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Data-driven boiling predictions: introducing the neural-gated mixture of engineering models approach

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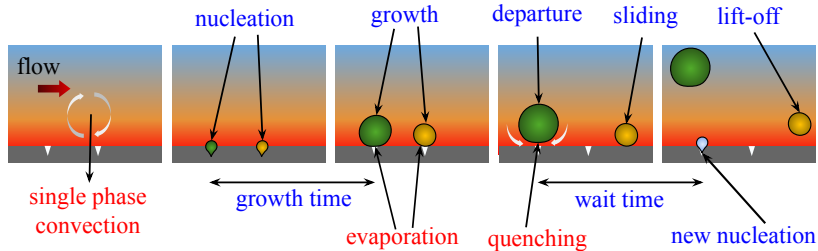
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Motivations

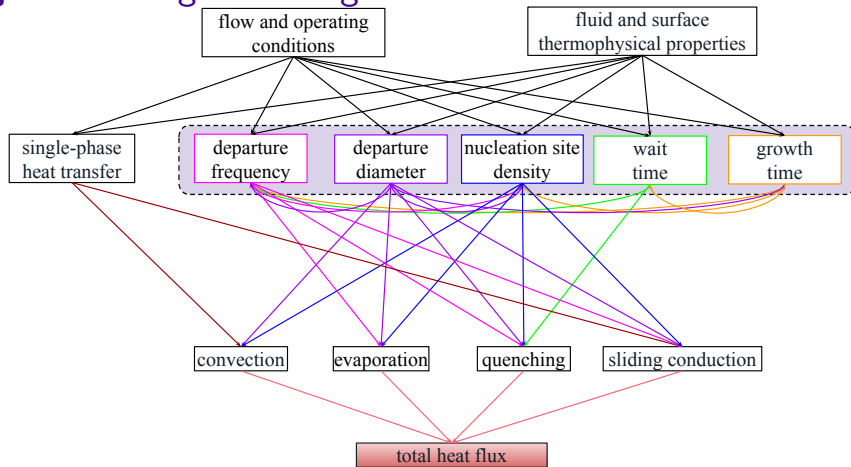
The **heat flux partitioning** approach to boiling modelling

- Boiling is central to many thermal-hydraulic applications



- Current E-E CFD approaches rely on heat flux partitioning (HFP)
 - Wall heat transfer decomposed into multiple **mechanisms**
 - Require numerous **bubble dynamics closures**: departure diameter, departure frequency, nucleation site density, growth and wait times

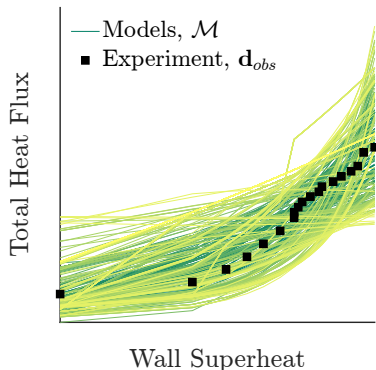
Challenges in boiling modelling



- Hundreds of available closure relations leading to thousands of combinations
- Strong interactions between sub-models
- Epistemic uncertainties

What we learned from XB0IL

- XB0IL: a point-averaged framework for systematic assessment of heat flux partitioning models and bubble-dynamics closures (Bidar and Colombo, Int. J. Heat Mass Transf. 2026)
- Assessed **16,848** boiling model configurations against **1,100+** experimental heat fluxes.
- Models can reproduce experimental heat flux predictions, but need to use the right combination of sub-models.
- No universal model configuration that adequately predicts for a broad (or even limited!) range of flow conditions.



Paper



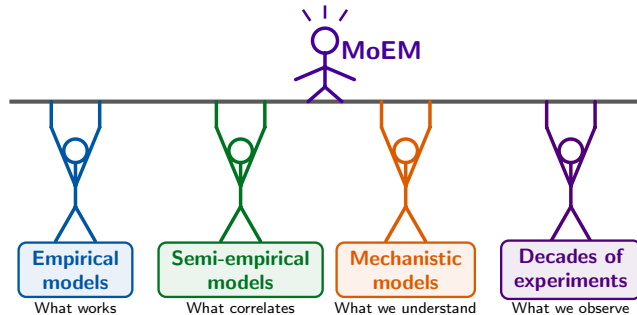
GitHub repo



Can we use machine learning to select the 'right' combination of models?

