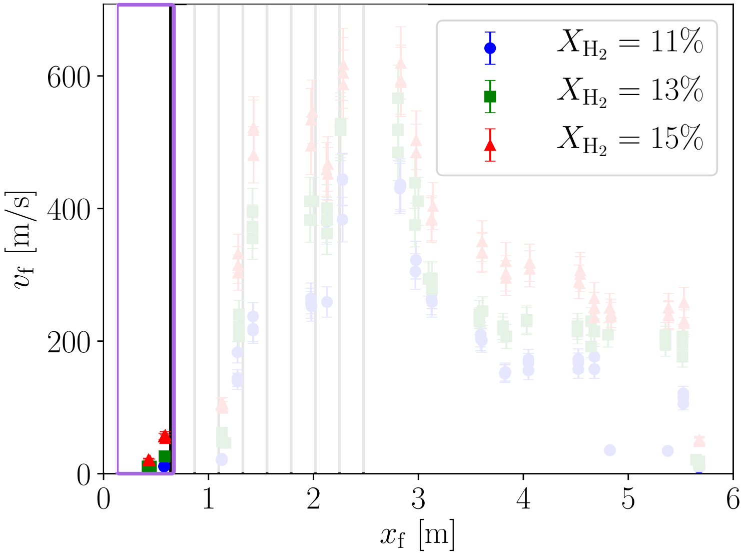


- Stretch effects
- Flame front instabilities

Mechanisms associated to lean H_2-air flames



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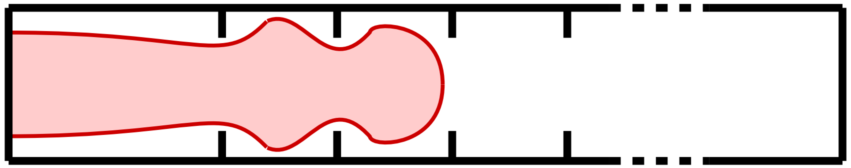

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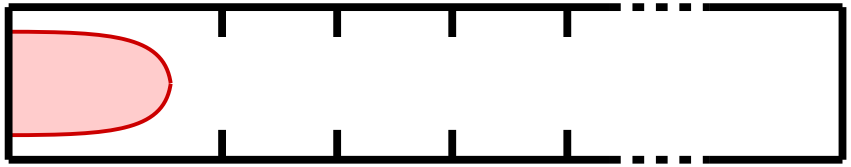

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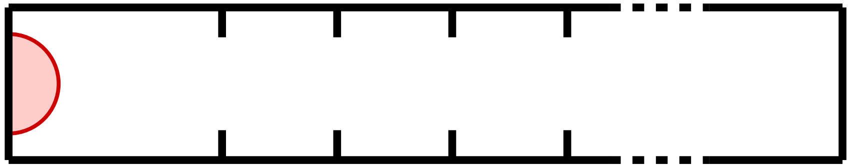

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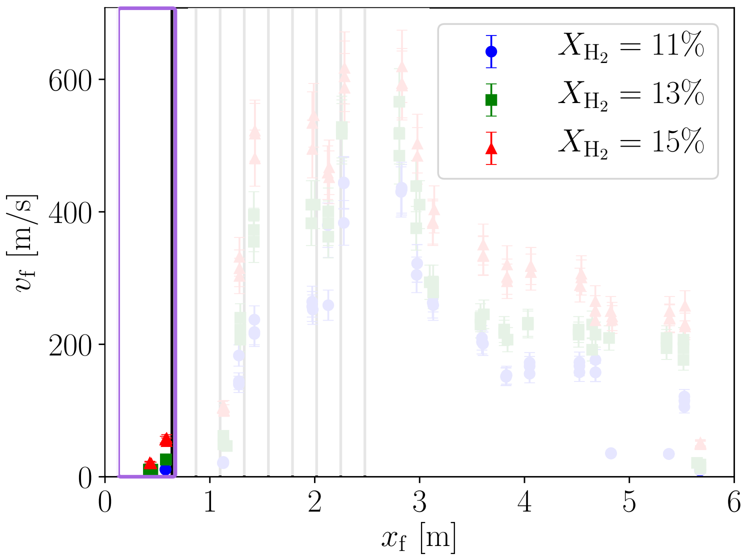

Are these H_2-related mechanisms well accounted for in the classical modelling approach?

Fundamentals of lean H_2-air flames

Thermo-diffusive (TD) instability[1-3]

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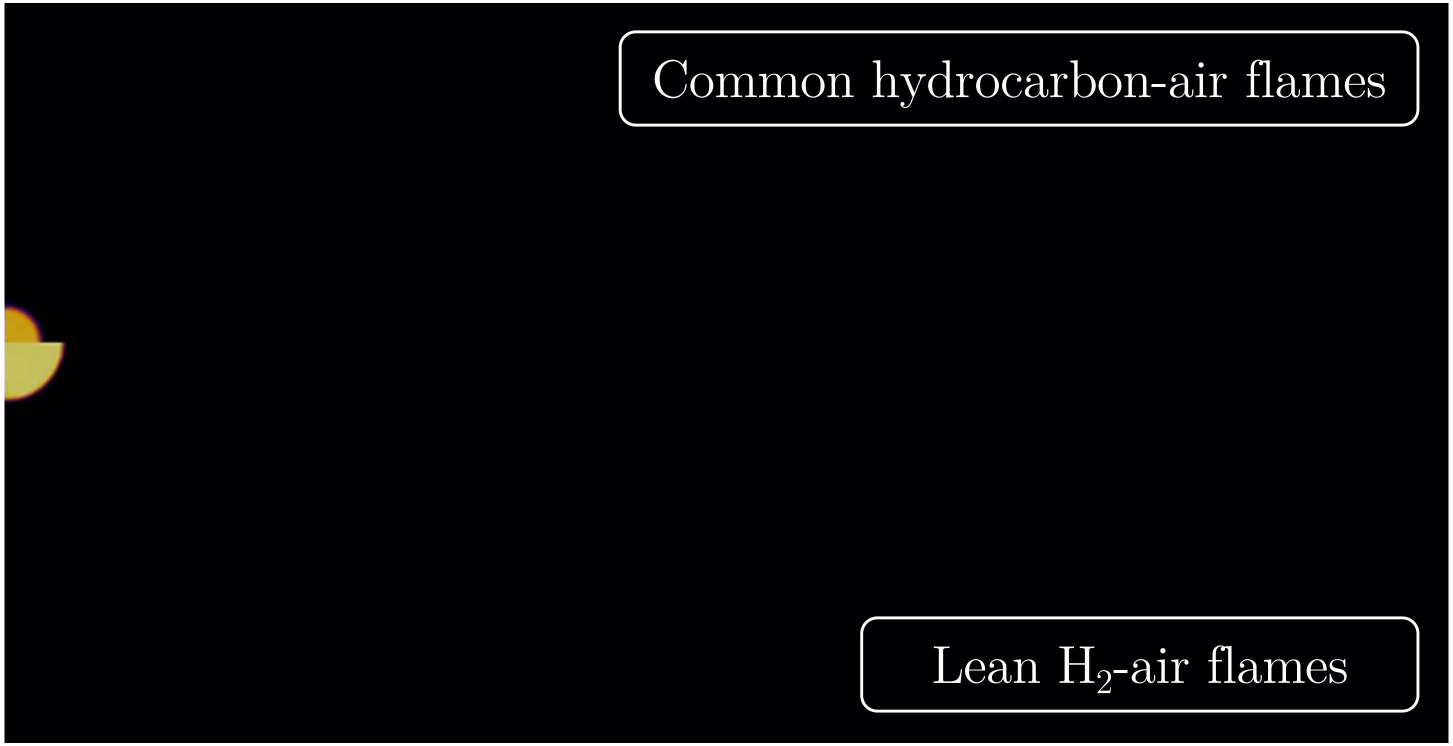

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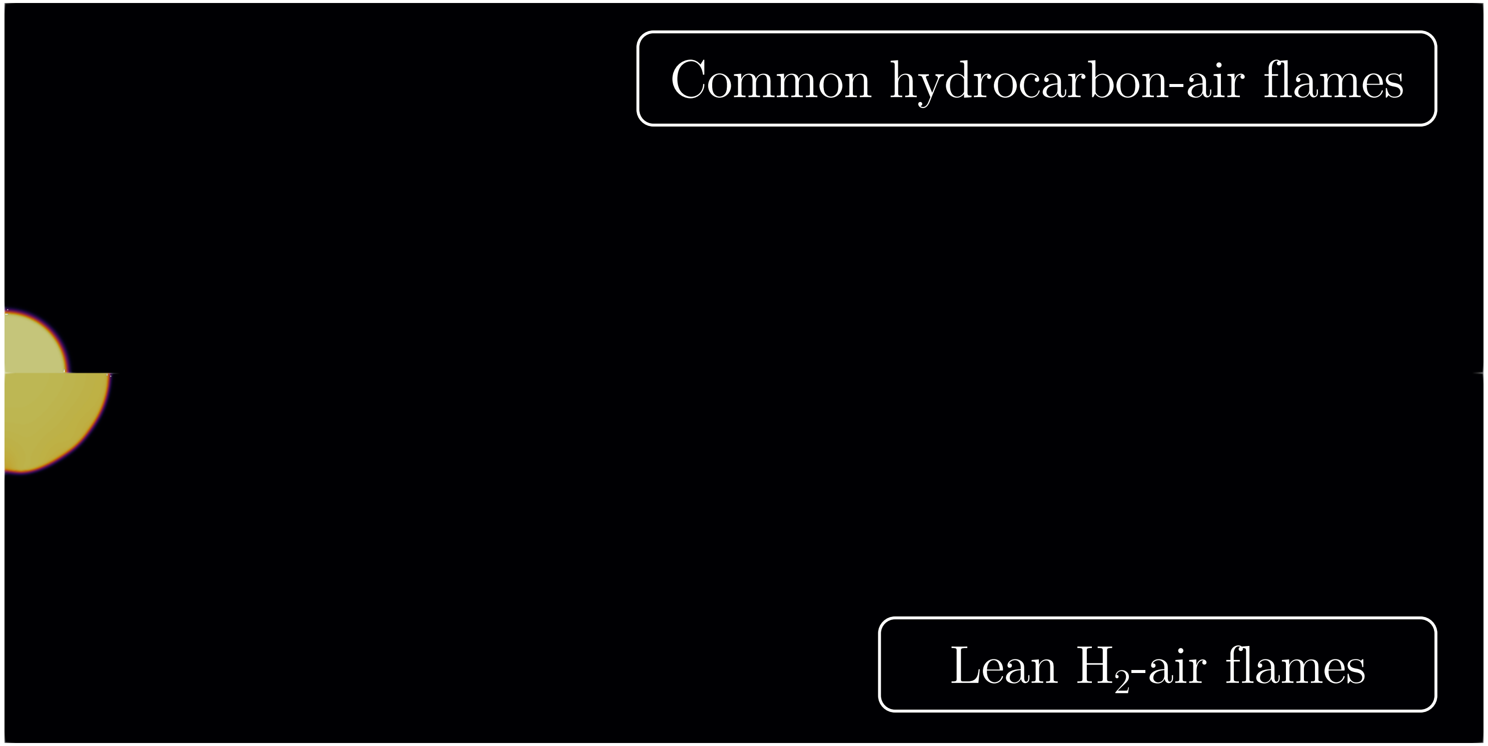

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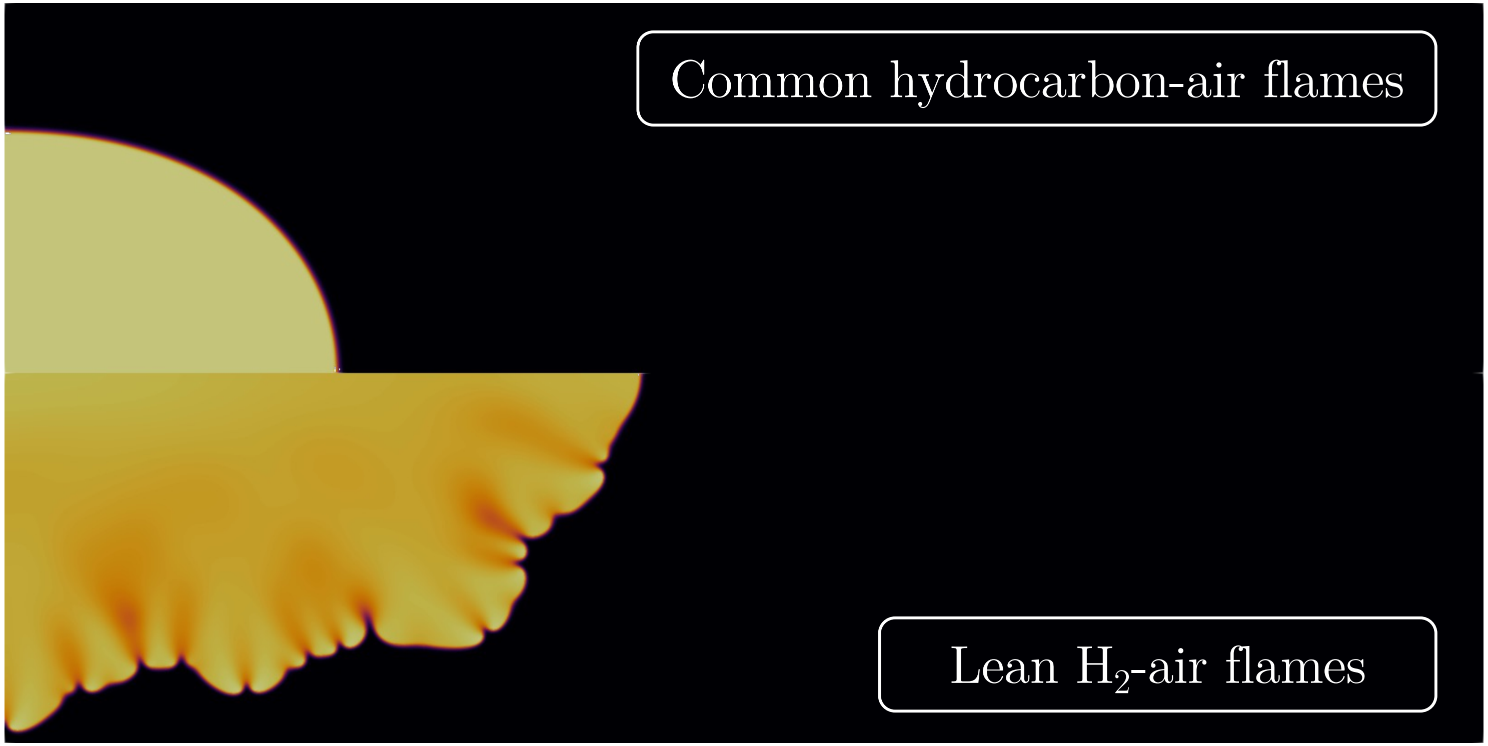

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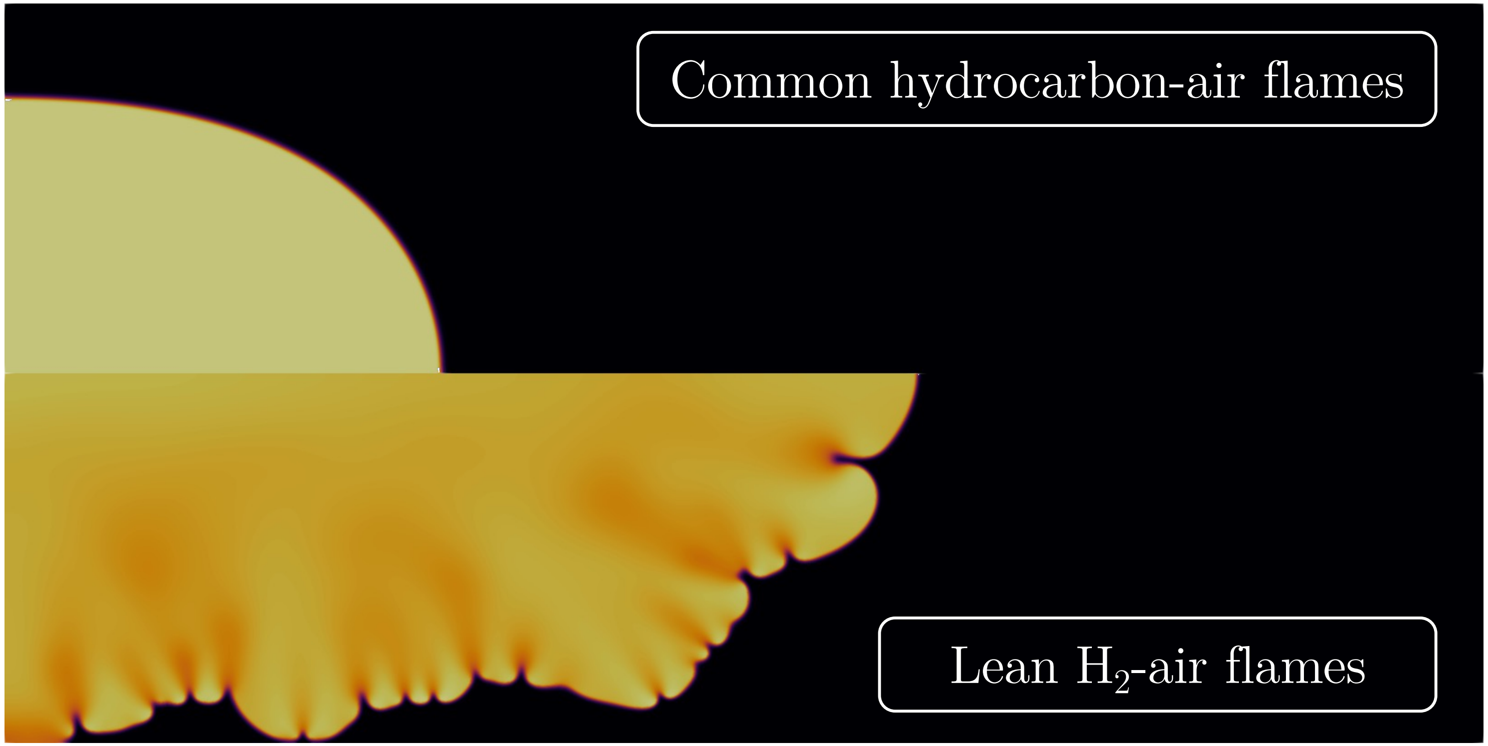

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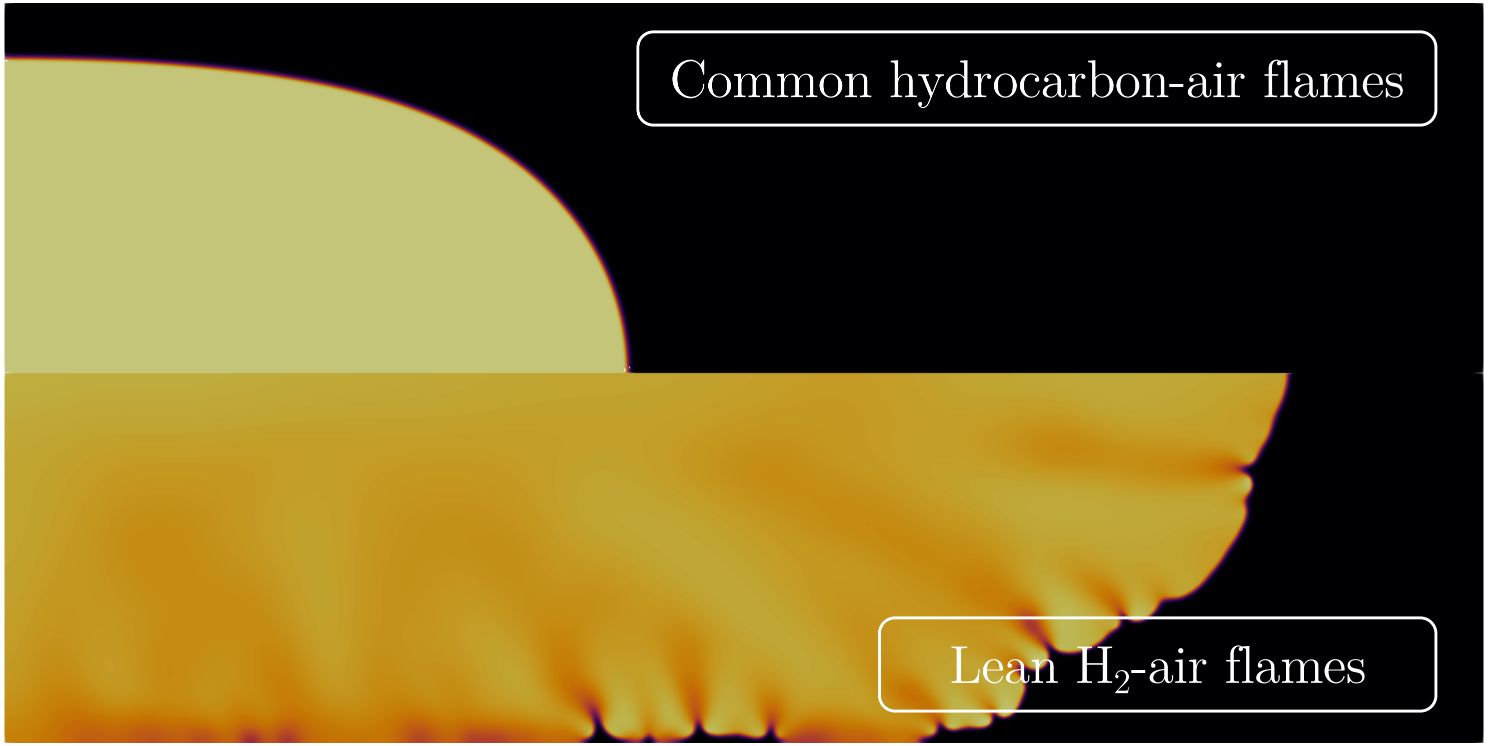

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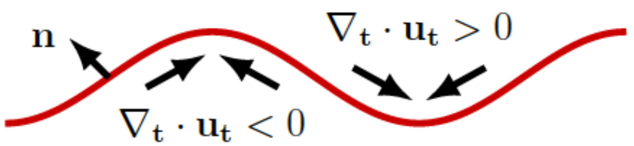
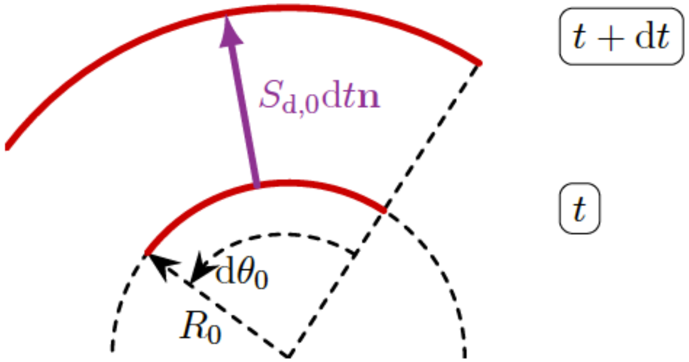
Stretch = rate of change in local flame surface area[1]





[1] Karlovitz et al., Symp. (Int.) Combust., 1953
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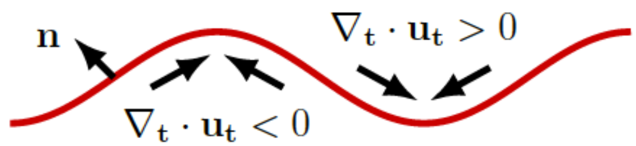
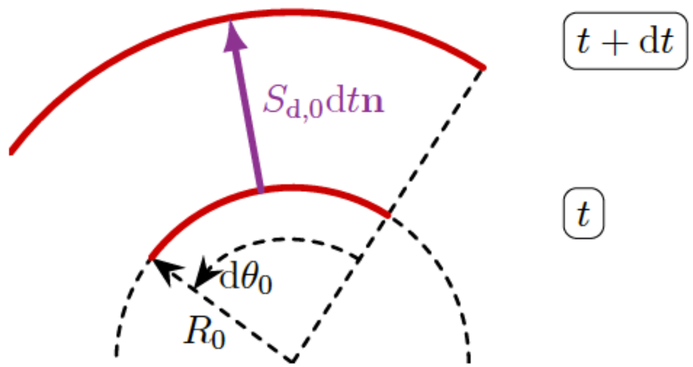
Fundamentals of lean H_2-air flames

Stretch = rate of change in local flame surface area[1]

→ Effect on flame speed at low stretch rates[2-4]:





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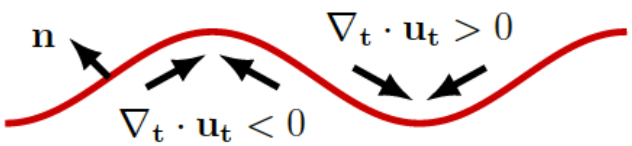

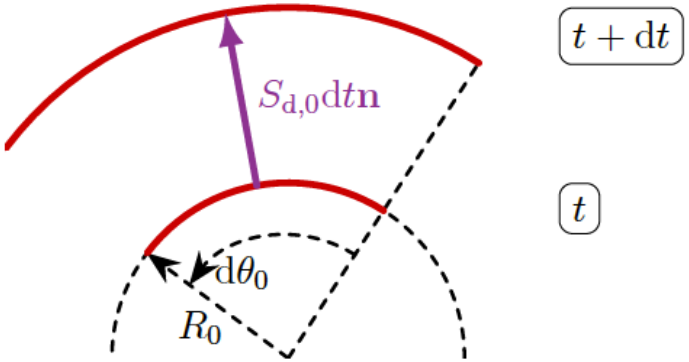

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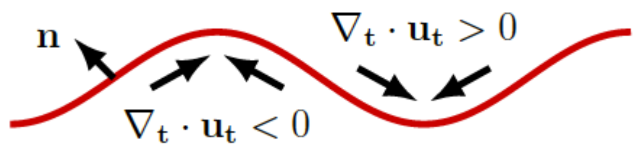

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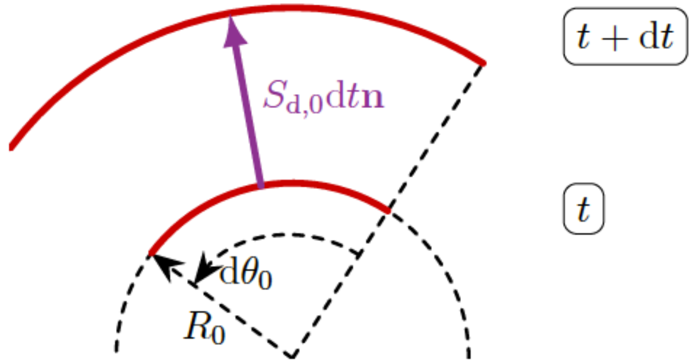
$$\frac{S_\mathrm{L}}{\boxed{S_\mathrm{L}^0}} = 1 - \mathcal{L}\frac{\mathbb{K}}{\boxed{S_\mathrm{L}^0}}$$

Unstretched laminar flame speed



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Fundamentals of lean H_2-air flames

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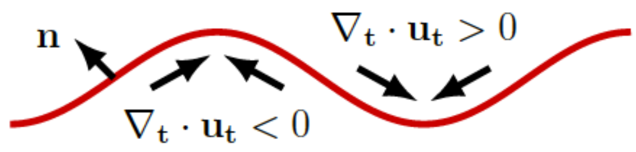

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Stretched laminar flame speed

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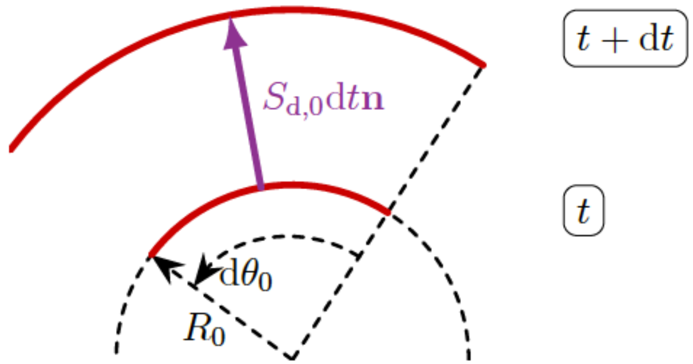

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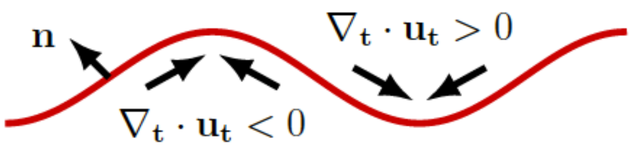

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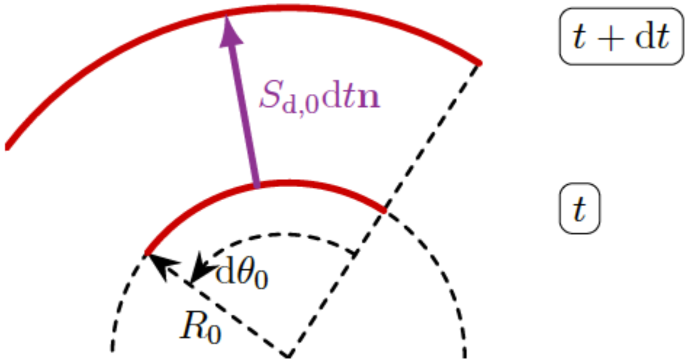
Flame stretch

Unstretched laminar flame speed



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Fundamentals of lean H_2-air flames

Stretch = rate of change in local flame surface area[1]

→ Effect on flame speed at low stretch rates[2-4]:

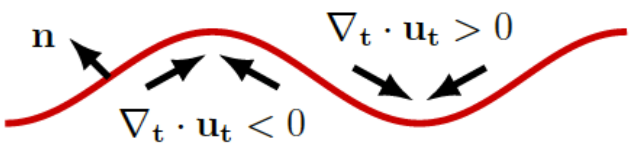
Markstein length

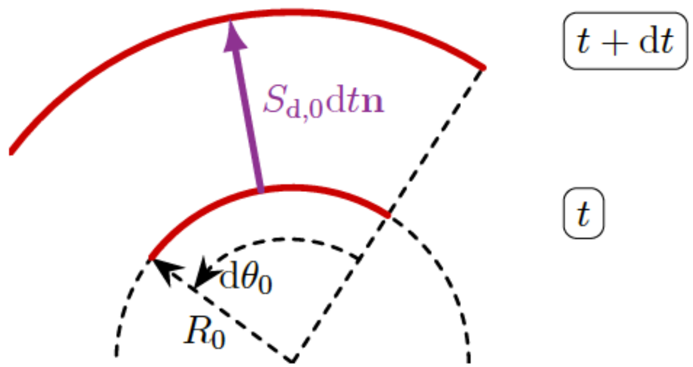
Stretched laminar flame speed

$$\frac{S_\mathrm{L}}{S_\mathrm{L}^0} = 1 - \mathcal{L}\frac{\mathbb{K}}{S_\mathrm{L}^0}$$

