EP/L015153/1

On the AI driven geometry optimisation of a stirred tank CFD model in laminar flow

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RSC SIG Formulation 4.0, 26th July 2024

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[1] School of Chemical Engineering, University of Birmingham.
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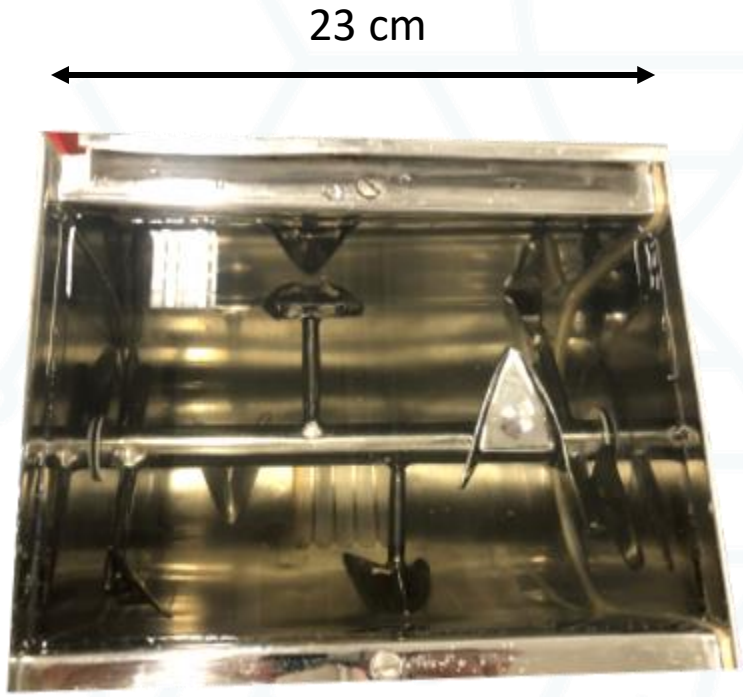
[3] Unilever R&D, Port Sunlight Laboratory.

Industrial mixing in a Ploughshare mixer

- Used in semi-solid and granular mixing.
- Poor axial mixing demonstrated for granulation [1-3]
- How to predict and improve viscous mixing?



Aims

1. Build a **CFD** model to predict single-phase liquid mixing.
2. **Validate** mixing using Positron Emission Projection Imaging.
3. Develop **predictive models** for mixing.
4. Optimise impeller geometry with a **data-driven** approach.

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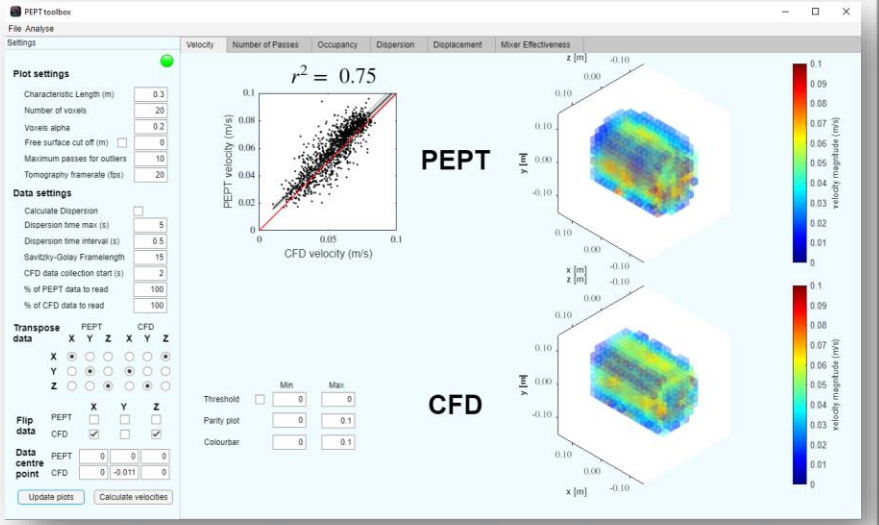
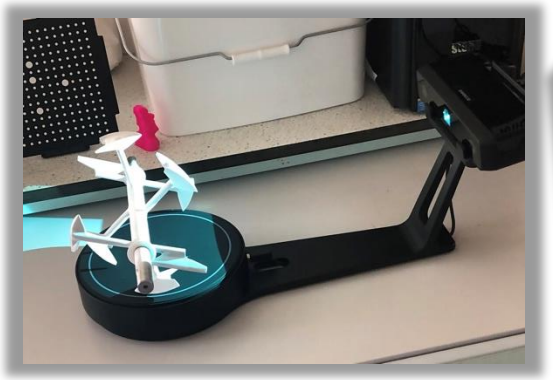
[1] Jones, J.R., et al 2007. Axial mixing in a ploughshare mixer. Powder Technology 178, 73–86.
[2] Laurent, B.F.C., Cleary, P.W., 2012. Comparative study by PEPT and DEM for flow and mixing in a ploughshare mixer. Powder Technology 228, 171-186.
[3] Forrest, S., et al, 2003. Flow patterns in granulating systems. Powder Technology 130, 91-96.

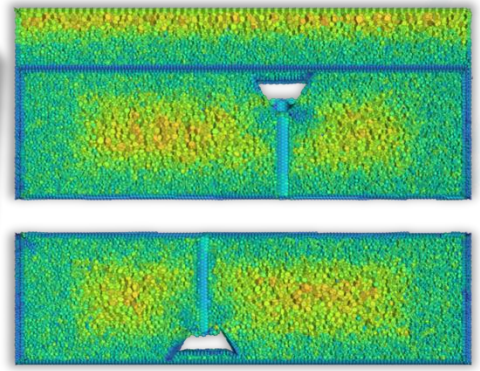
CFD model

- Viscous mixing in laminar flow
- Sliding mesh, single-phase liquid.
- Velocity fields validated using PEPT in previous work [4]
- **Passive scalar tracers** used to predict mixing performance.

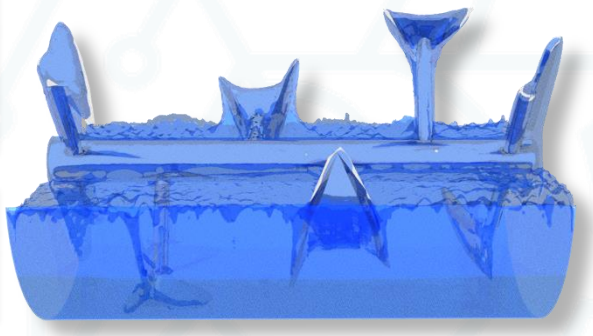




3d scanned impeller



1.1 M cells



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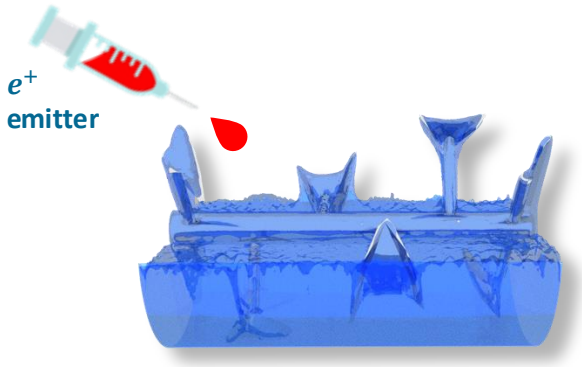
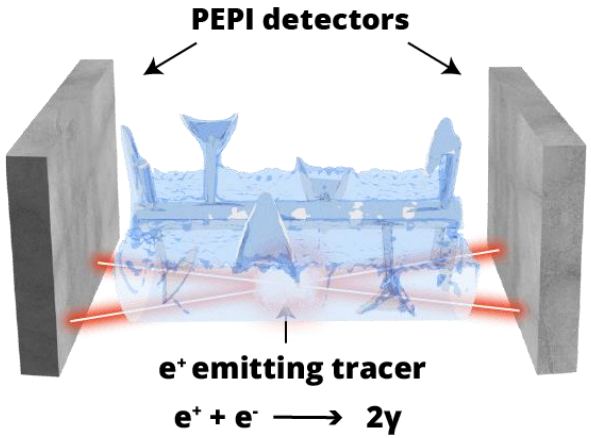
[4] Hart-Villamil, R., et al 2024. On the autonomous validation and comparison of particle models for a Newtonian laminar flow mixing model using PEPT. Chemical Engineering Research and Design 206, 139–150.

