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A data-driven approach to correct the cell reacting fraction in the partially-stirred reactor closure for LES of premixed flames

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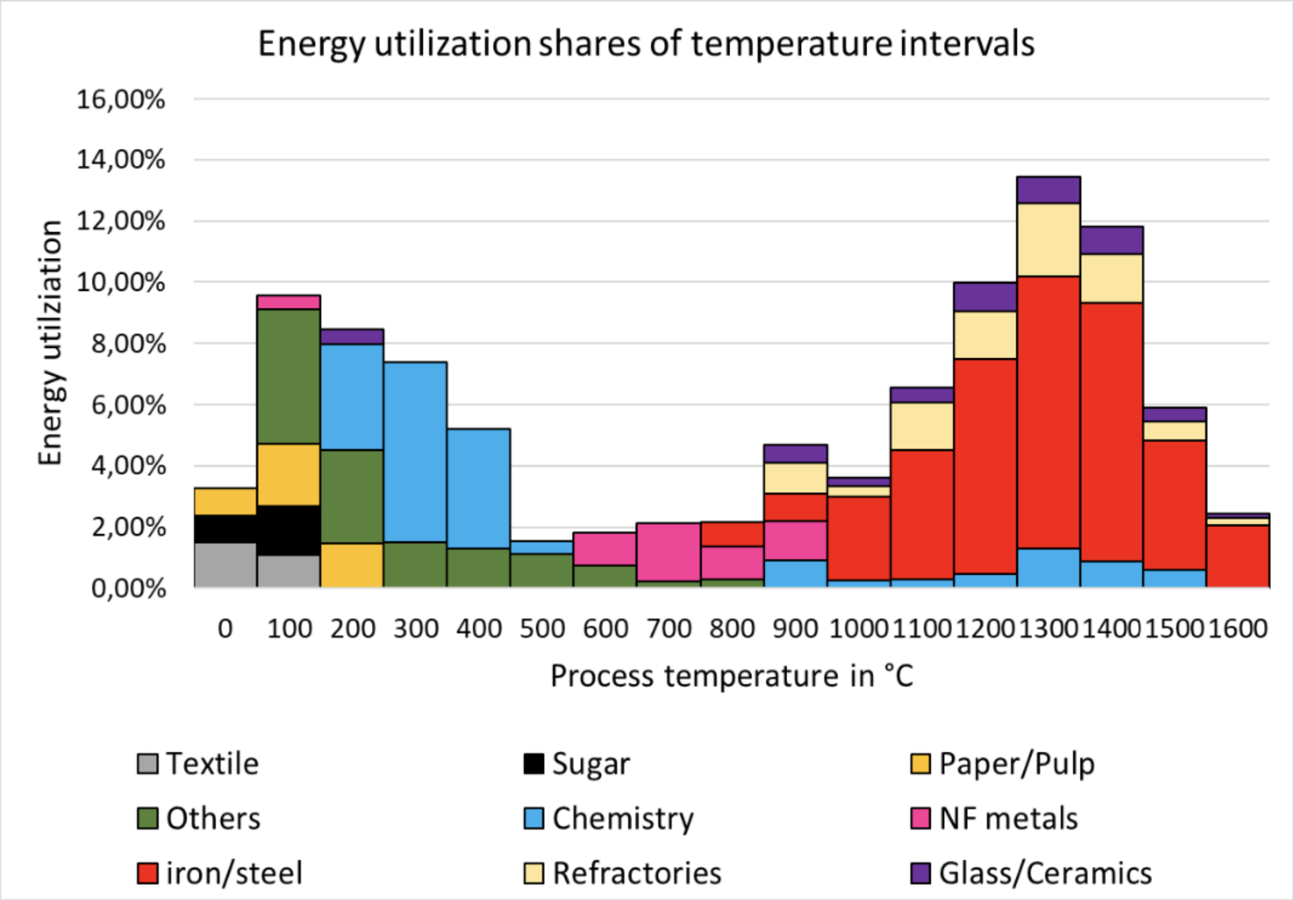
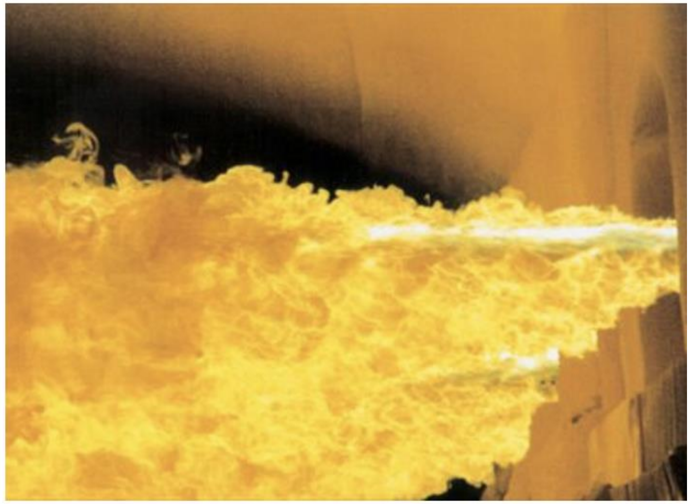
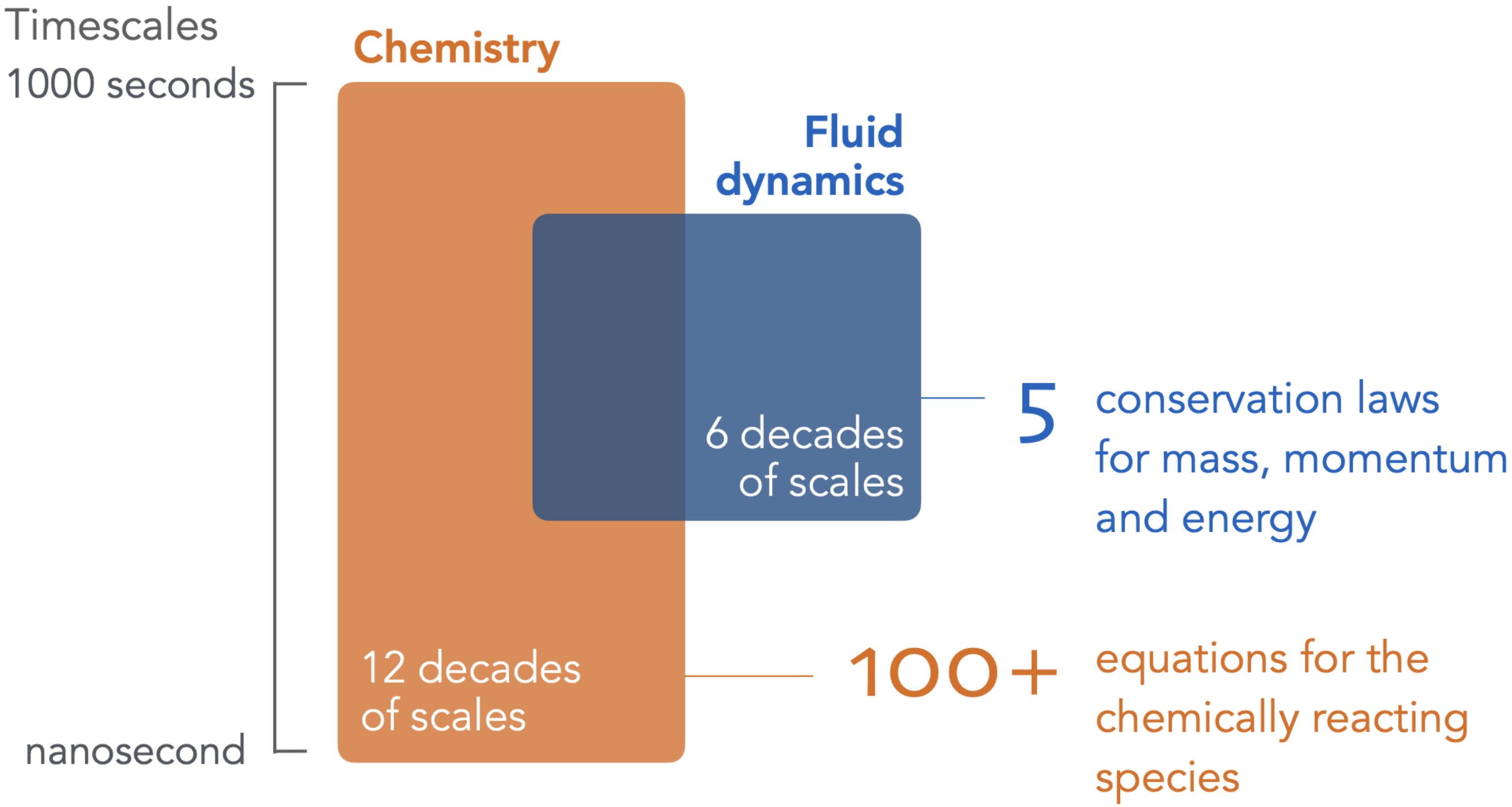
Manufacturing processes require high temperatures that cannot be reached without combustion



https://www.dena.de/fileadmin/dena/Dokumente/Pdf/9283_dena_Study_Integrated_Energy_Transition.PDF



Combustion systems are characterized by multiple scales and multi-physics processes



Turbulent combustion CFD codes are becoming more common across industries, but their current predictive capabilities fail to meet the standards needed. The prediction of **pollutant concetrations** and **stability** of the flame can be improved