Flame stretch

Unstretched laminar flame speed





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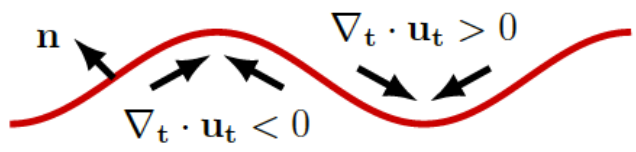

→ Effect on flame speed at low stretch rates[2-4]:

Markstein length

Stretched laminar flame speed

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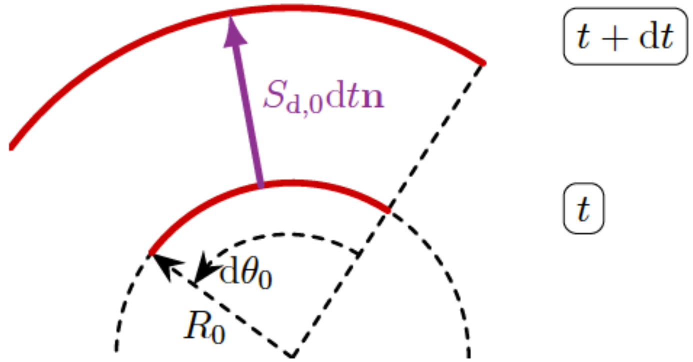
Flame stretch

Unstretched laminar flame speed



$$\mathcal{L} \propto (\mathrm{Le_{eff}} - 1)\ \delta_L^0$$

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Fundamentals of lean H_2-air flames

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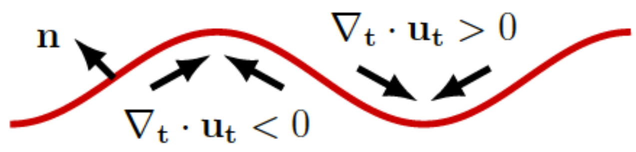

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Markstein length

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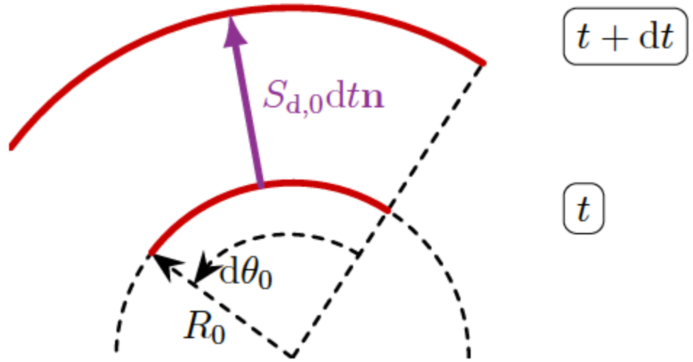
Flame stretch

Unstretched laminar flame speed



$$\mathcal{L} \propto (\mathrm{Le}_{\mathrm{eff}} - 1) \boxed{\delta_L^0}$$

Flame thickness

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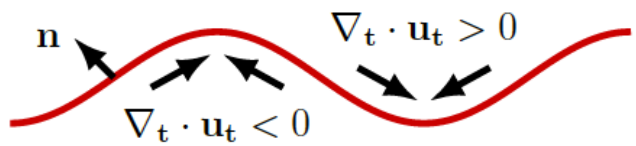


→ Effect on flame speed at low stretch rates[2-4]:

Stretched laminar flame speed

Markstein length

Flame stretch

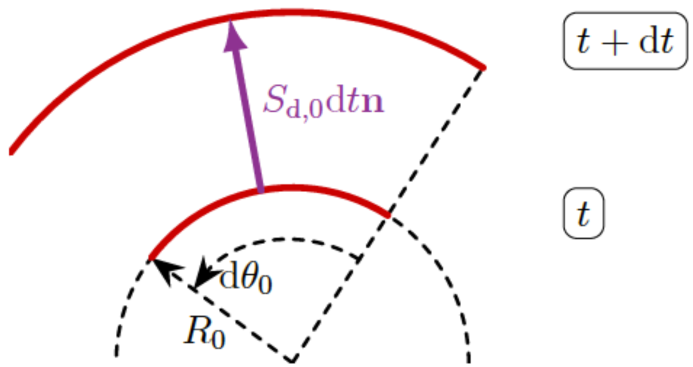
$$\frac{\boxed{S_L}}{\boxed{S_L^0}} = 1 - \boxed{\mathcal{L}}\frac{\boxed{\mathbb{K}}}{\boxed{S_L^0}}$$

Unstretched laminar flame speed

Mixture effective Lewis number

$$\mathcal{L} \propto (\boxed{\mathrm{Le}_{\mathrm{eff}}} - 1)\,\boxed{\delta_L^0}$$

Flame thickness



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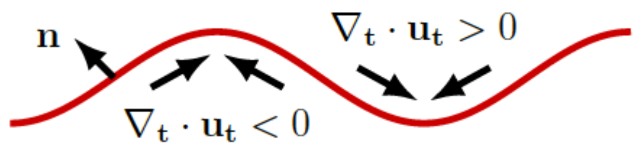

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Unstretched laminar flame speed

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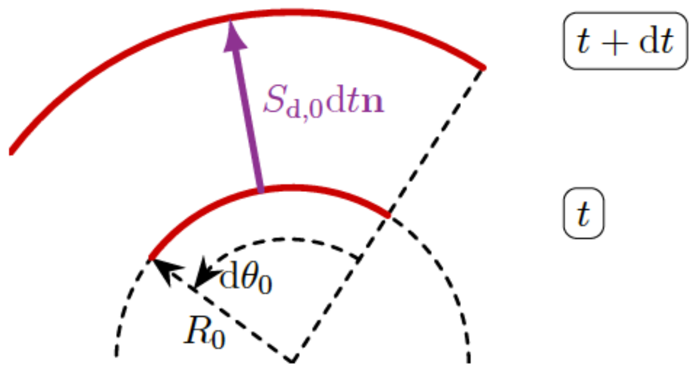
Flame thickness



Lean H_2-air flames

$$\mathrm{Le_{eff}} < 1 \implies \mathcal{L} < 0 \implies S_\mathrm{L} > S_\mathrm{L}^0 \text{ for } \mathbb{K} > 0$$

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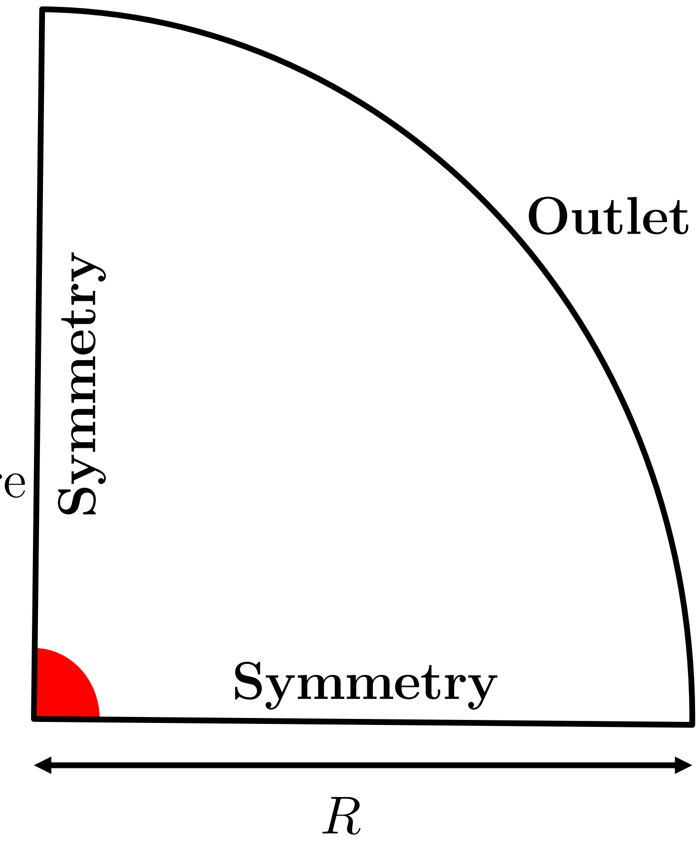
2D spherical flame set-up

Geometry, boundary and initial conditions:



Chemistry: simple mechanism reproducing

- Laminar flame properties (S_L^0, δ_L^0)
- Flame response to stretch

Operating conditions: ambient (T_u, p), lean mixture

$(\Phi = 0.4)$

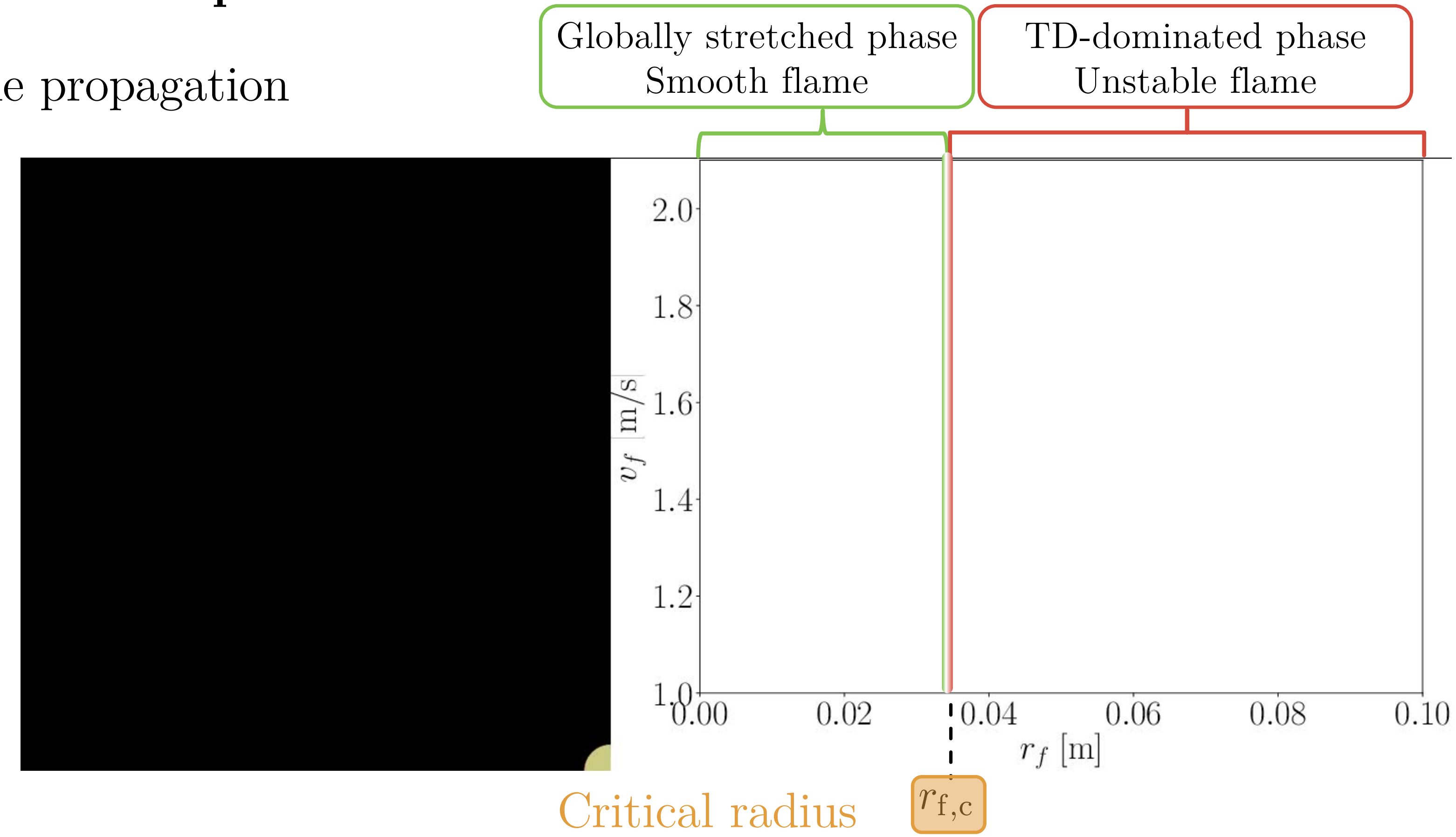
S_L^0 [m/s]	δ_L^0 [μm]	T_{ad} [K]
0.24	580	1420

DNS of the spherical flame

Flame propagation

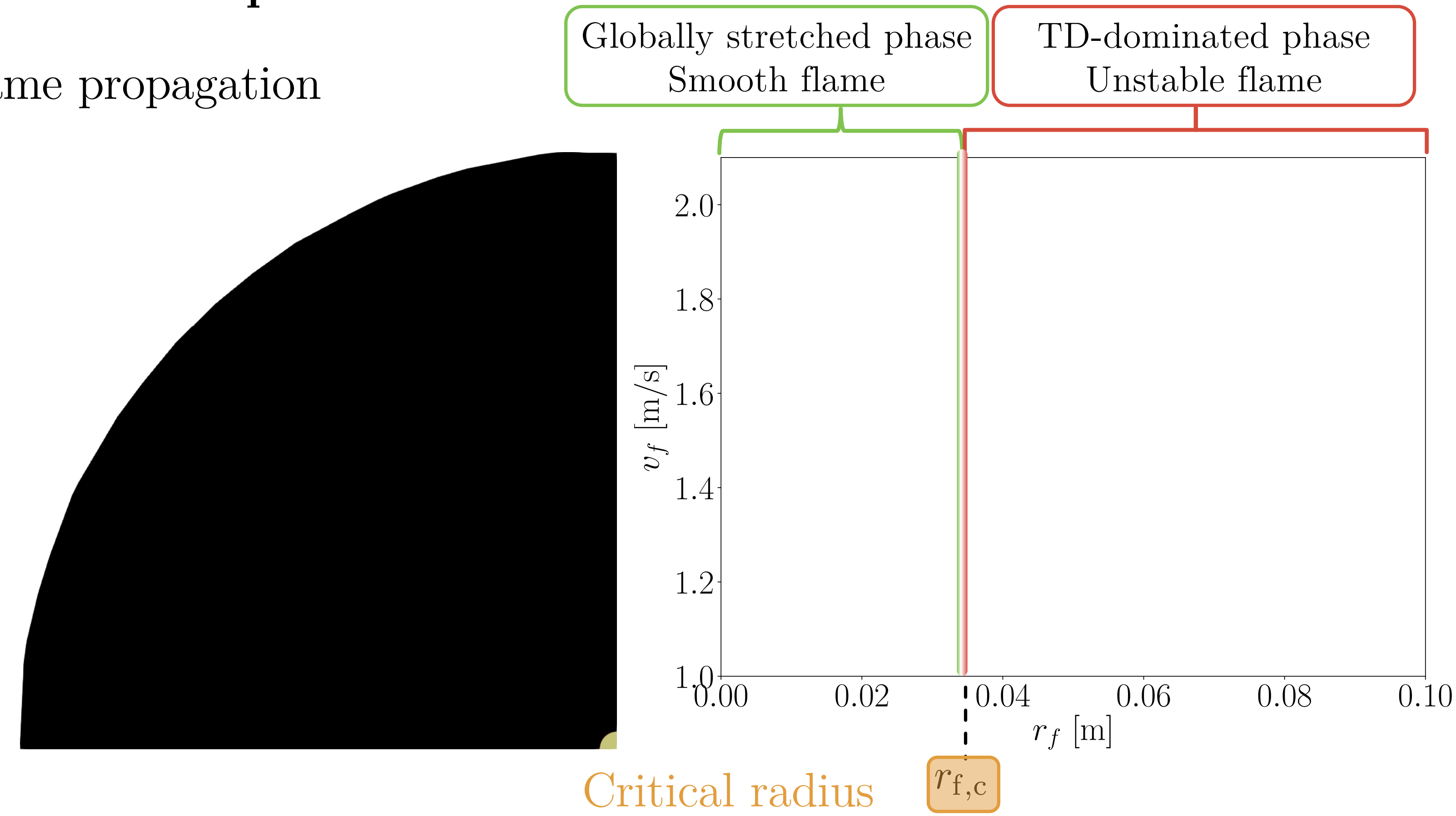
DNS of the spherical flame

Flame propagation



DNS of the spherical flame

Flame propagation



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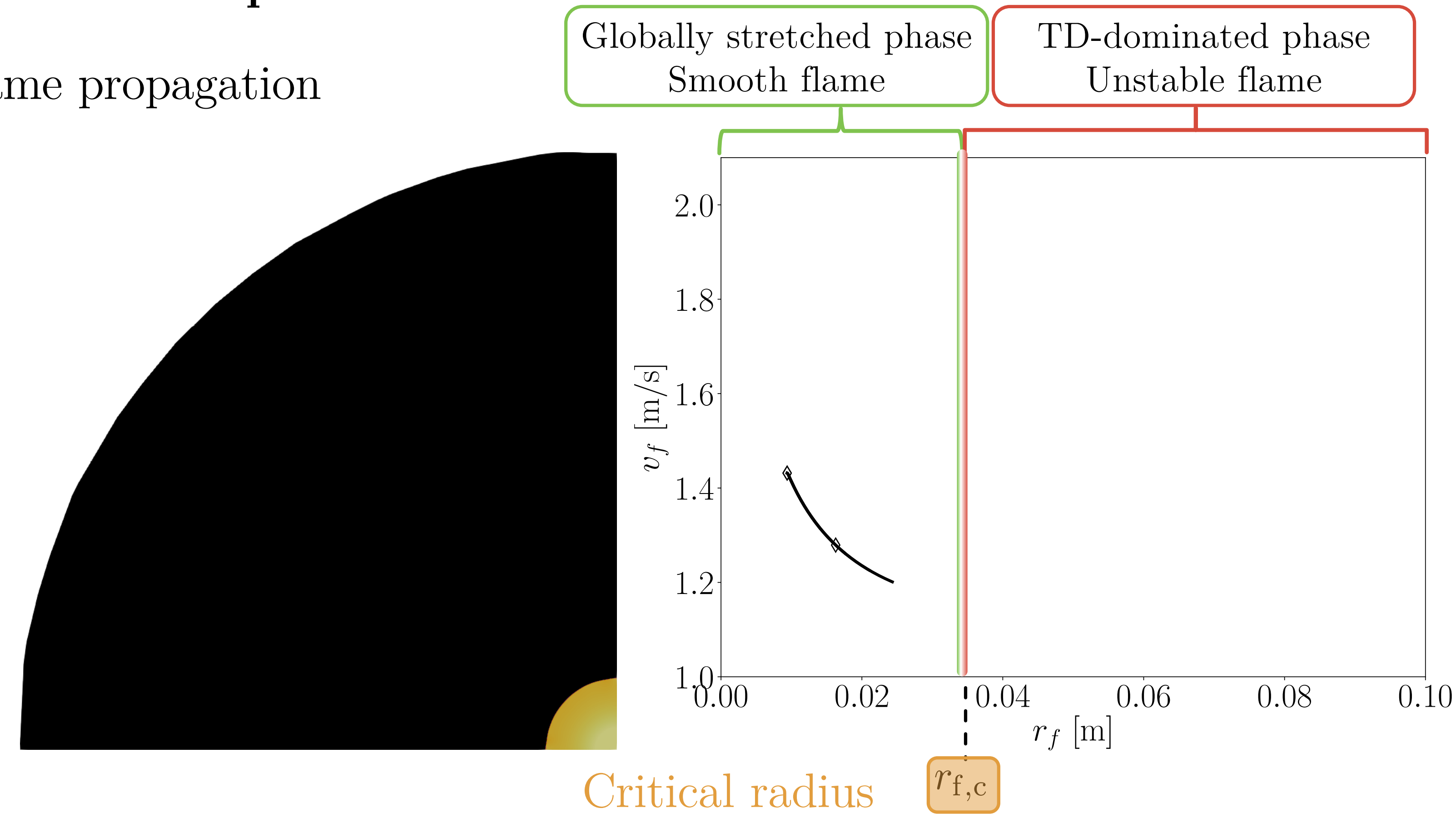

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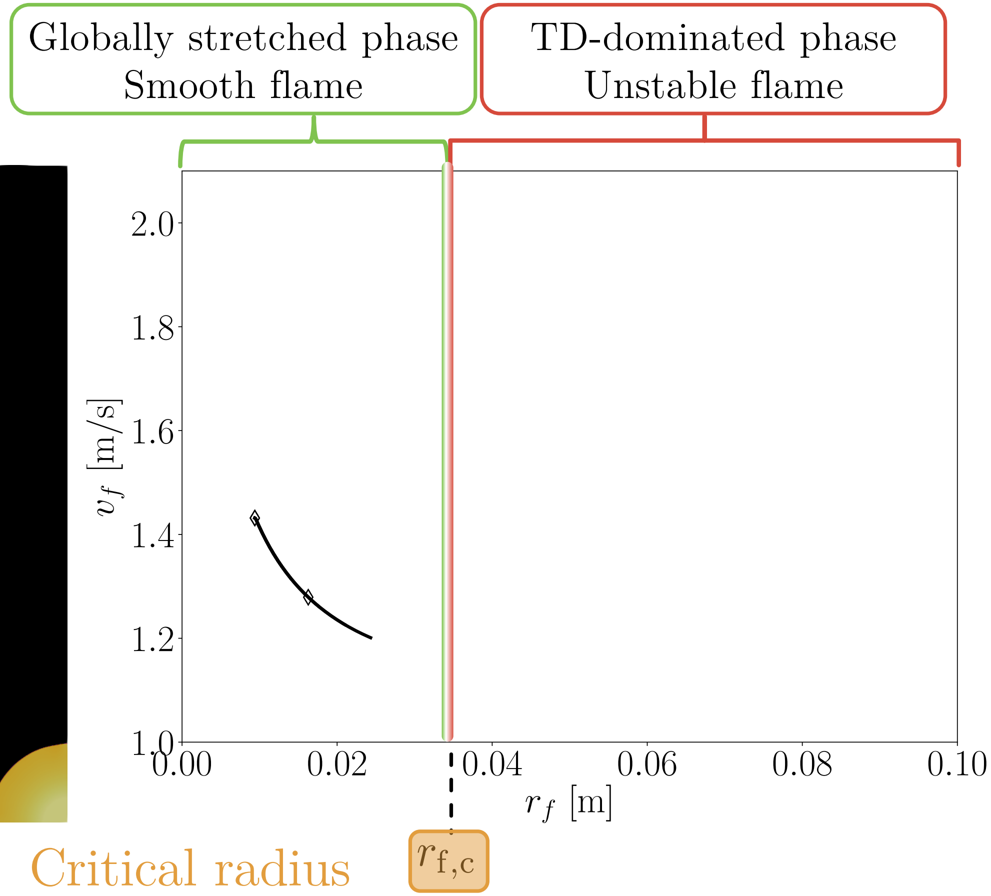

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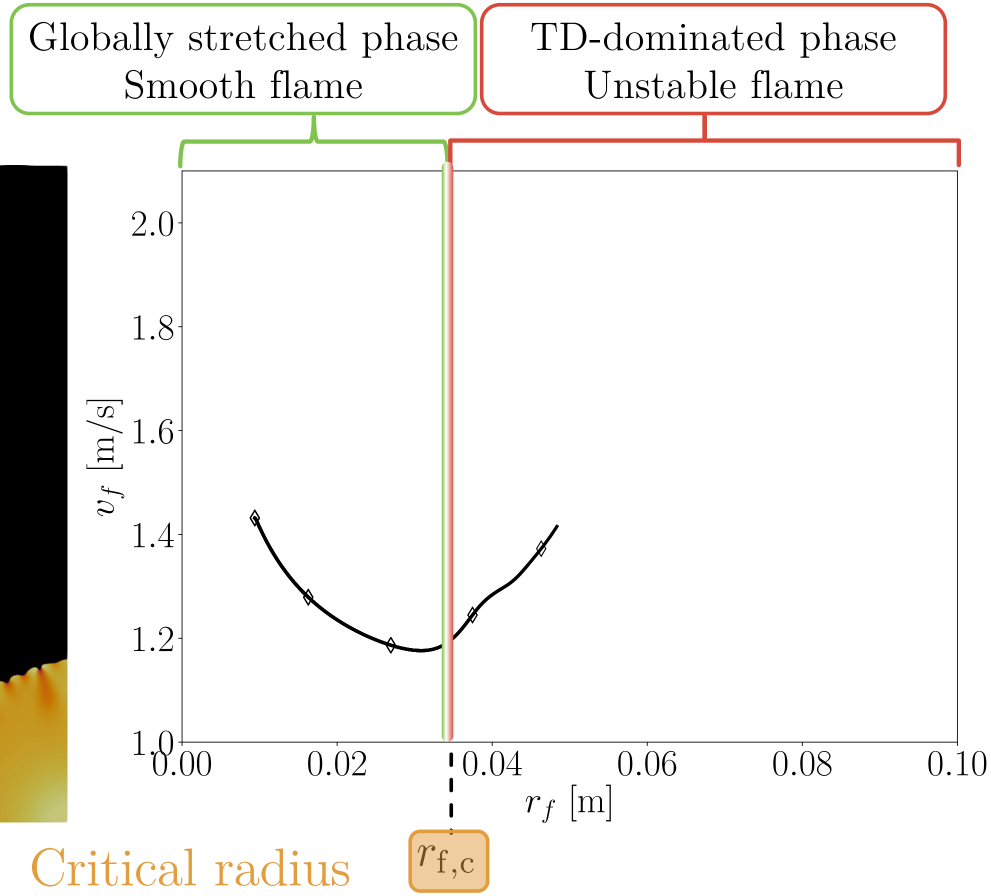

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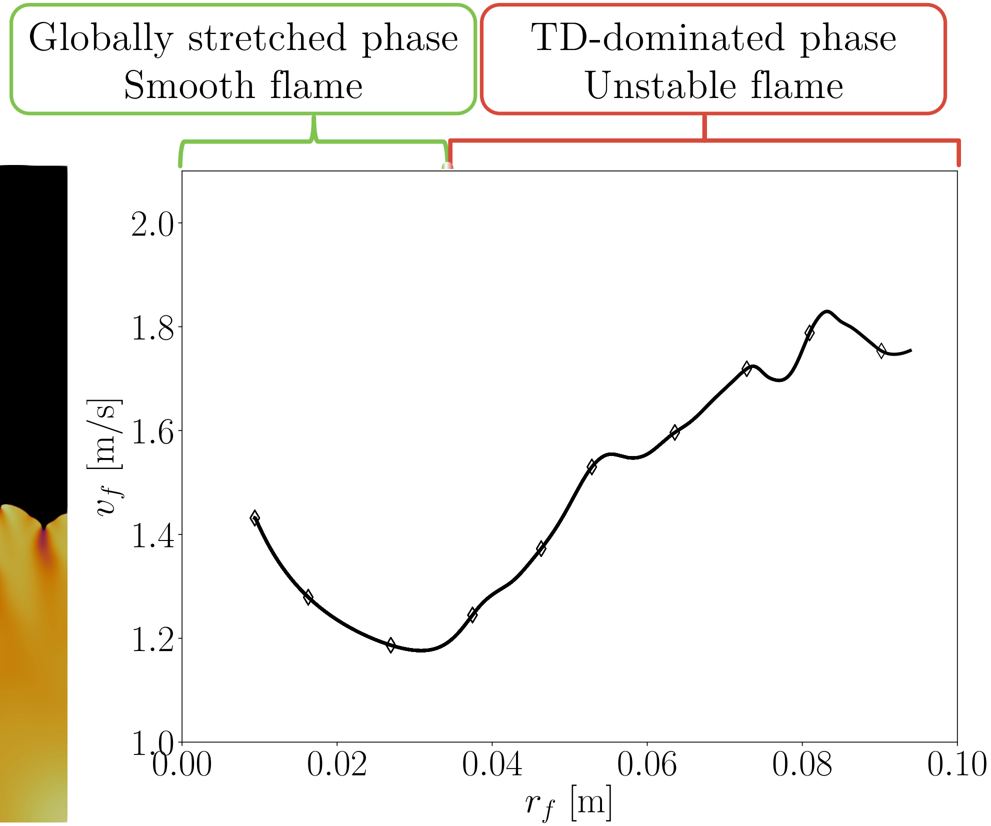

Critical radius $r_{f,c}$

LES of the spherical flame using the classical TF model

Mesh:

- Resolution decreased from DNS to LES-like

$\delta_{\mathrm{L}}^{0}/\Delta x$
21
3.50
1.75
1.17
0.87
0.7

[1] Butler et al., Symp. (Int.) Combust., 1977

[2] O'Rourke et al., J. Comp. Phys., 1979

LES of the spherical flame using the classical TF model

Mesh:

- Resolution decreased from DNS to LES-like
- Use of the Thickened Flame (TF) model[1-2] to resolve the flame structure

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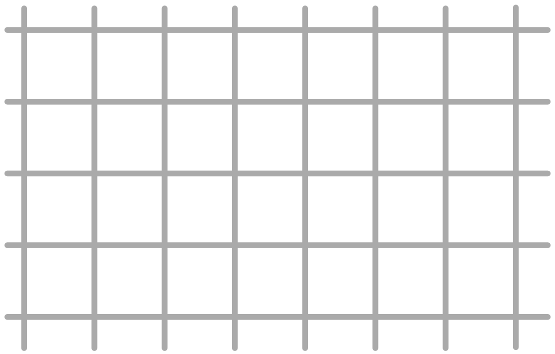

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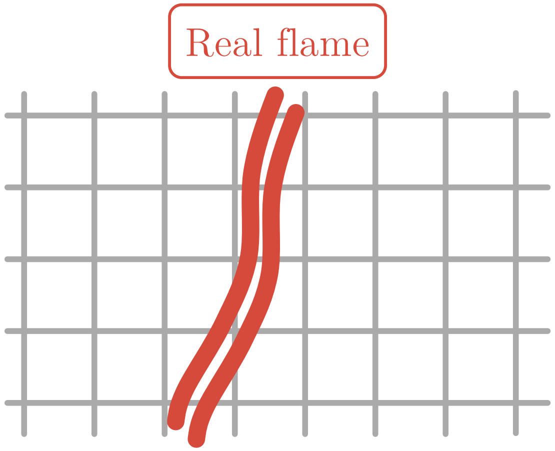