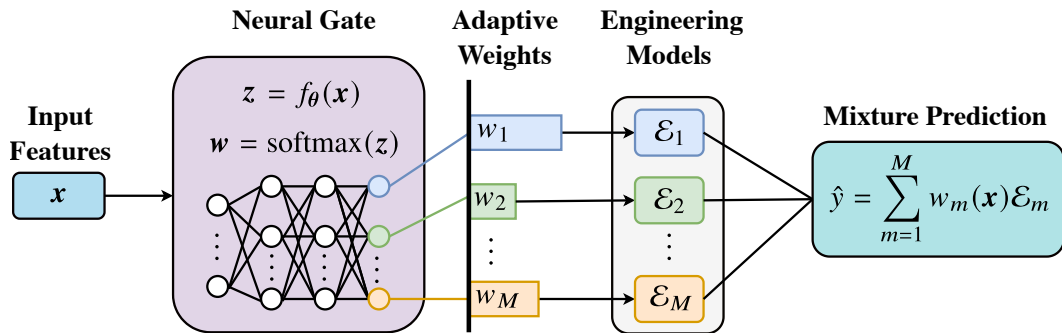
Neural-Gated Mixture of Engineering Models

Standing on the shoulders of giants?



- Decades of research have produced a diverse library of engineering models describing boiling phenomena.
- Rather than replacing these models, the MoEM learns how to blend their predictions informed by experimental data.
- The resulting prediction combines established physical knowledge with data-driven adaptation.
- Potential? If multiple models already exist for a phenomenon, MoEM provides a route to leverage their collective knowledge.

The architecture



- Experimental data are used to train the neural gate to assign adaptive weights to engineering models based on local operating conditions.
- Retains interpretability: model contributions remain explicit through the learned weights.

Examples of input features, x

Interfacial/Surface

Surface tension competition and wettability control bubble attachment and detachment.

$$\alpha_{\text{eff}} = 1 + \cos \theta_c$$

Effective wettability

$$Bo = \frac{g(\rho_l - \rho_v)D_h^2}{\sigma}$$

Bond number (buoyancy vs surface tension)

$$We = \frac{\rho_l U_l^2 D_h}{\sigma}$$

Weber number (inertia vs surface tension)

$$Ca = \frac{\mu_l U_l}{\sigma}$$

Capillary number (viscous vs surface tension)

Flow/Intertia

Hydrodynamic forces control momentum transport, shear and bubble detachment.

$$Re = \frac{\rho_l U_l D_h}{\mu_l}$$

Reynolds number (inertial vs viscous)

$$Fr = \frac{U_l^2}{g D_h}$$

Froude number (inertial vs gravitational)

Interfacial - Thermal

(overlap)

Surface properties influence microlayer evaporation and thermal boundary conditions; wettability affects heat transfer.

Interfacial - Flow

(overlap)

Inertial and viscous forces act against surface tension, affecting bubble shape and detachment.

Thermal - System

(overlap)

Thermal driving depends on pressure and thermophysical properties.

Flow - System

(overlap)

Flow regime interact with geometry and gravity; contains characteristic length scale.

$$p_r = \frac{p}{p_{\text{crit}}}$$

Non-dimensional pressure

$$Su = \frac{\rho_l \sigma D_h}{\mu_l^2}$$

Suratman number (capillary-inertial-viscous group)

ϕ Channel inclination angle

Thermal

Thermal driving and energy transfer govern bubble growth and phase change processes.

$$Ja = \frac{c_{p,l} \Delta T_{\text{sub}}}{h_{lv}}$$

$$Ja_{\Delta T_w} = \frac{c_{p,l} \Delta T_w}{h_{lv}}$$

Jakob number based on subcooling and wall superheat.

$$\frac{\Delta T_w}{T_{\text{sat}}}$$

Non-dimensional wall superheat.

$$Pr = \frac{c_{p,l} \mu_l}{k_l}$$

Prandtl number (momentum vs thermal diffusivity)

Geometry/Pressure/System

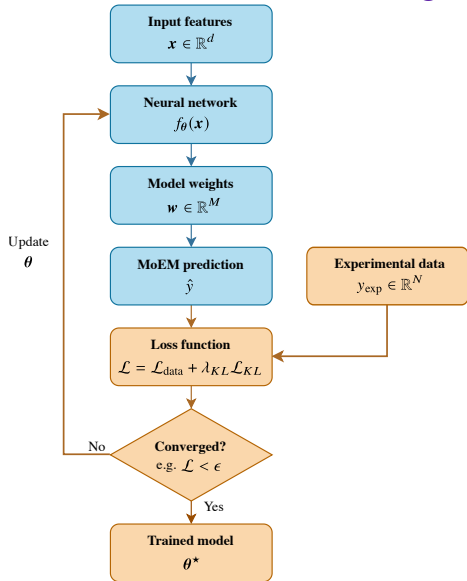
System dimensions, and pressure define the operating envelope.

All features ultimately depend on common underlying variables.