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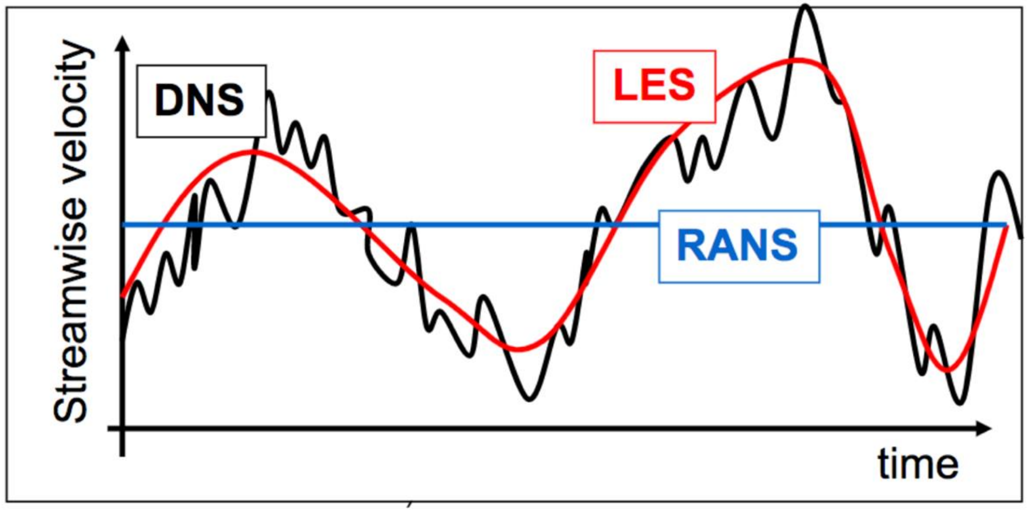
Challenge: modelling of Turbulence-Chemistry Interaction

Turbulent fluctuations can have a significant effect on chemical source terms

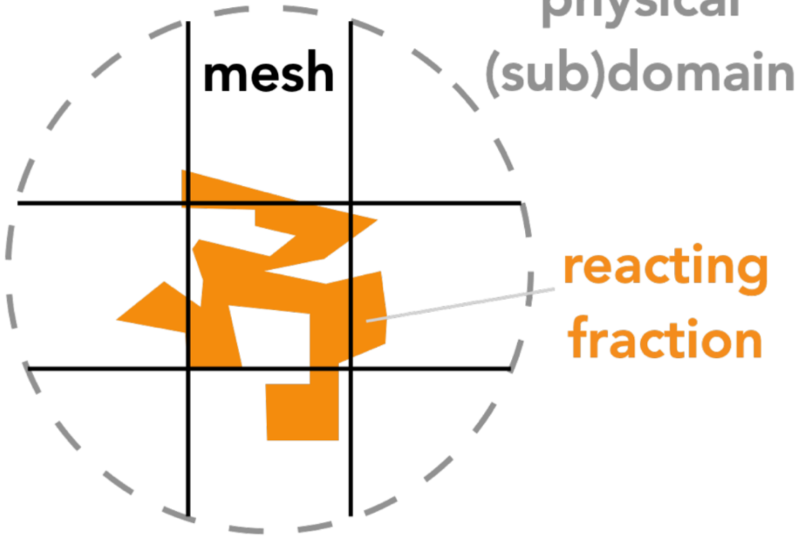


$$\overline{\dot{\omega}_k(T,Y)} \neq \dot{\omega}_k(\bar{T},\bar{Y})$$

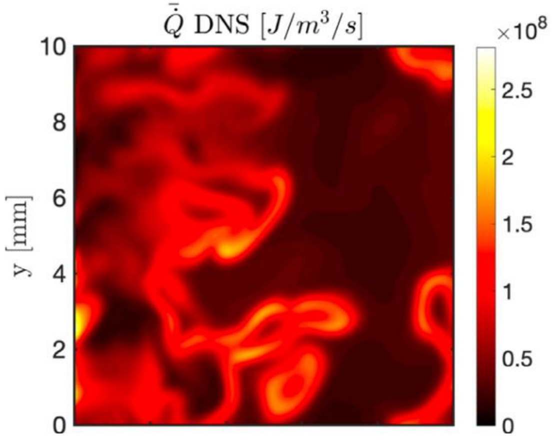
Need for a model to describe the effect of turbulent mixing on the mean reaction rates

The Partially Stirred Reactor (PaSR) showed some limitations in modelling the turbulence-chemistry interaction (TCI)

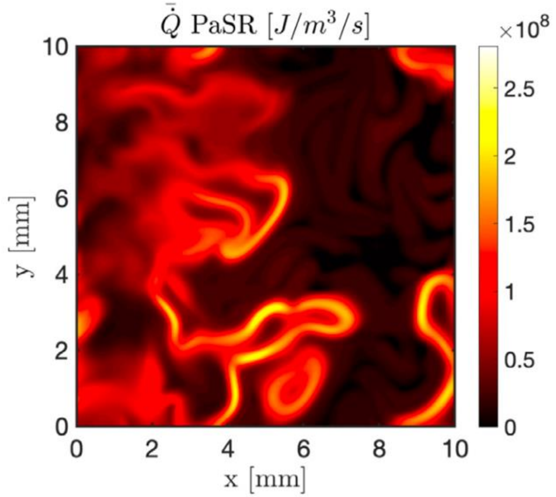
$$\bar{\dot{\omega}}_{k,\mathrm{PaSR}} = \underbrace{\frac{\tau_c}{\tau_c + \tau_m}}_{} \bar{\dot{\omega}}_{k,LFR} = \underbrace{\gamma_{PaSR}}_{} \bar{\dot{\omega}}_{k,LFR}$$



(a)



(b)



[1] Iavarone, Salvatore & Péquin, Arthur & Chen, Zhi & Doan, N. Anh Khoa & Swaminathan, N. & Parente, Alessandro. (2020). An a priori assessment of the Partially Stirred Reactor (PaSR) model for MILD combustion. Proceedings of the Combustion Institute

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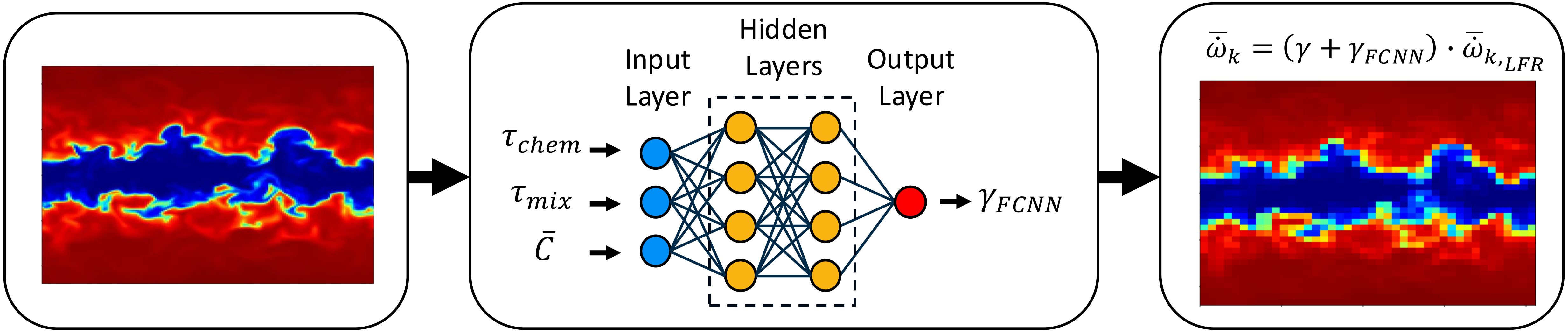
Objective: Improve PaSR using DNS data

DNS

Fully Connected Neural Network (FCNN)

LES



$$\bar{\dot{\omega}}_k = (\gamma + \gamma_{FCNN}) \cdot \bar{\dot{\omega}}_{k,LFR}$$

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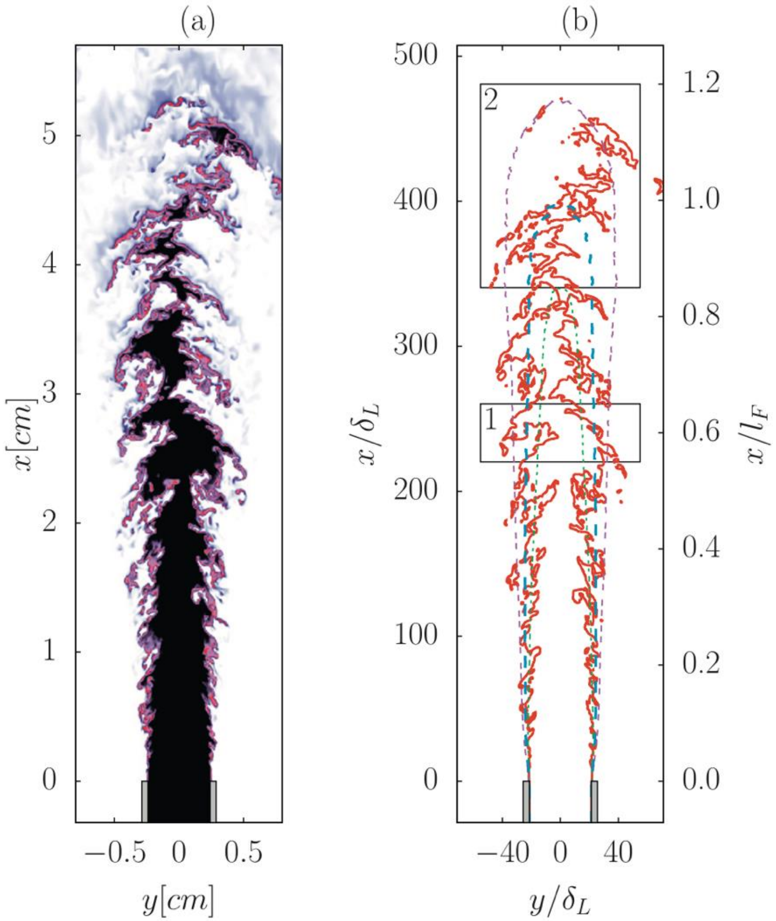
DNS dataset used to train the model

Slot turbulent **CH4 premixed jet flame.**

Data provided by Professor Antonio Attili

- **Equivalence ratio:** $\phi = 0.7$
- **Inlet temperature:** 800 K
- **Laminar flame speed:** 1 m/s
- **Thermal thickness:** 110 μm → 6 DNS cells
- **Jet velocity:** 100 m/s
- **Coflow velocity:** 15 m/s



[2] A. Attili, S. Luca, D. Denker, F. Bisetti, H. Pitsch. Turbulent flame speed and reaction layer thickening in premixed jet flames at constant Karlovitz and increasing Reynolds numbers. Proceedings of the Combustion Institute. 2020

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Fully Connected Neural Network (FCNN) Architecture and training parameters

The filtering of the DNS data was performed by Dr. Arthur Pequin, a first setup of the FCNN is provided by Dr. Rodolfo Freitas.