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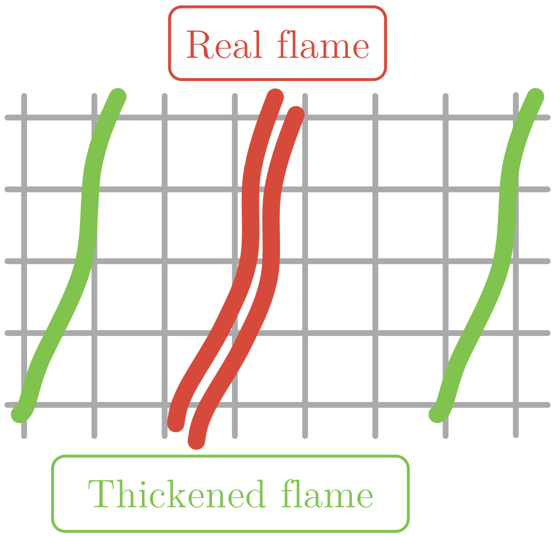

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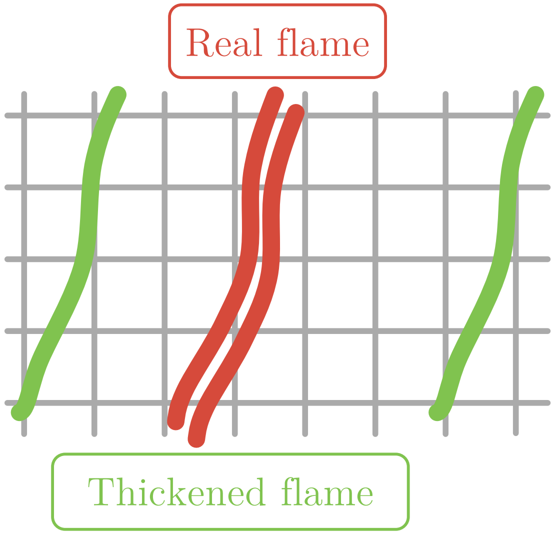

$\delta_L^0/\Delta x$	F	$F\delta_L^0/\Delta x$
21	-	21
3.50	2	7
1.75	4	7
1.17	6	7
0.87	8	7
0.7	10	7

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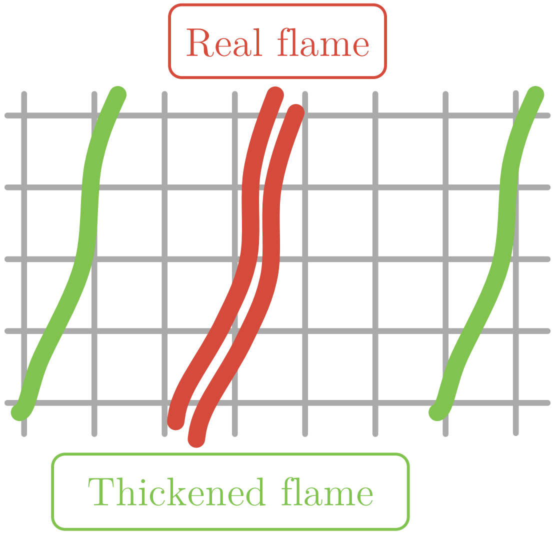

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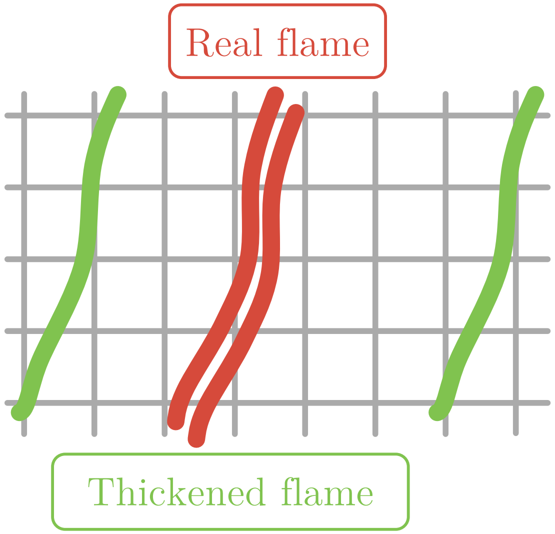

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TF model activated

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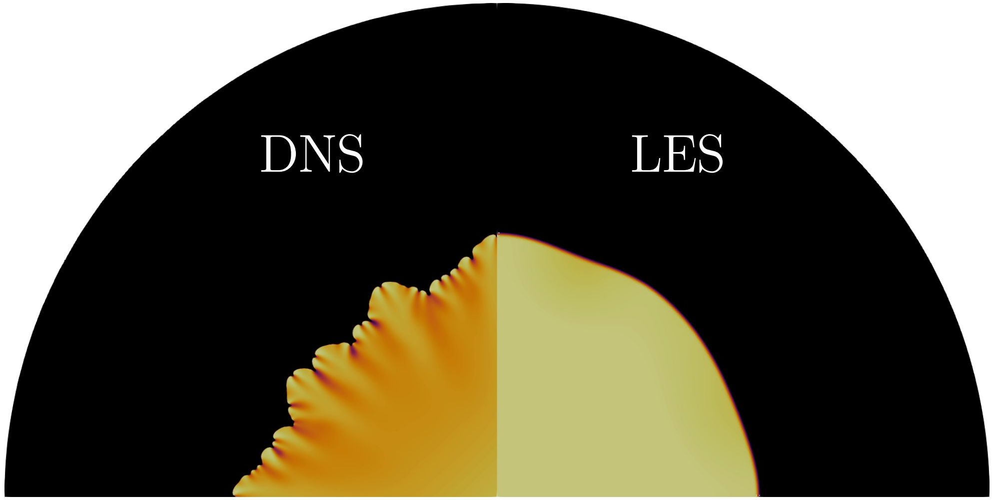
LES of the spherical flame using the classical TF model

Visual analysis:



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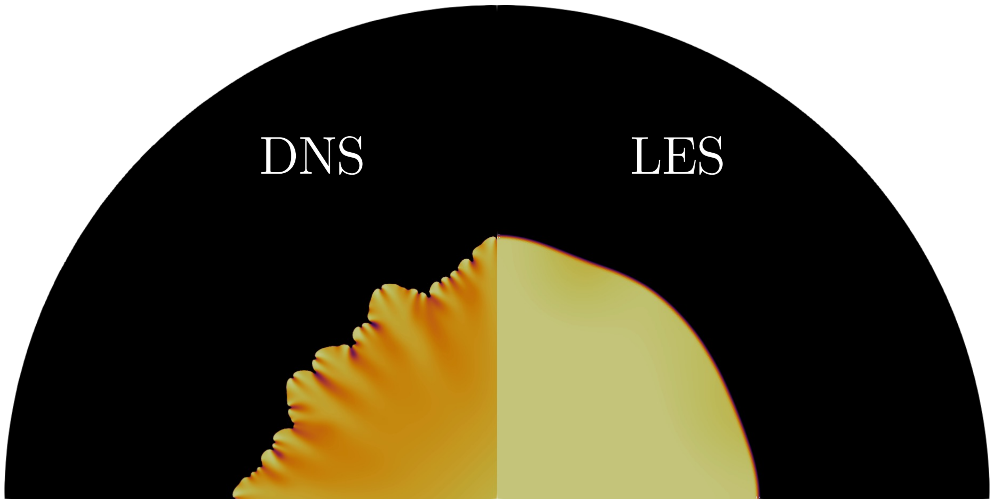

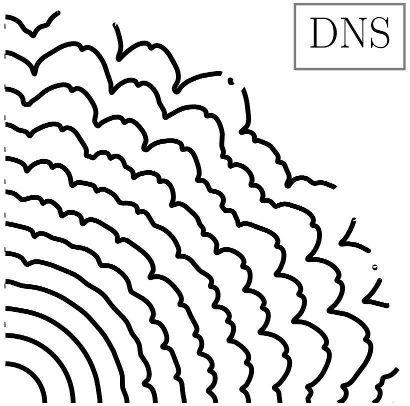

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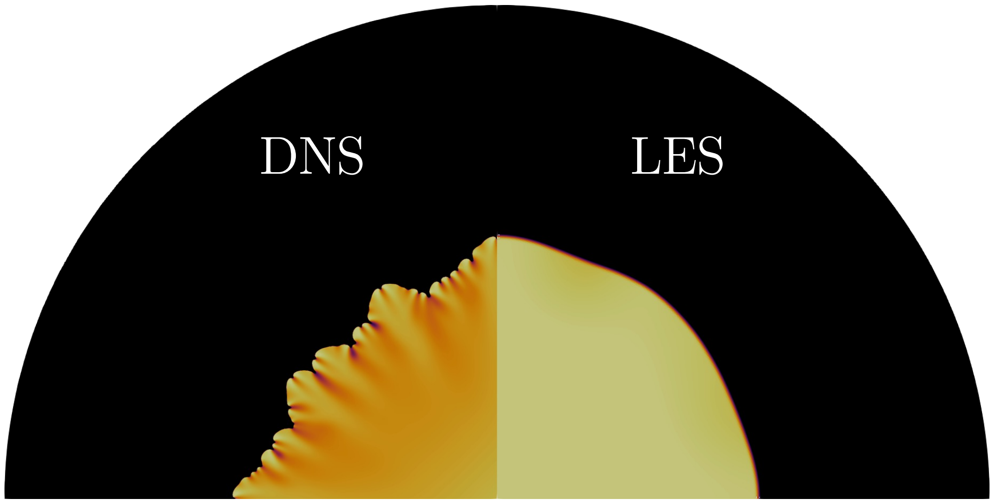

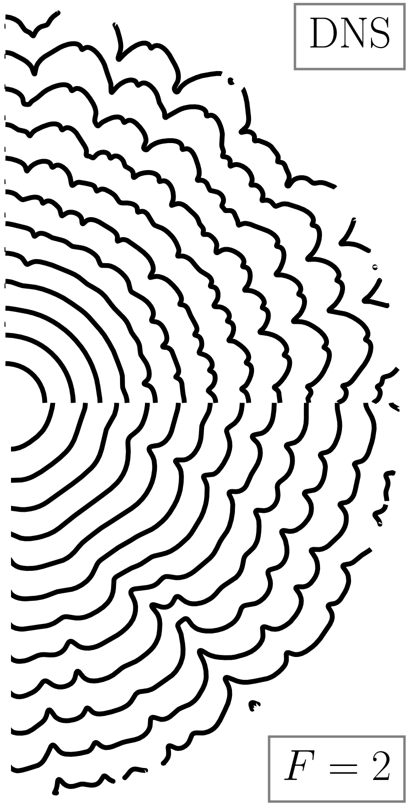

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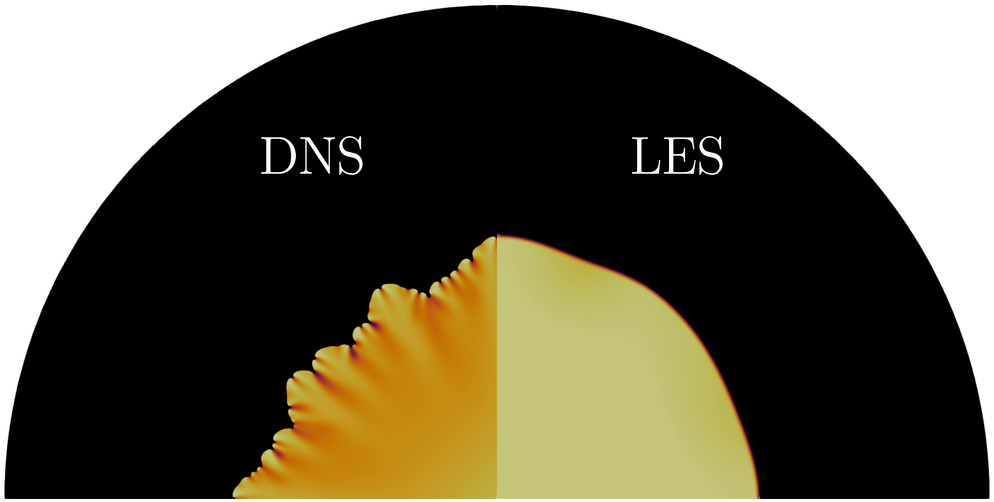

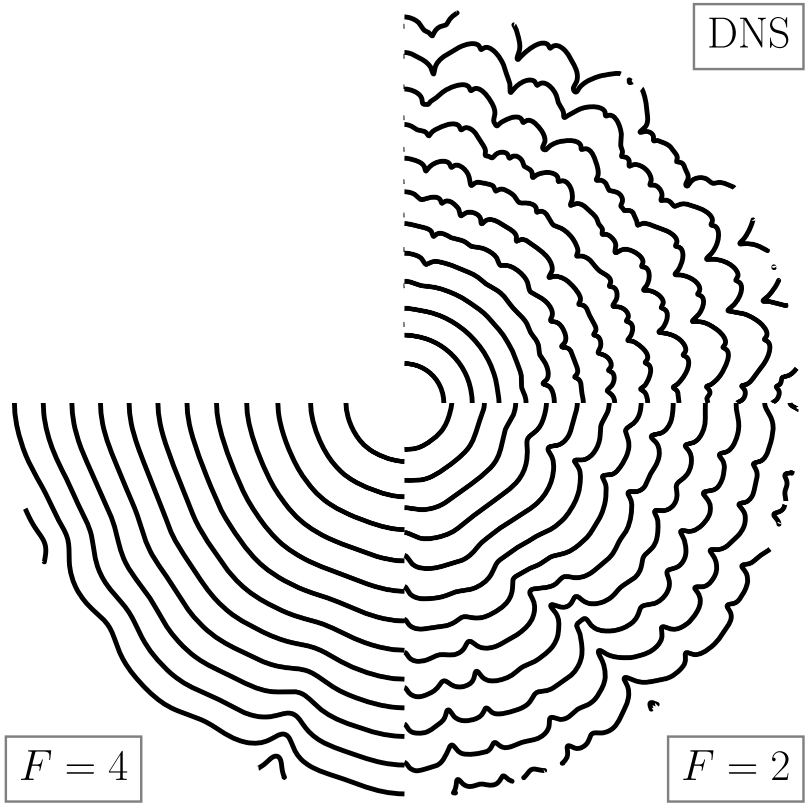

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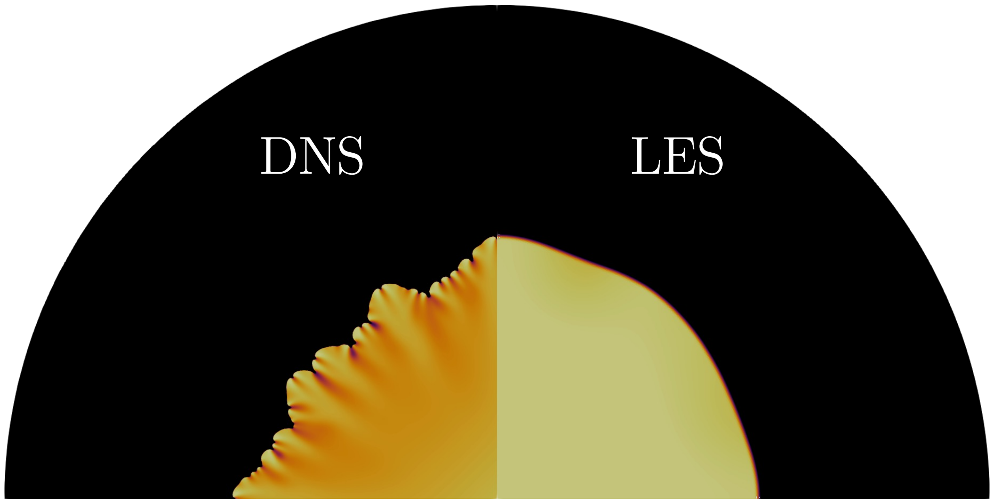
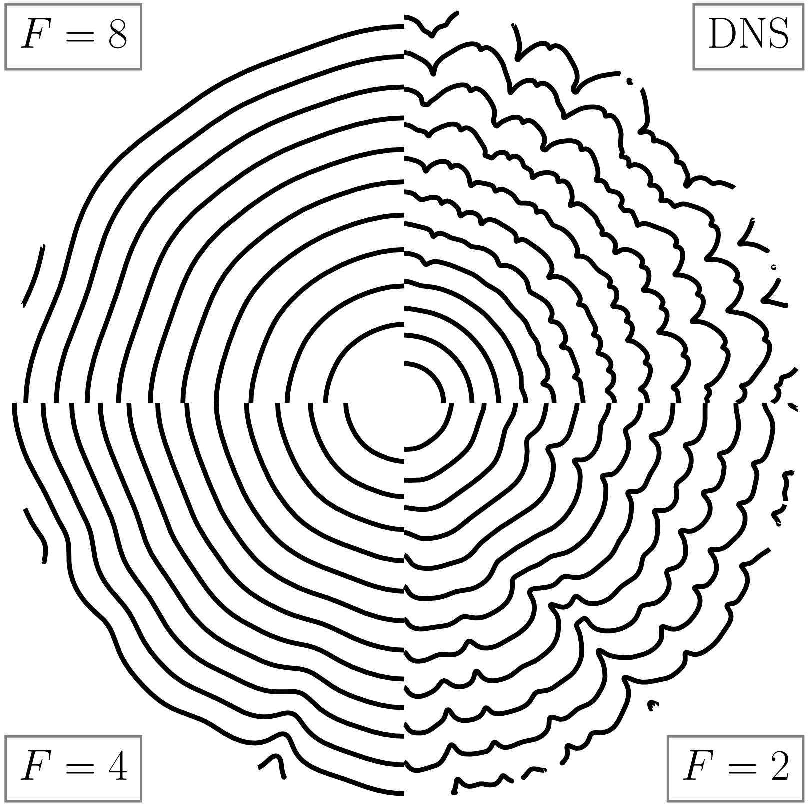
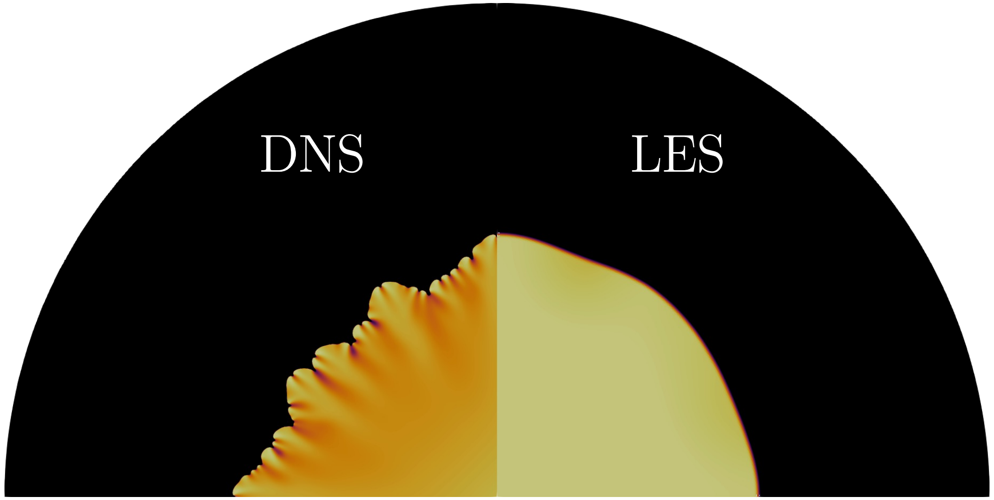
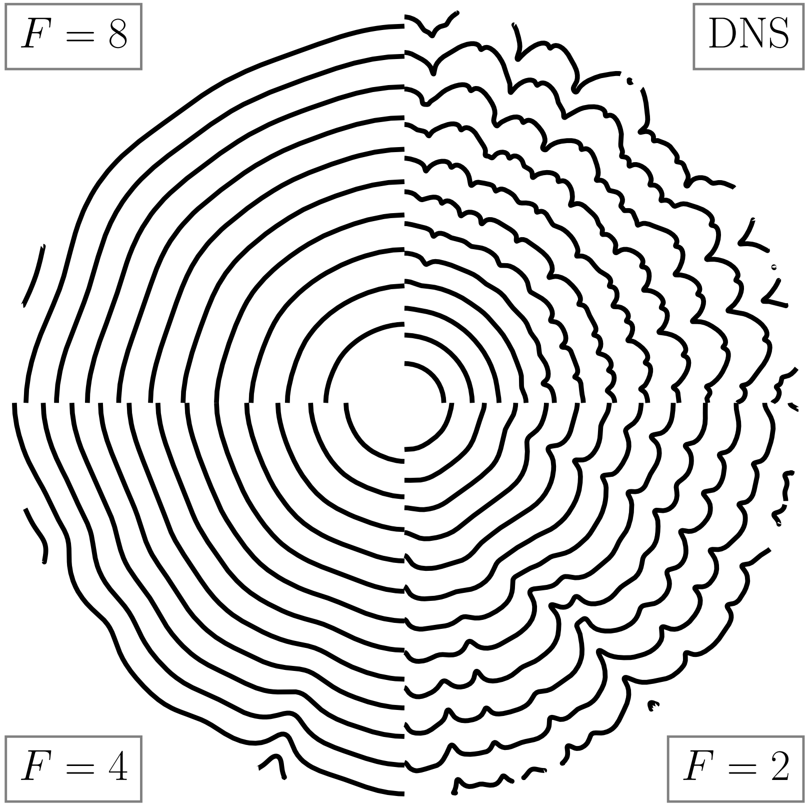




LES of the spherical flame using the classical TF model

Visual analysis:





- Progressive loss of flame wrinkling when decreasing the mesh resolution/increasing the thickening factor

LES of the spherical flame using the classical TF model

Flame propagation:

r_f [m]

LES of the spherical flame using the classical TF model

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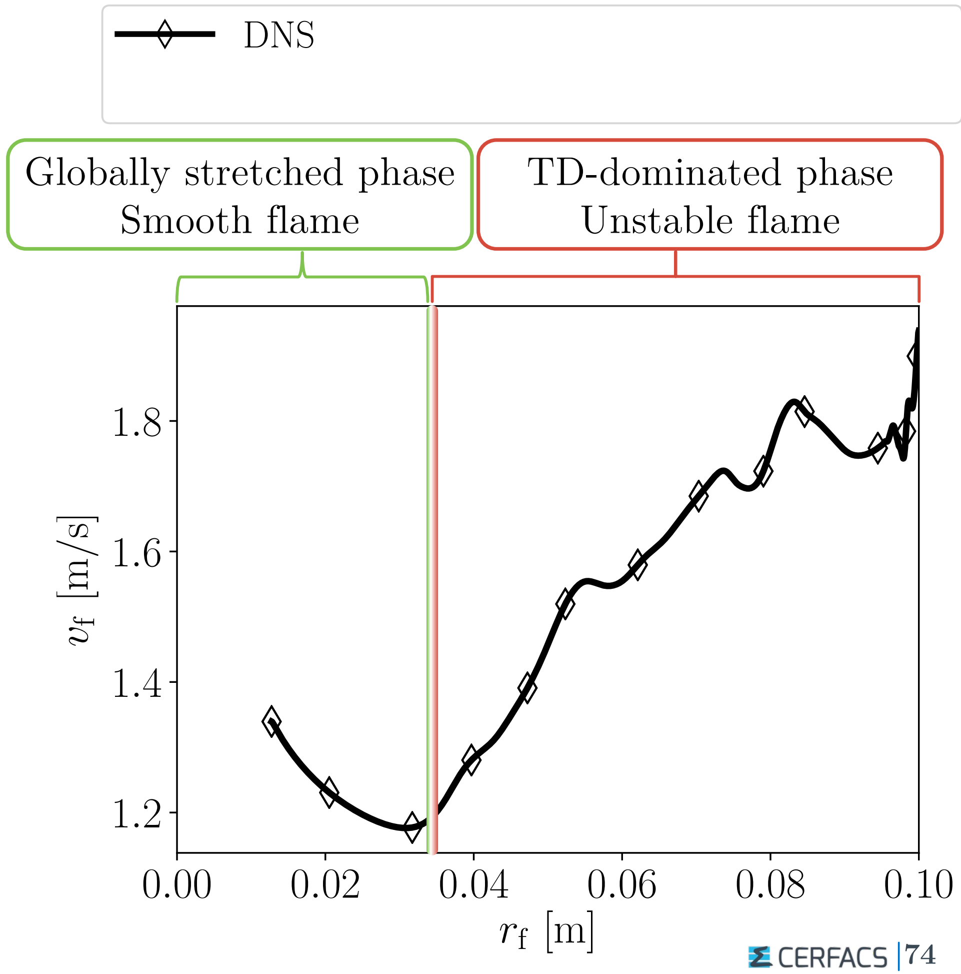

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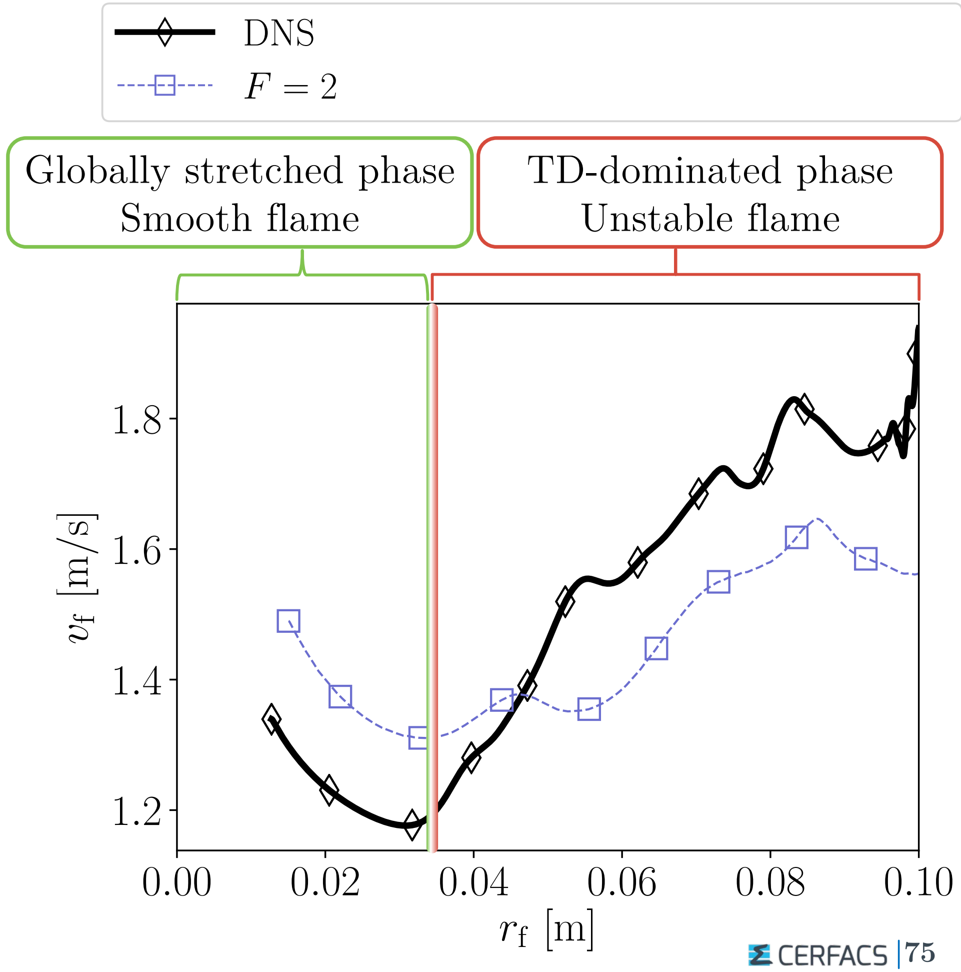

LES of the spherical flame using the classical TF model

Flame propagation:

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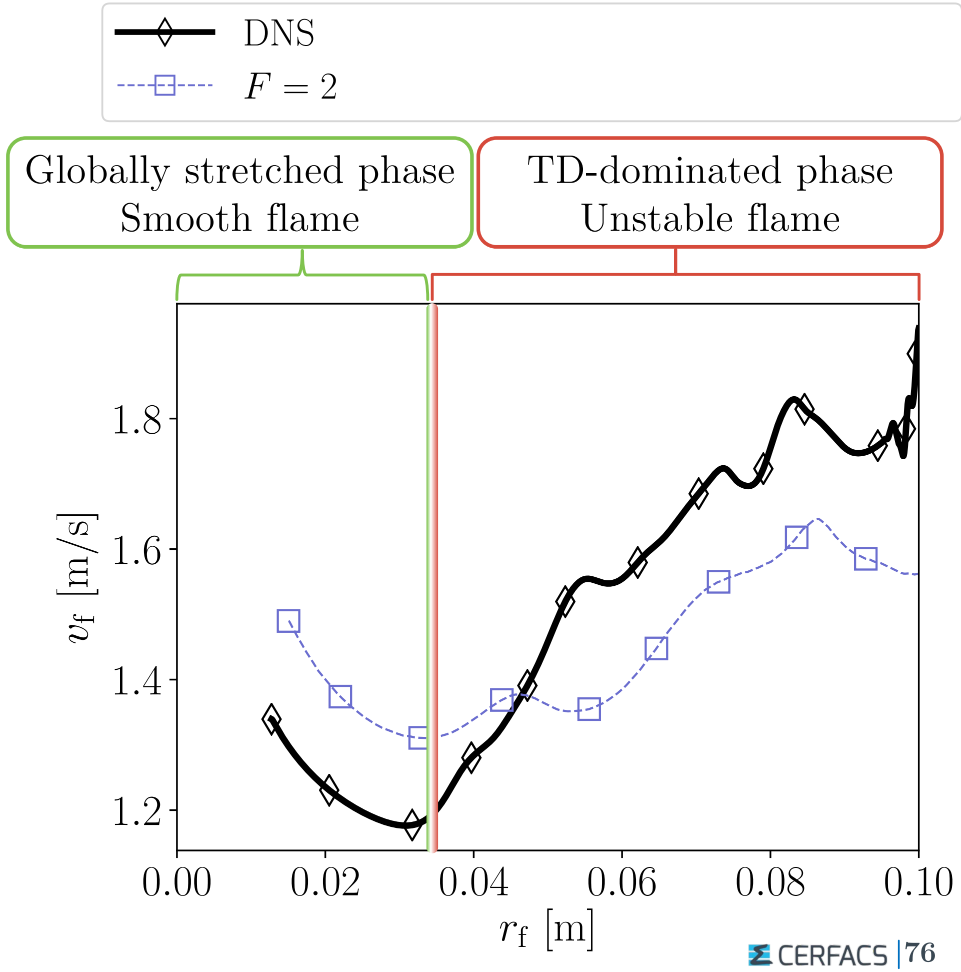