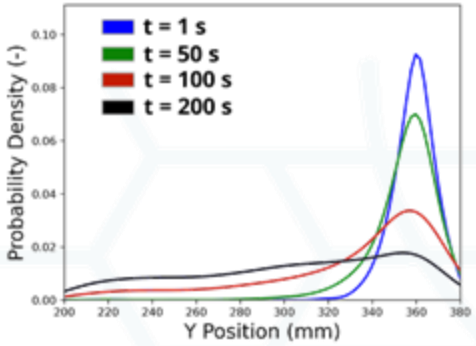
What is Positron Emission Projection Imaging (PEPI)?

- Direct tracking of **species concentration** using gamma photons.
- It allows us to **'see inside' opaque systems**.
- ~ 2 mm spatial and ~1 s temporal resolution

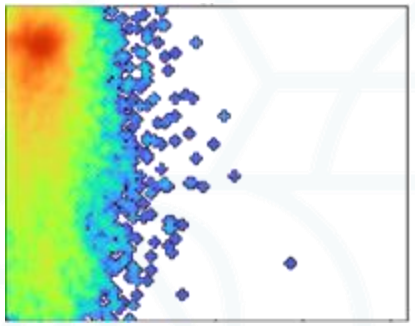




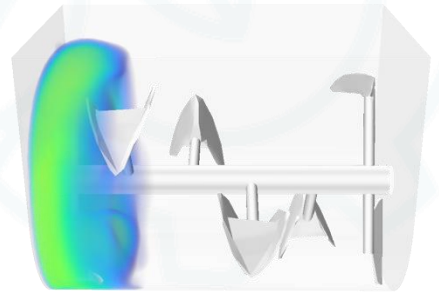
Mass distributions



Concentration fields



In-silico comparison



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[5] Windows-Yule et al., 2022. *PEPT, a Comprehensive Guide*, IoP eBooks, ISBN 9780750330718

Validating the simulation

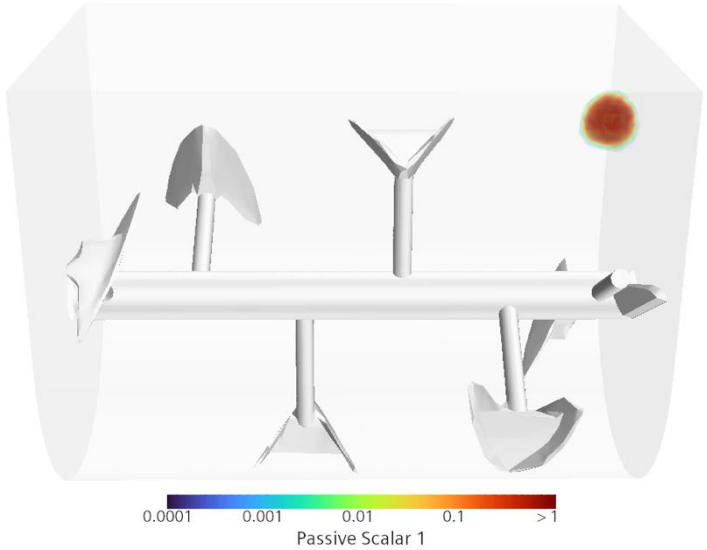
Glycerol in laminar flow

$N = 33\ rpm$

$\mu = 1.4\ Pa\ s$

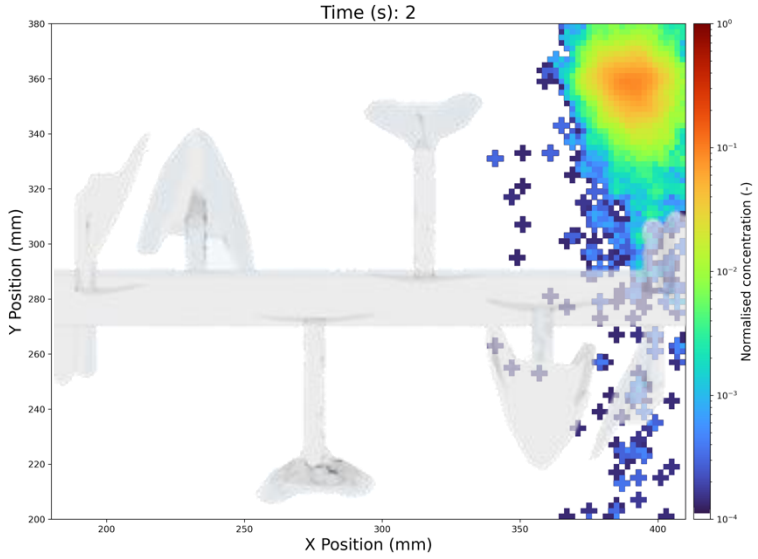
$\rho = 1256\ kg\ m^{-3}$

$Re = 10$



Solution Time 0.04 (s)

CFD model



Positron Emission Projection Imaging

Exploring how ρ N K n Impacts Torque, Mixing

rotation rate

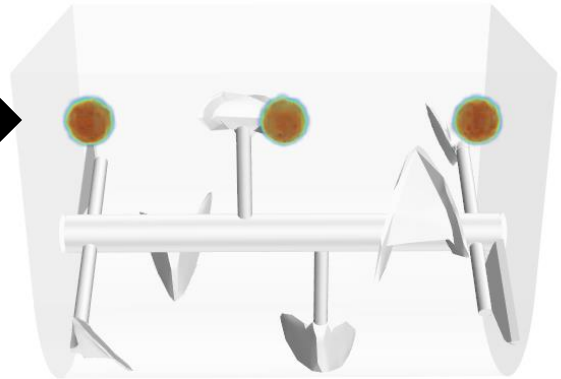
flow index

density

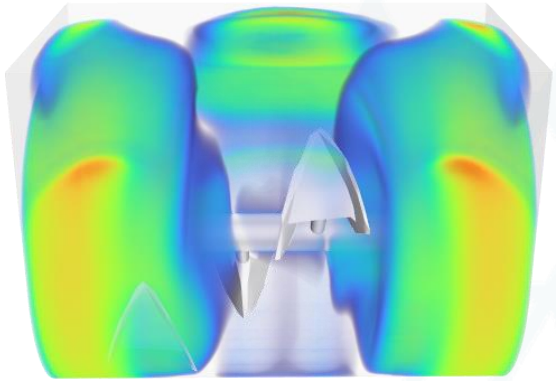
flow consistency

- 60 parameter combinations sampled with Latin Hypercube

scalar tracers



$t = 0$



$t = 30\ s$

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Equation discovery via symbolic regression

- Similar functionality to ANNs, but not a “black box”
- Closed-form mathematical equations
- Improved understanding
- Reduced dimensionality means almost **zero inference costs**

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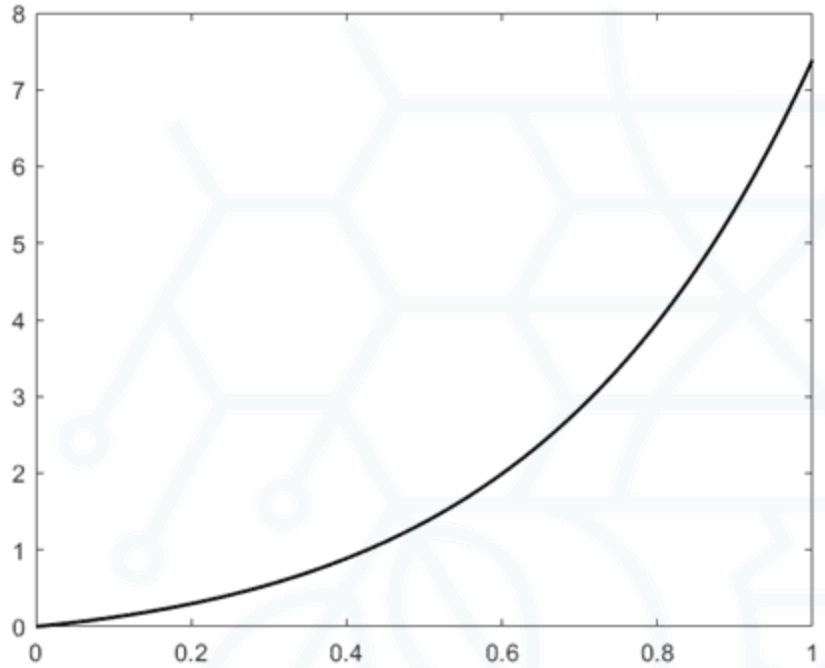