- **Input:** Progress Variable $\bar{C}$, Chemical Timescale τ_c, Mixing Timescale τ_m.
- **Output:** Cell reacting fraction correction γ_{FCNN}.
- **Architecture:** 3 input, 6 hidden layers, 64 neurons per layer, 1 output.
- **Learning Rate:** 1e-3, **Number of epochs:** 1000.
- **Loss function:** $\left\| \bar{\dot{Q}}_{pred} - \bar{\dot{Q}}_{DNS} \right\|_2$

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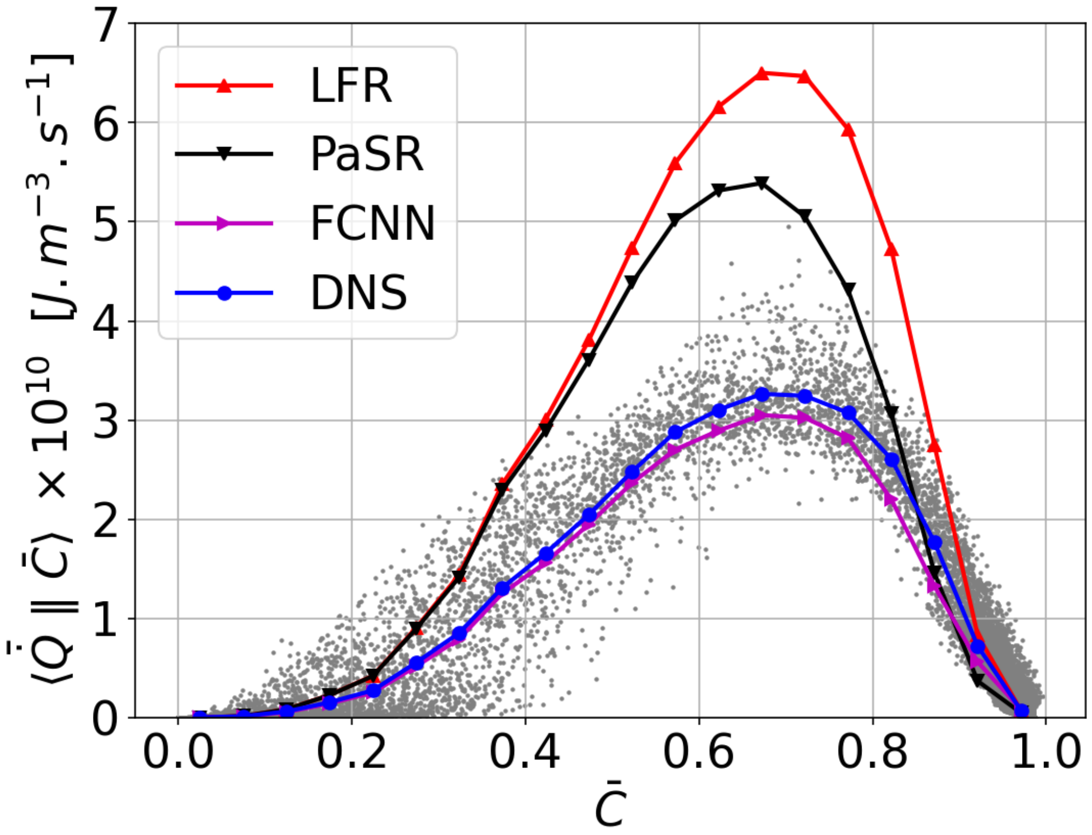
The Machine Learning-Enhanced PaSR can drastically improve the predictions compared with classic PaSR

Model 1

Input: $\bar{C}$ τ_c τ_m

Training: $\Delta = 6$

Train-Test split:
70% - 30%



$\Delta = 6$

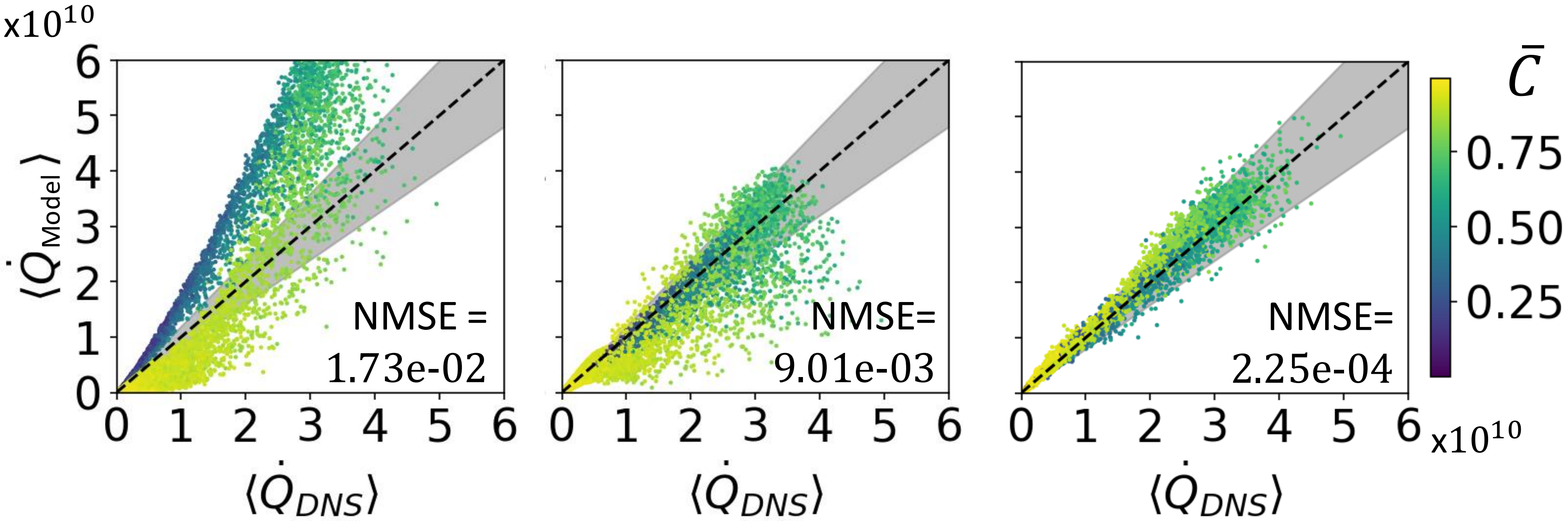
Can this model still be improved?

Adding spatial information improves the performance of the model

PaSR **Model 1** **Model 2**

Model 1: $\bar{C}$ τ_c τ_m

Model 2: $\nabla^2\bar{C}$ $\nabla\bar{C}$ $\bar{C}$ τ_c τ_m



$$\Delta = 6$$

$\dot{Q}$ = heat release rate

$[\dot{Q}] = [J \cdot m^{-3} \cdot s^{-1}]$

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Adding spatial information improves the performance of the model

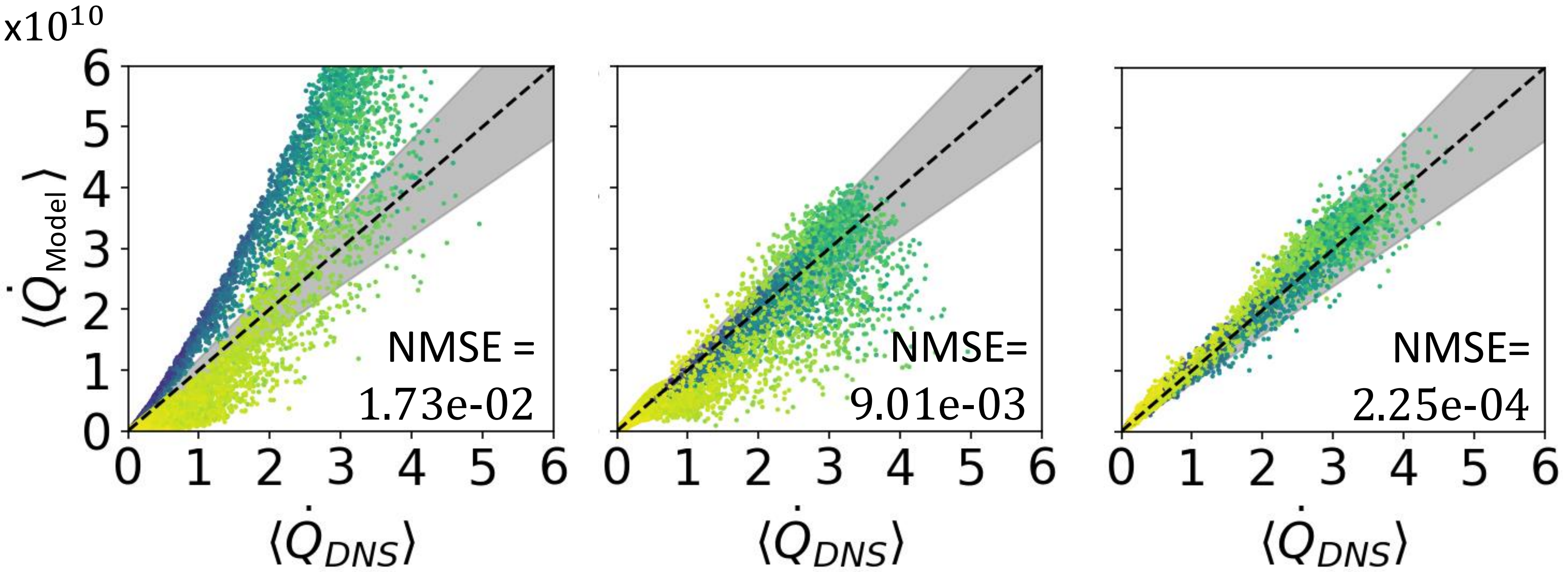
PaSR

Model 1

$\bar{C}$ τ_c τ_m

Model 2

$\nabla^2\bar{C}$ $\nabla\bar{C}$ $\bar{C}$ τ_c τ_m



How does the model generalize on different filter widths?