LES of the spherical flame using the classical TF model

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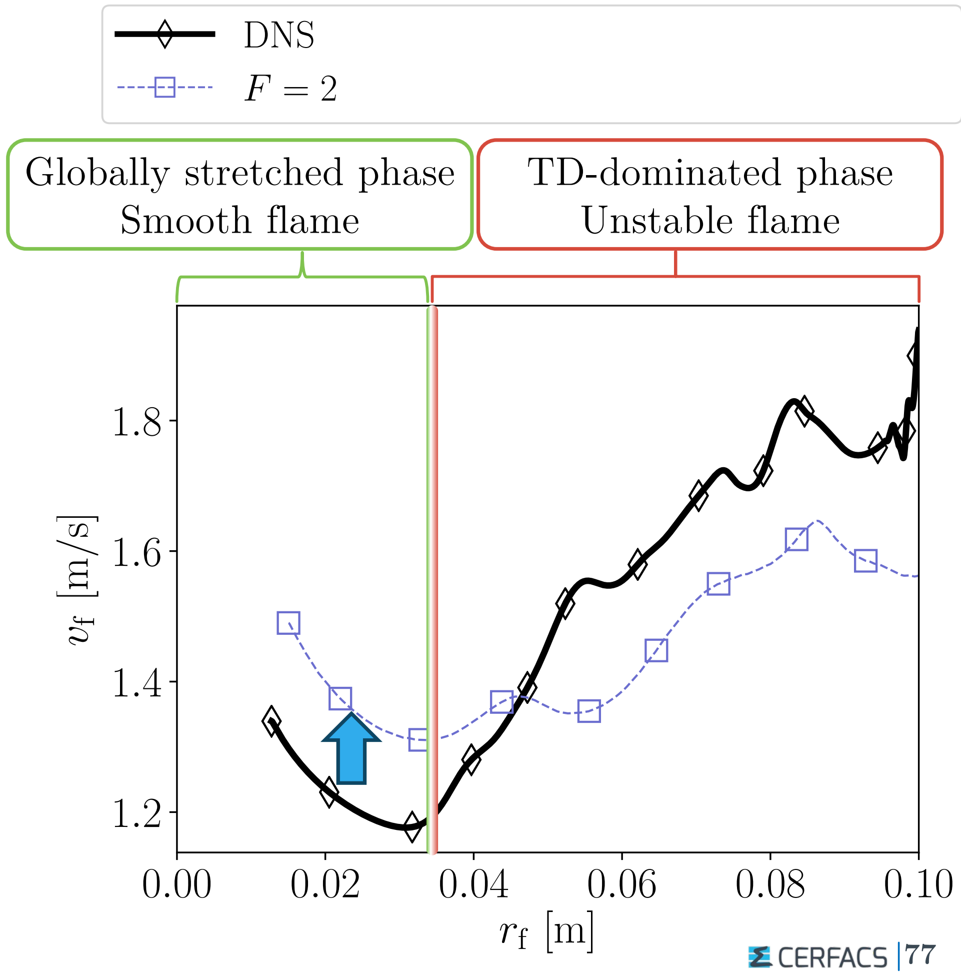

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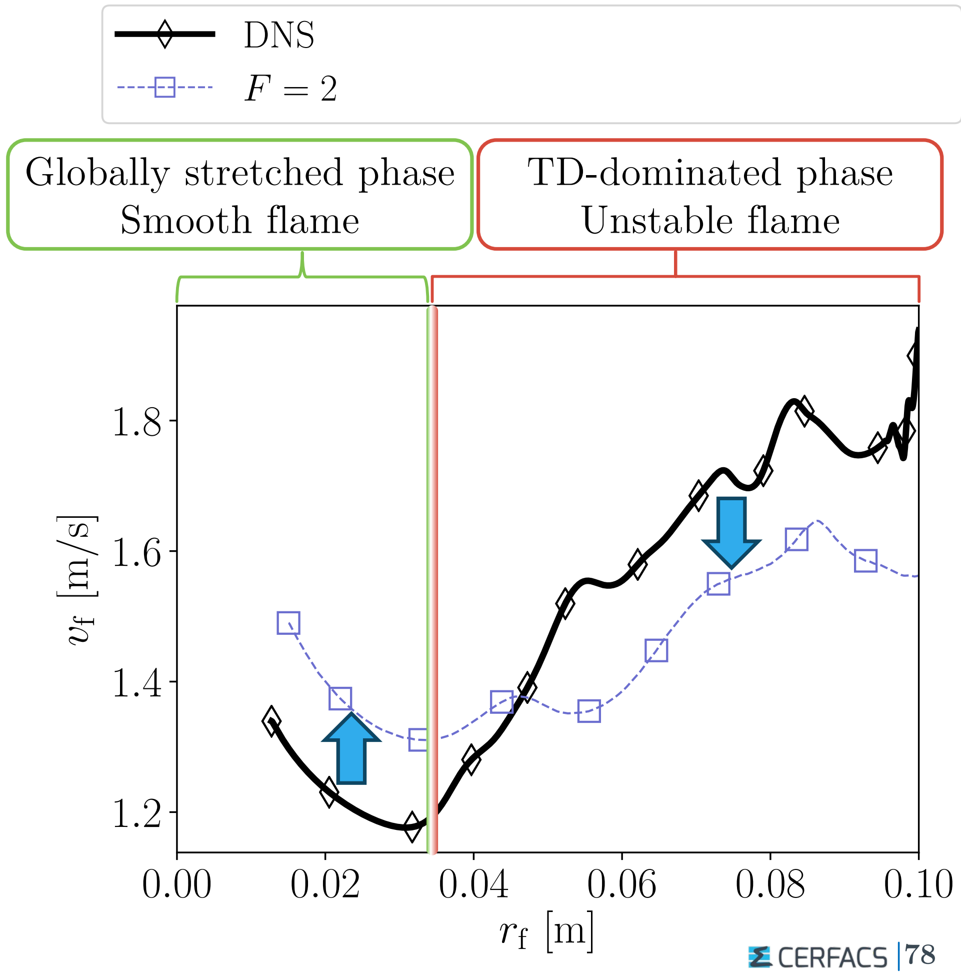

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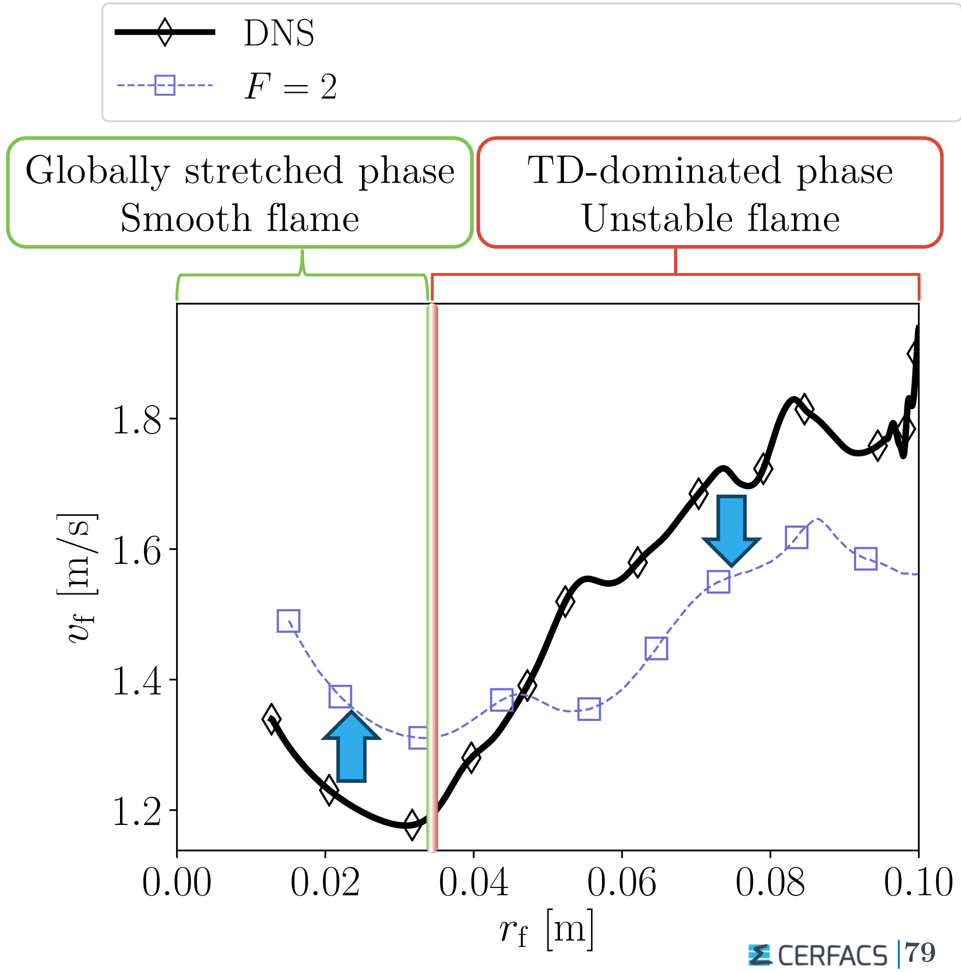

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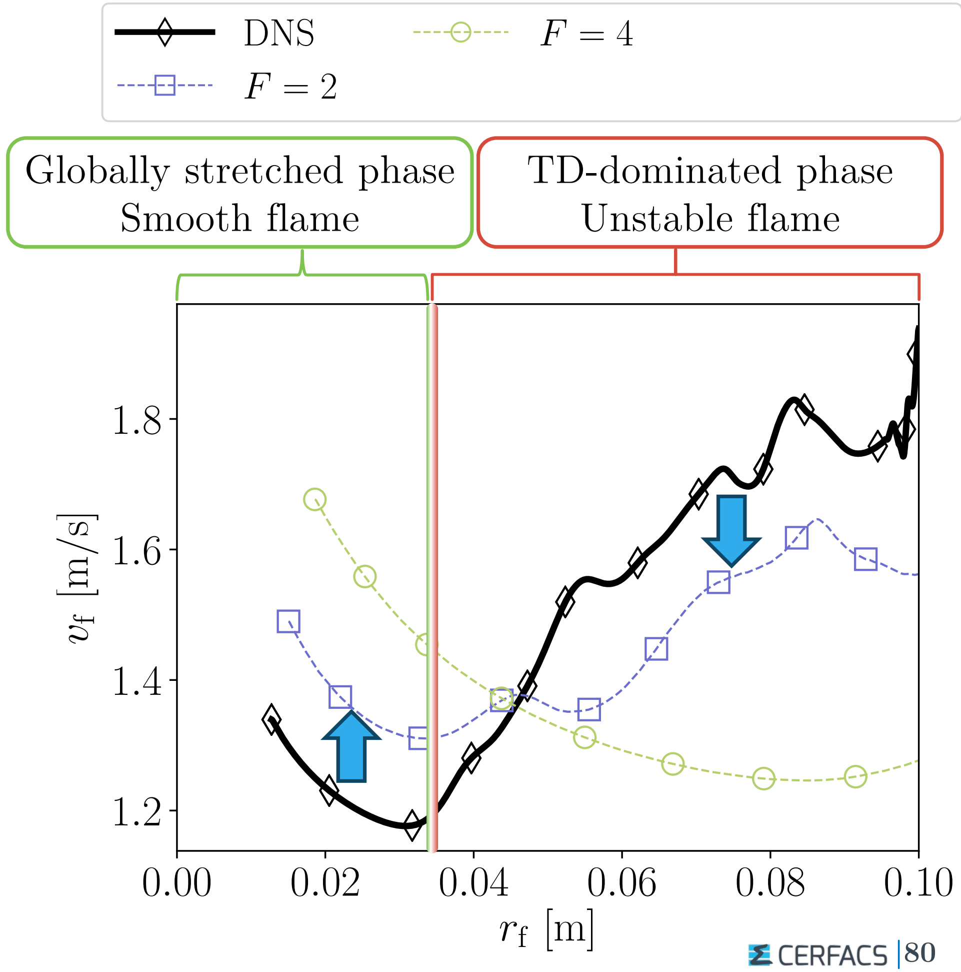

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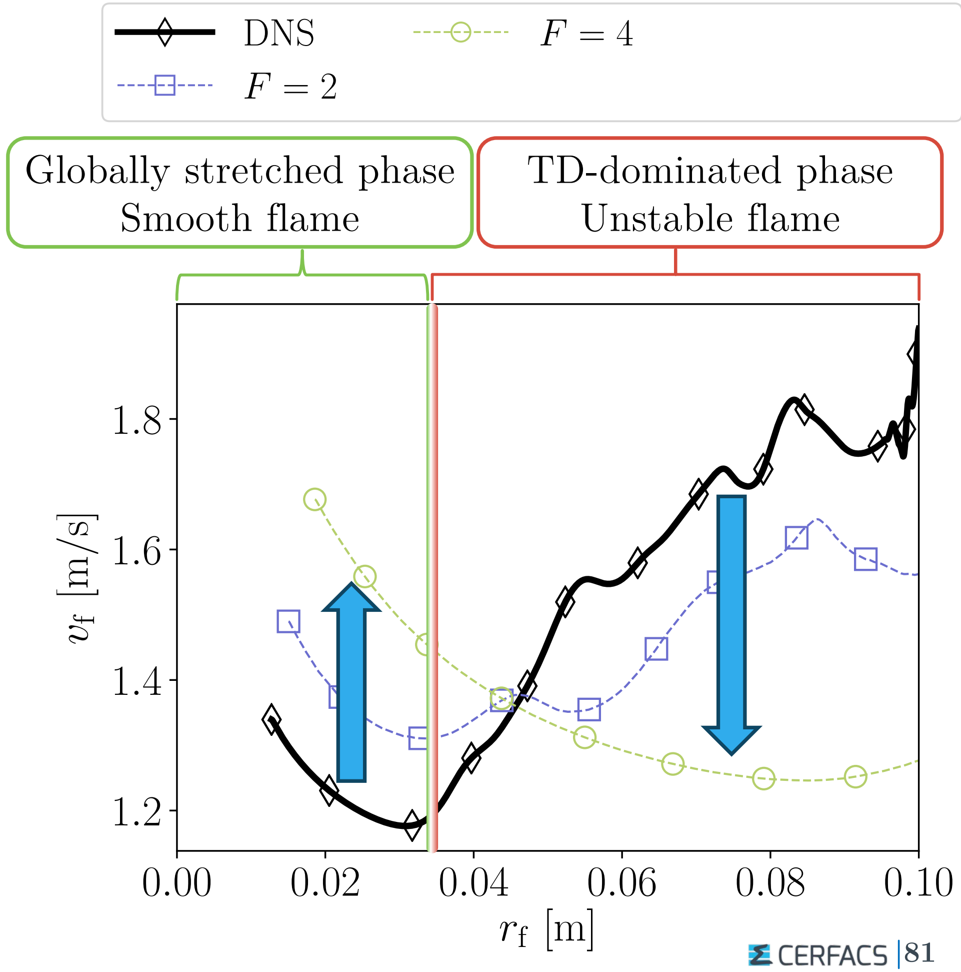
- ***P1*** and ***P2*** intensify with thickening



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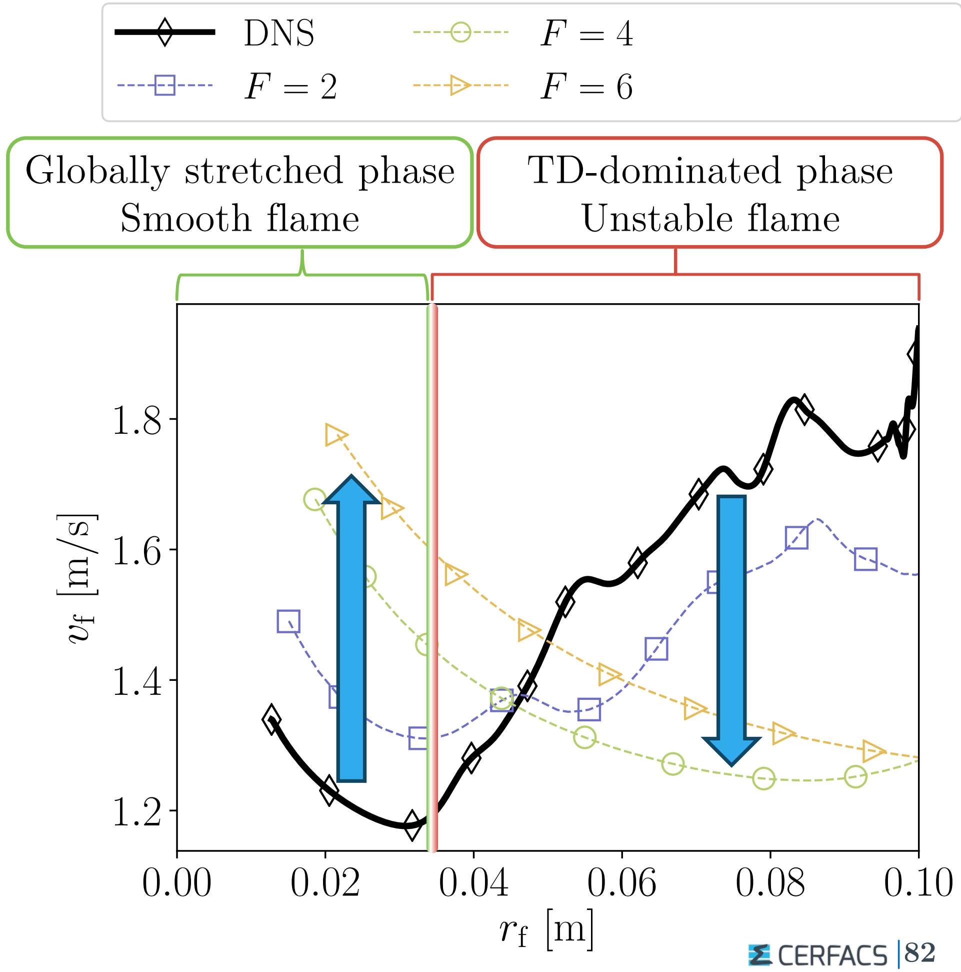

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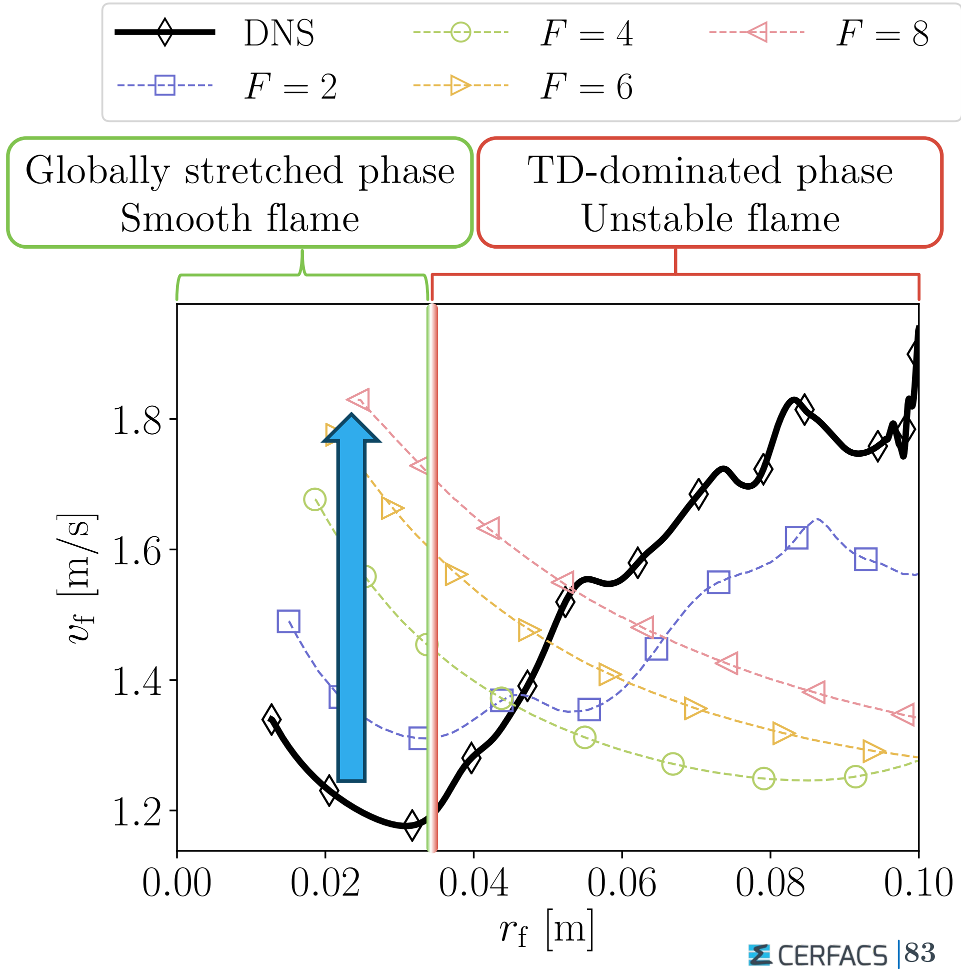

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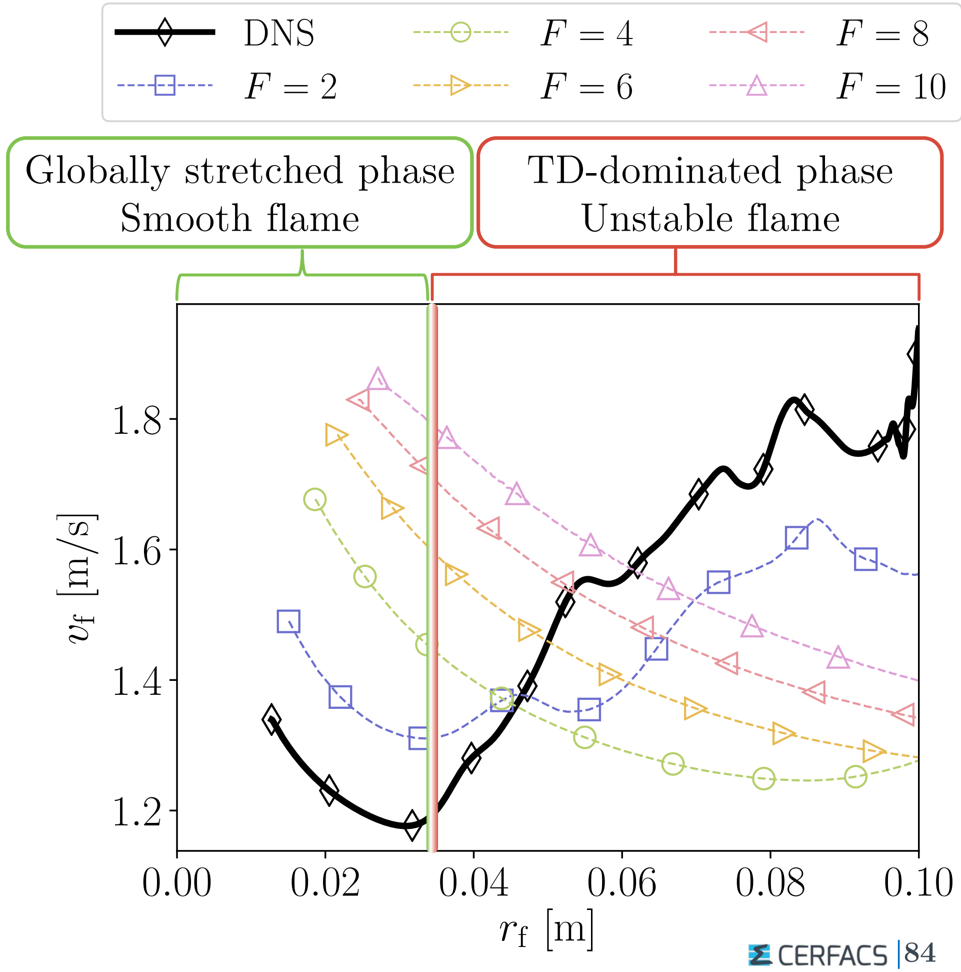

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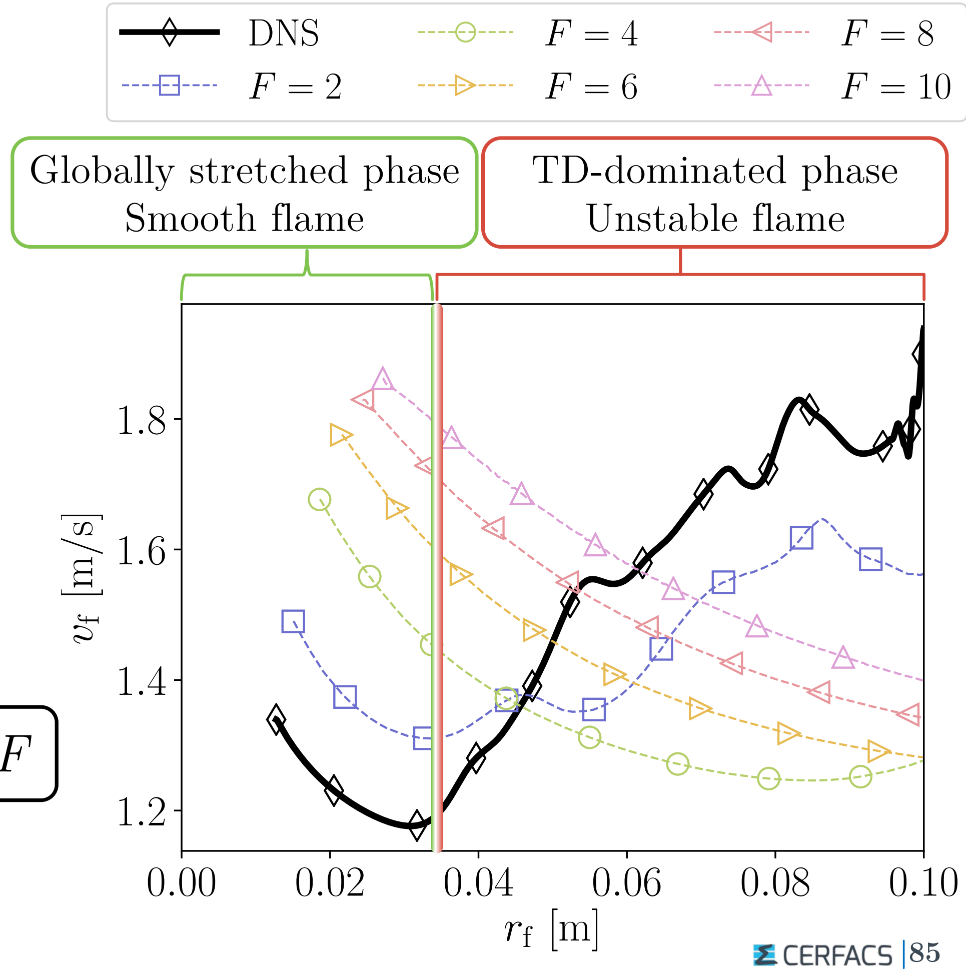
Leads to a strong mesh dependency with TF



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Flame propagation:

- Two deficie... due to thickening...