Underlying physical and thermophysical variables

ρ_l, ρ_v	μ_l	σ	$c_{p,l}$	k_l	h_{lv}	U_l	g	D_h	p
Densities	Viscosity	Surface tension	Specific heat capacity	Thermal conductivity	Latent heat	Characteristic velocity	Gravity	Characteristic length	Pressure

How do we train the neural gate?



$$\theta^* = \arg \min_{\theta} \left[\underbrace{\frac{1}{N} \sum_{i=1}^N \ell(y_{\text{exp},i} - \hat{y}_i)}_{\mathcal{L}_{\text{data}} : \text{fit data}} + \underbrace{\lambda_{\text{KL}} \frac{1}{N} \sum_{i=1}^N \sum_{m=1}^M \tilde{w}_{im} \log \left(\frac{\tilde{w}_{im}}{w_m(\mathbf{x}_i; \theta)} \right)}_{\mathcal{L}_{\text{KL}} : \text{model-guidance regularisation}} \right]$$

$$\tilde{w}_{im} = \frac{\exp[-\ell(y_{\text{exp},i} - \hat{y}_{im}) / \tau]}{\sum_{j=1}^M \exp[-\ell(y_{\text{exp},i} - \hat{y}_{ij}) / \tau]}$$

$\tilde{w}_{im}$: data-informed target weight from each model's error.

$w_m(\mathbf{x}_i; \theta)$: neural-gate weight assigned to model m .

λ_{KL} : strength of model-guidance regularisation.

τ : tuning param; smaller values concentrate weight on the best-performing models.

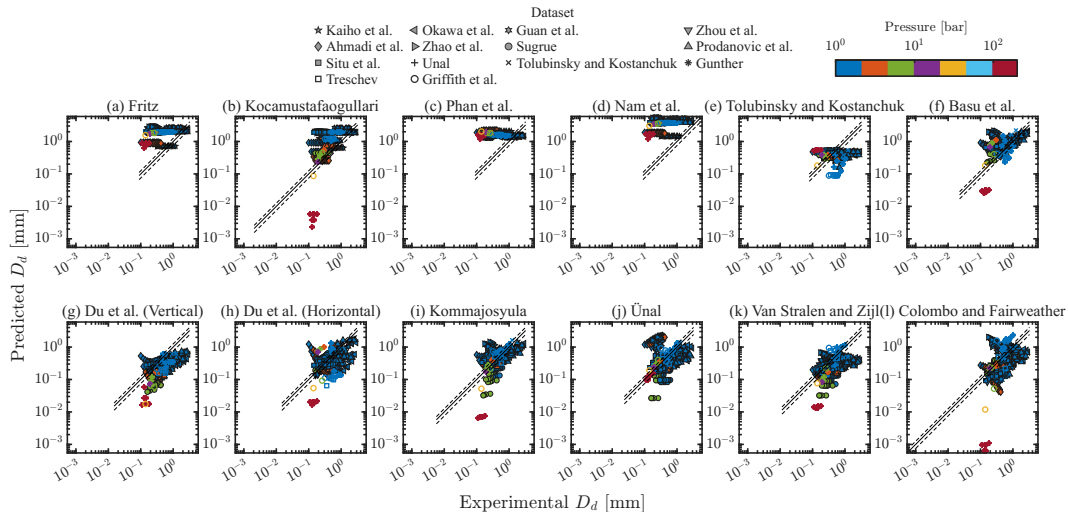
Application 1:
bubble departure diameter

Bubble departure diameter **dataset** and **model library**

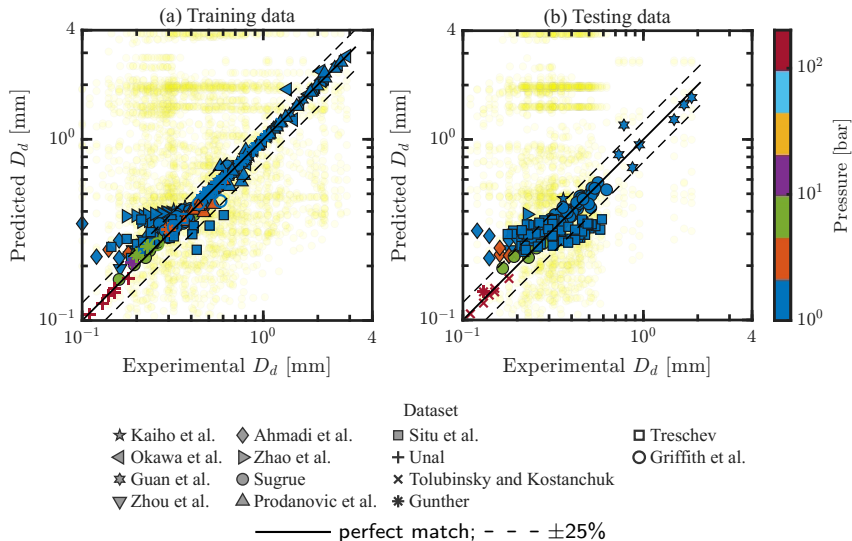
- Bubble departure diameter, D_d , is a key closure in wall-boiling models, affecting vapour generation, interfacial area, and heat-transfer prediction.
- Dataset: **14 experimental flow-boiling datasets** with **452 measurements**, covering different surfaces, geometries, orientations, pressures, mass fluxes, and subcooling levels.
- Model library: **12 literature departure-diameter models**, including empirical, semi-empirical, and mechanistic formulations.