$$\Delta = 6$$

$\dot{Q}$ = heat release rate
$[\dot{Q}] = [J \cdot m^{-3} \cdot s^{-1}]$

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Testing on different filter sizes shows poor generalizability

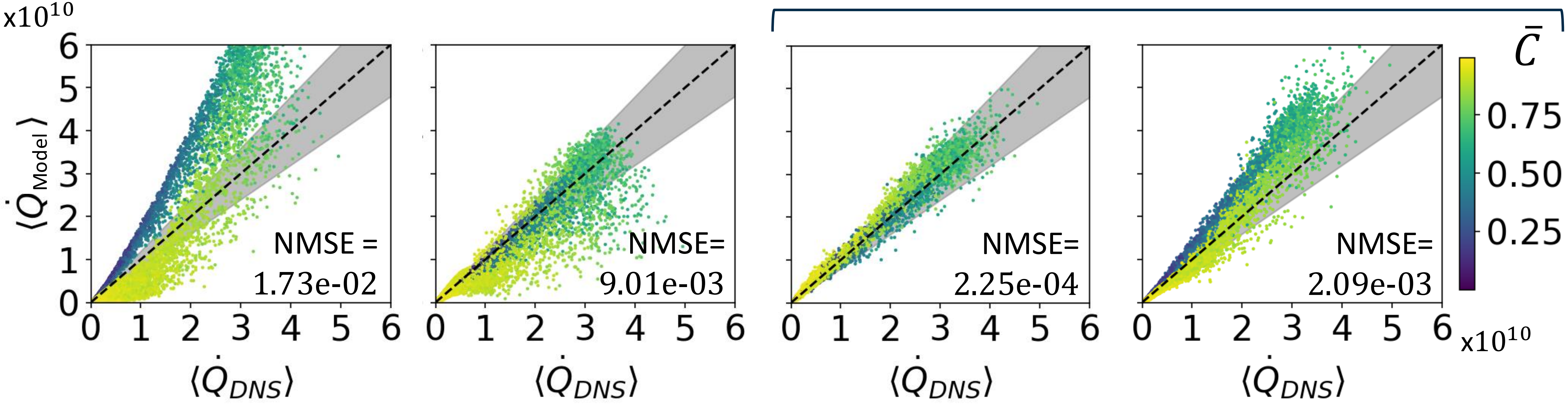
PaSR

Model 1

$\bar{C}$ τ_c τ_m

Model 2

$\nabla^2\bar{C}$ $\nabla\bar{C}$ $\bar{C}$ τ_c τ_m



$\Delta = 6$

$\Delta = 3 \rightarrow \Delta = 6$

$\dot{Q}$ = heat release rate
$[\dot{Q}] = [J \cdot m^{-3} \cdot s^{-1}]$

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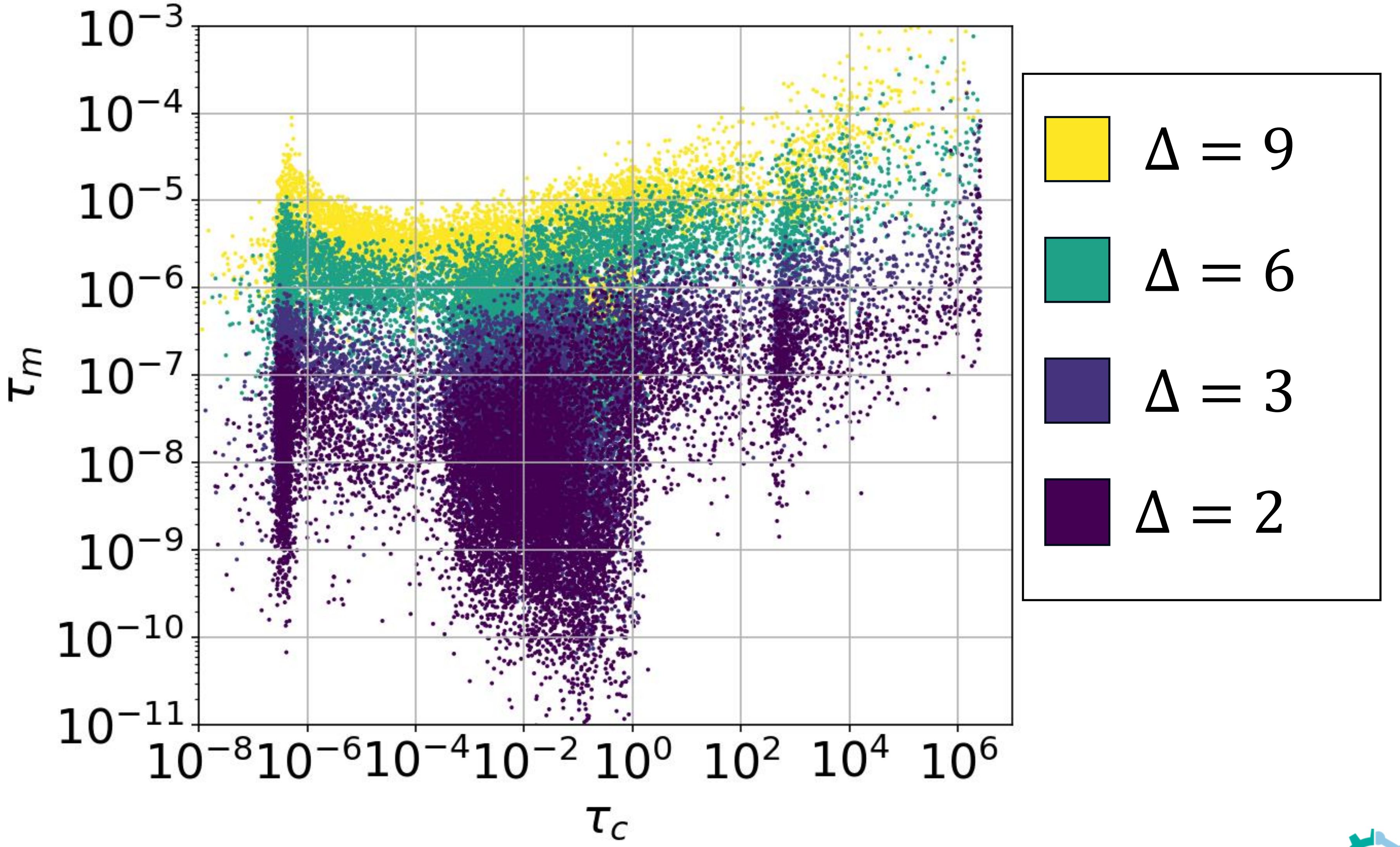
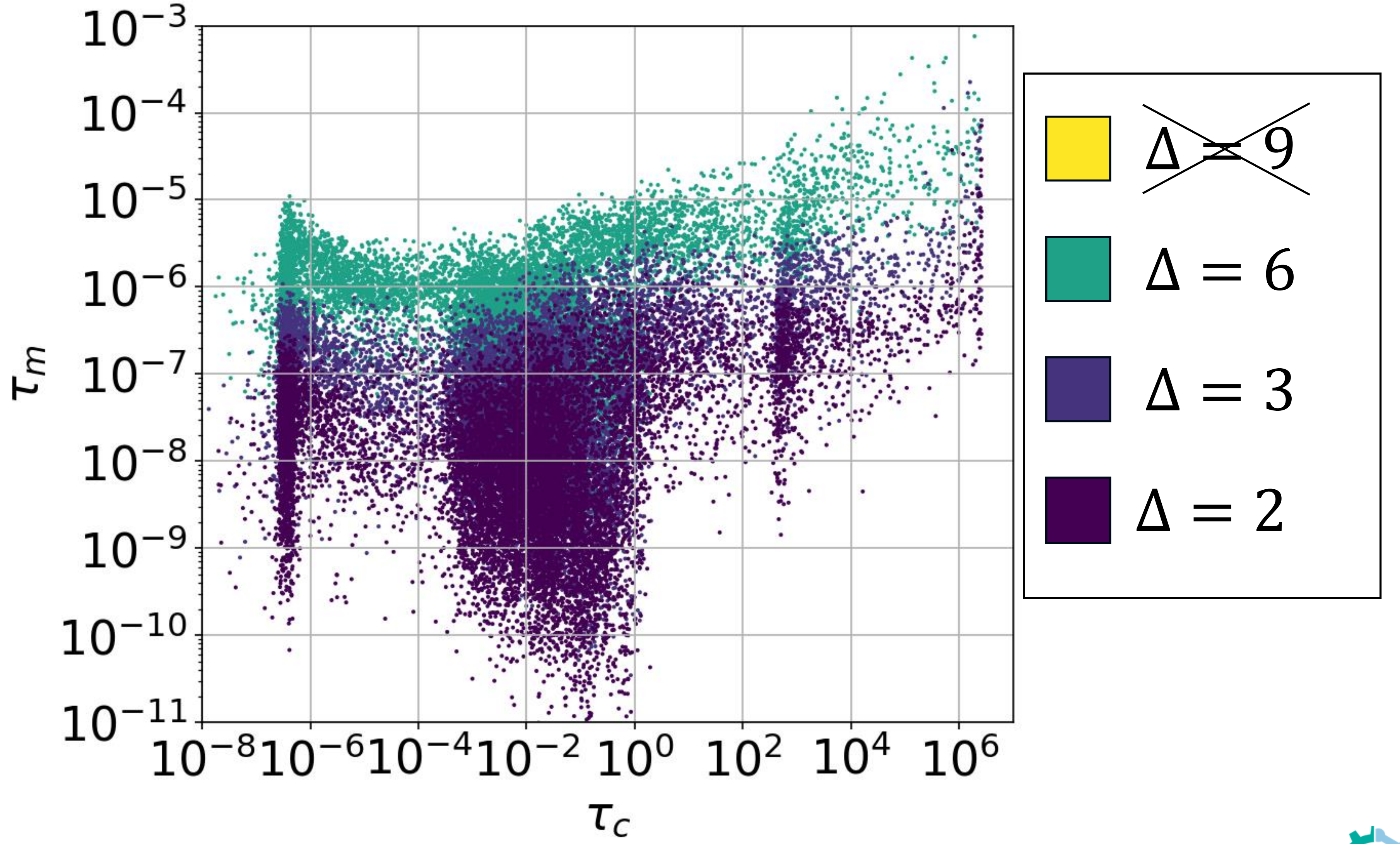
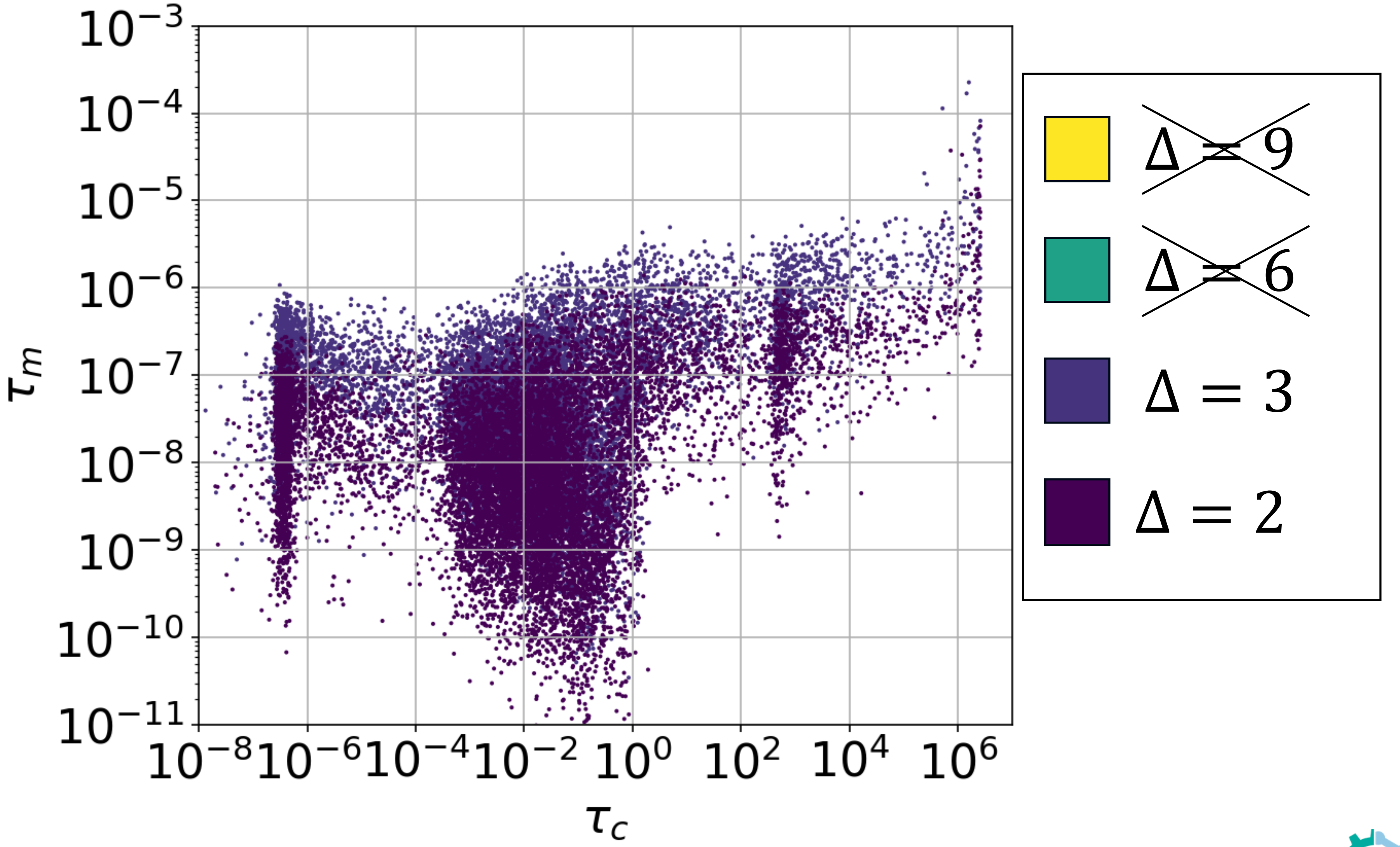
Why did we obtain poor generalizability? Input Parameters Space