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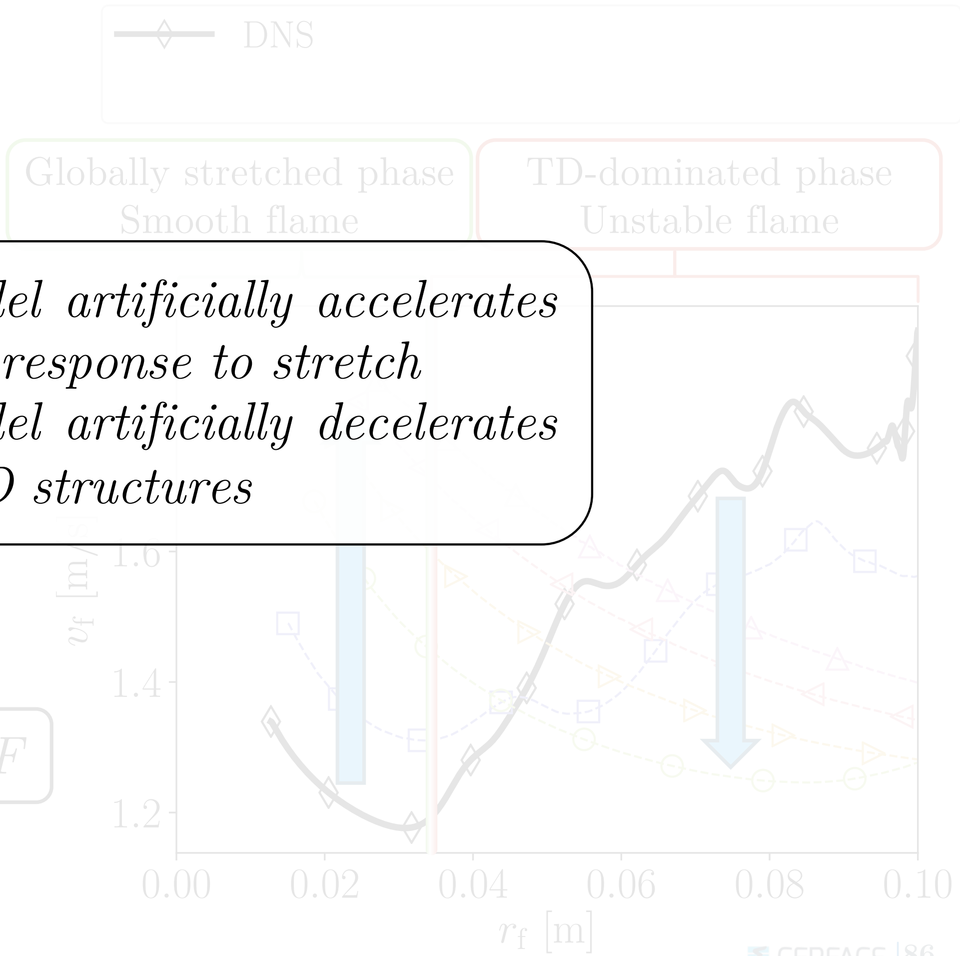

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Development of a correction: solution for *P1*

S1. Stretched-Thickened Flame (S-TF) model[1-2]

- Extension of the classical TF model, using:

[1] **Hok J.-J.**, Dounia O., Detomaso N., Jaravel T., Douasbin Q. & Vermorel O., Int. J. Hydrogen Energ., 2024
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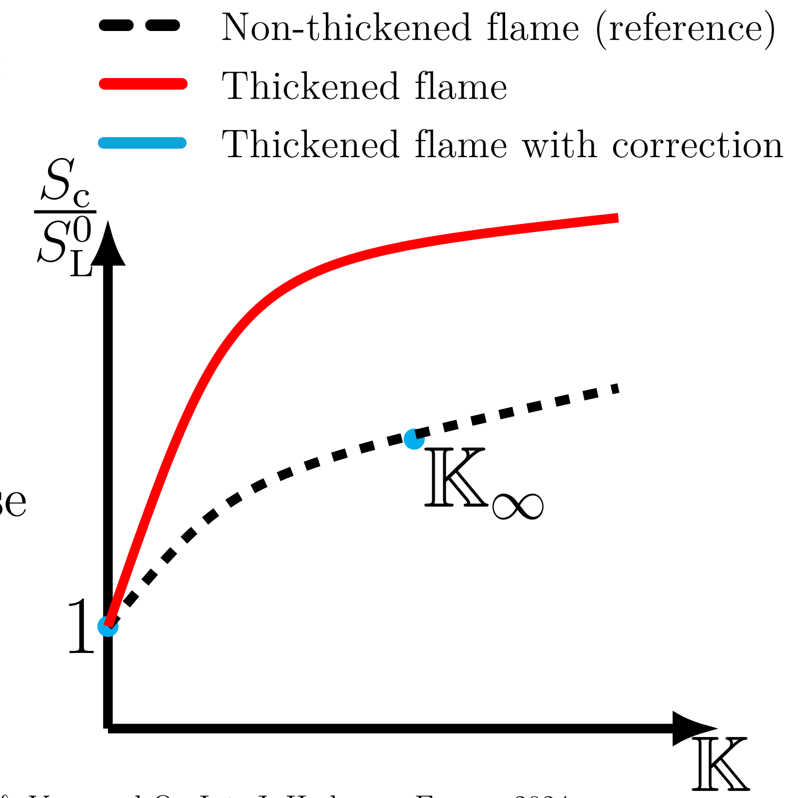

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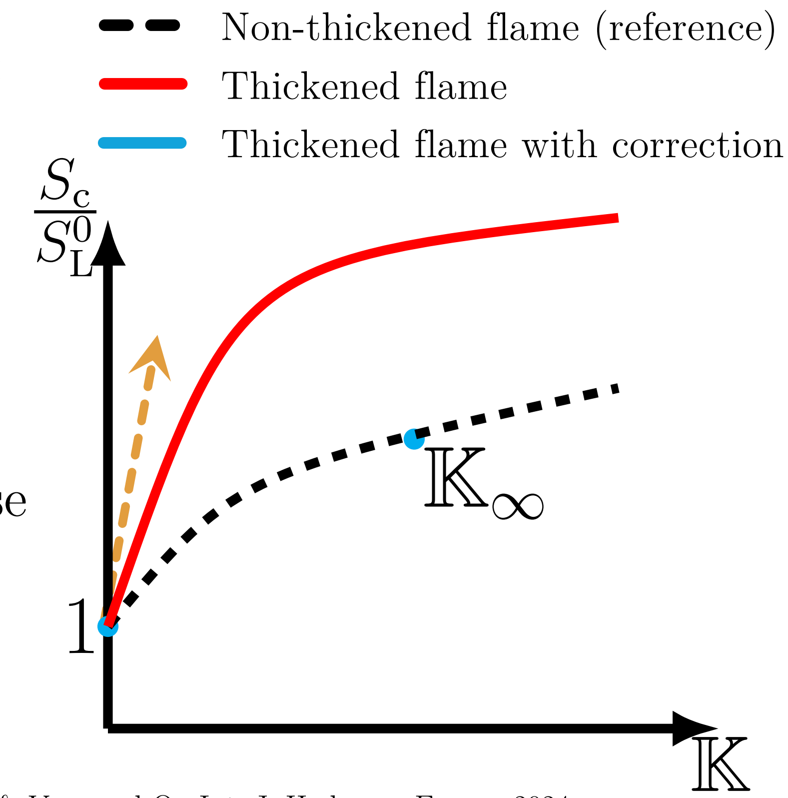

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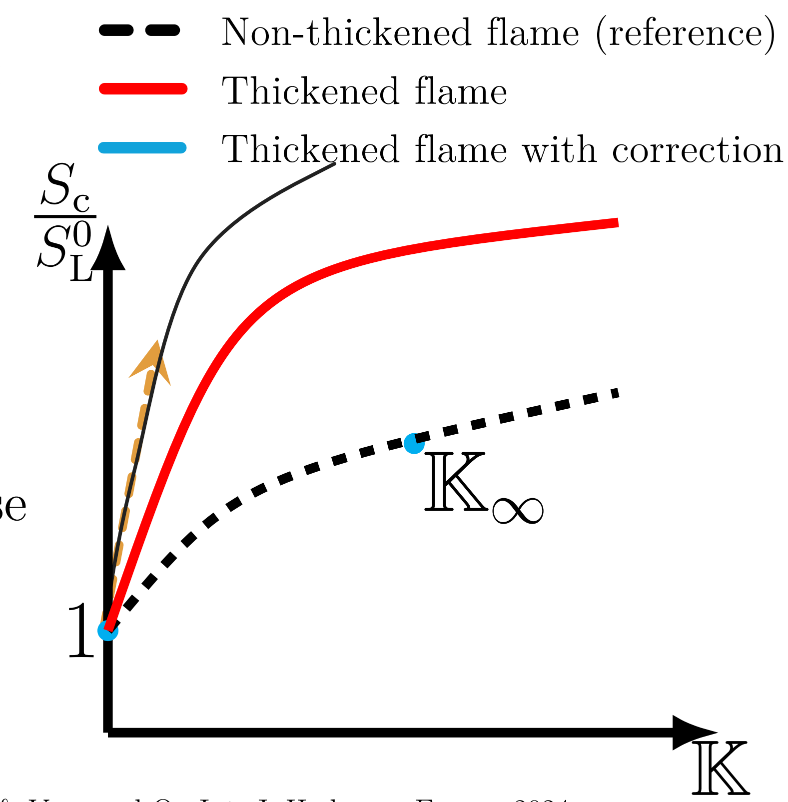

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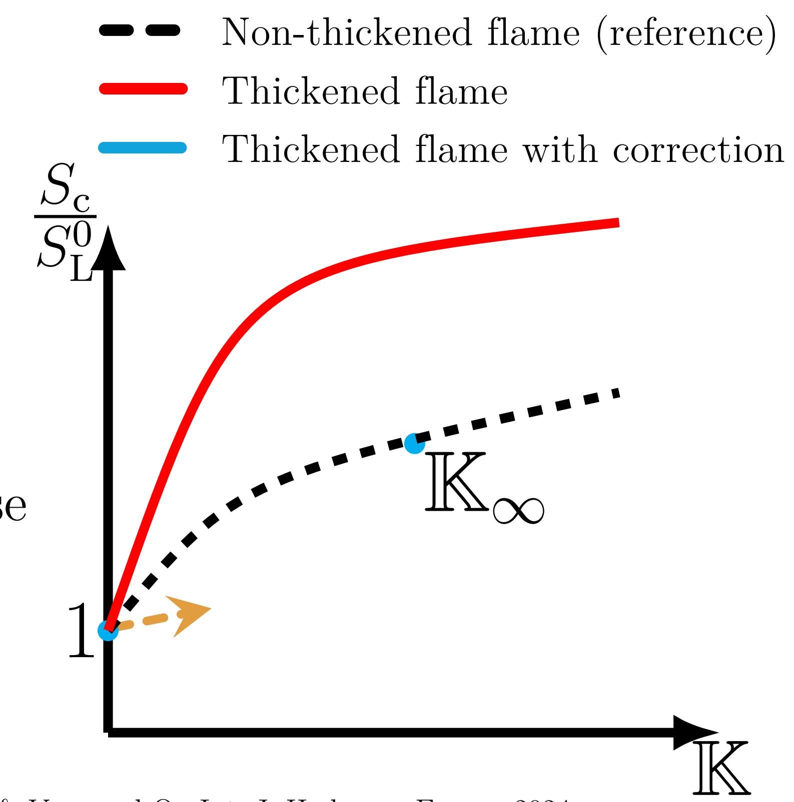

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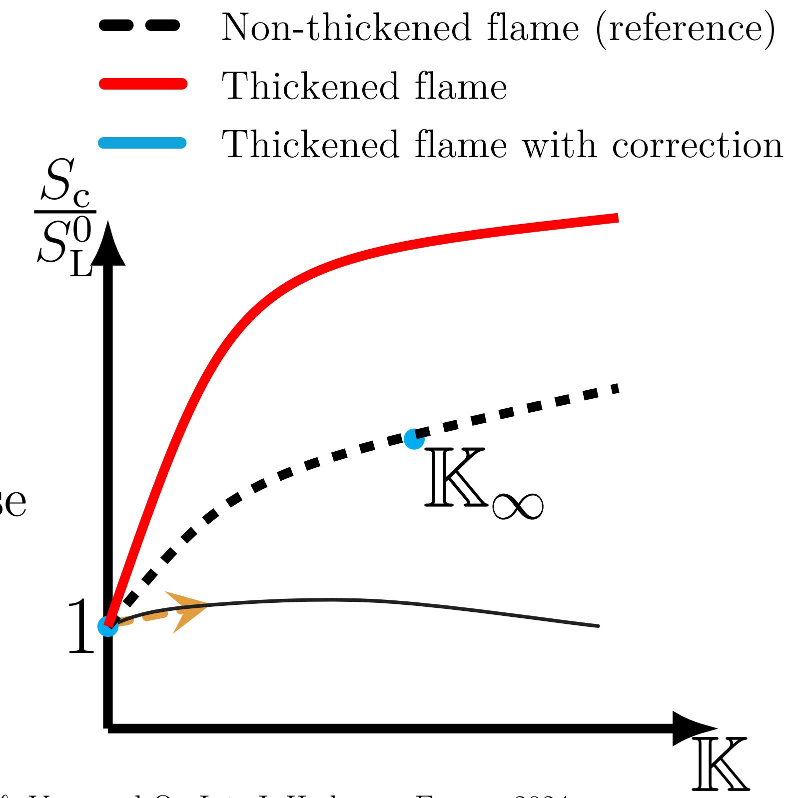

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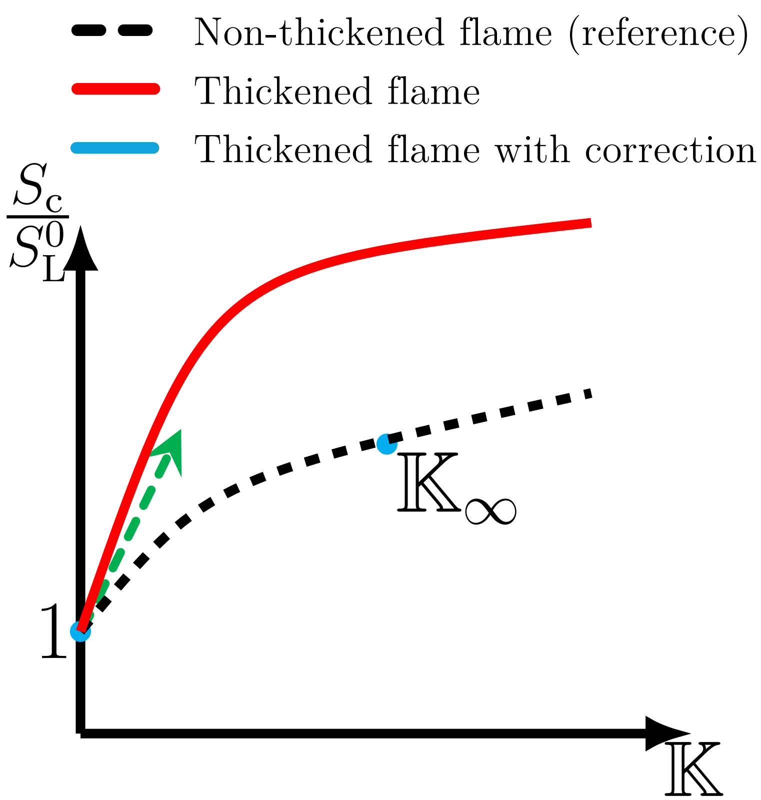

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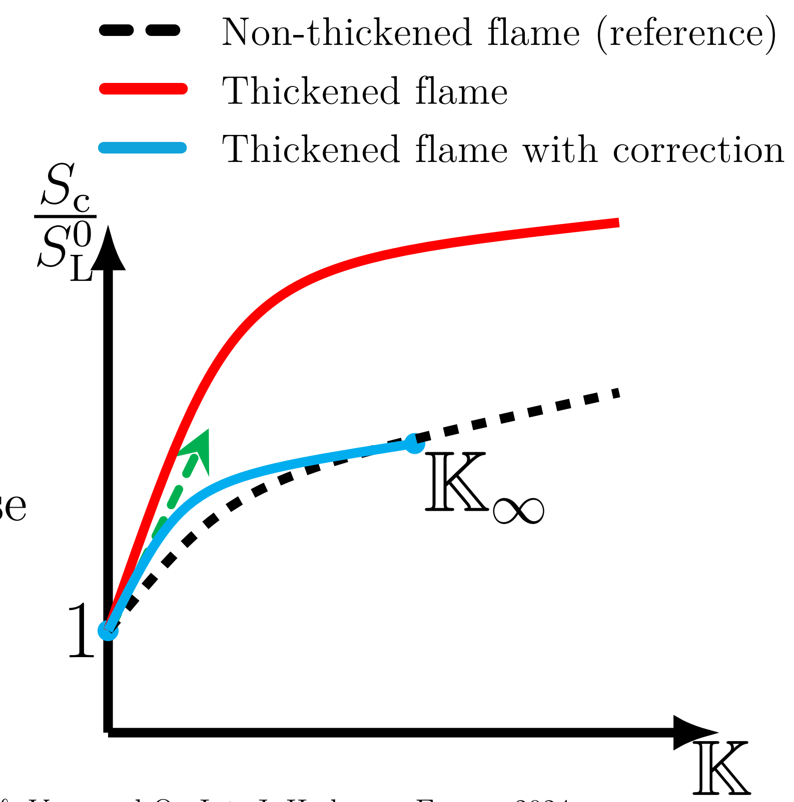

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Application of the correction *S1*: the S-TF model[1]

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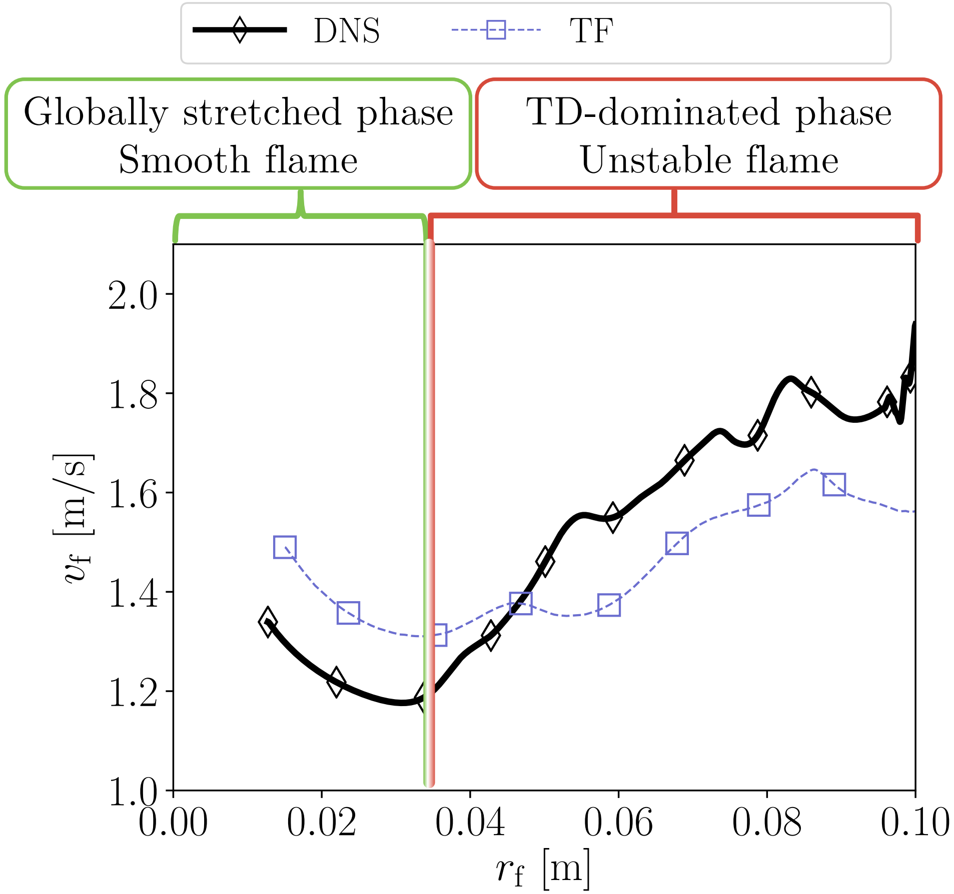

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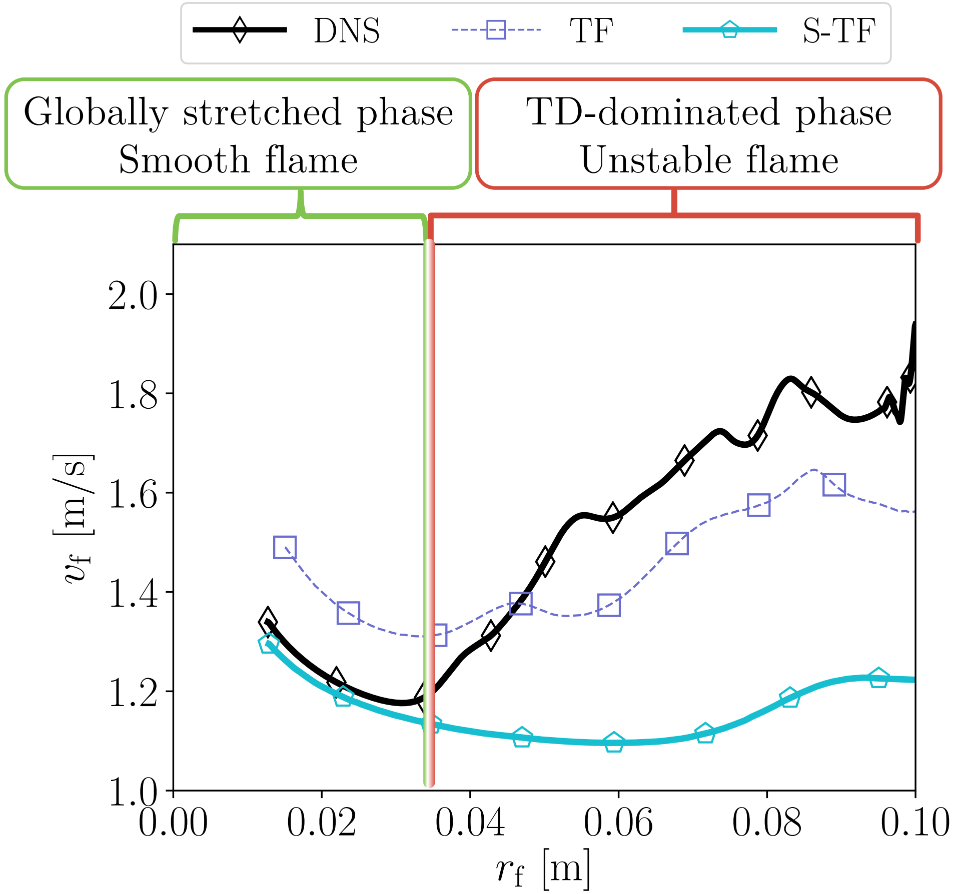

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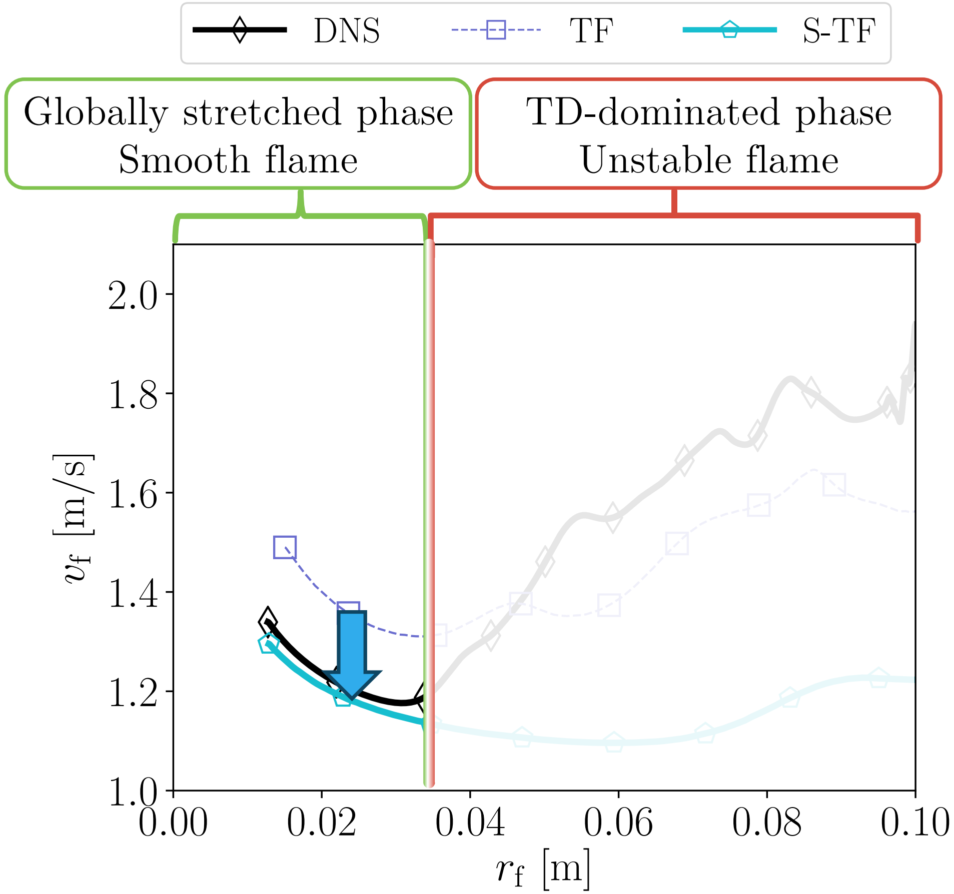

✓ *The S-TF model effectively solves the amplification of stretch effects by thickening factor;*

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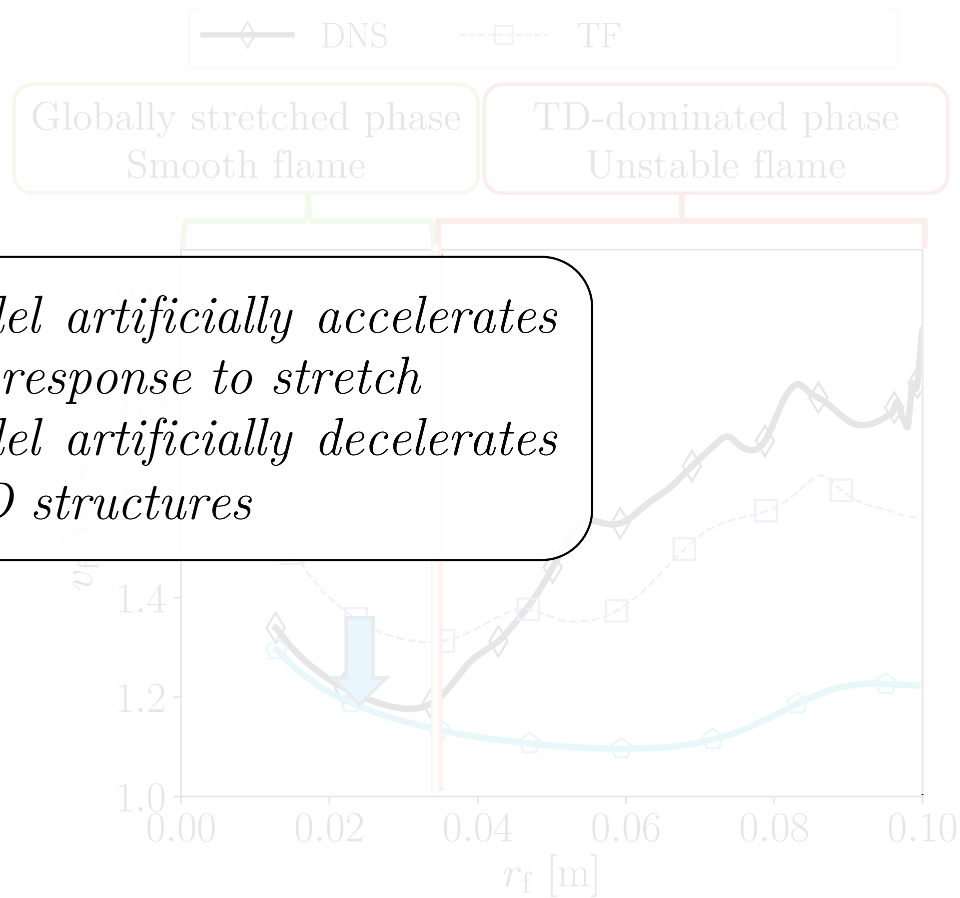
amplification
thickening fa



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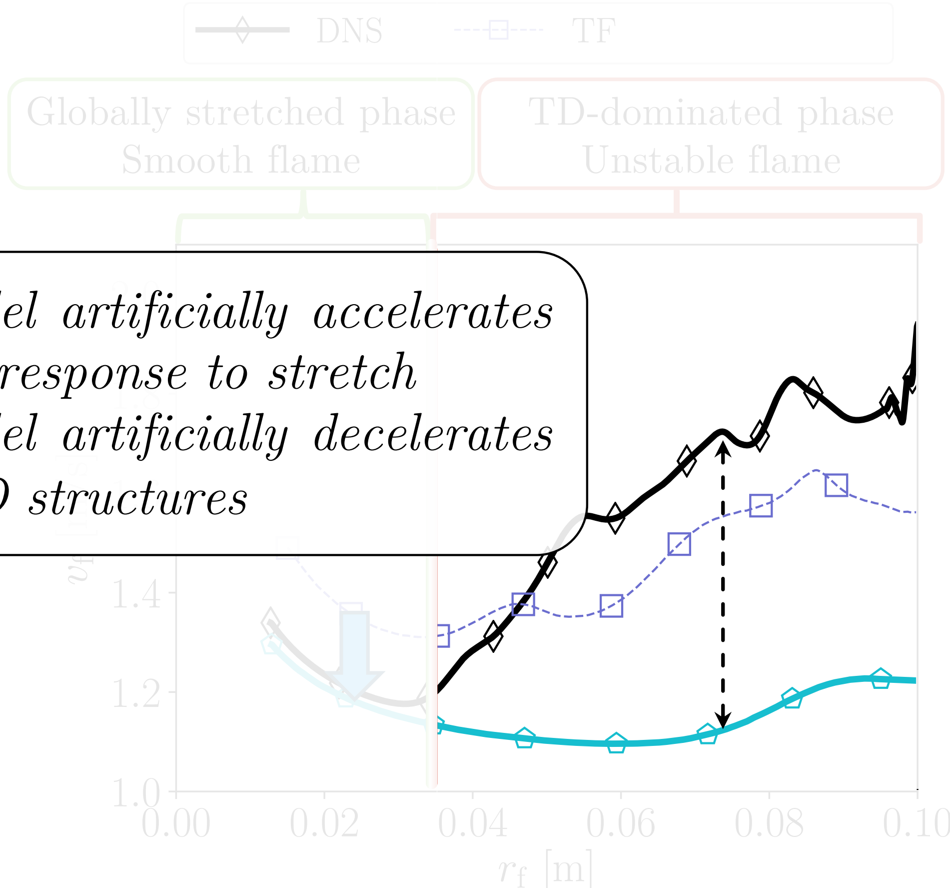

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Development of a correction: solution for *P2*

[1] Goulier, Thesis, 2015

Development of a correction: solution for ***P2***

S2. *Subgrid model (efficiency)*

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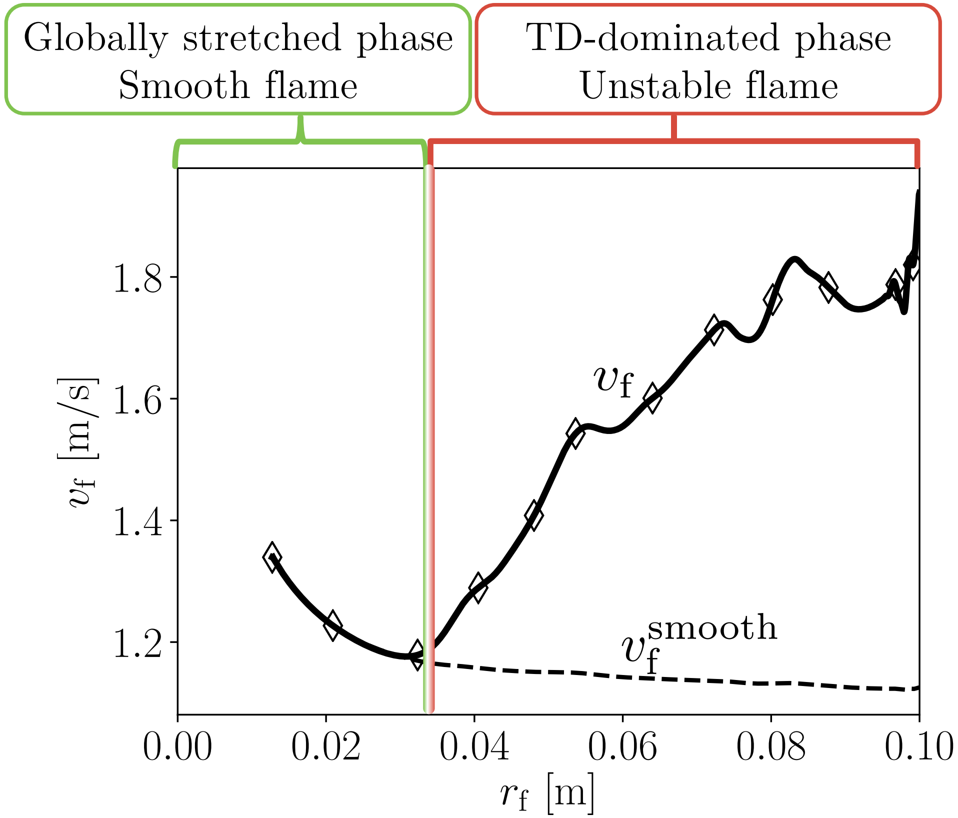