$f_1(x) =$

$f_2(x) =$

$a \quad x \quad x^{\alpha} \quad e^{\alpha x} \quad \sin \alpha x \quad \cos \alpha x \quad \tan \alpha x \quad \log \alpha x \quad \ln \alpha x$

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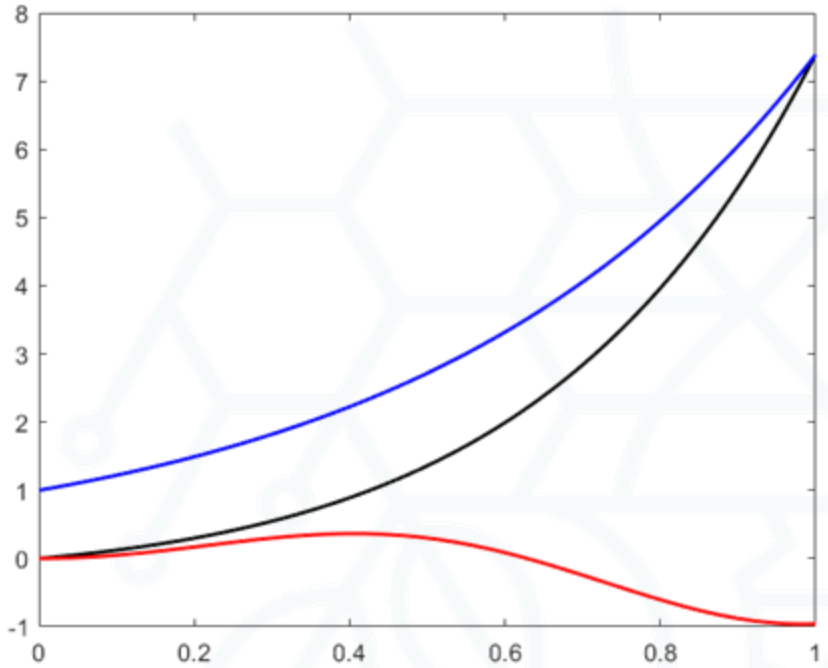

$$f_1(x) = x \sin \alpha x$$

$$f_2(x) = a e^{\alpha x}$$

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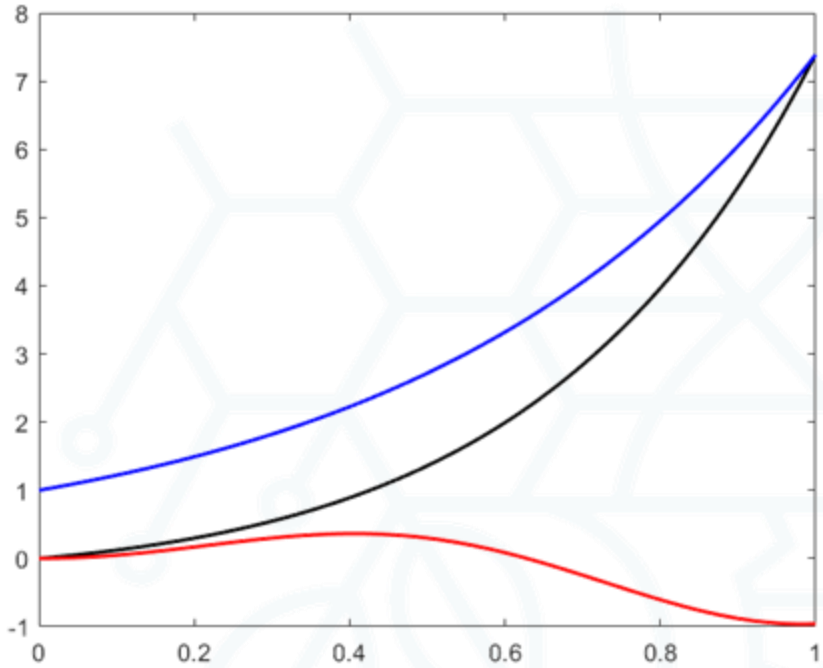

~~$f_1(x) =$~~

$f_2(x) = a e^{\alpha x}$

a x x^{α} $e^{\alpha x}$ $\sin \alpha x$ $\cos \alpha x$ $\tan \alpha x$ $\log \alpha x$ $\ln \alpha x$

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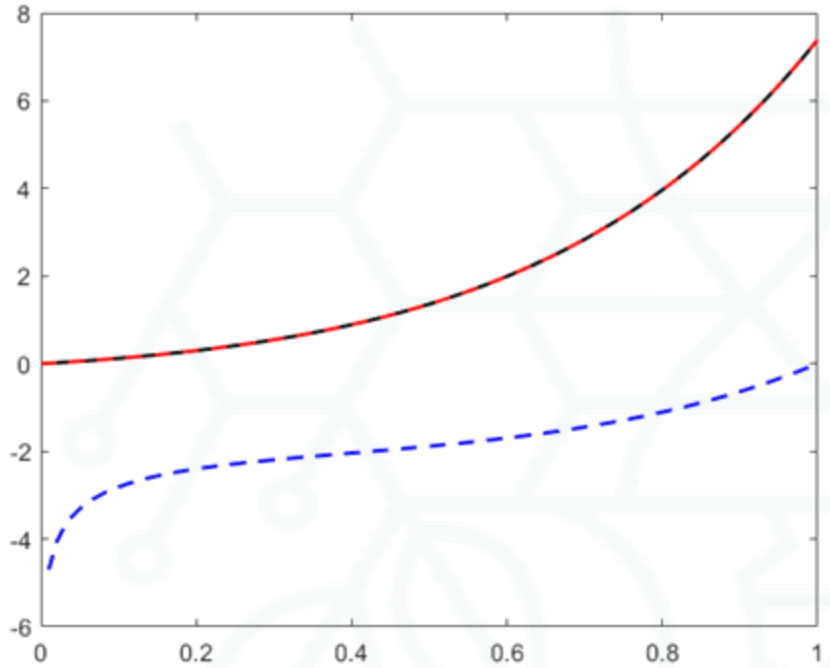

~~$f_1(x) =$~~

$f_2(x) = a e^{\alpha x}$

$f_3(x) = a x e^{\alpha x}$

$f_4(x) = \ln \alpha x \; e^{\alpha x}$

$a \quad x \quad x^{\alpha} \quad e^{\alpha x} \quad \sin \alpha x \quad \cos \alpha x \quad \tan \alpha x \quad \log \alpha x \quad \ln \alpha x$

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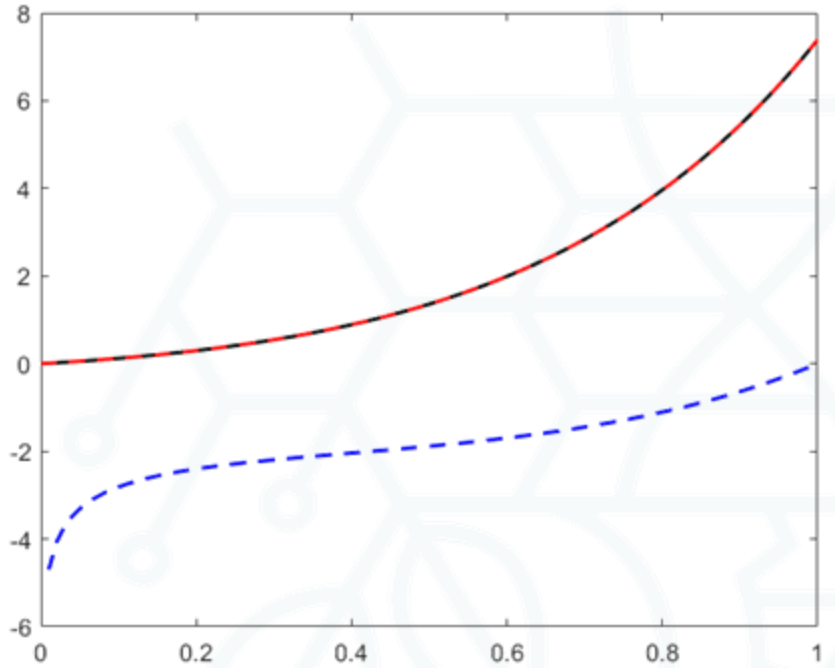