Why did we obtain poor generalizability? Input Parameters Space

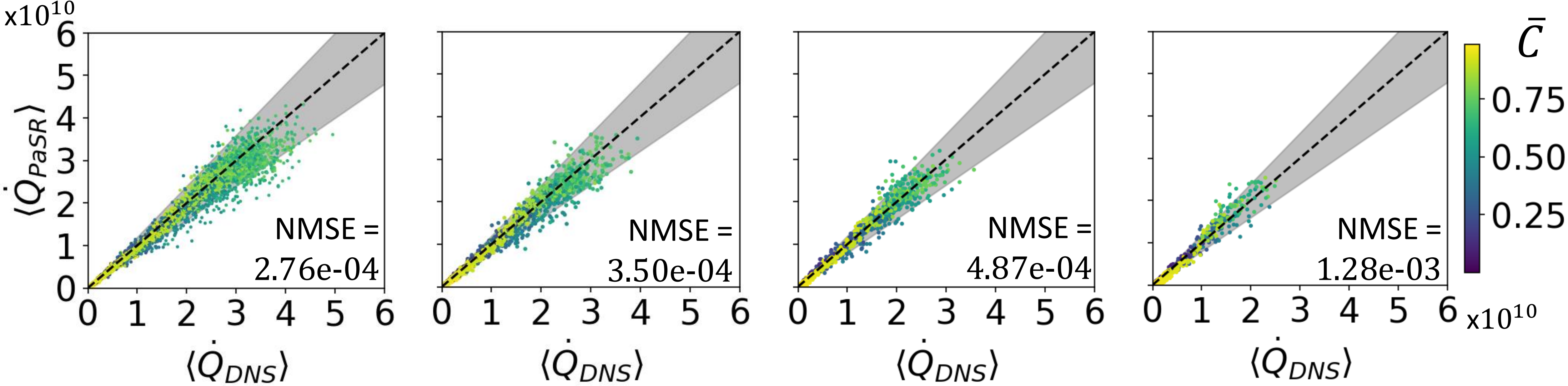


Why did we obtain poor generalizability? Input Parameters Space



Training on different filter sizes (2, 3, 6, 9) extends the generalizability of the model

Model 3 Input: $\nabla^2\bar{C}$ $\nabla\bar{C}$ $\bar{C}$ τ_c τ_m Training: $\Delta = 2, 3, 6, 9$



$\Delta = 6$ $\Delta = 9$ $\Delta = 12$ $\Delta = 18$

Seen data

Unseen data

$\dot{Q}$ = heat release rate
$[\dot{Q}] = [J \cdot m^{-3} \cdot s^{-1}]$

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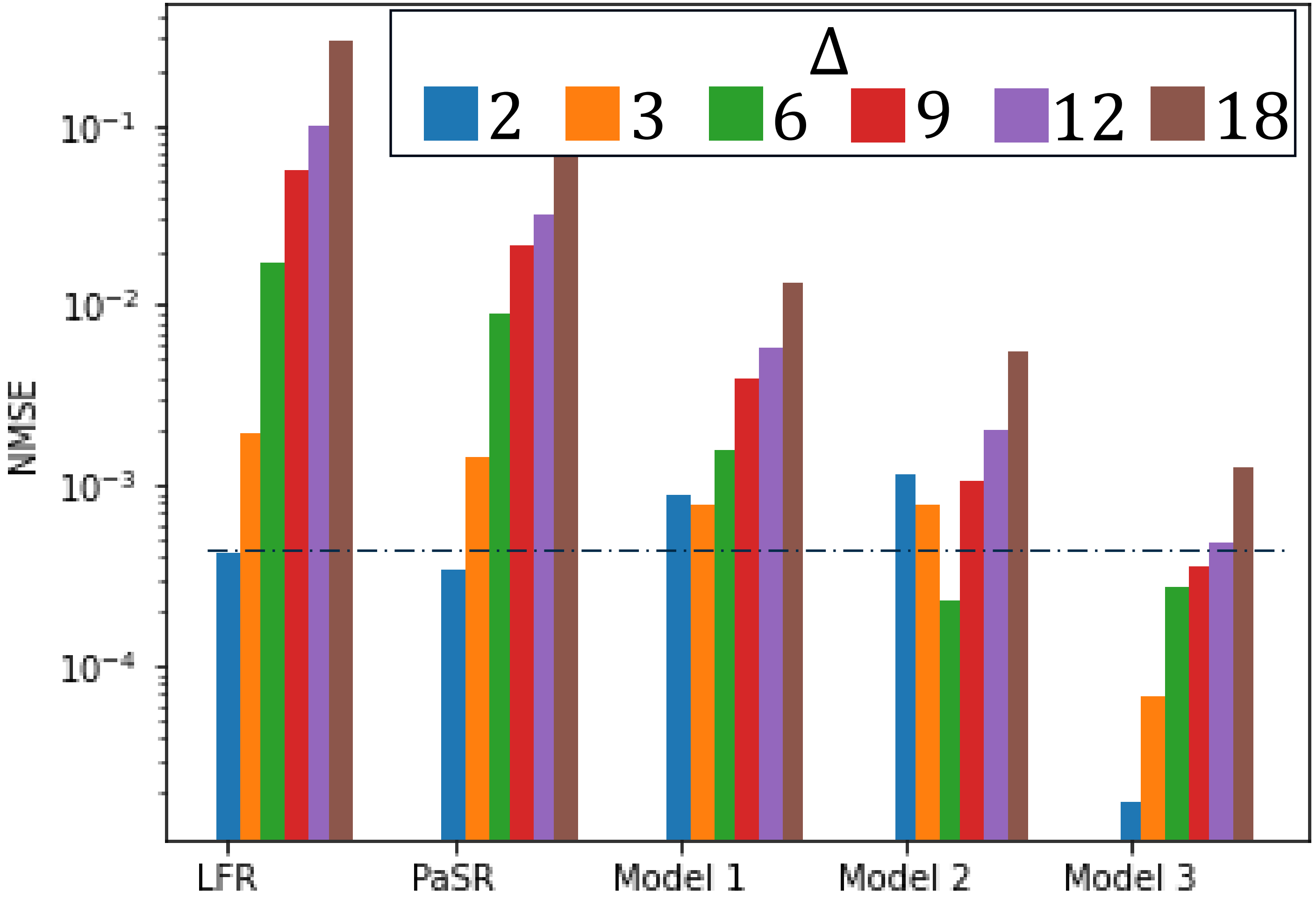
The model accuracy is improved with the Machine Learning Enhanced closure