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"Total =
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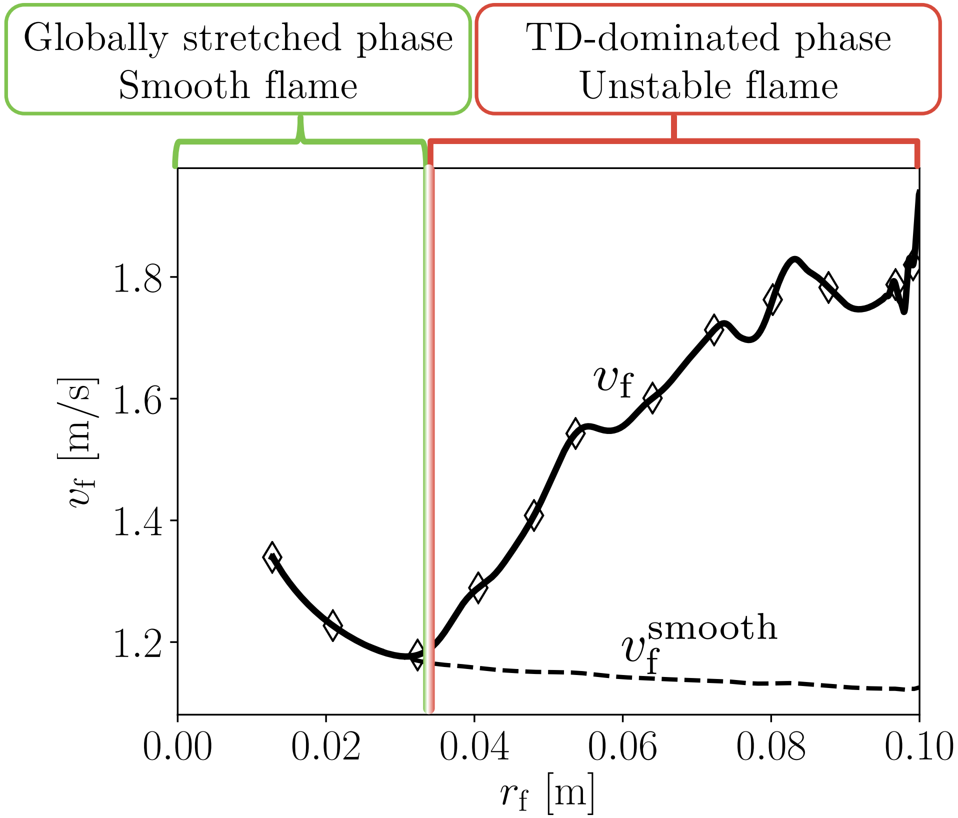

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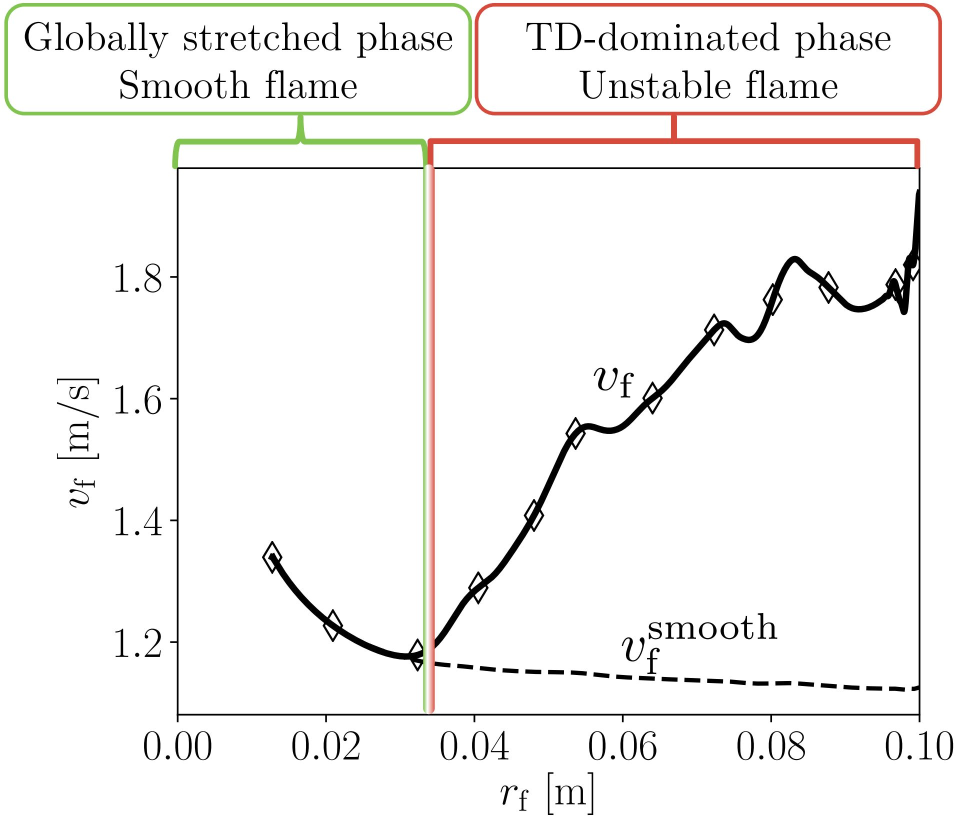

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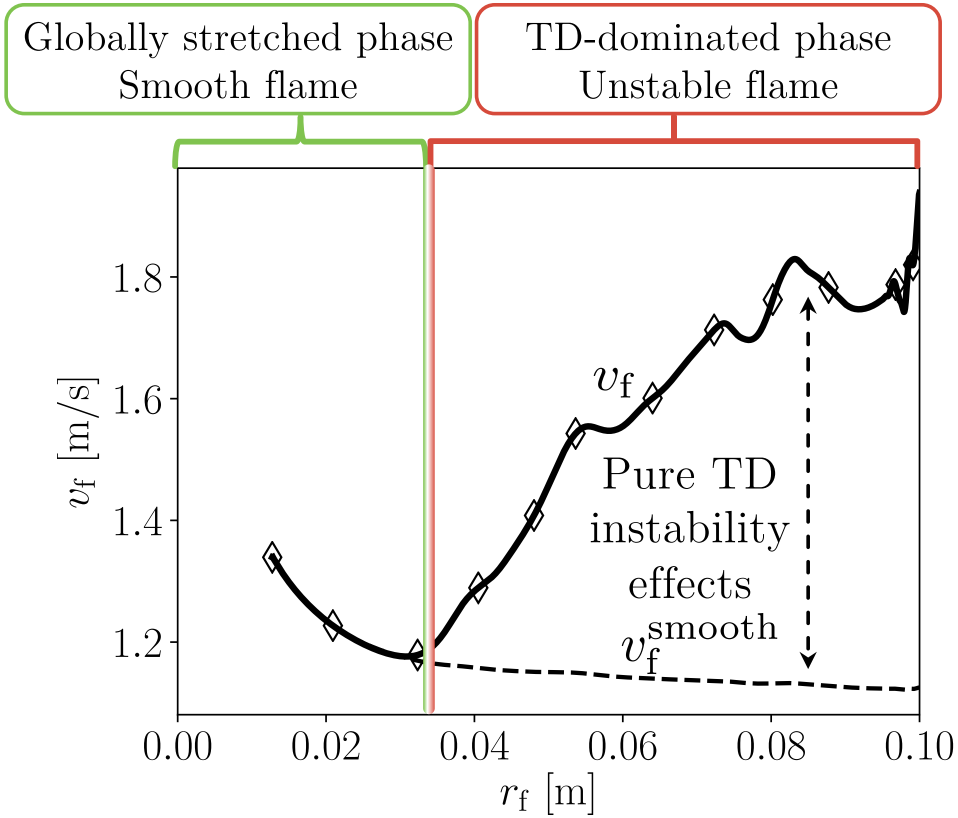

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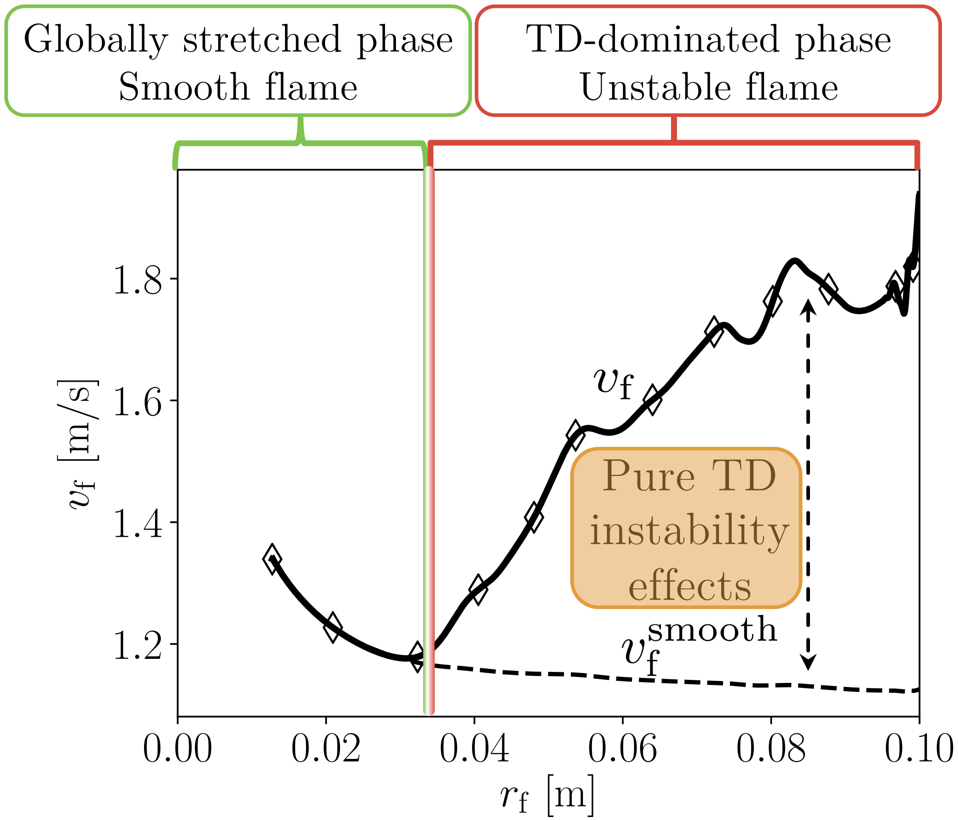

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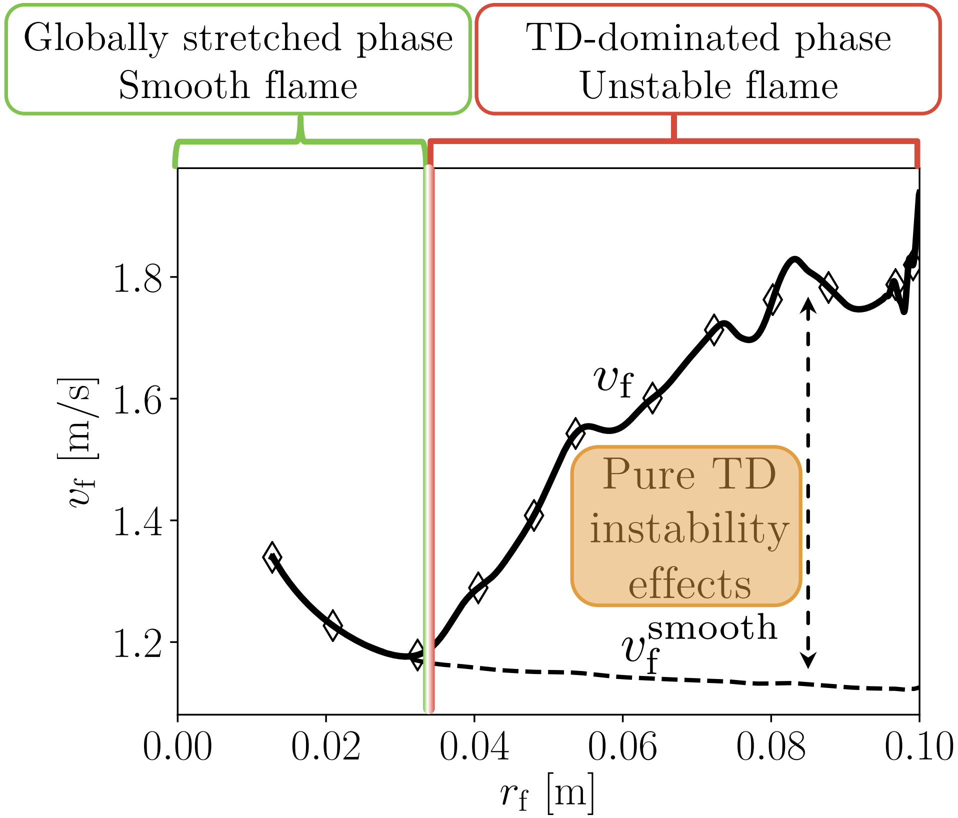
S-TF model

$$E_{\mathrm{TDS}} = \frac{v_{\mathrm{f}}}{v_{\mathrm{f}}^{\mathrm{smooth}}}$$



[1] Goulier, Thesis, 2015

Development of a correction: solution for *P2*

S2. *Subgrid model (efficiency)*

"*Total* = *Resolved stretch effects* + *Pure TD instability effects*"

Resolved stretch effects → S-TF model

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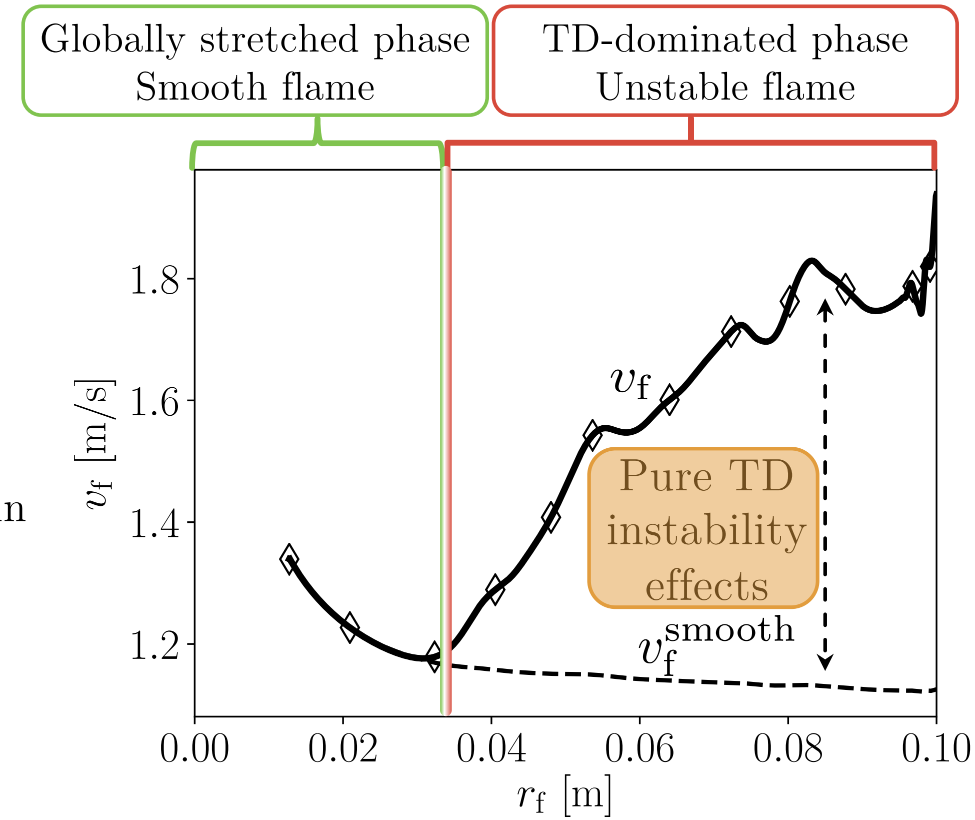
→ taken from experimental correlations, verified in DNS in a wide range of conditions



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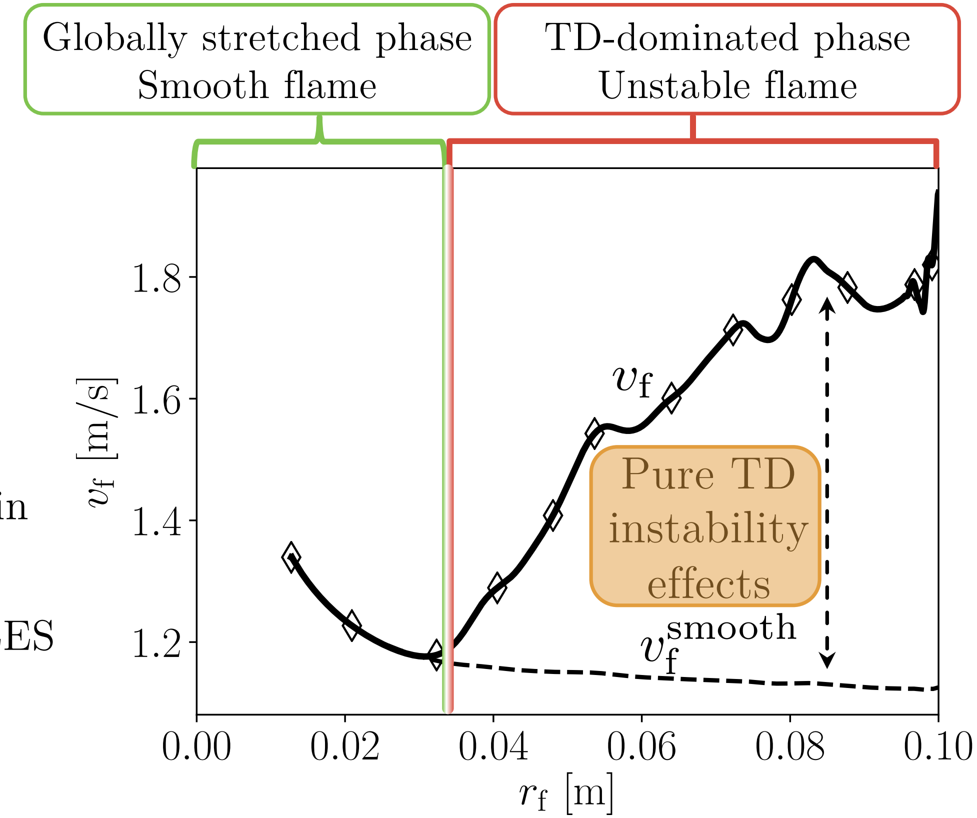
Hypothesis: no TD structure is resolved in the LES and all TD instability effects are modelled



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Application of the correction *S1*+*S2*: the TD-S-TF model[1]

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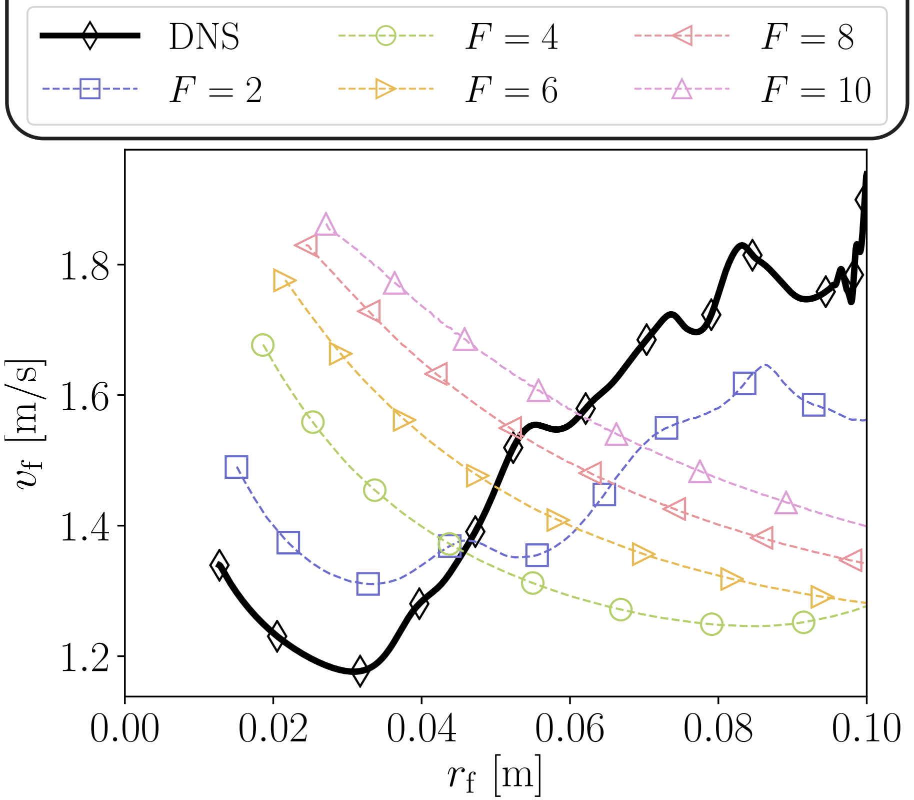
Classical TF approach



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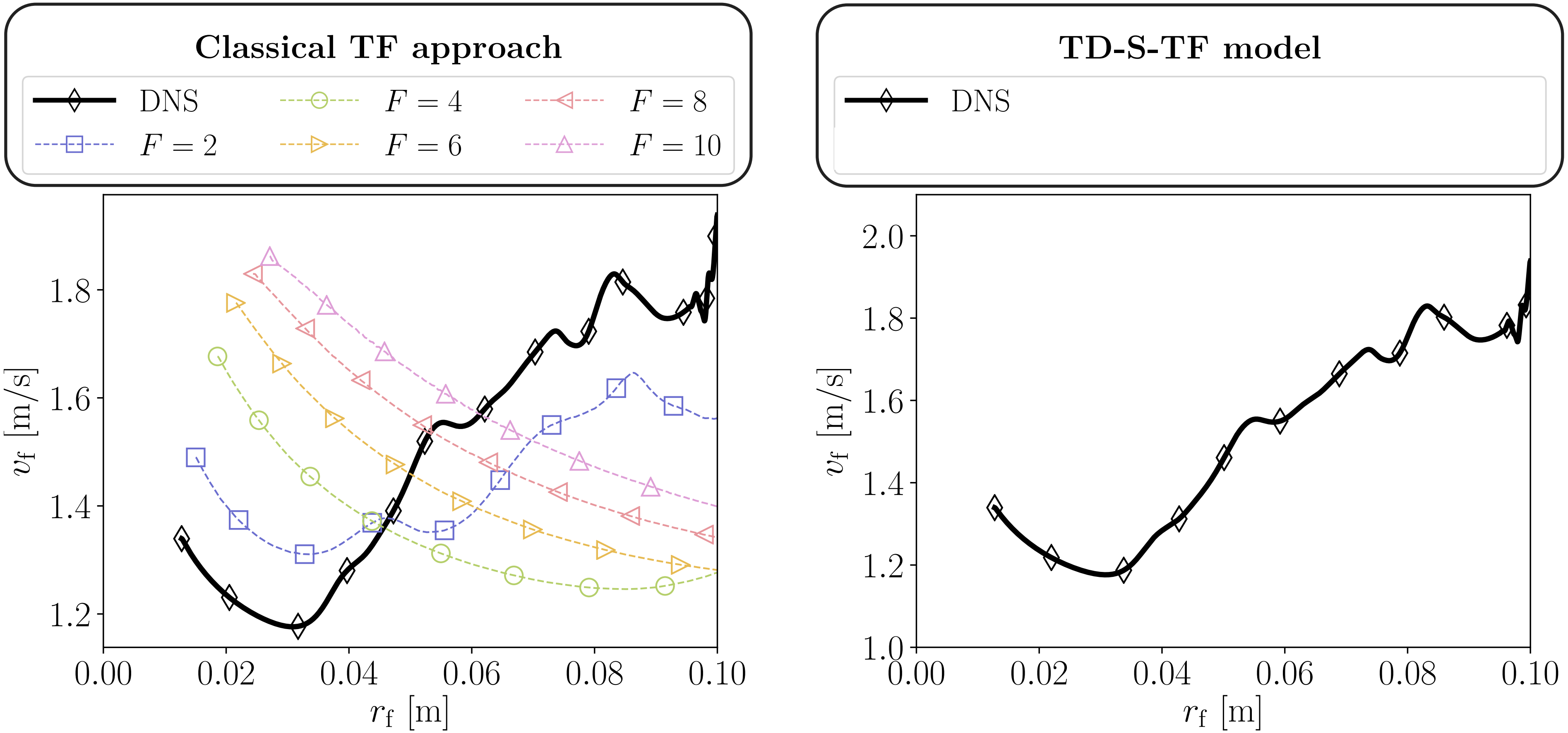

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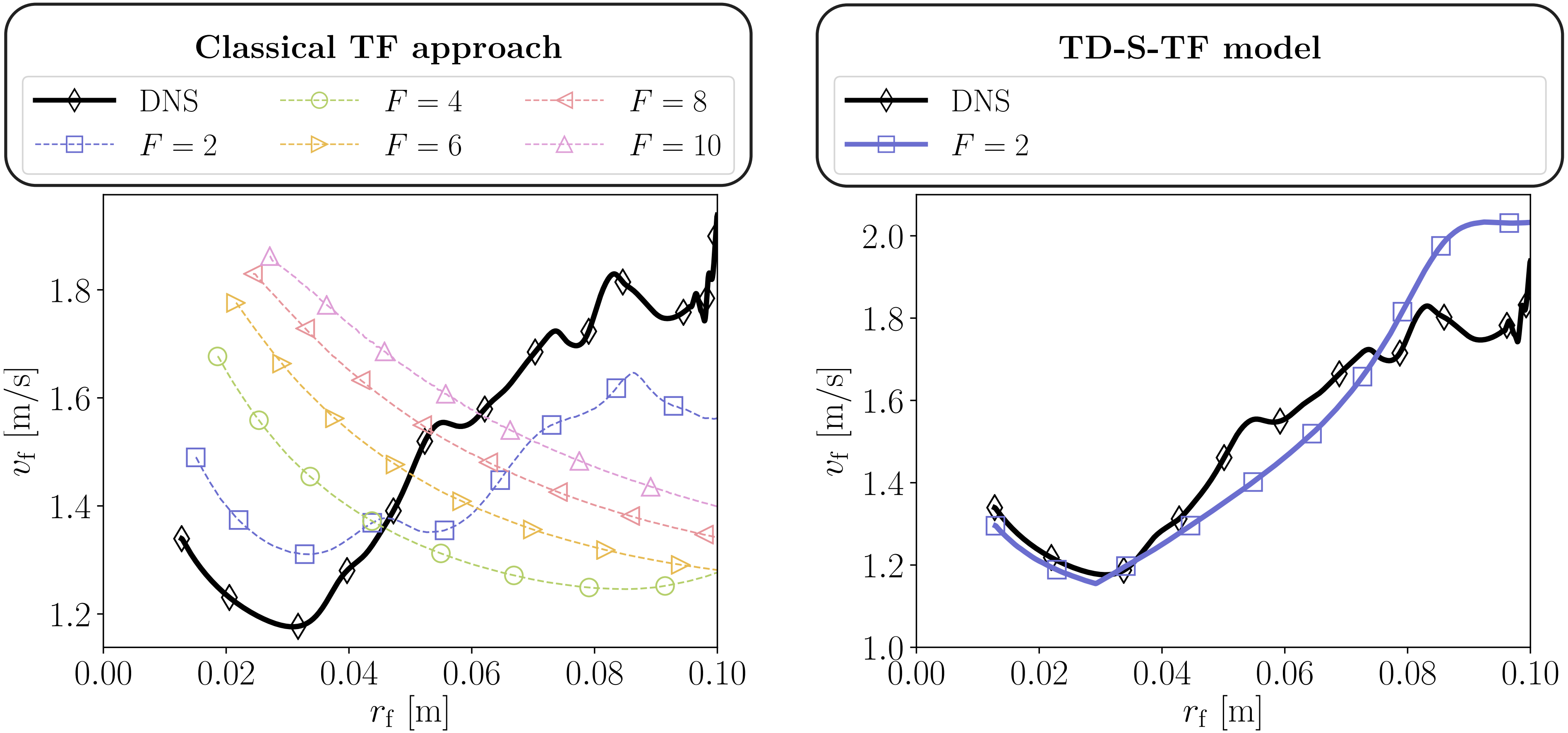

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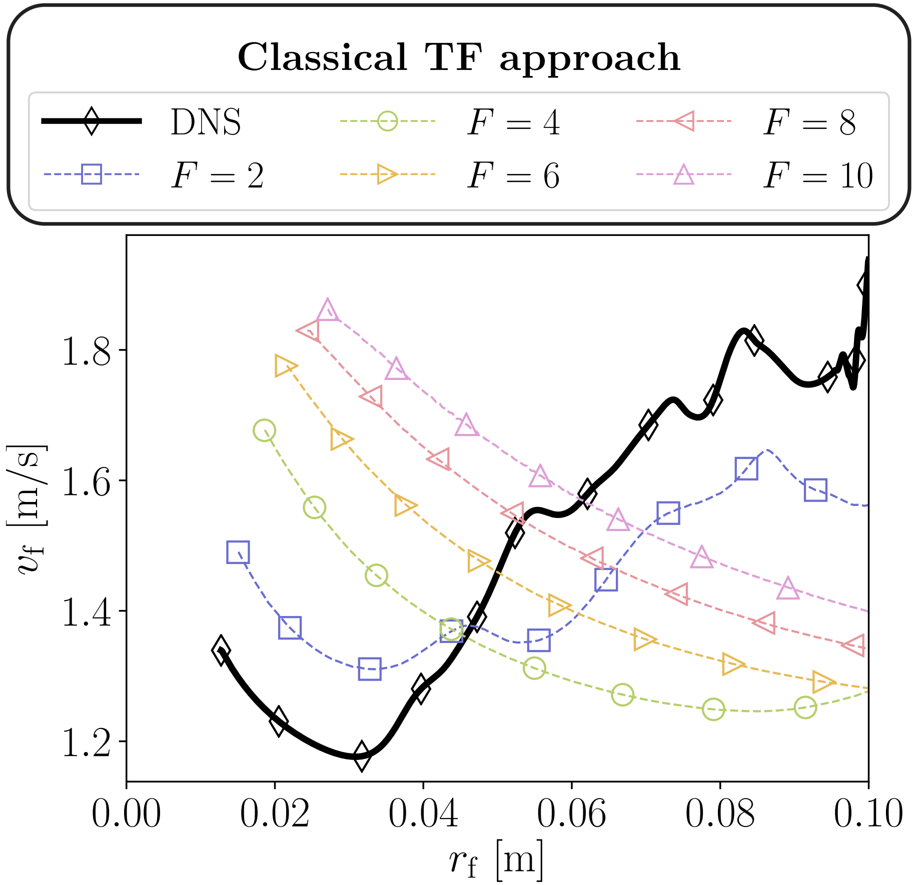