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$f_4(x) =$

…

a x x^{α} $e^{\alpha x}$ $\sin \alpha x$ $\cos \alpha x$ $\tan \alpha x$ $\log \alpha x$ $\ln \alpha x$

Exploring how ρ N K n Impacts Torque, Mixing

left $Nt_m = 401$ revs

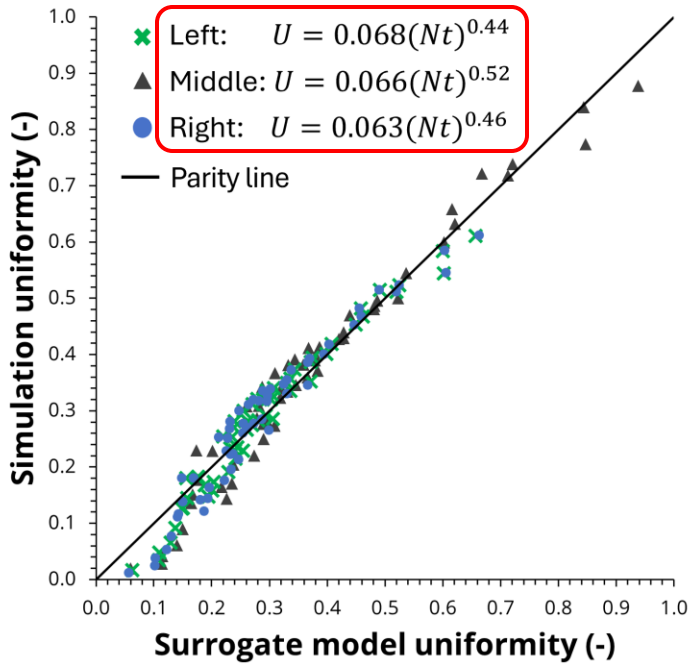
middle $Nt_m = 169$ revs

right $Nt_m = 365$ revs

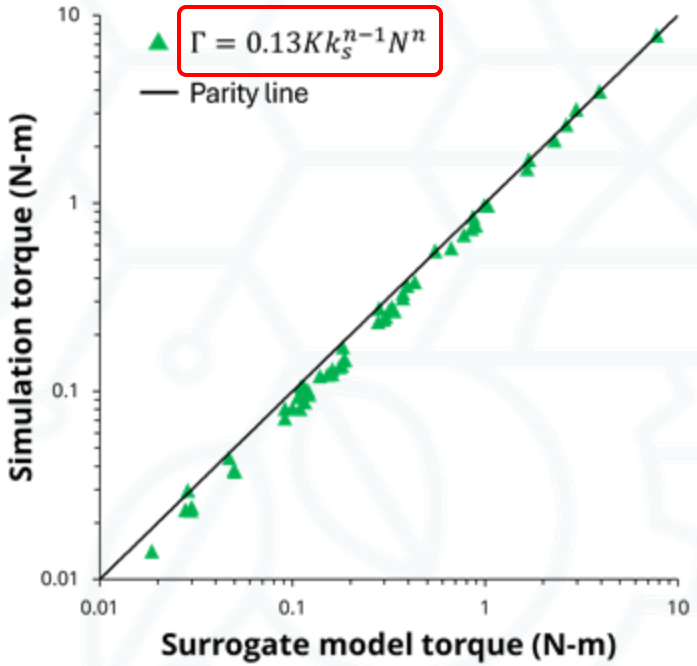
$$W_m = \frac{0.13 K k_s^{n-1} N^{n+1} t_m}{\rho V}$$

Mixing energy

Mixing parity plot



Torque parity plot



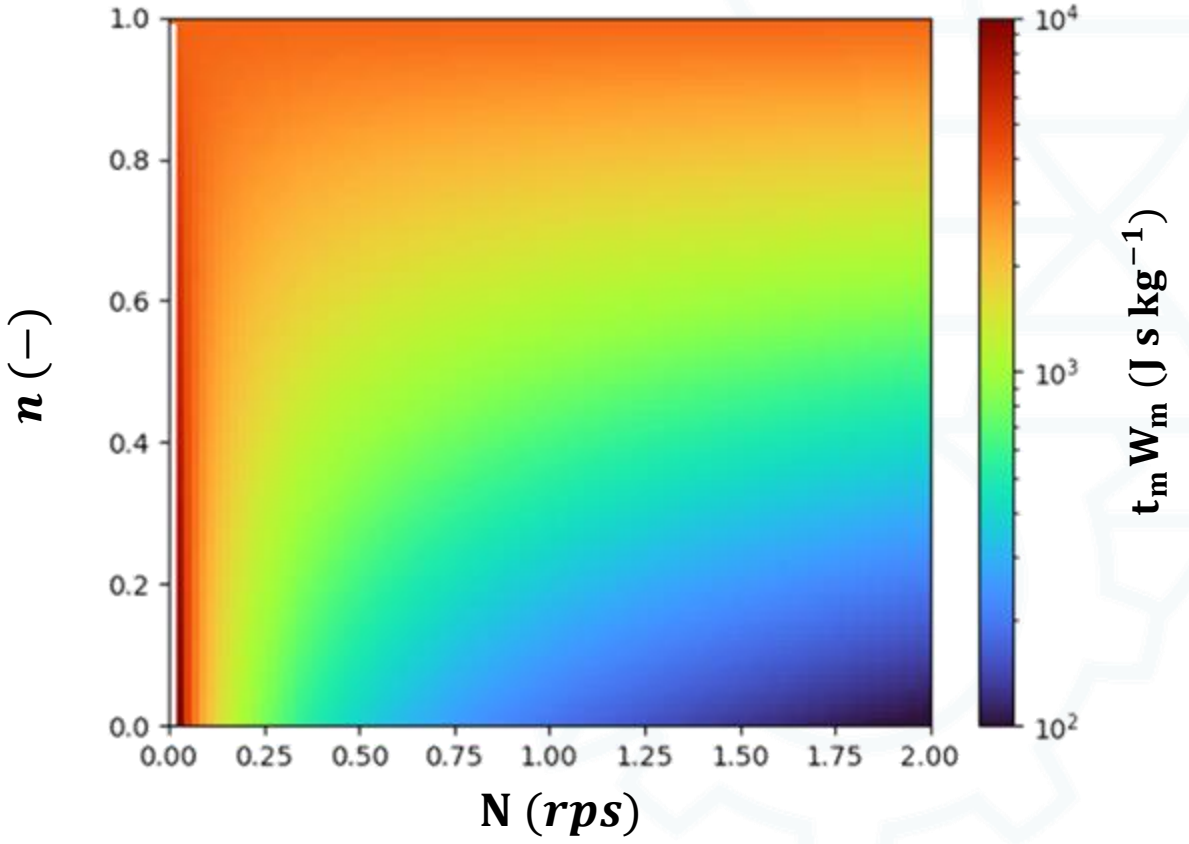
[6] Tatterson, 1991. Fluid Mixing and Gas Dispersion in Agitated Tanks, McGraw-Hill, New York.
[7] Kresta, S. M., et al 2016. Advances in Industrial Mixing. John Wiley & Sons.
[8] Metzner, A. B., Otto, R. E., 1957. Agitation of non-Newtonian fluids. AIChE J., 3: 3-10.
[9] Nicusan 2023. MEDEq Library. https://med.readthedocs.io
[10] Laplante, P. et al 2015. Demulsifier performance in froth treatment. Fuel Processing Technology, 138: 361-367.