Model 1

Input: $\bar{C}$ τ_c τ_m

Training: $\Delta = 6$

Model 2

Input: $\nabla^2\bar{C}$ $\nabla\bar{C}$ $\bar{C}$ τ_c τ_m

Training : $\Delta = 6$

Model 3

Input: $\nabla^2\bar{C}$ $\nabla\bar{C}$ $\bar{C}$ τ_c τ_m

Training: $\Delta = 2, 3, 6, 9$

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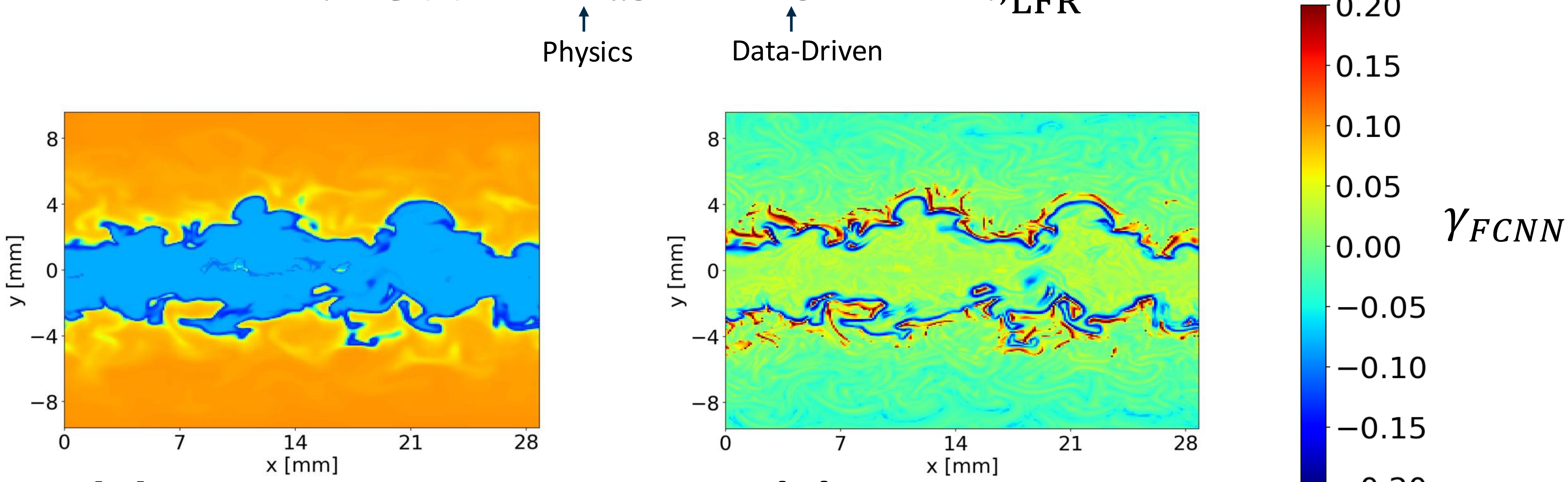
Adding spatial information improves the sparsity of the model

$$(\bar{\dot{\omega}}_k)_{\mathrm{FCNN}} = (\underset{\substack{\uparrow \\ \text{Physics}}}{\gamma_{PaSR}} + \underset{\substack{\uparrow \\ \text{Data-Driven}}}{\gamma_{FCNN}}) \cdot \bar{\dot{\omega}}_{k,\mathrm{LFR}}$$



Model 1

Input: $\bar{C}$ τ_c τ_m

Training: $\Delta = 6$

Model 3

Input: $\nabla^2\bar{C}$ $\nabla\bar{C}$ $\bar{C}$ τ_c τ_m

Training: $\Delta = 2, 3, 6, 9$

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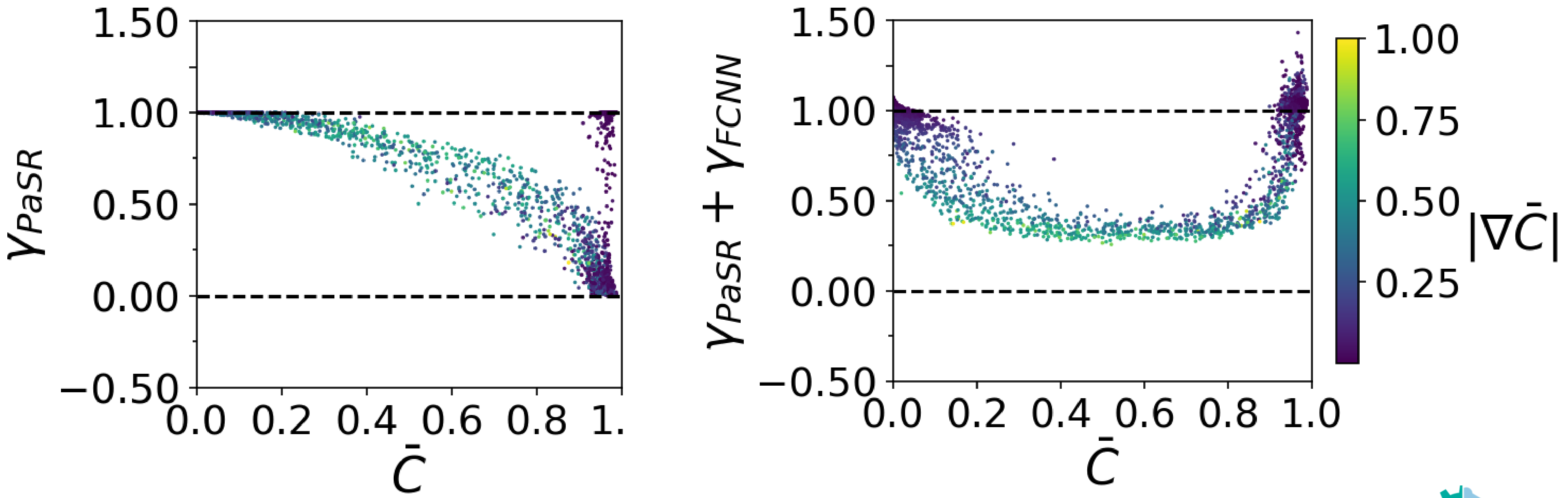
To obtain optimal results we need values of the cell reacting fraction that outbound the physical limits (between 0 and 1)

$$(\bar{\dot{\omega}}_k)_{\mathrm{FCNN}} = (\underset{\uparrow}{\gamma_{PaSR}} + \underset{\uparrow}{\gamma_{FCNN}}) \cdot \bar{\dot{\omega}}_{k,\mathrm{LFR}}$$

Physics

Data-Driven



Key Takeaways

- Using **spatial information** based on the progress variable as inputs of the FCNN improved the accuracy and the sparsity of the model

- **Training on different filter sizes** improved the generalizability of the model, without explicitly using the filter size as input

- Optimal results require the cell reacting fraction to **outbound its physical limits** (between 0 and 1)

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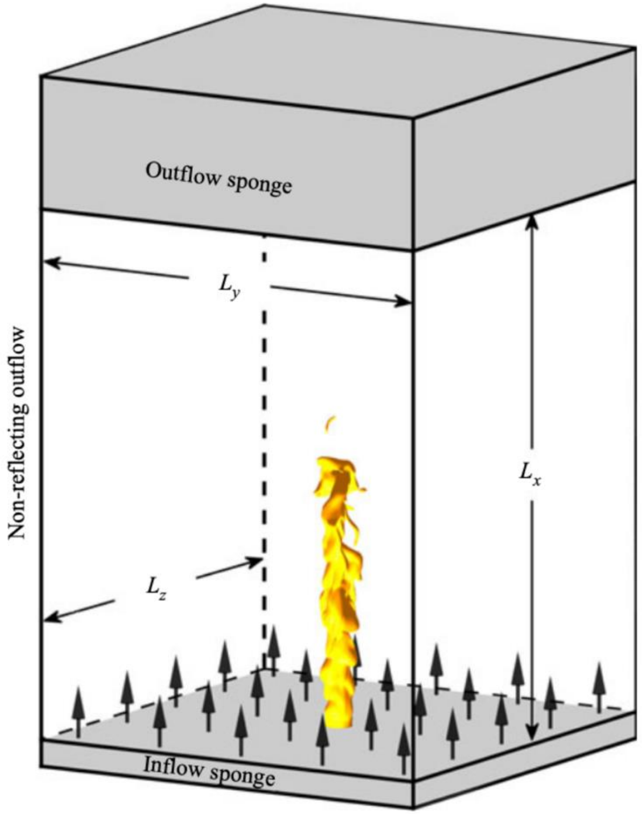
Further Steps

- Test the model a-priori on another flame

  (Premixed CH4) [4]

- Test the model a-posteriori

- Try the same approach on non-premixed flames



[4] Brouzet D, Talei M, Brear MJ, Cuenot B. The impact of chemical modelling on turbulent premixed flame acoustics. *Journal of Fluid Mechanics*. 2021.
[5] Chung, Wai Tong, Matthias Ihme, Ki Sung Jung, Jacqueline H. Chen, Jack Guo, Davy Brouzet, Mohsen Talei, et al. 'Blastnet Simulation Dataset'. Zenodo, 27 February 2024. https://doi.org/10.5281/zenodo.10732791.