Variable	Minimum	Maximum
Mass flux, G [$\text{kg m}^{-2} \text{s}^{-1}$]	73	6070
Liquid velocity, u [m s^{-1}]	0.08	6.10
Subcooling, ΔT_{sub} [K]	1	86
Pressure, p [bar]	1.00	177
Orientation, ϕ [$^\circ$]	0	90
Contact angle, θ_c [$^\circ$]	13.8	55
Hydraulic diameter, D_h [mm]	5.1	20

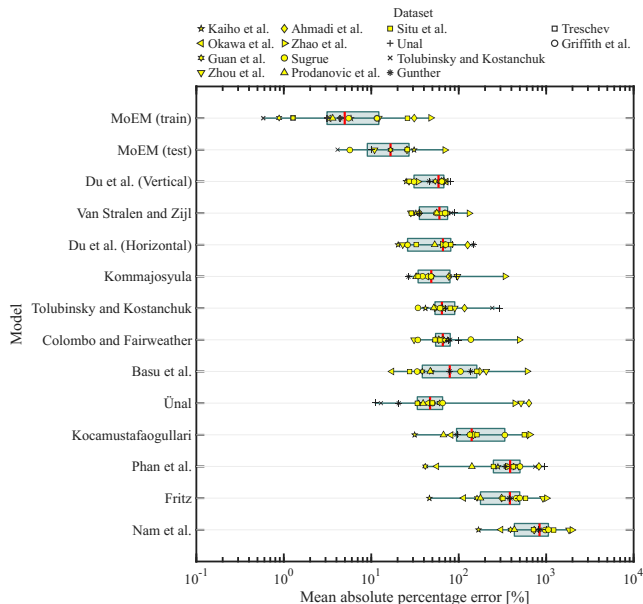
Predictions by **existing models**; many models, many predictions.