Exploring how ρ N K n Impacts Torque, Mixing

What conditions for fastest mixing at lowest energy?

- Operate at $\min(t_m \times W_m)$
- For **Newtonian** liquid there are equal trade-offs.
- If more **shear-thinning**, better to increase rpm.

But what if you **can't** increase rotation rate or change fluid?



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Optimisation

Objectives

- Maximise **axial mixing**
- Modify **geometry** using evolutionary algorithms
- Retain **plough-like** features

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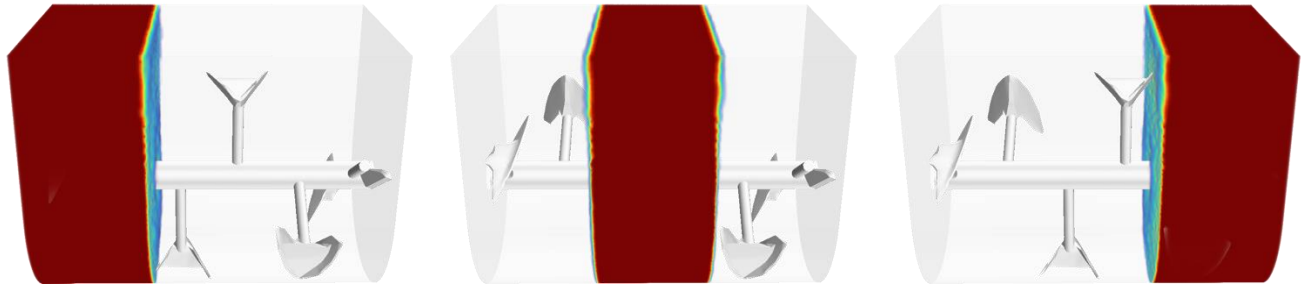
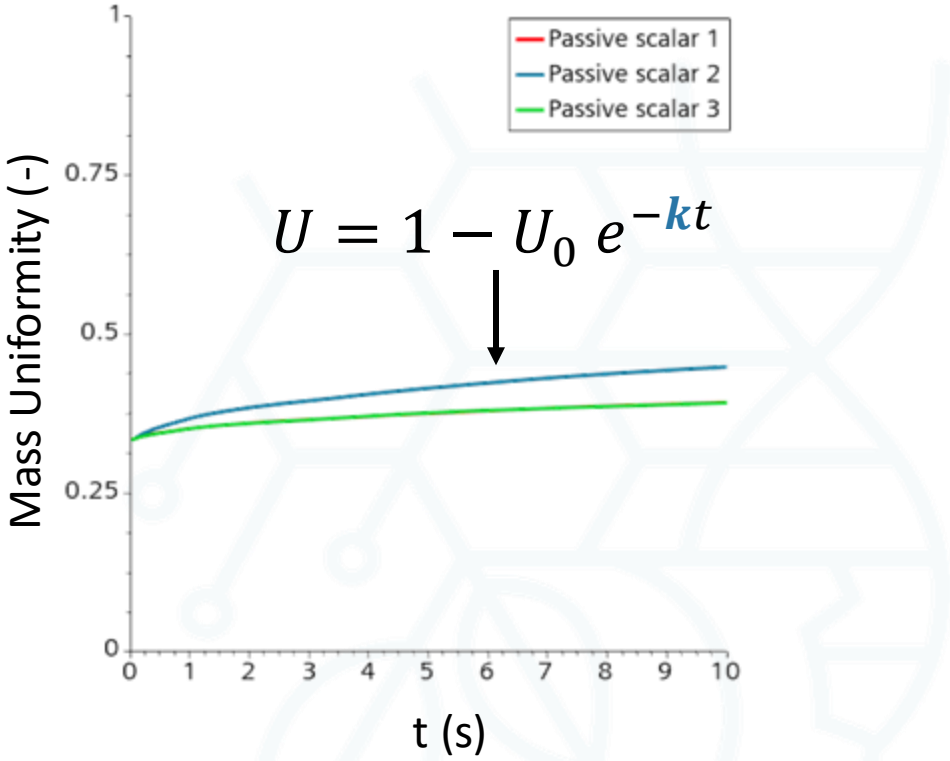
Optimisation

- **Evaluating axial mixing**



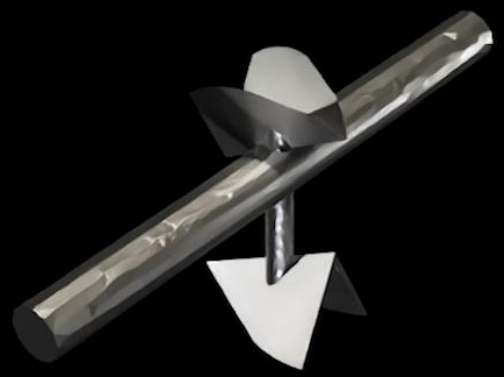


Maximise rate constant $\boldsymbol{k}$

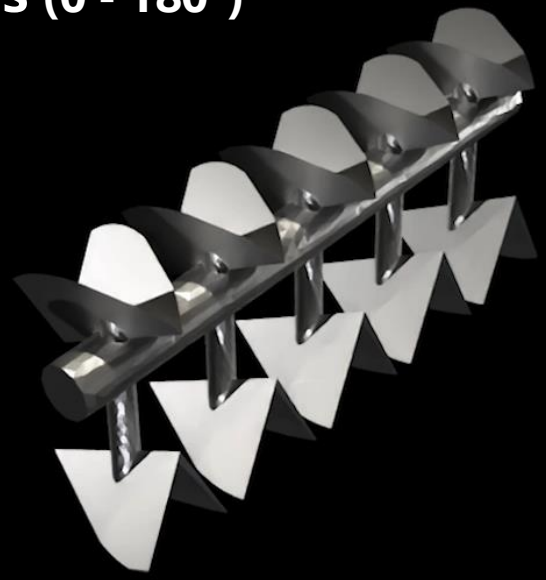
=

Error function → Minimise $t_{1/2} = \frac{\ln 2}{\boldsymbol{k}}$

Number of plows (1-12)

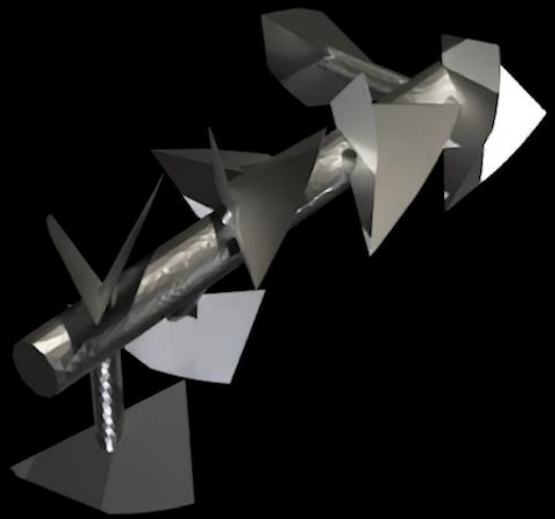


Bias (0 - 180°)



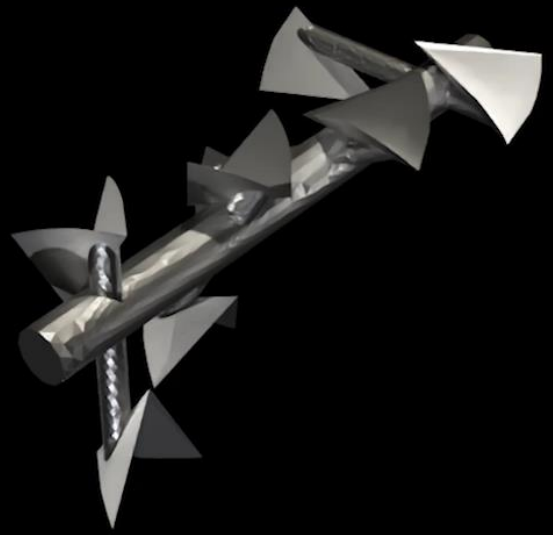
Side angle (-45 – 45°)