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Thank you for your attention 😃

Any questions?

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Backup Slides

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The inputs selected for the FCNN describe turbulence, chemistry, and the flame structure

Chemical Timescale

$$\frac{1}{\tau_c} = \max\left(\frac{-\bar{\dot{\omega}}_F}{\bar{Y}_F}, \frac{-\bar{\dot{\omega}}_O}{\bar{Y}_O}\right)/\rho$$

Mixing Timescale

$$\tau_m = \frac{\overline{C''}}{\bar{\epsilon}_C} = \frac{C_z|\nabla\,\bar{C}|^2}{2(D + D_t)|\nabla\,\bar{C}|^2}$$

Progress Variable

$$\bar{C} = \frac{\bar{Y}_{O2} - \bar{Y}_{O2_u}}{\bar{Y}_{O2_b} - \bar{Y}_{O2_u}}$$

[4] Raman, V., Pitsch, H. A consistent LES/filtered-density function formulation for the simulation of turbulent flames with detailed chemistry. Proceedings of the Combustion Institute 31 (2007)

[5] Chomiak, J., 1990. Combustion a study in theory, fact and application.

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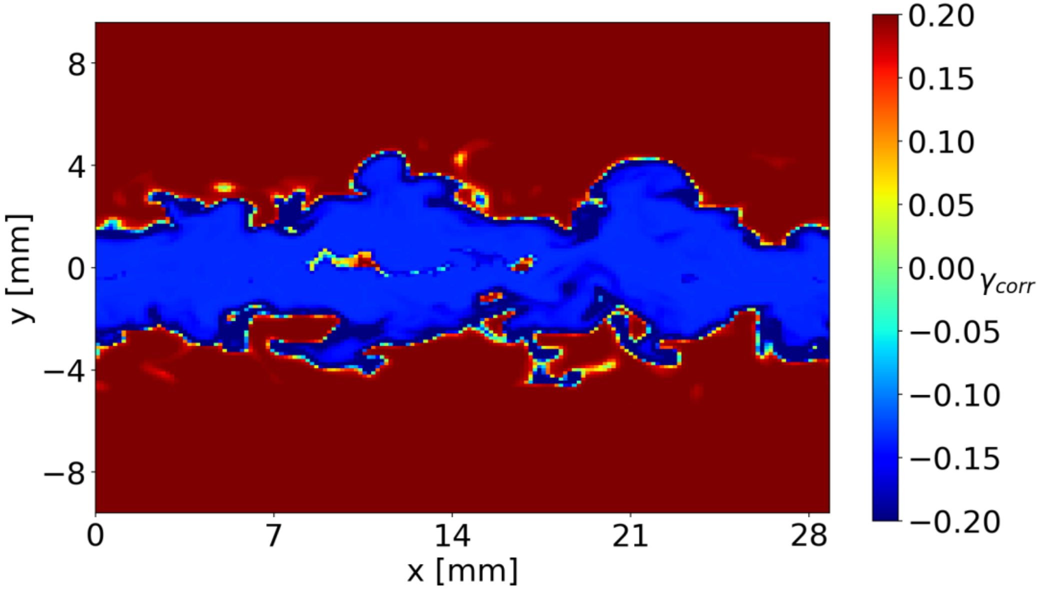
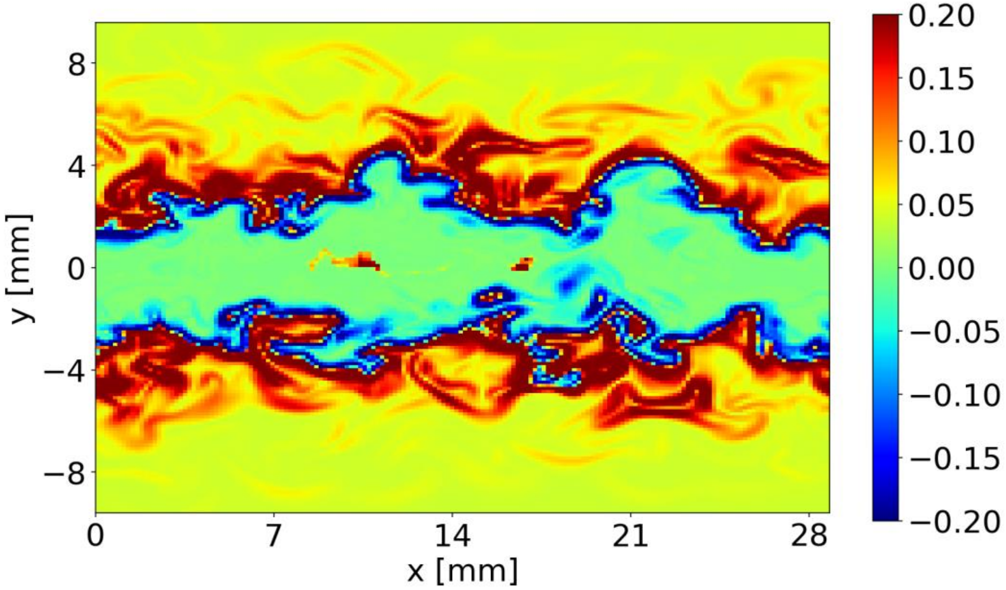
Why a FCNN?

1. Pointwise calculation, easy to implement in CFD
2. Capability of understanding spatial patterns if we input the derivative terms (already computed in CFD codes)



Input parameters: $T, \tau_{chem}, \tau_{mix}$



Input parameters: $T, |\nabla T|, \tau_{chem}, \tau_{mix}$

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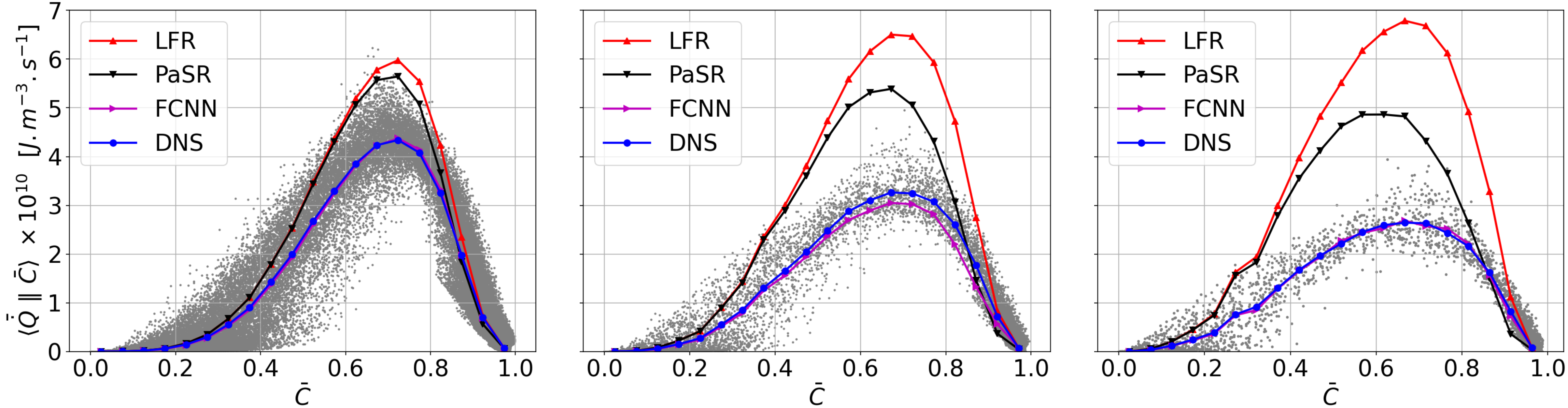
A FCNN can drastically improve the predictions compared with classic PaSR

Input parameters: $\bar{\text{C}}, \tau_{chem}, \tau_{mix},$

Train-Test split: 70% - 30%



$\Delta = 3$

$\Delta = 6$

$\Delta = 9$

Can this model still be improved?