MoEM predictions



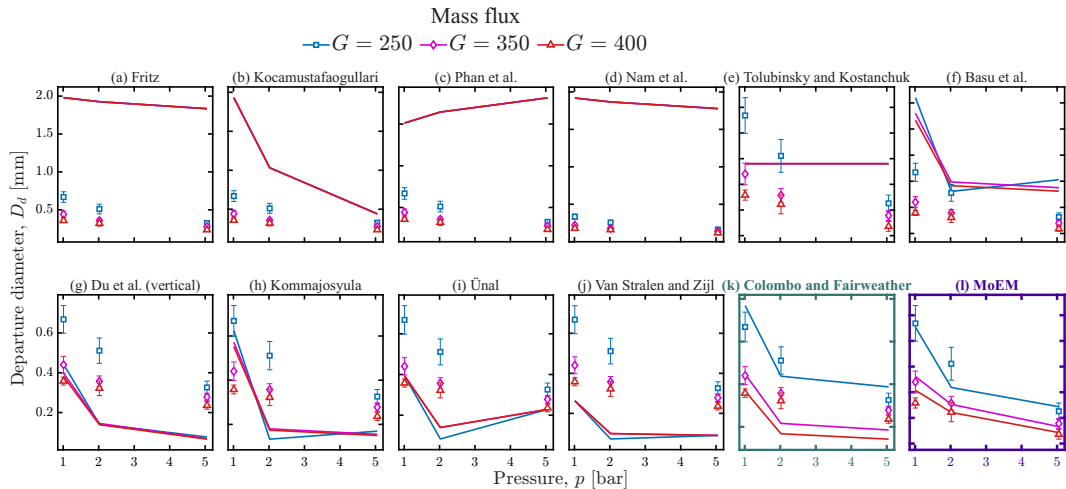
Errors



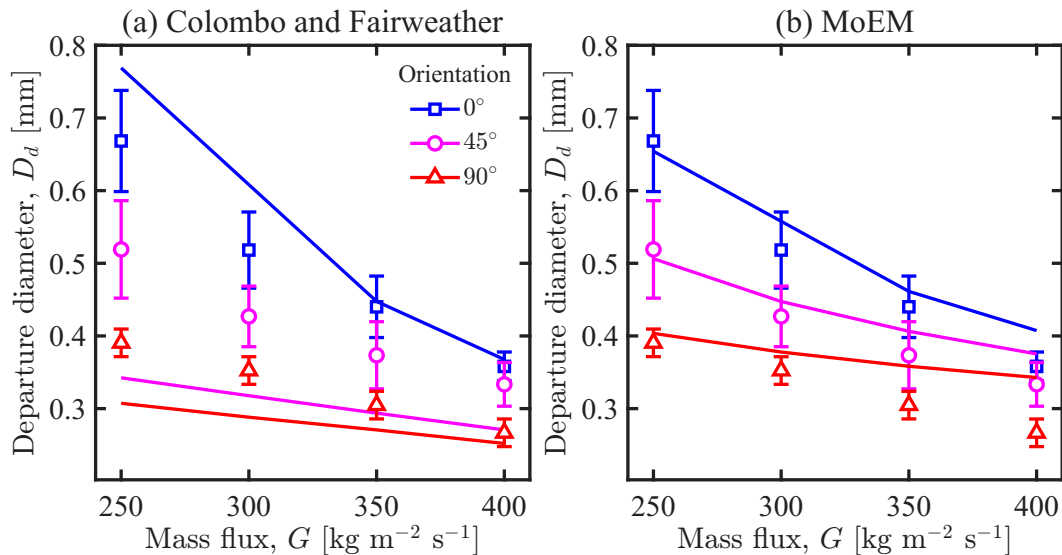
Mean MAPE

- MoEM (train): 11.2%
- MoEM (test): 22.1%
- Best existing model: 52.0%
- Worst existing model: 892.3%

Model performance for pressure and mass flux variations



Model performance for mass flux and channel inclination



Application 2:
heat flux predictions
(boiling curves)

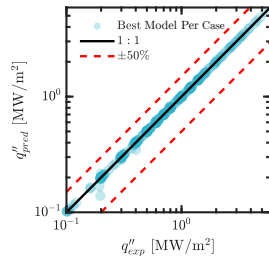
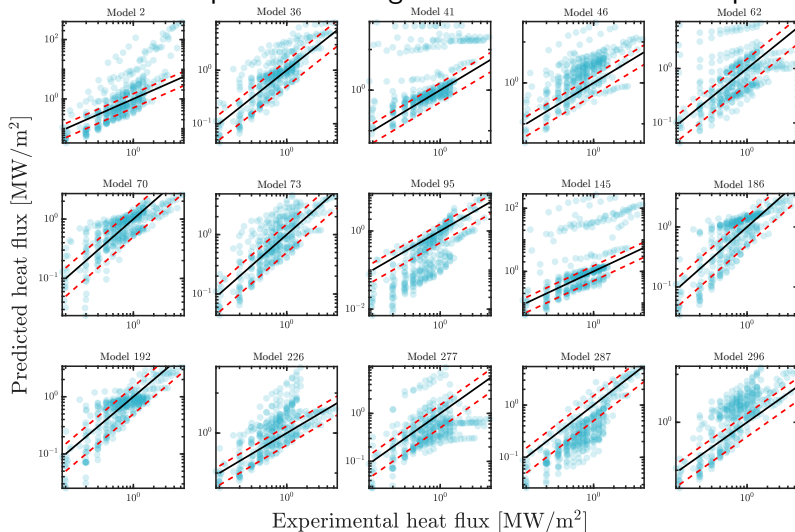
Boiling heat-flux prediction **dataset** and **model library**

- Experimental database: **67 flow-boiling curves** comprising **603 measurements**
- Operating conditions span a broad range of pressures, velocities, subcooling levels and channel geometries representative of saturated and subcooled flow boiling.
- Model library generated using XBOIL
- More than **16,000 model combinations** were constructed by combining alternative heat-flux partitioning formulations and bubble-dynamics closures from the literature.
- After performance and diversity filtering, a representative pool of approximately **350 boiling-model experts** was retained for MoEM training.

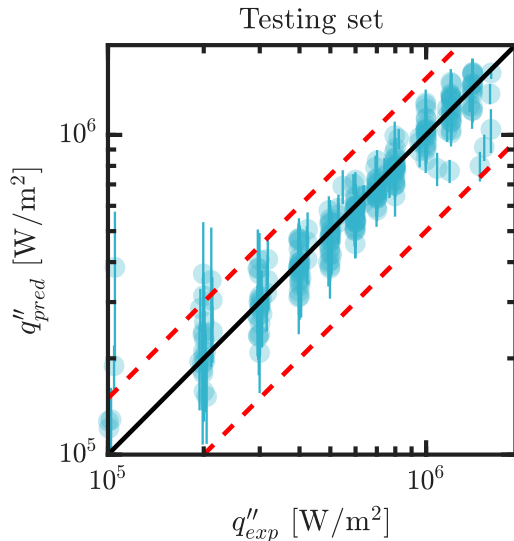
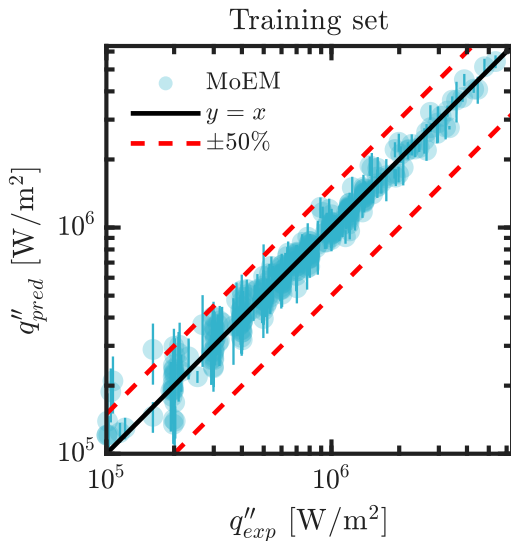
Variable	Minimum	Maximum
Pressure [bar]	1.05	6.0
Velocity [m s^{-1}]	0.16	3.66
Subcooling [K]	5	83.3
Hydraulic diameter [mm]	10	18.5
Heat flux [MW m^{-2}]	0.003	5.4