Twist angle (-45 - 45°)



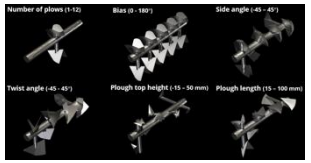
Plough top height (-15 – 50 mm)

Plough length (15 – 100 mm)



Optimisation

Input parameters



Optimiser

HARPPP

EvoPhase+

HPC

Closed loop epoch

Error function

$t_{1/2}$

Post-processing

Simulation

STAR-CCM+

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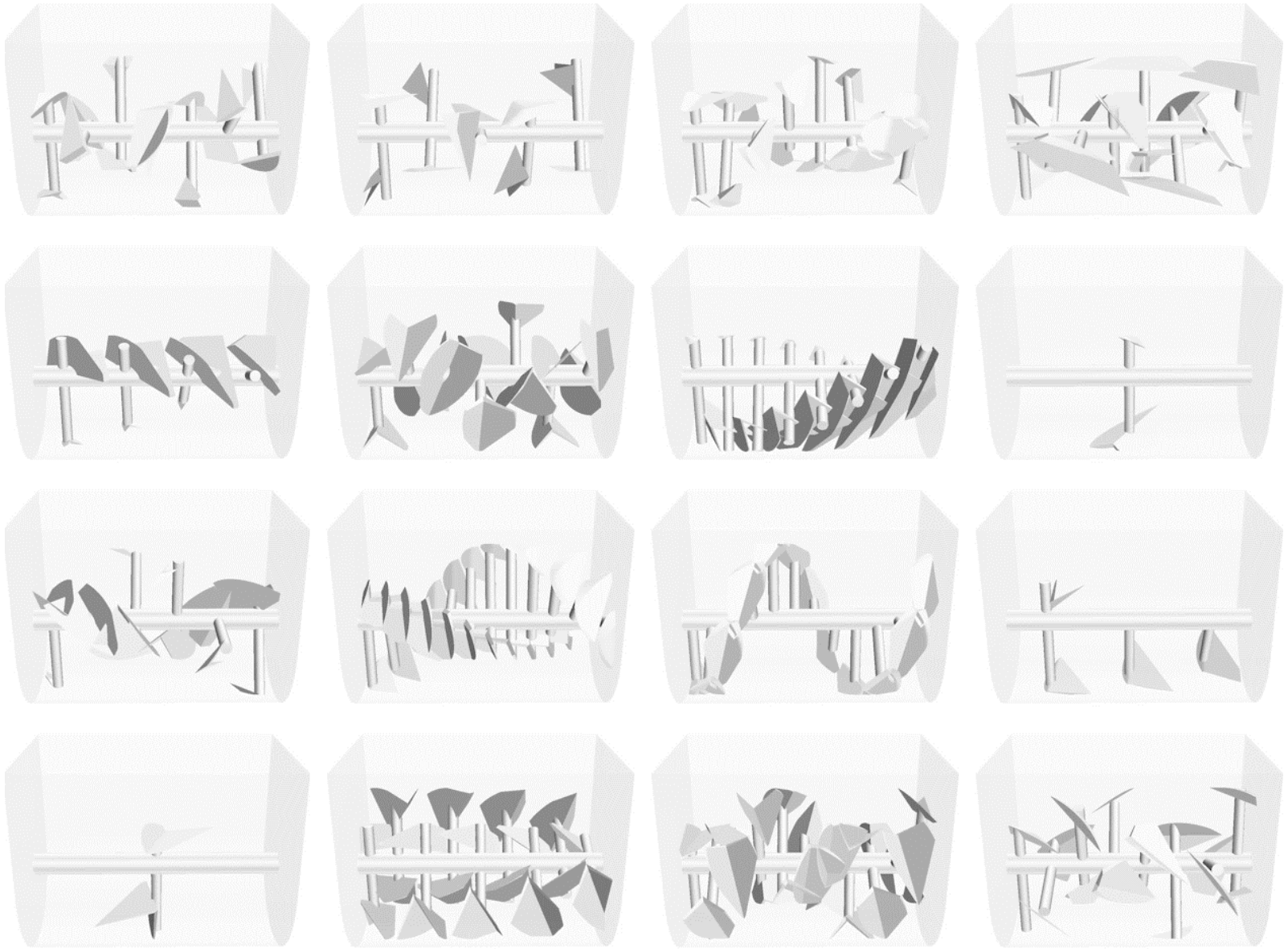
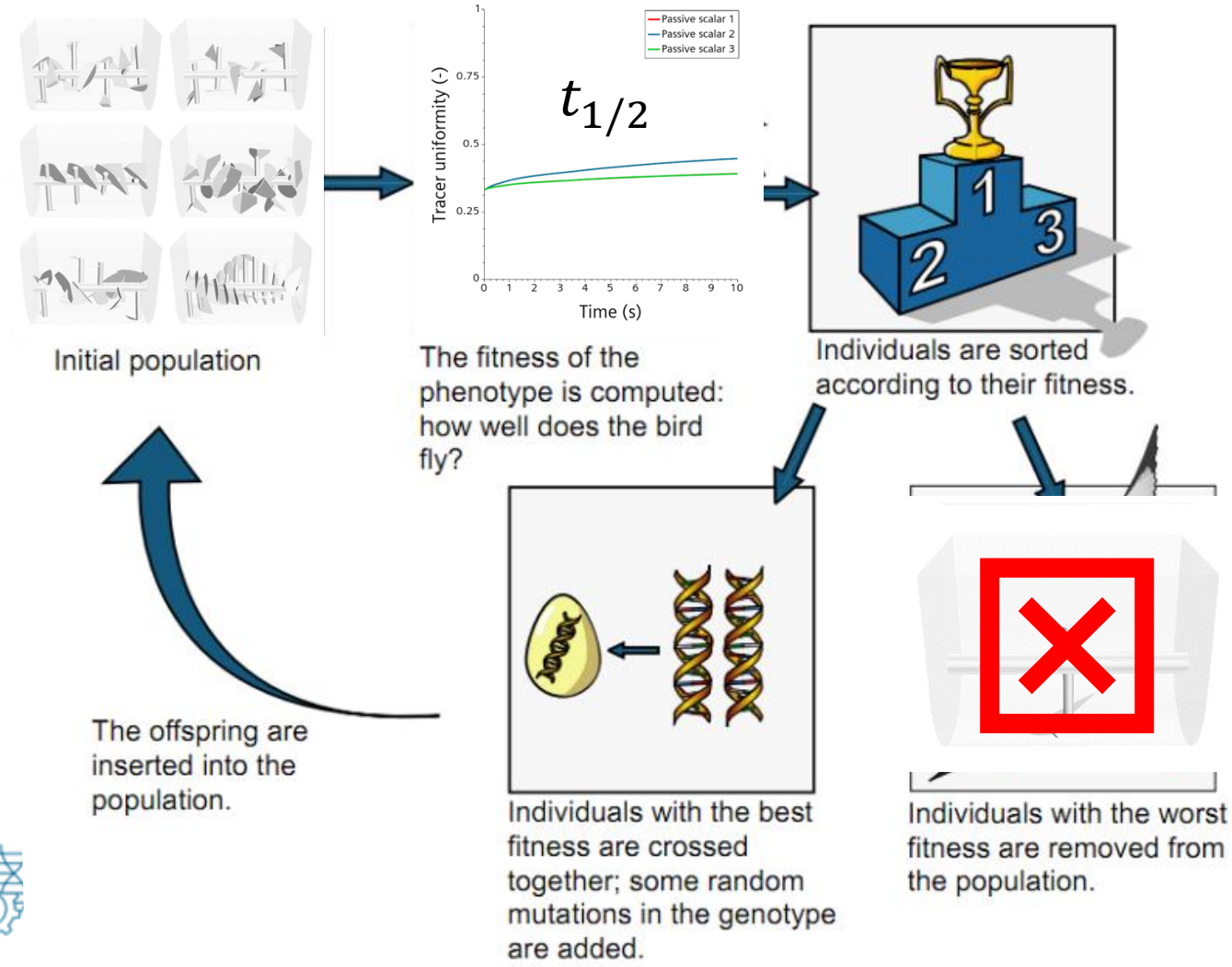
Optimisation