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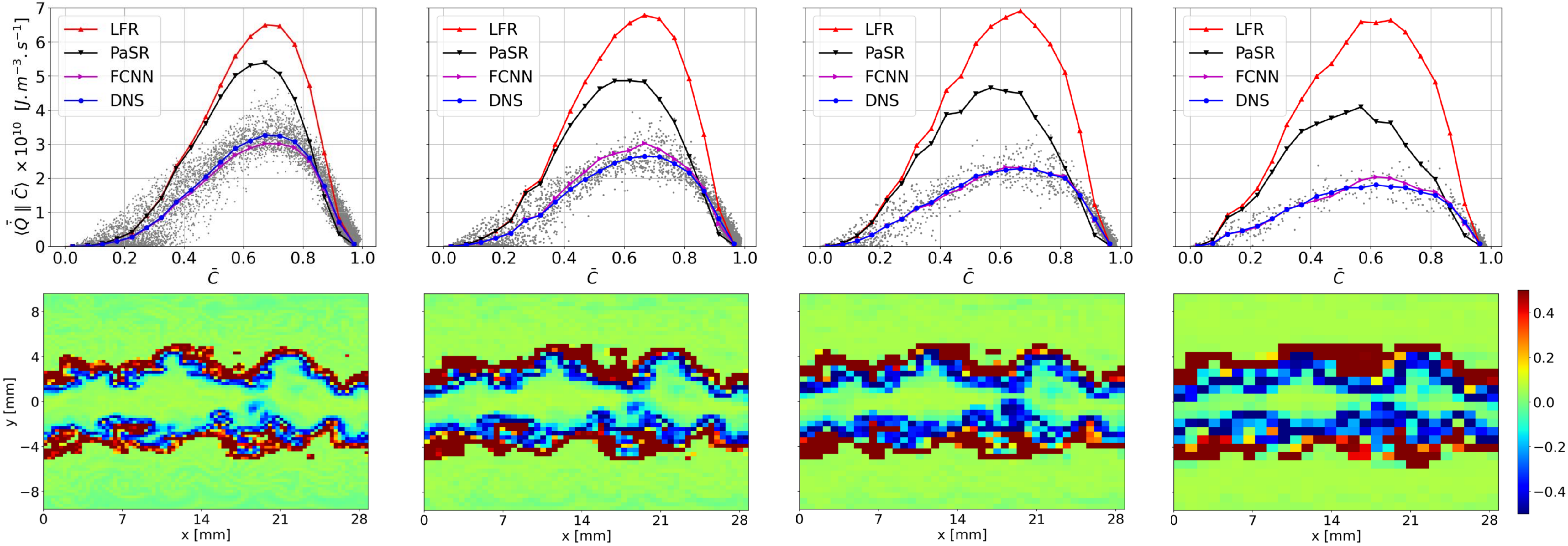
Training on different filter sizes (2, 3, 6, 9) extends the generalizability of the model

Input parameters: C, $|\nabla C|$, $\nabla^2 C$, τ_{chem}, τ_{mix}



$\Delta = 6$ $\Delta = 9$ $\Delta = 12$ $\Delta = 18$

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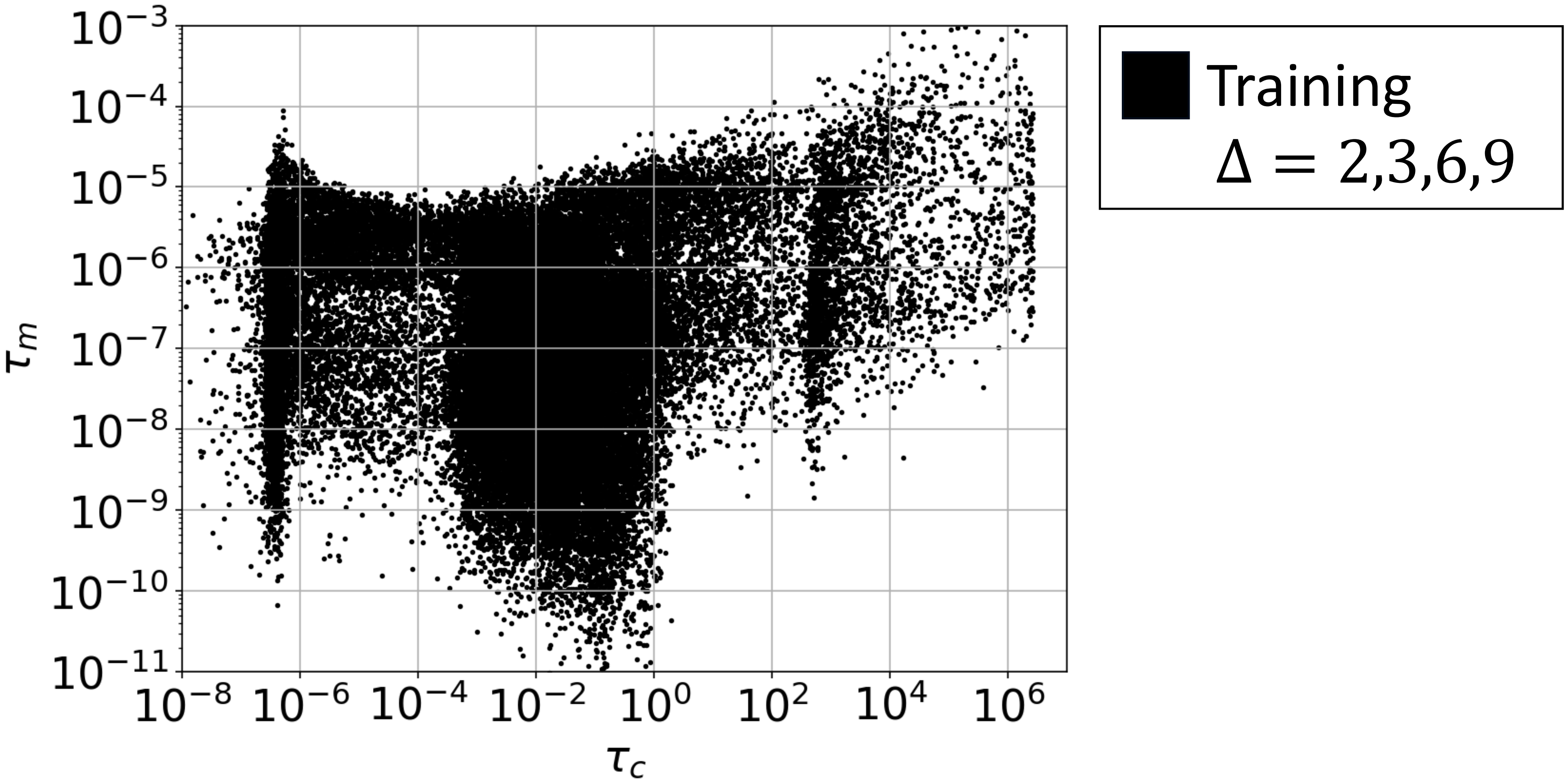
Training on different filter sizes (2, 3, 6, 9) extends the generalizability of the model



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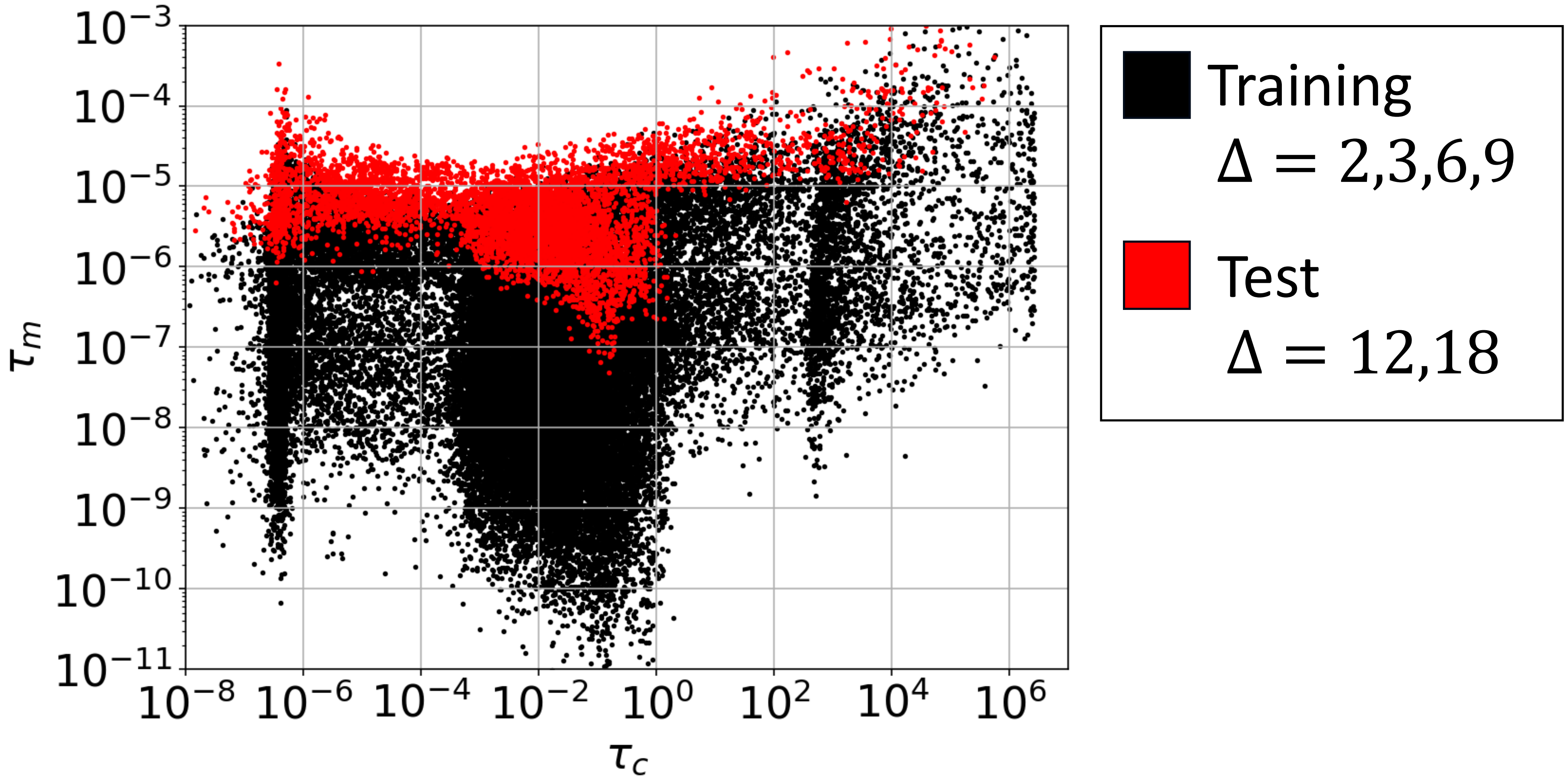

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