Example (existing) model predictions

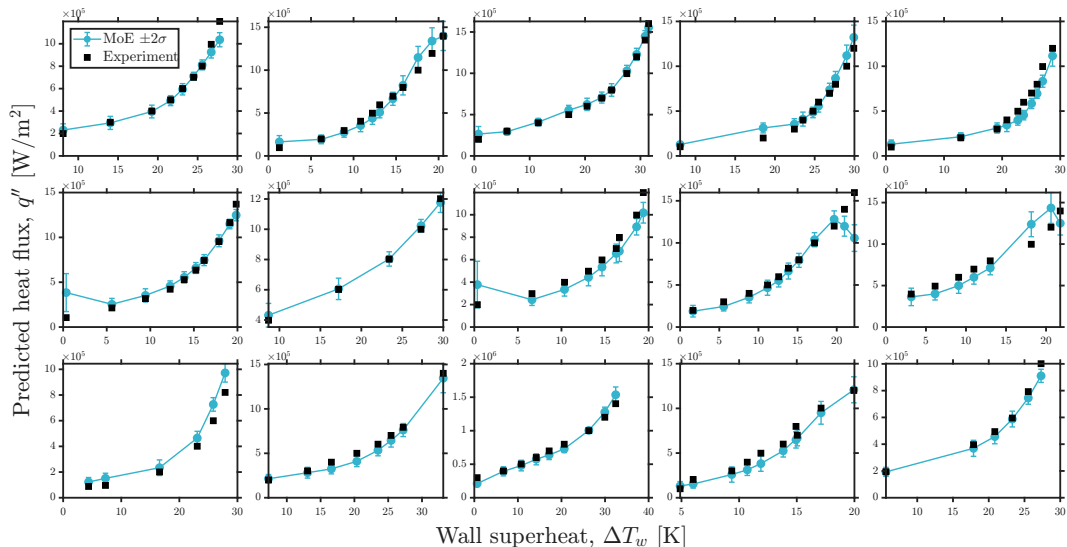
Each *model* represent a configuration of 7 sub-models required: HFP, D_d , $\bar{N}_b$, f etc.



MoEM results: scatter plots



MoEM results: **boiling curves** (random samples from test dataset)