Evolutionary algorithms



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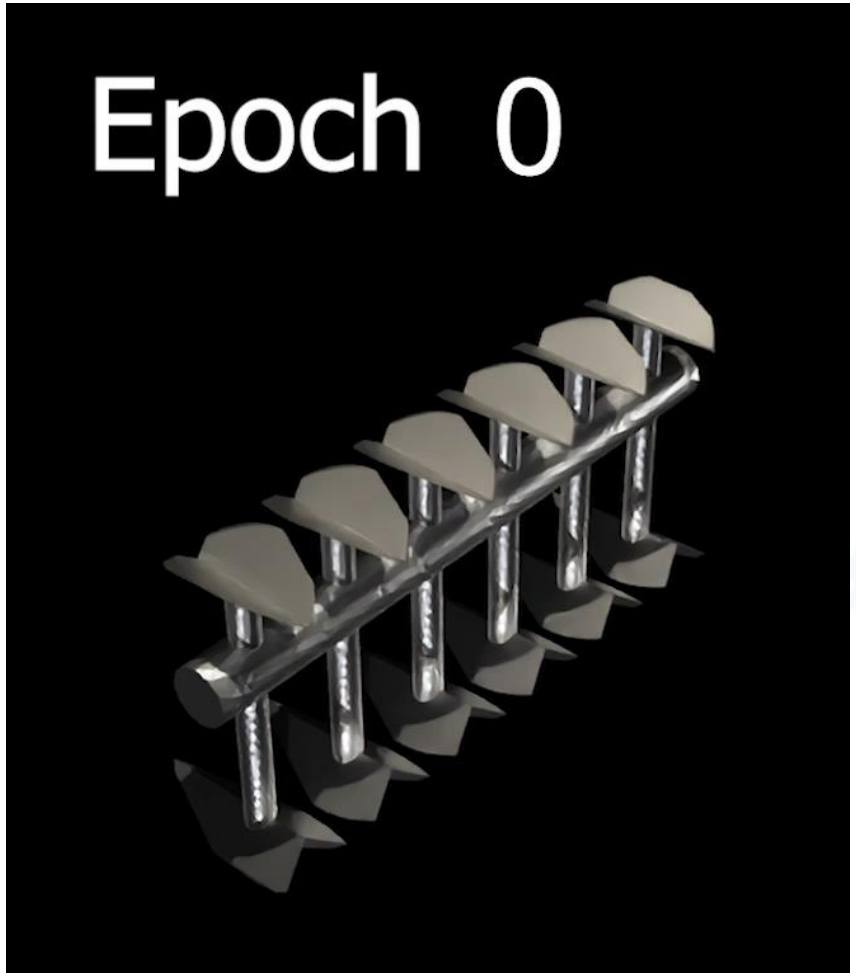
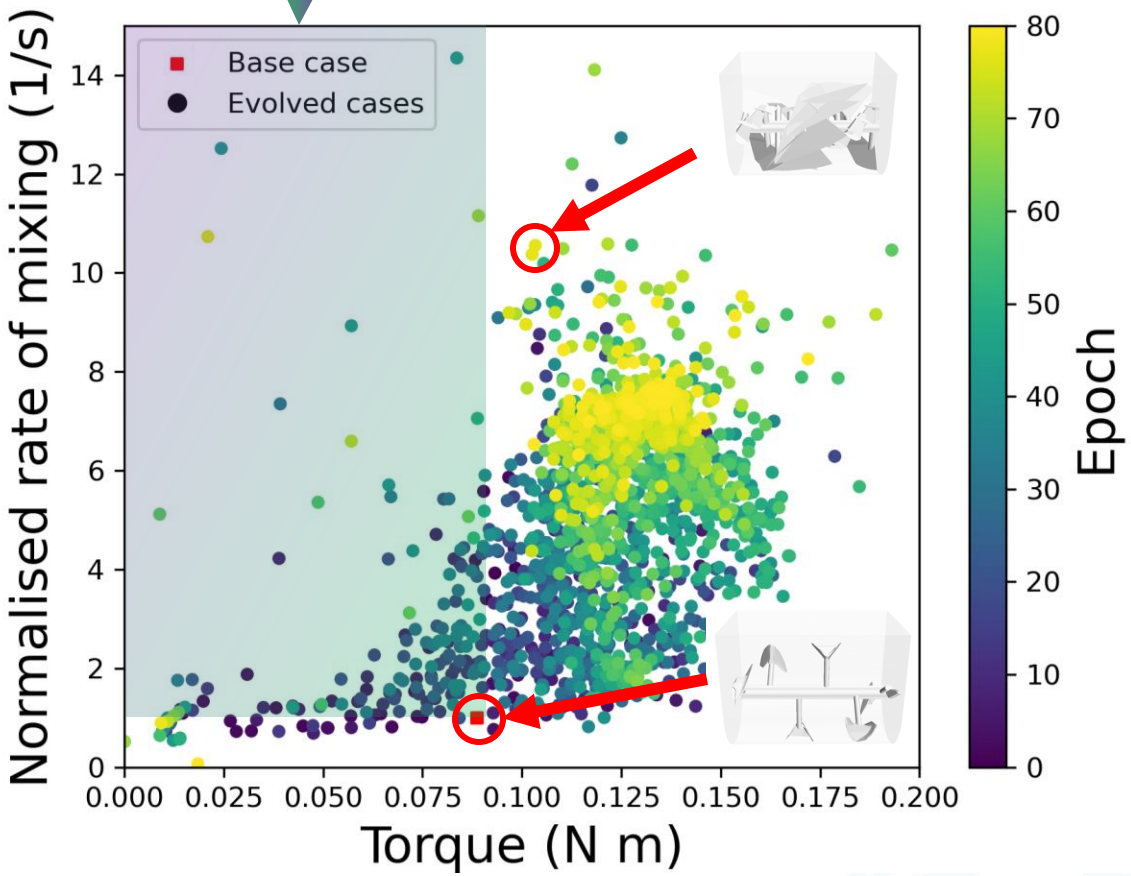
Optimisation



Optimisation

Increased profit + improved sustainability

increasing throughput (Profit)



Decreasing energy use (Sustainability)

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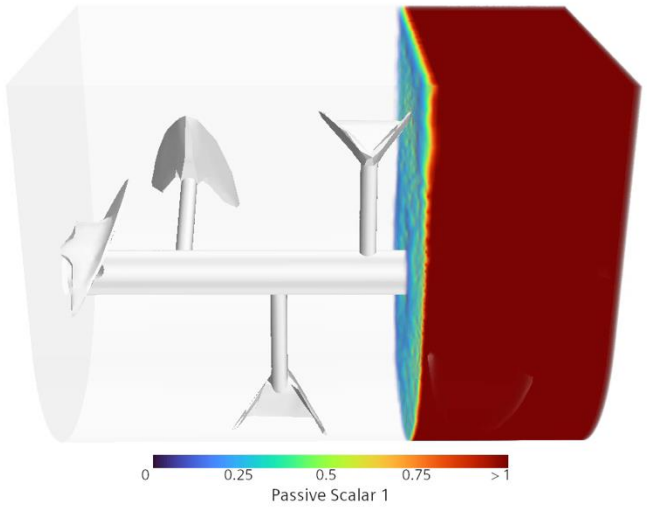
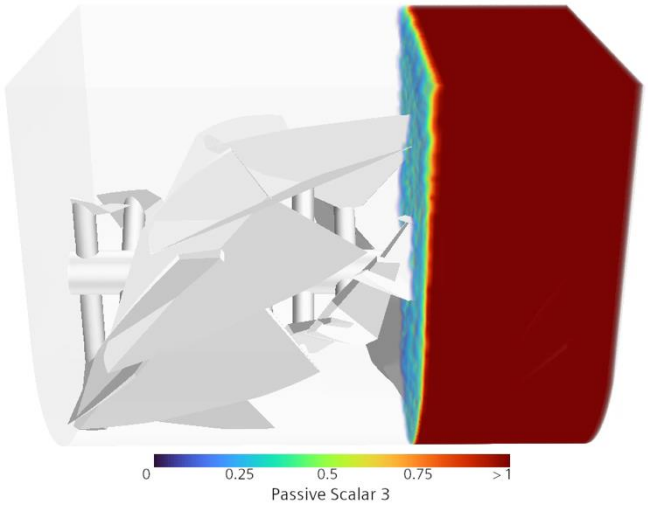
Optimisation