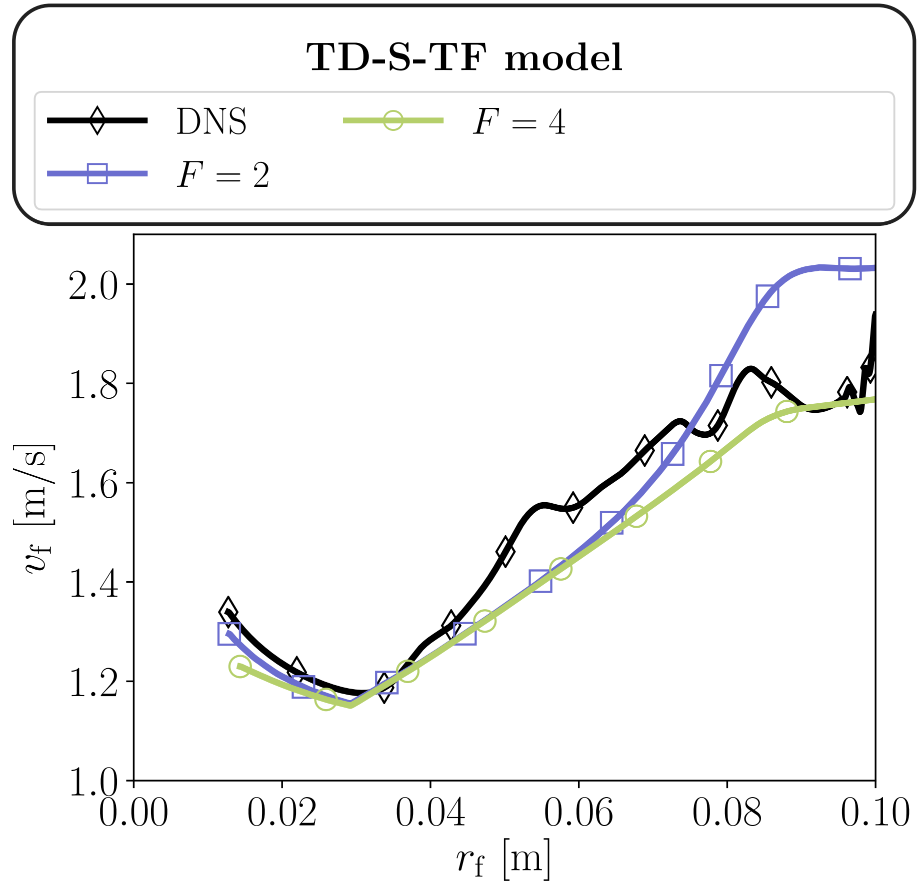

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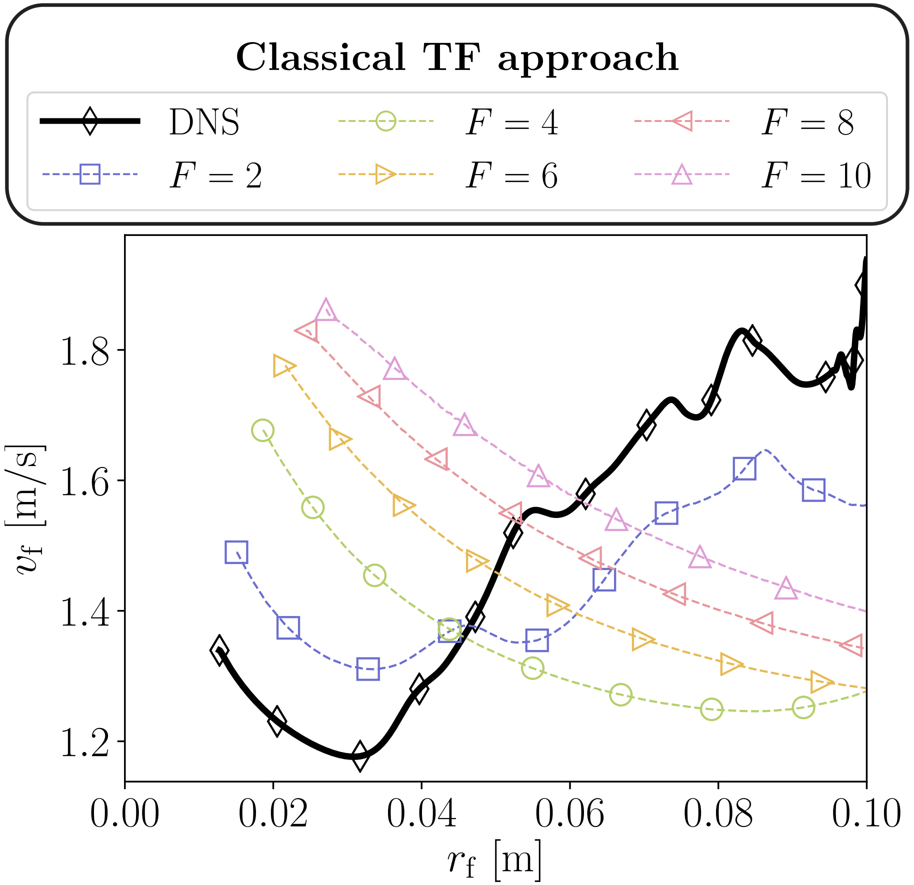

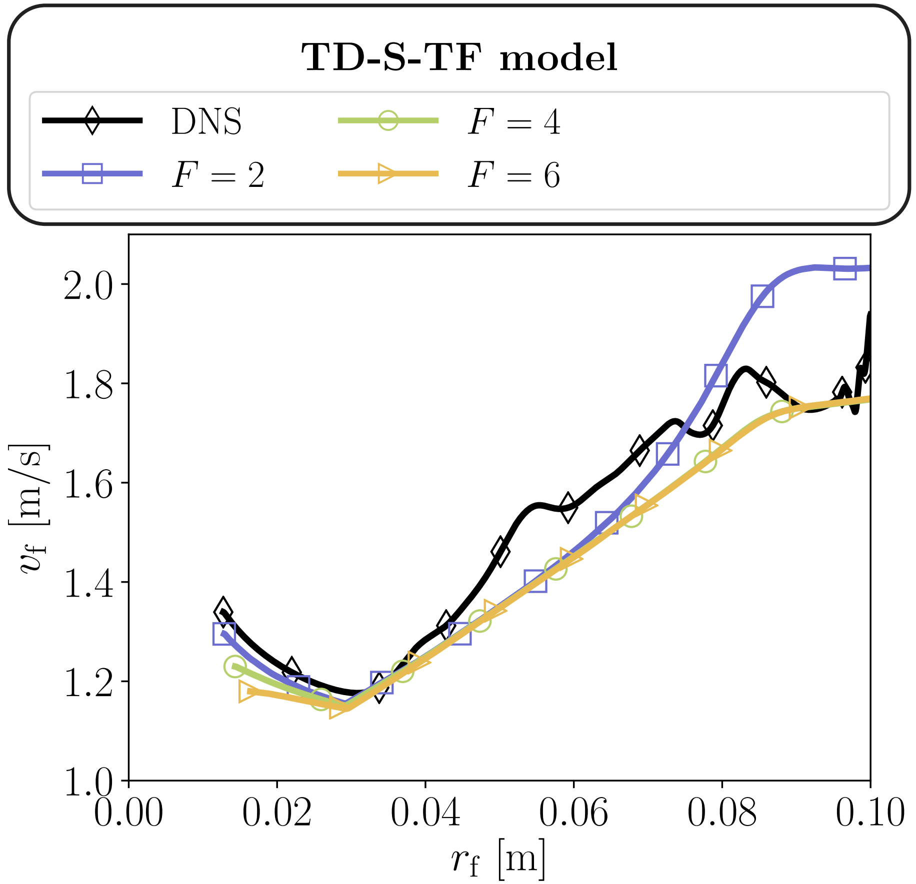

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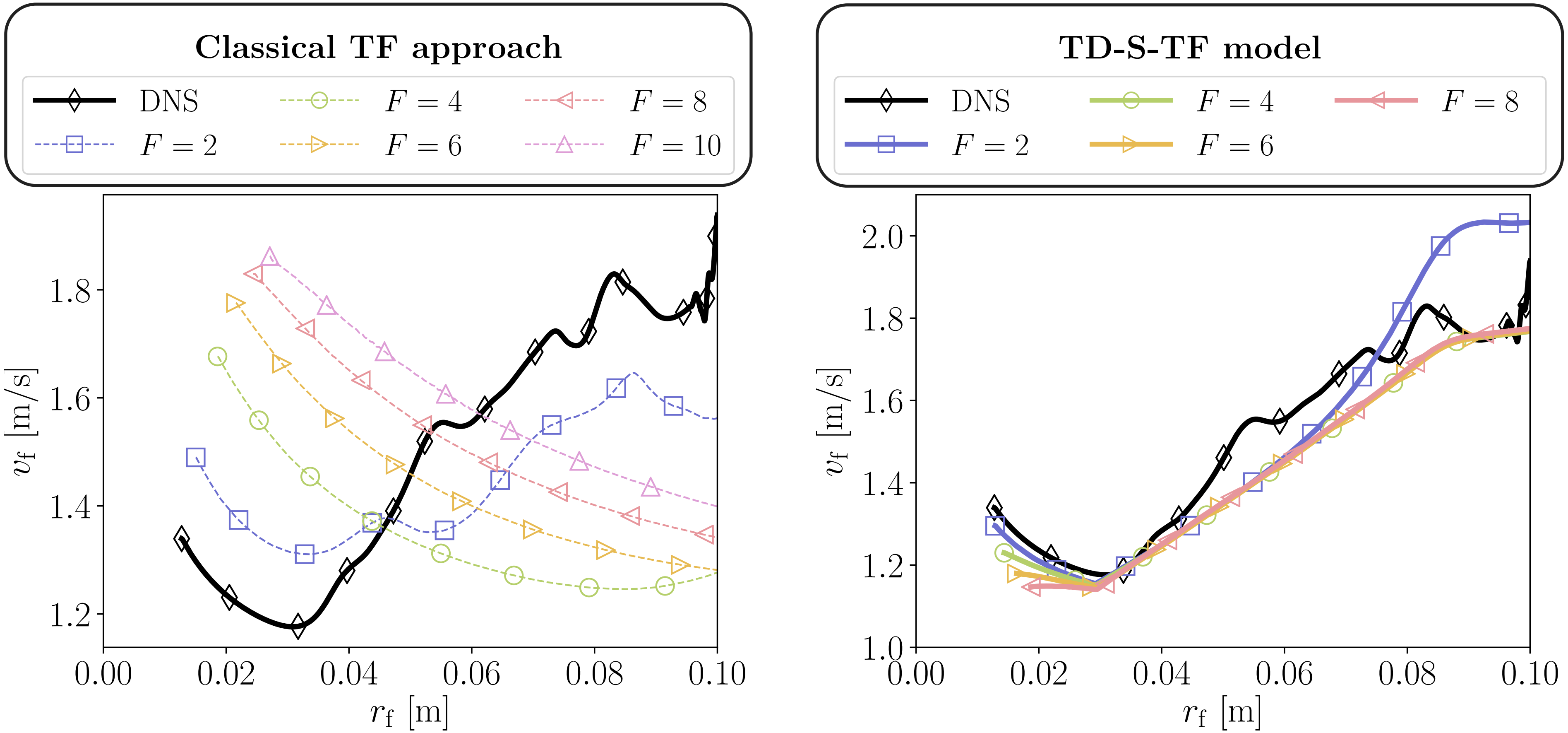

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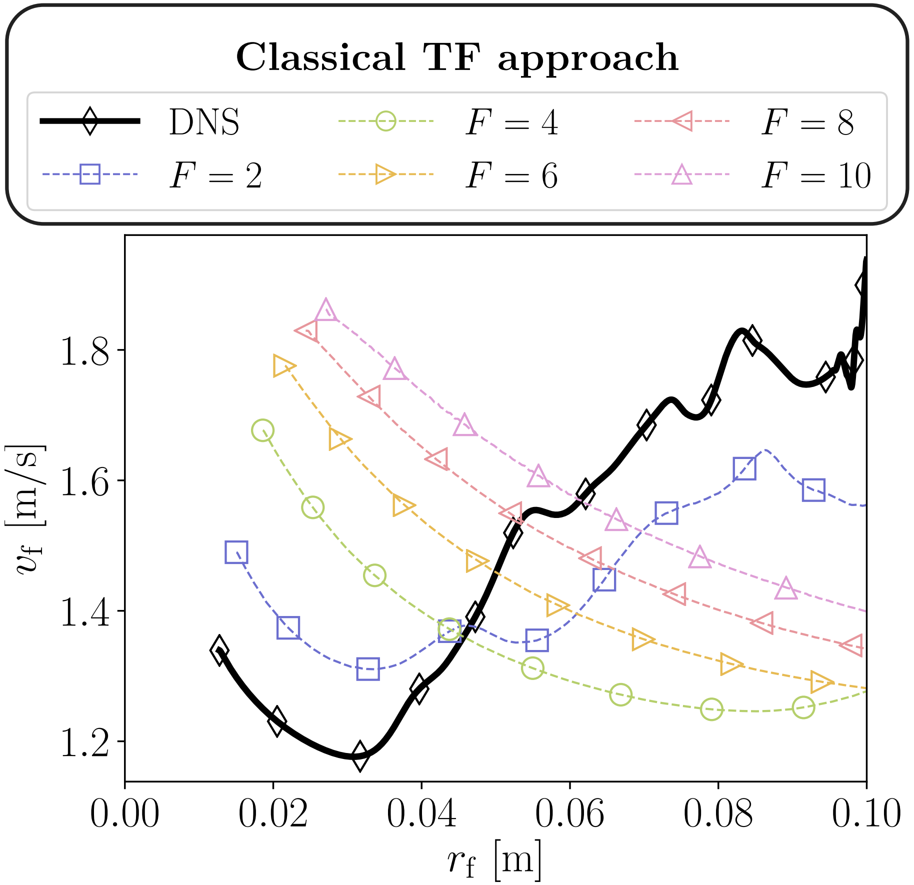

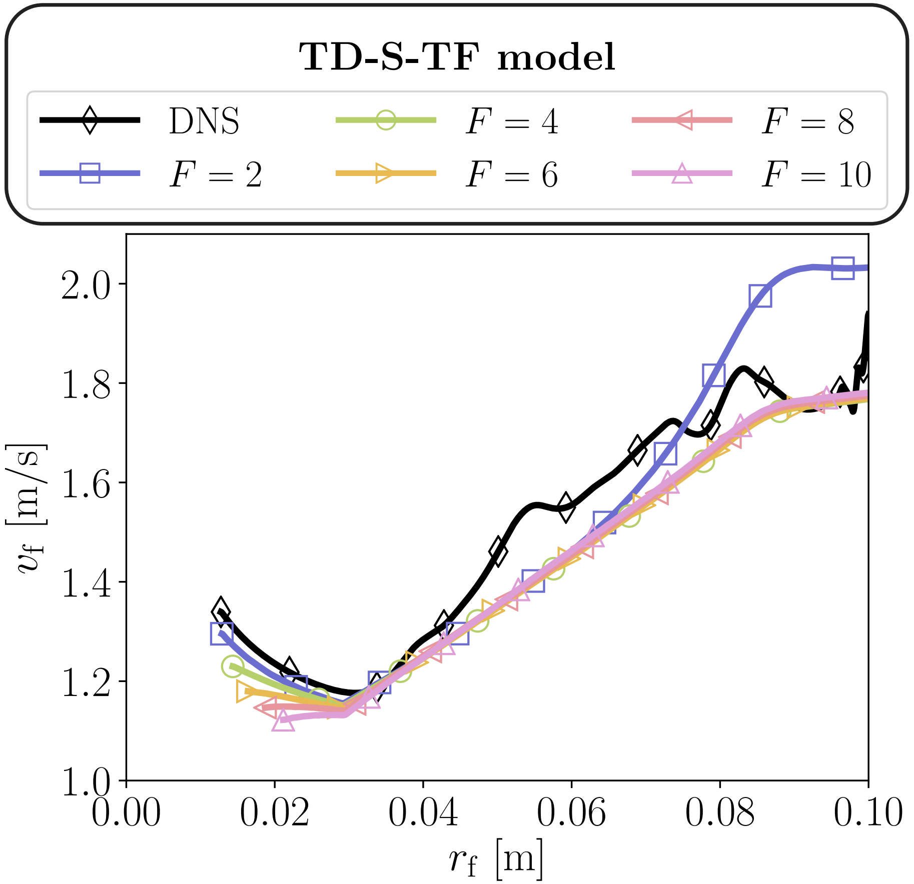

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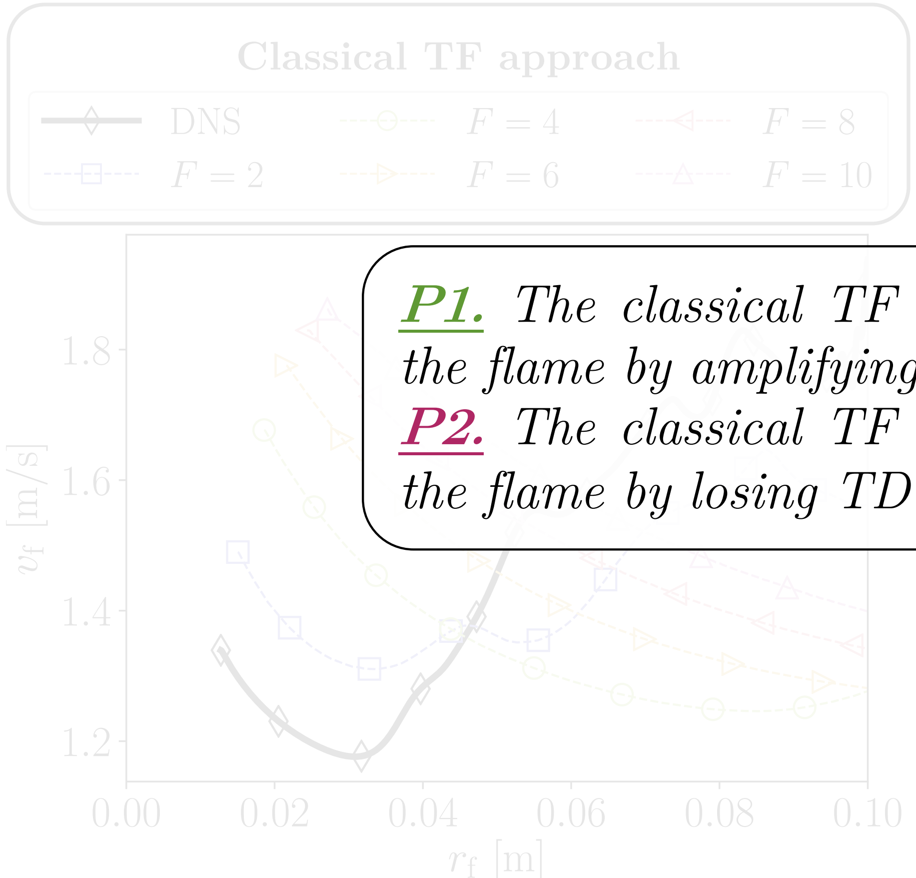

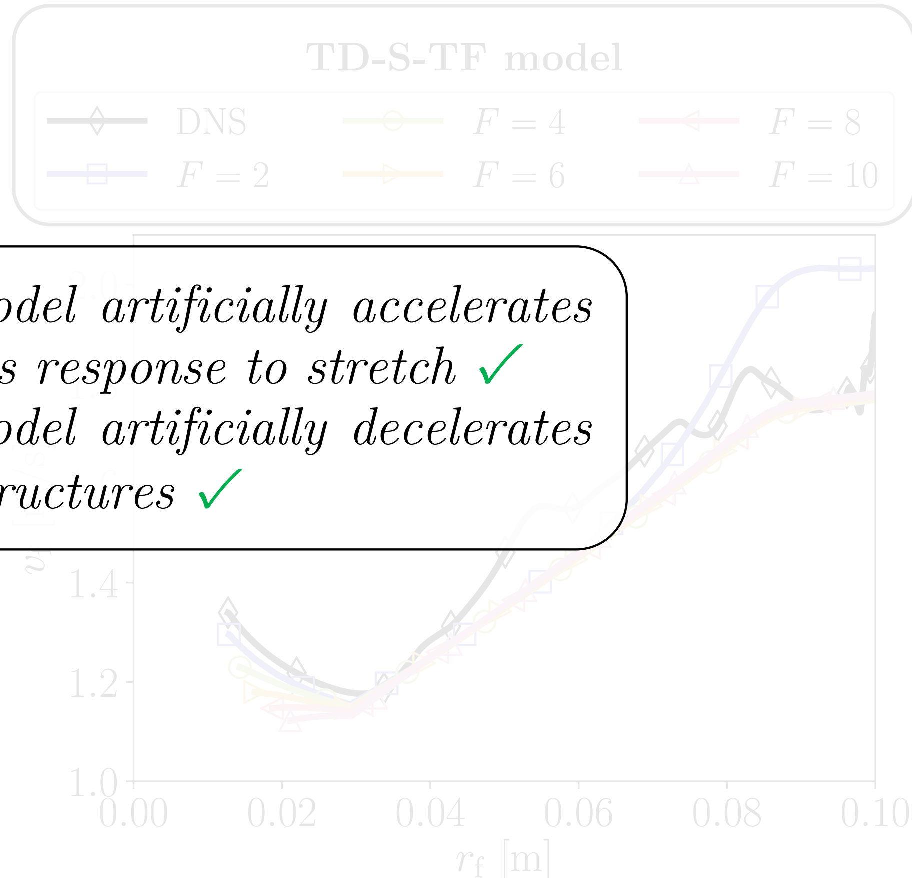

P1. *The classical TF model artificially accelerates the flame by amplifying its response to stretch* ✓

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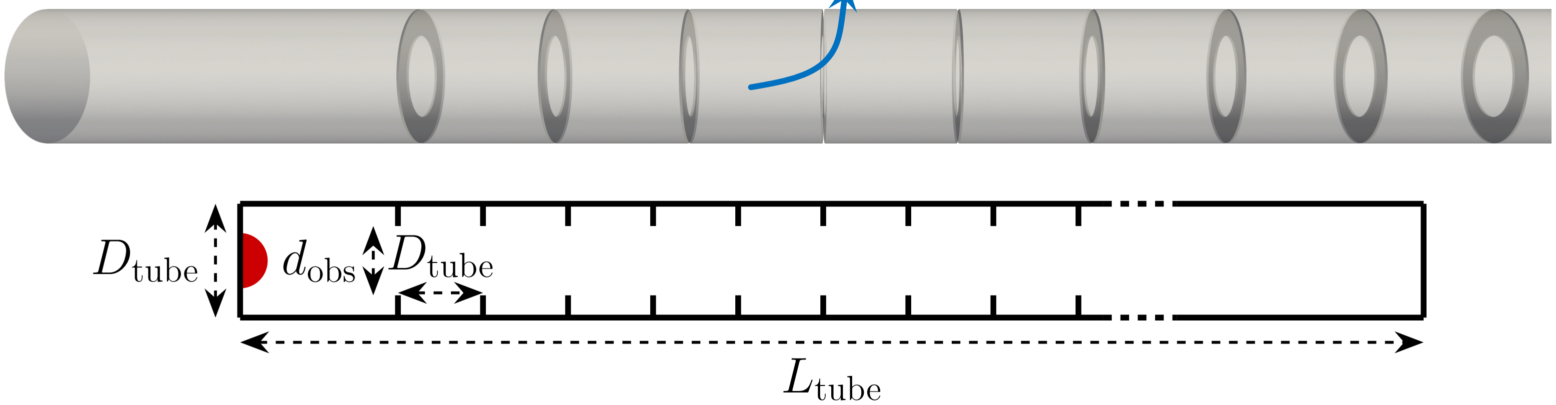
The ENACCEF2 explosion

Geometry, boundary and initial conditions:

All walls: law of the wall, isothermal



- $L_{\text{tube}} = 7.65\text{m},\ D_{\text{tube}} = 0.23\text{m},\ d_{\text{obs}} = 0.14\text{m}$

Photo of ENACCEF2 test rig[1].

[1] Grosseuvres, Thesis, 2018

Application of the TD-S-TF model

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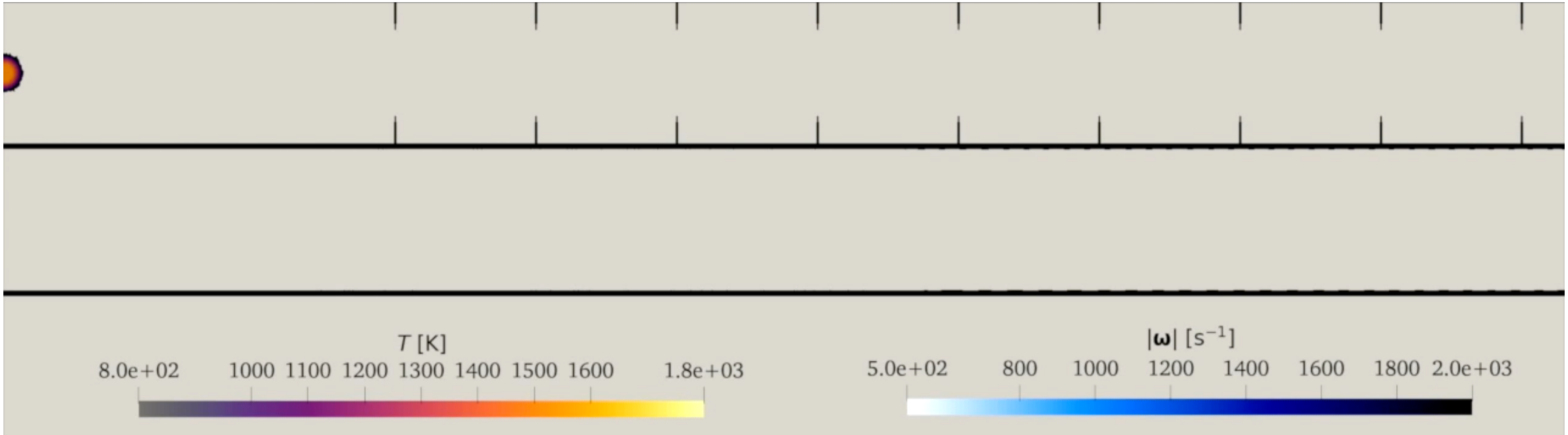

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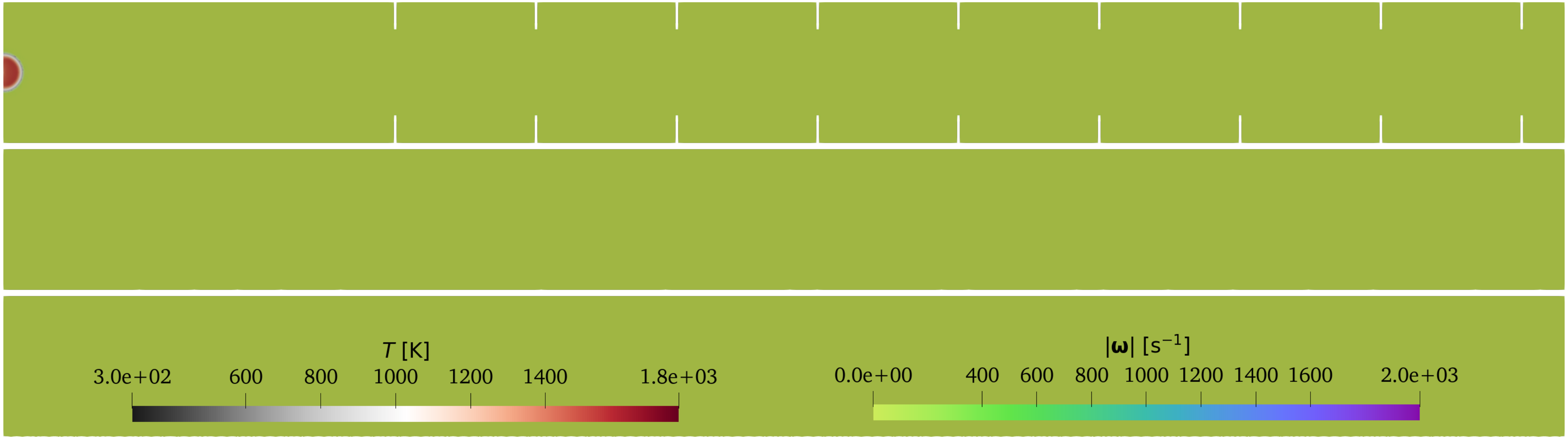

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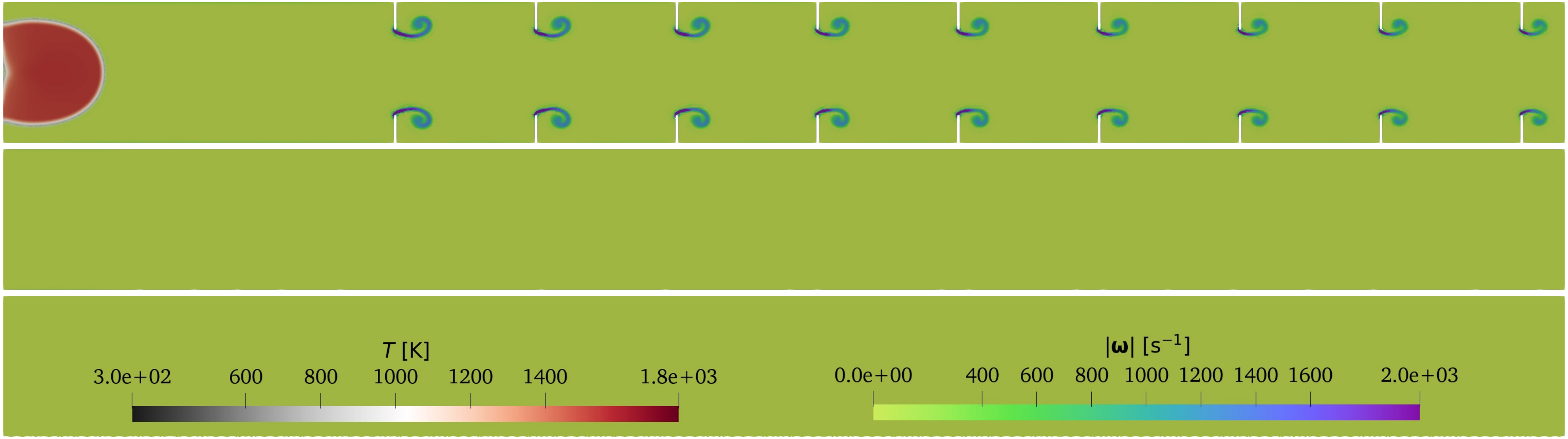