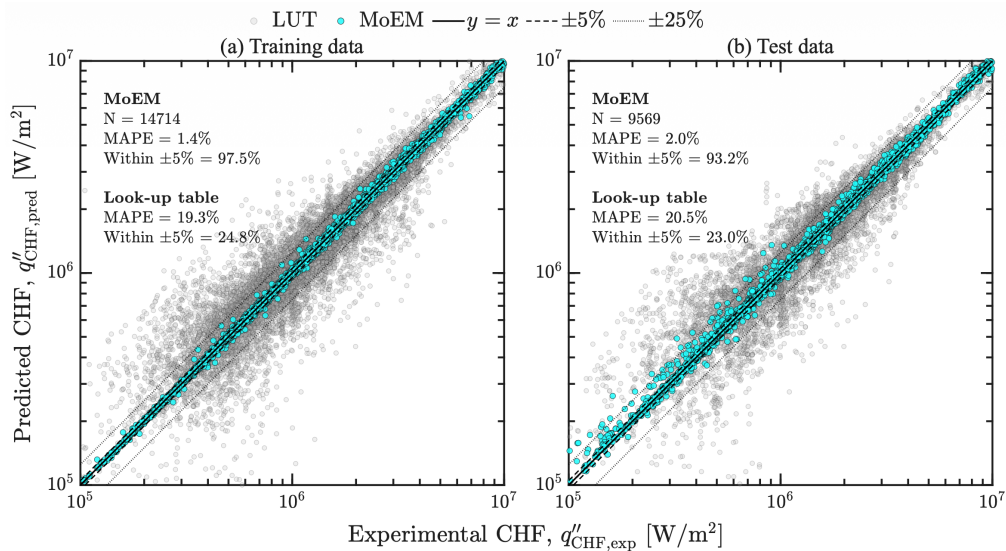
Application 3: **critical heat flux**

CHF benchmark dataset and model library

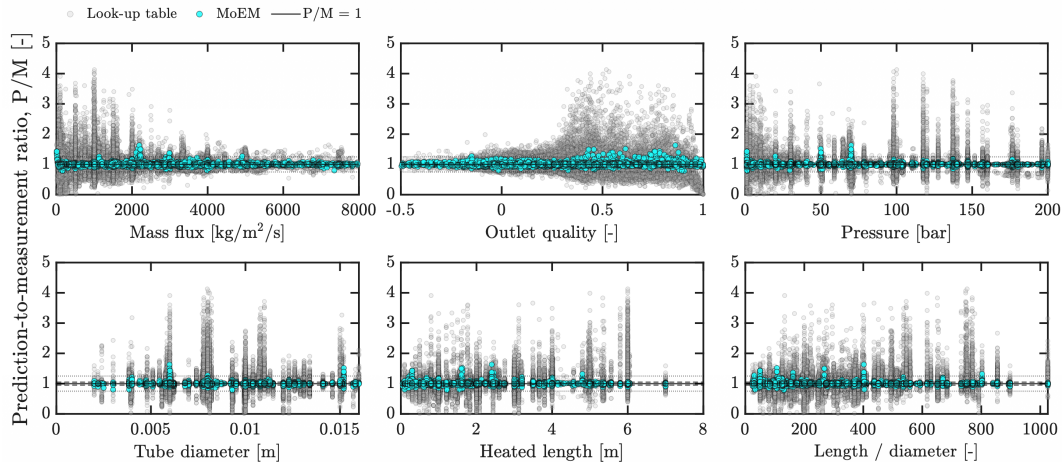
- **66 CHF models**/correlations were implemented from literature and used as candidate models within the MoEM framework.
- NRC CHF database containing over **24,000 experimental measurements**.
- The same database was used to develop the Groeneveld 2006 CHF Look-Up Table (LUT).

Variable	Minimum	Maximum
CHF [kW m^{-2}]	50	16 339
Pressure [kPa]	100	20 000
Mass flux [$\text{kg m}^{-2} \text{s}^{-1}$]	8.2	7 964
Equilibrium quality [-]	-0.497	0.999
Tube diameter [m]	2×10^{-3}	16×10^{-3}
Heated length [m]	0.05	20

MoEM results: scatter plots



Prediction-to-measurement CHF ratio across operating conditions



Take-home messages

- ❶ Decades of boiling research have produced many useful models, but no universally reliable model.
- ❷ The MoEM learns how to combine existing engineering models rather than replacing them.
- ❸ Across three boiling applications, the framework consistently improves agreement with experimental data; retaining interpretability?

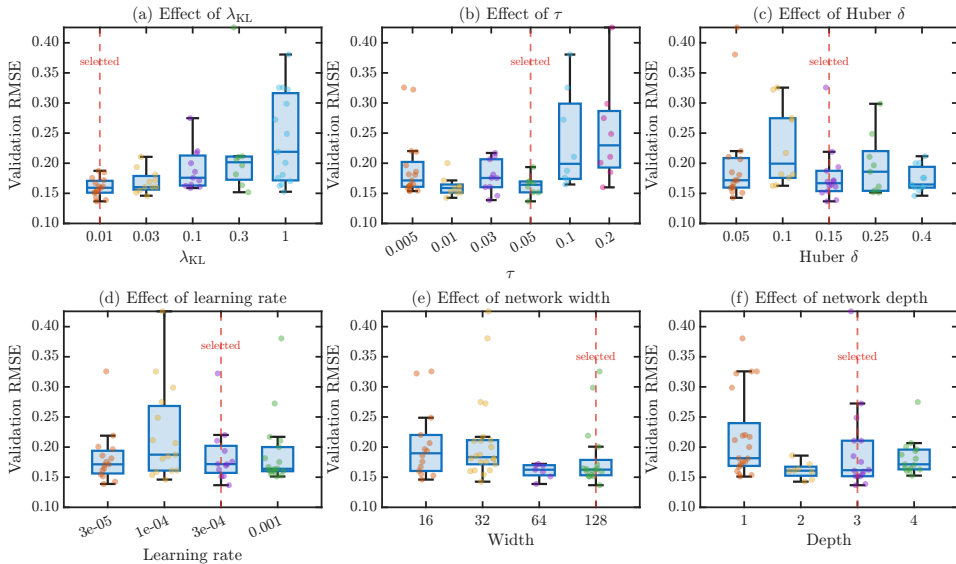
Looking forward:

- *Credibility-aware models*: quantify prediction confidence using model validity and applicability limits
- *Beyond weighted averaging*: explore regime-aware and physics-constrained model selection to determine when model switching may be more appropriate than continuous blending
- Application within CFD
- Where else could a mixture of engineering models approach be useful?