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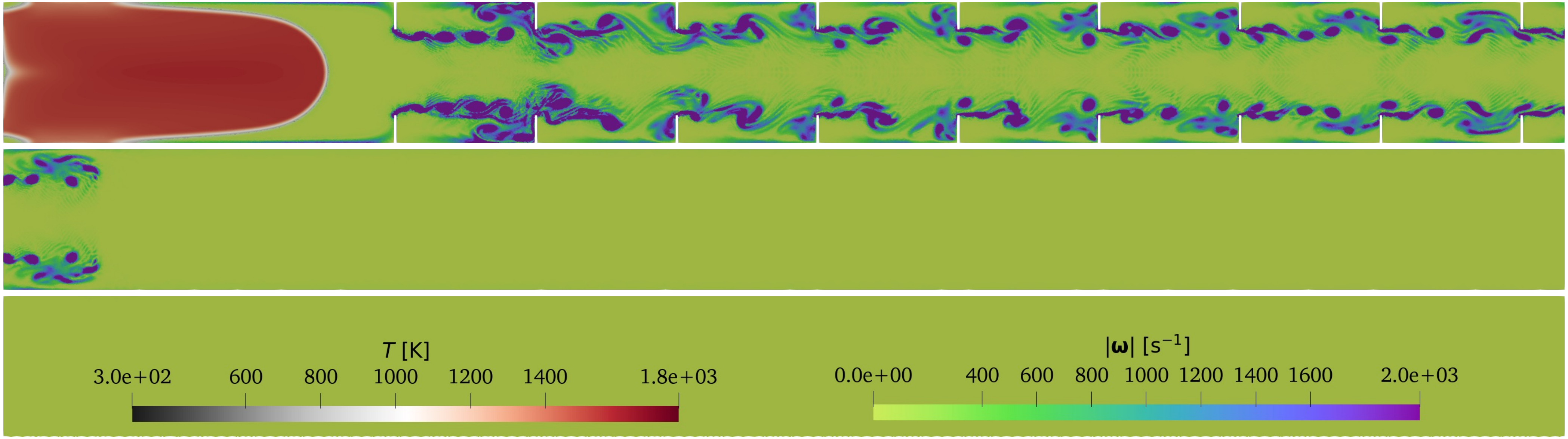

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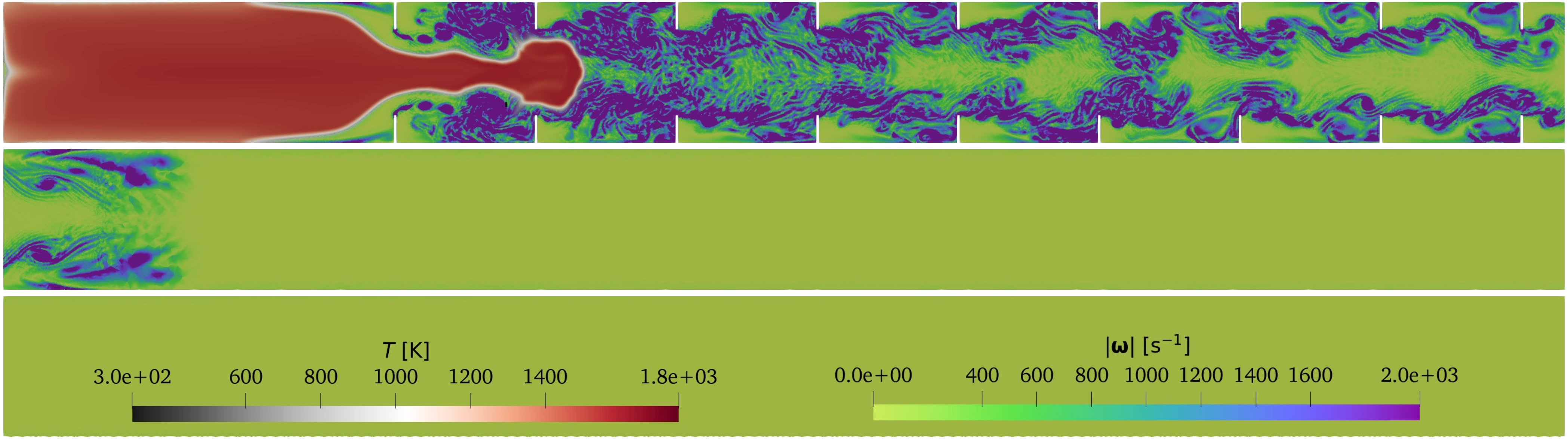

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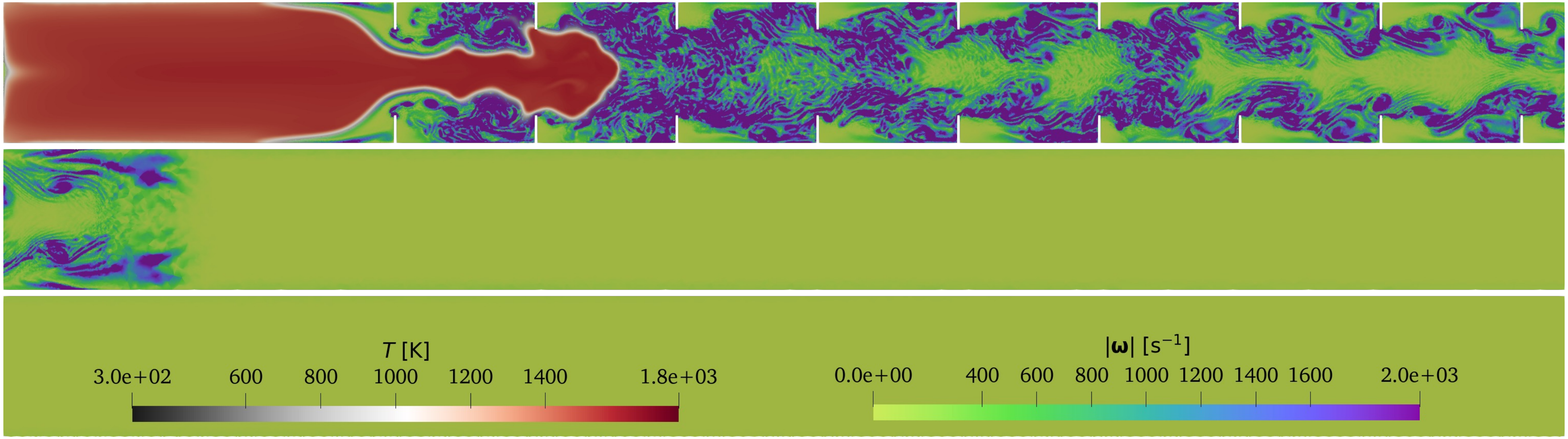

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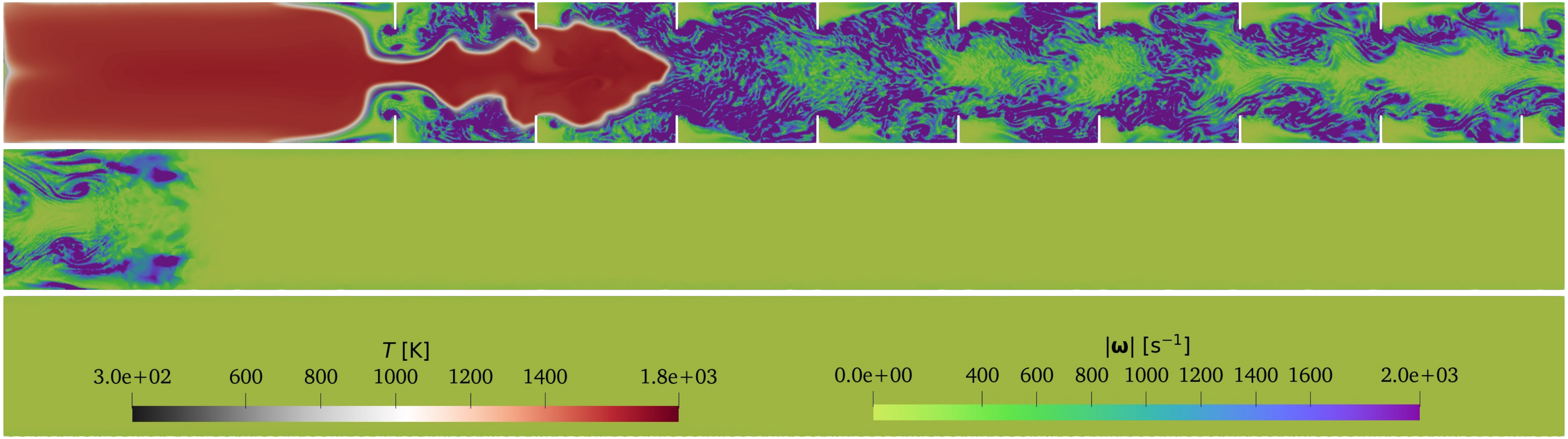

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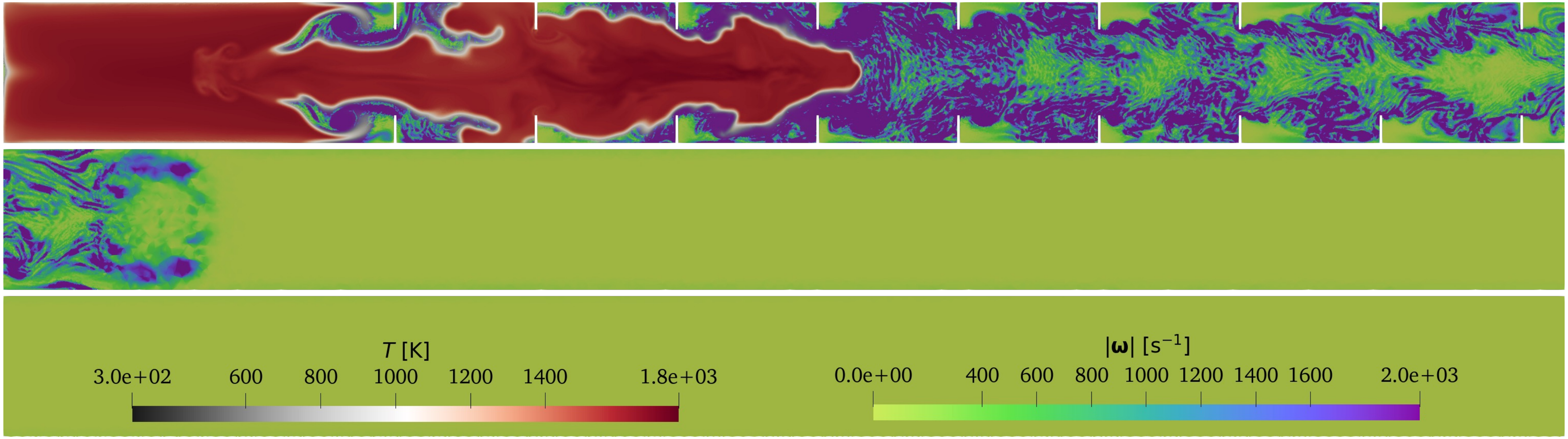

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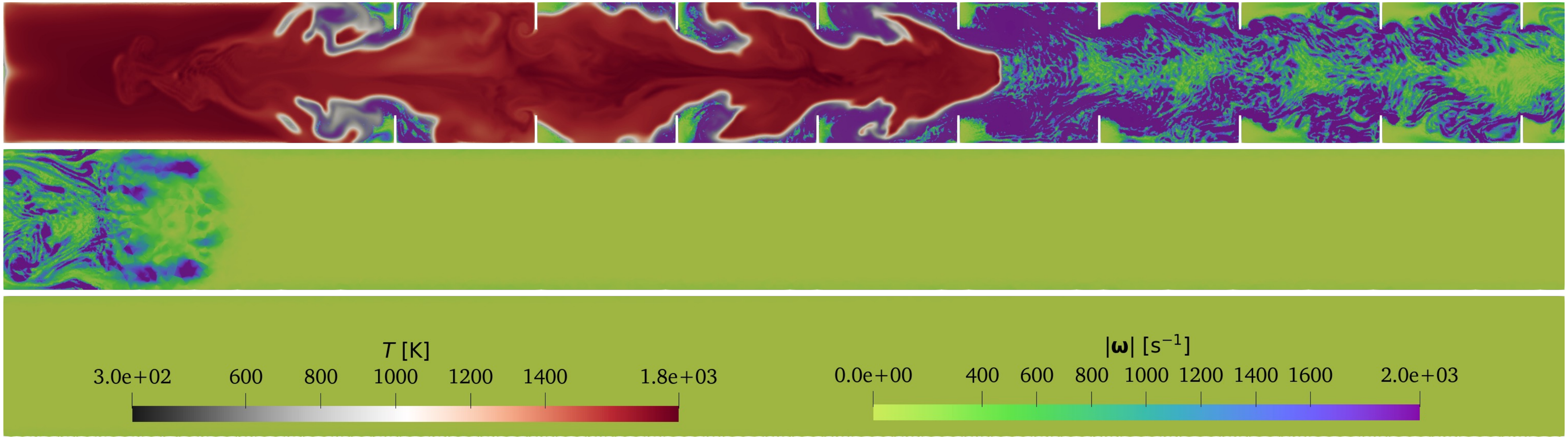

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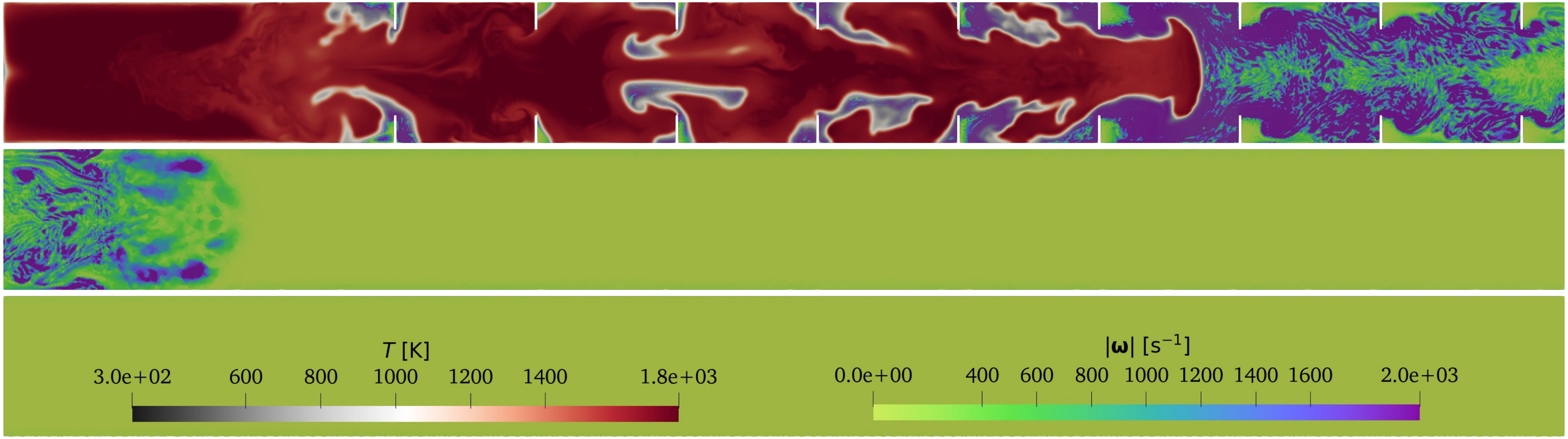

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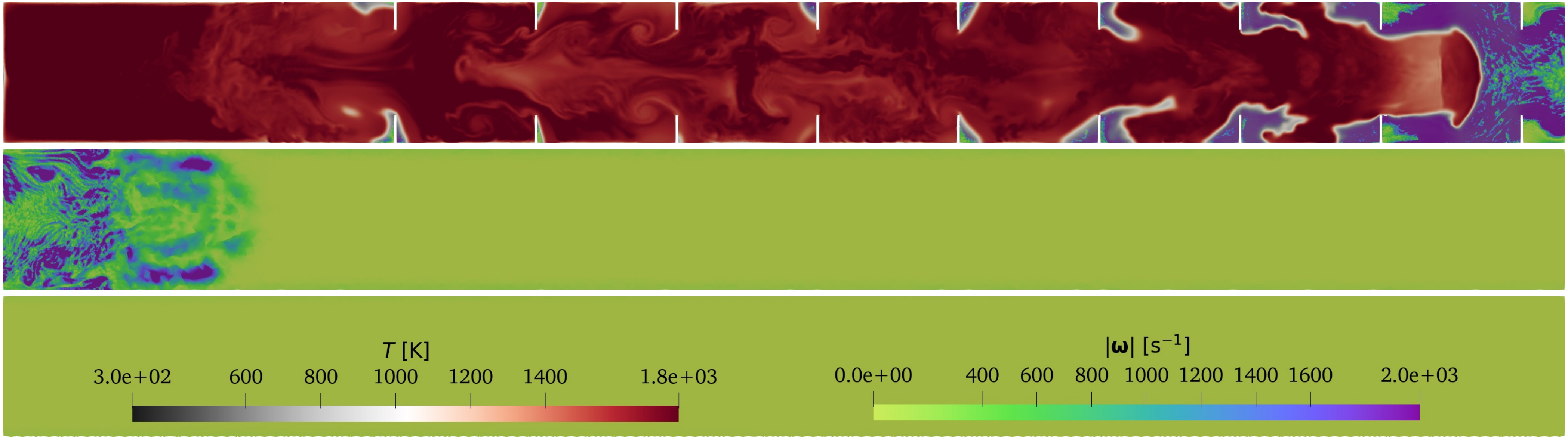

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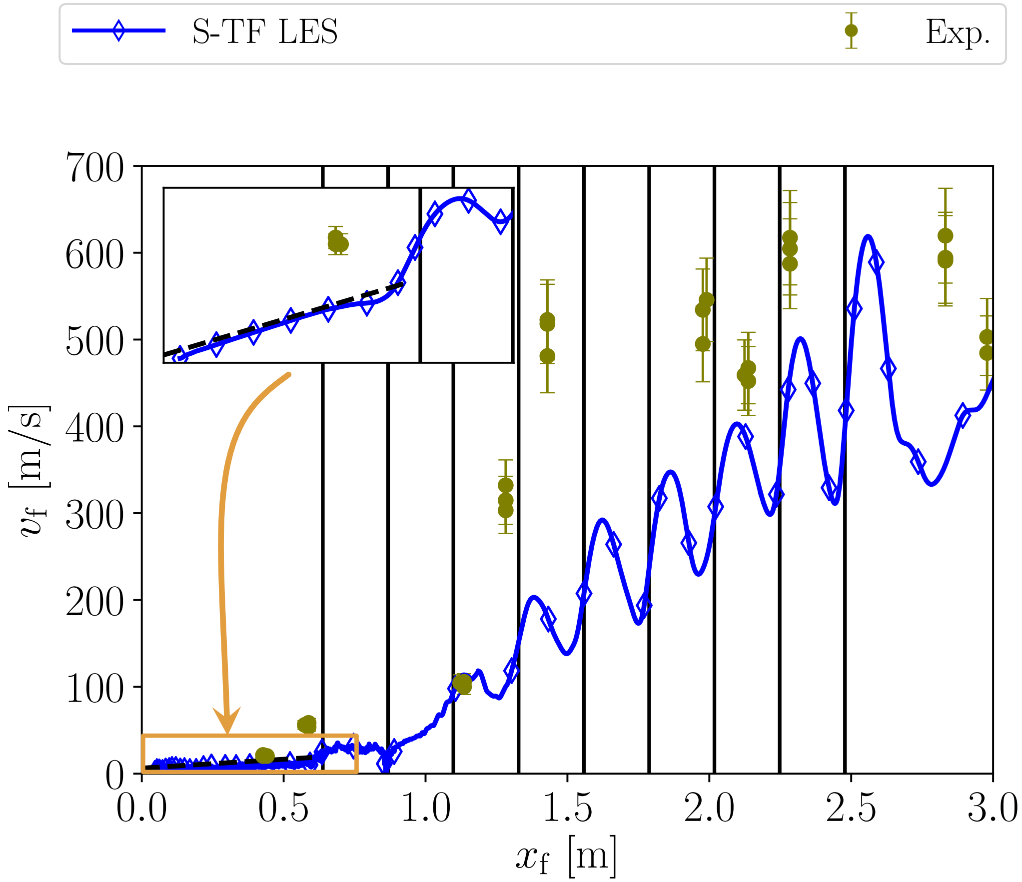
S-TF LES (correction ***S1*** only):

✗ Flame speeds too low (no account for TD instability effects)



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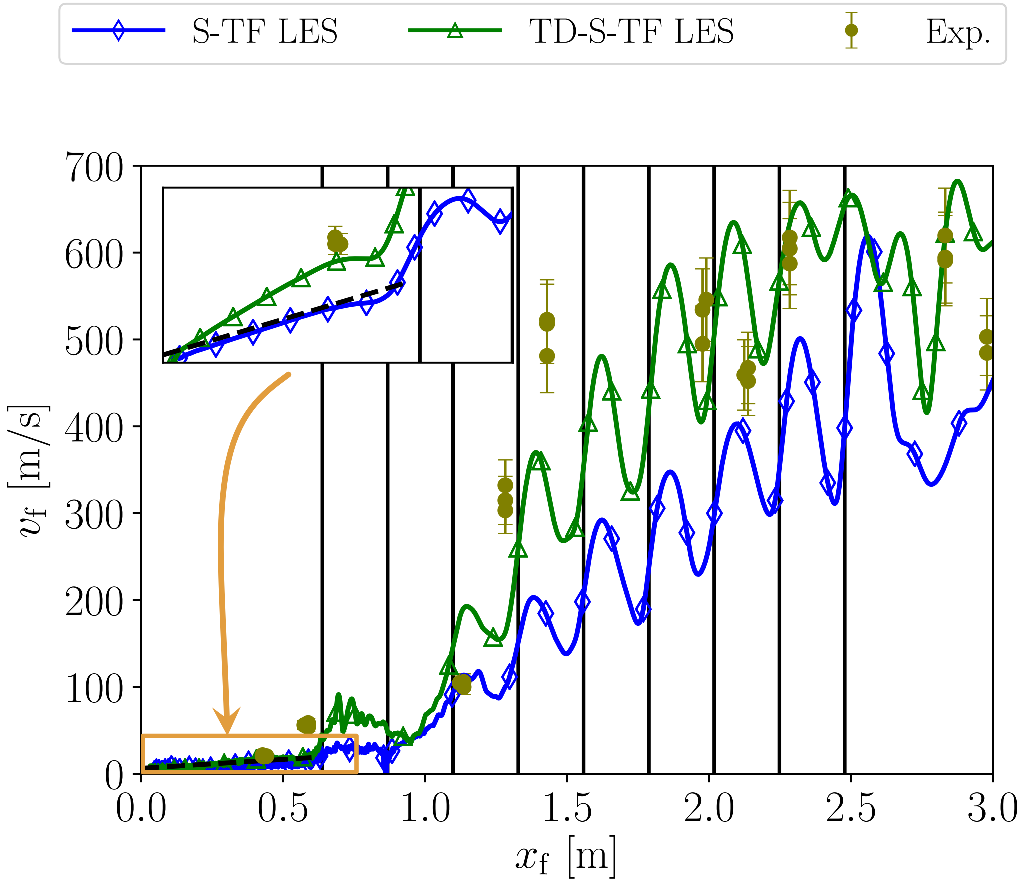

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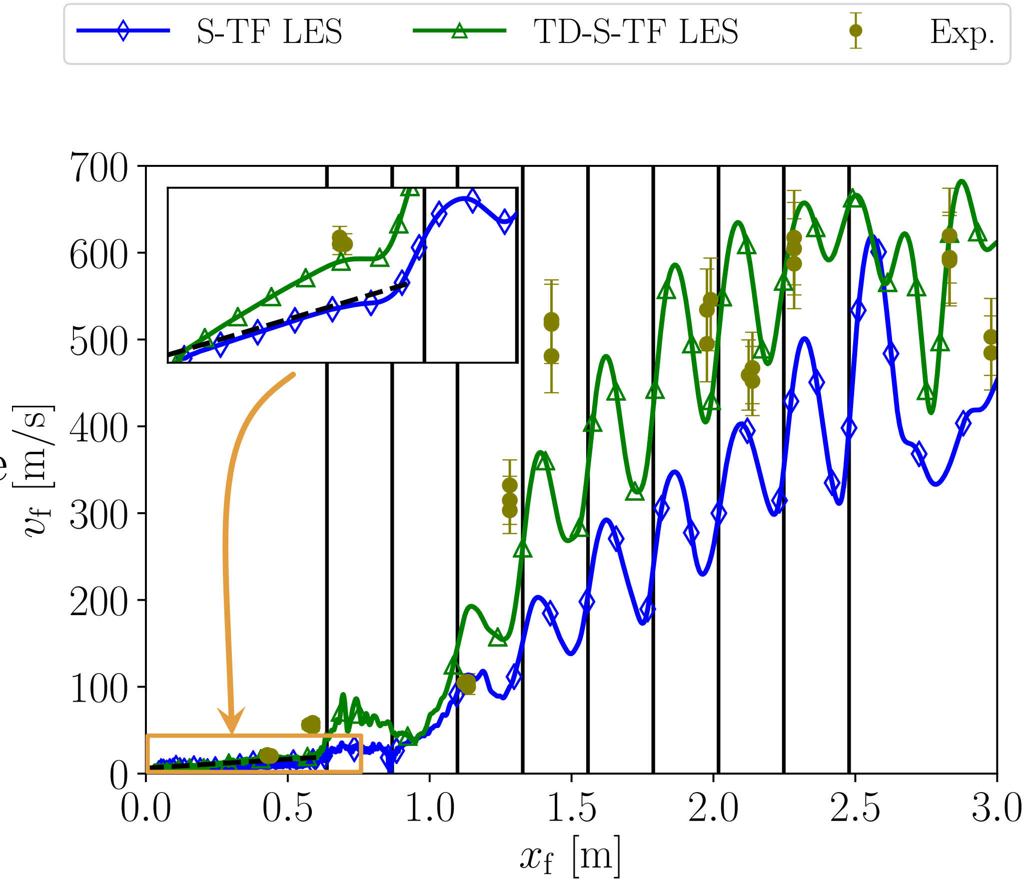
TD-S-TF LES (corrections ***S1*** and ***S2***)

✓ Correct reproduction of progressive flame acceleration scenario

✓ Right flame speed levels

- Before the obstructed region (laminar)
- Within the obstructed region



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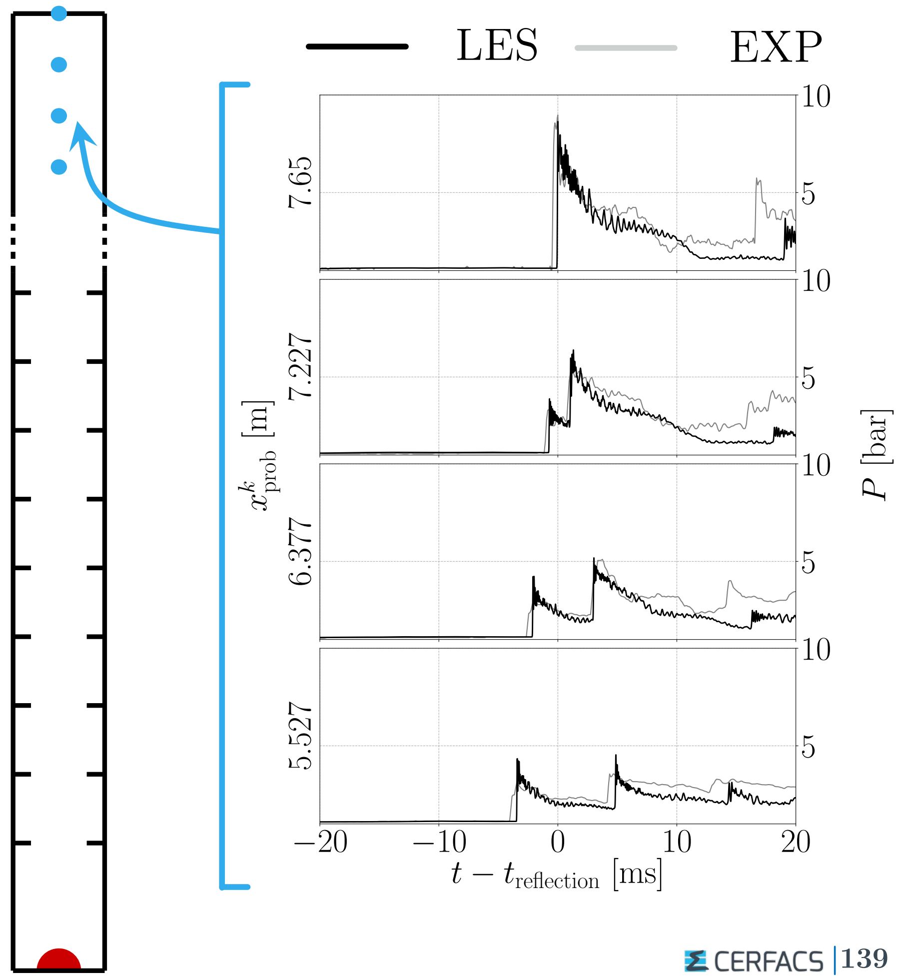
Application of the TD-S-TF model

TD-S-TF LES

- ✓ Correct reproduction of progressive flame acceleration scenario
- ✓ Right flame speed levels
- ✓ *Right pressure levels → correct prediction of the explosion damage*



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- The resulting mesh dependency questions the predictability of the standard approach and calls for new models;

Conclusions

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  ✓ Industrial-like confined and obstructed explosions.

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List of publications and communications

Publications in scientific journals

- Detomaso N., **Hok J.-J.**, Dounia O., Laera D., & Poinsot T. (2023). A generalization of the Thickened Flame model for stretched flames. *Combustion and Flame*, *258*, 113080;
- **Hok J.-J.**, Dounia O., Detomaso N., Jaravel T., Douasbin Q. & Vermorel O. (2024). A modelling strategy for the Thickened Flame simulation of propagating lean hydrogen-air flames. *International Journal of Hydrogen Energy*.
- **Hok, J.-J.**, Dounia, O., & Vermorel, O. (2025). A thickened flame model extension for the simulation of lean hydrogen-air explosions in confined environments. *Combustion and Flame*

Conferences

- **Hok J.-J.**, Dounia O., Vermorel O. & Jaravel T. (2021). « Modelling of hydrogen-air explosions in confined environments: effect of flame front thermo-diffusive instability on flame acceleration in a tube », MATHIAS TotalEnergies conference, Paris;
- **Hok J.-J.**, Vermorel O., Jaravel T. & Douasbin Q. (2022). « Modelling of hydrogen-air explosions in confined environments: on the interplay of stretch effects and thermo-diffusive instabilities », MATHIAS TotalEnergies conference, Paris;
- **Hok J.-J.**, Dounia O., Vermorel O., & Jaravel T. (2022). Effect of Flame Front Thermo-Diffusive Instability on Flame Acceleration in a Tube. *Proceedings of the 28th International Colloquium on the Dynamics of Explosions and Reactive Systems*, Napoli (Italy).
- Matas Mur, E., **Hok, J.-J.**, Dounia, O., & Douasbin, Q. (2025). A posteriori Evaluation of the Stretched-Thickened Flame Model for Accurate LES of Hydrogen Flames. *Proceedings of the 12th European Combustion Meeting*.
- Dounia, O., **Hok, J.-J.**, Meziat, F., Douasbin, Q., Jaravel, T., & Vermorel, O. (2025). Towards the large-scale modeling of turbulent combustion in fast deflagrations. *Proceedings of the 30th International Colloquium on the Dynamics of Explosions and Reactive Systems*, Ottawa (Canada).

THANK YOU


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