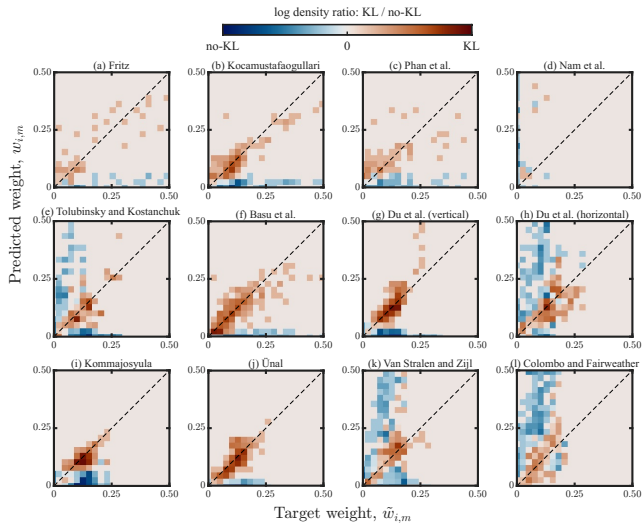
Questions?



Hyper-parameter optimisation: D_d example

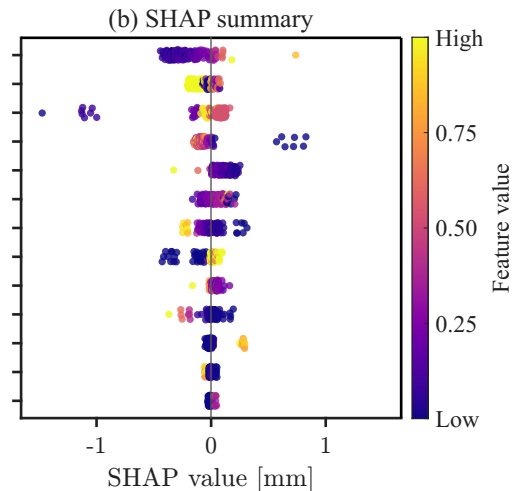
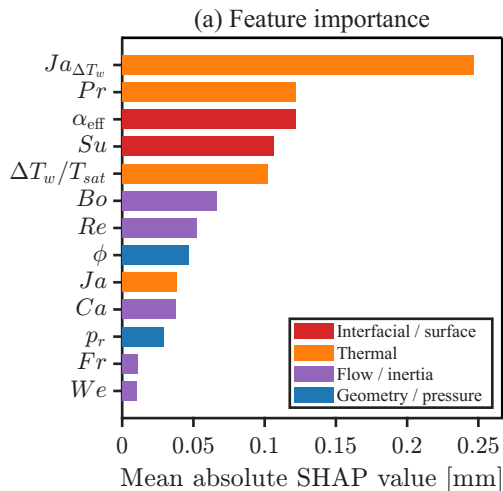


Impact of the **Kullback-Leibler** regularisation: D_d example

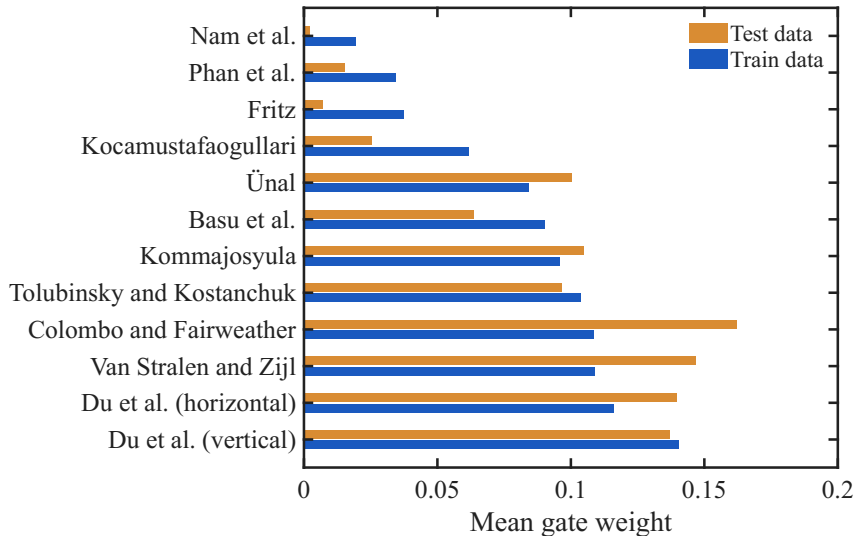


- Each point compares the weight suggested by experimental performance with the weight learned by the neural gate.
- KL regularisation moves the predictions towards the diagonal, meaning the gate better reflects which engineering models perform well in each regime.

Feature importance analysis: D_d example



Average gate weights per model: D_d example



Effective number of experts: D_d example