Base case



Solution Time 0.04 (s)

Evolved design



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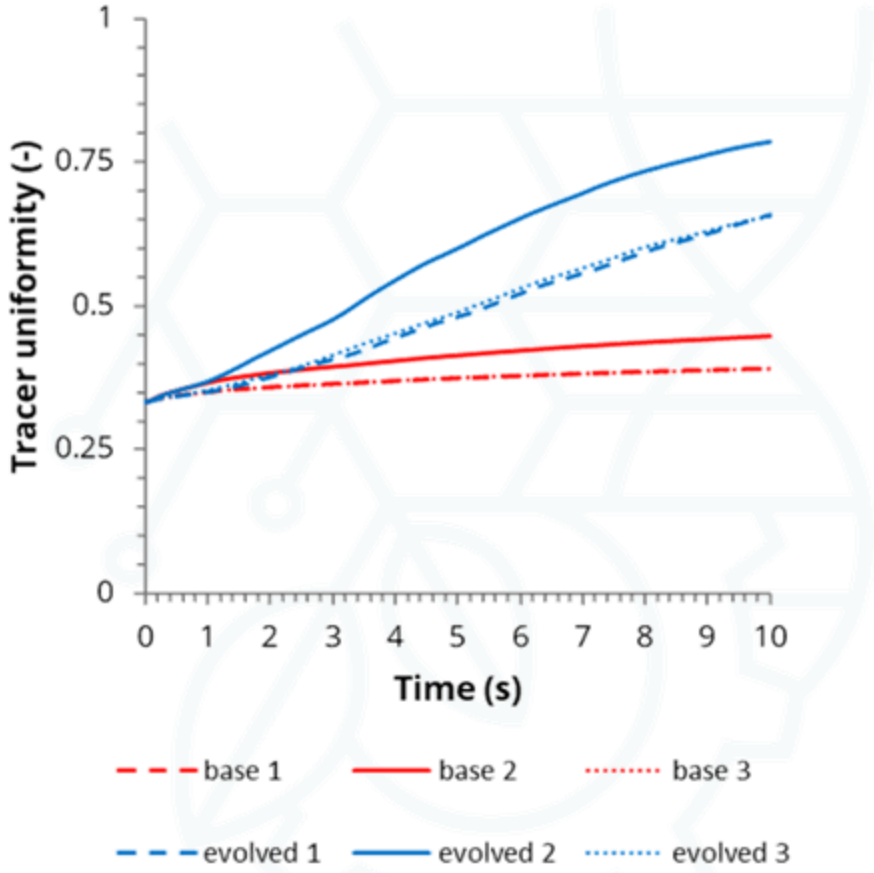

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[10] Yang, Z., et al 2018. Design and Performance of Helical Ribbon and Screw Impeller Aerobic Compost Bioreactor. International Journal of Environmental Science and Development 9.12. 385-389.

Impeller comparison

3-D printed design

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PEPI experiments

Glycerol in laminar flow

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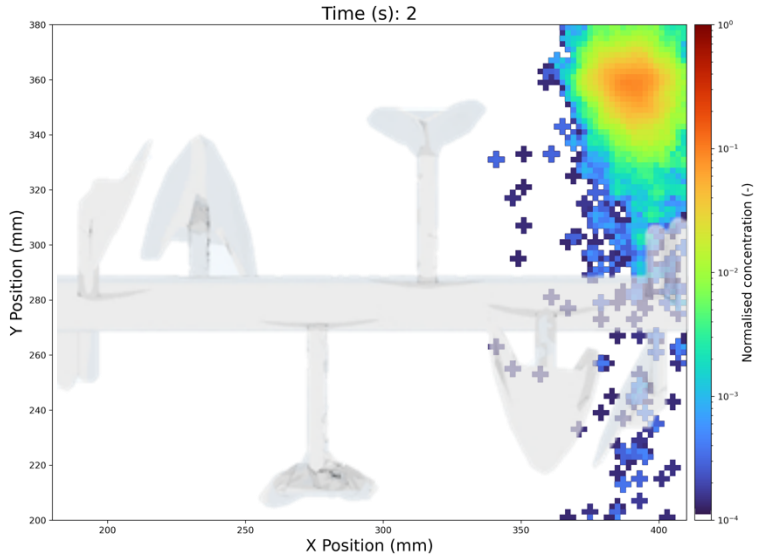

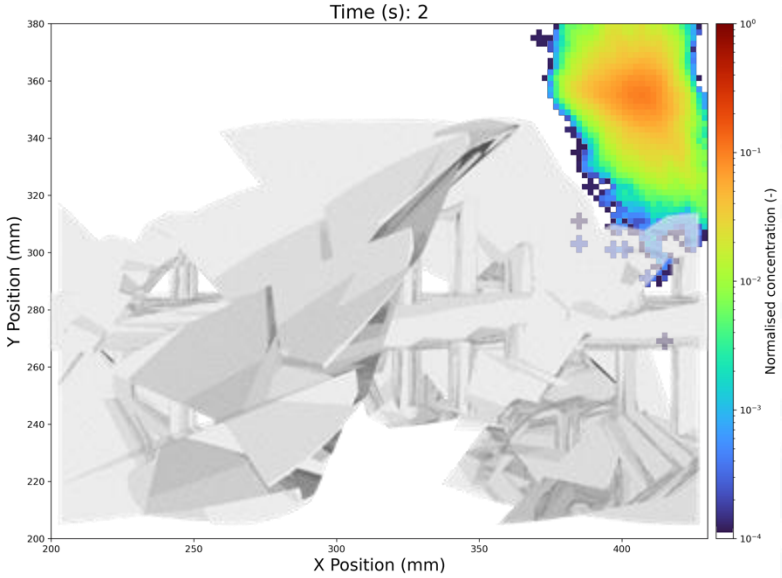

Original design

Evolved design

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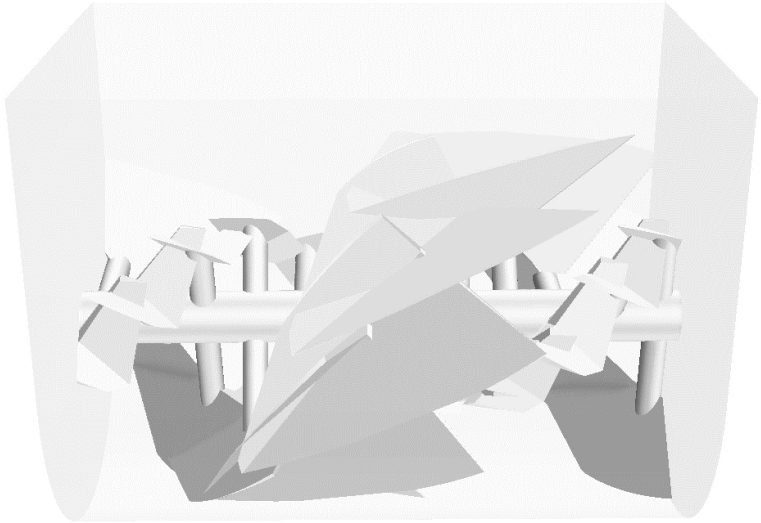
Conclusions

- PEPI can **validate** model predictions.
- Symbolic regression can discover **predictive models** without prior knowledge
- **General** data-driven approach for autonomous geometry optimisation.
- **Verified >10x** improved rate of axial mixing at similar torque.



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Thanks for your time

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School of Chemical Engineering

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Referenced work

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[2] Laurent, B.F.C., Cleary, P.W., 2012. Comparative study by PEPT and DEM for flow and mixing in a ploughshare mixer. Powder Technology 228, 171-186.

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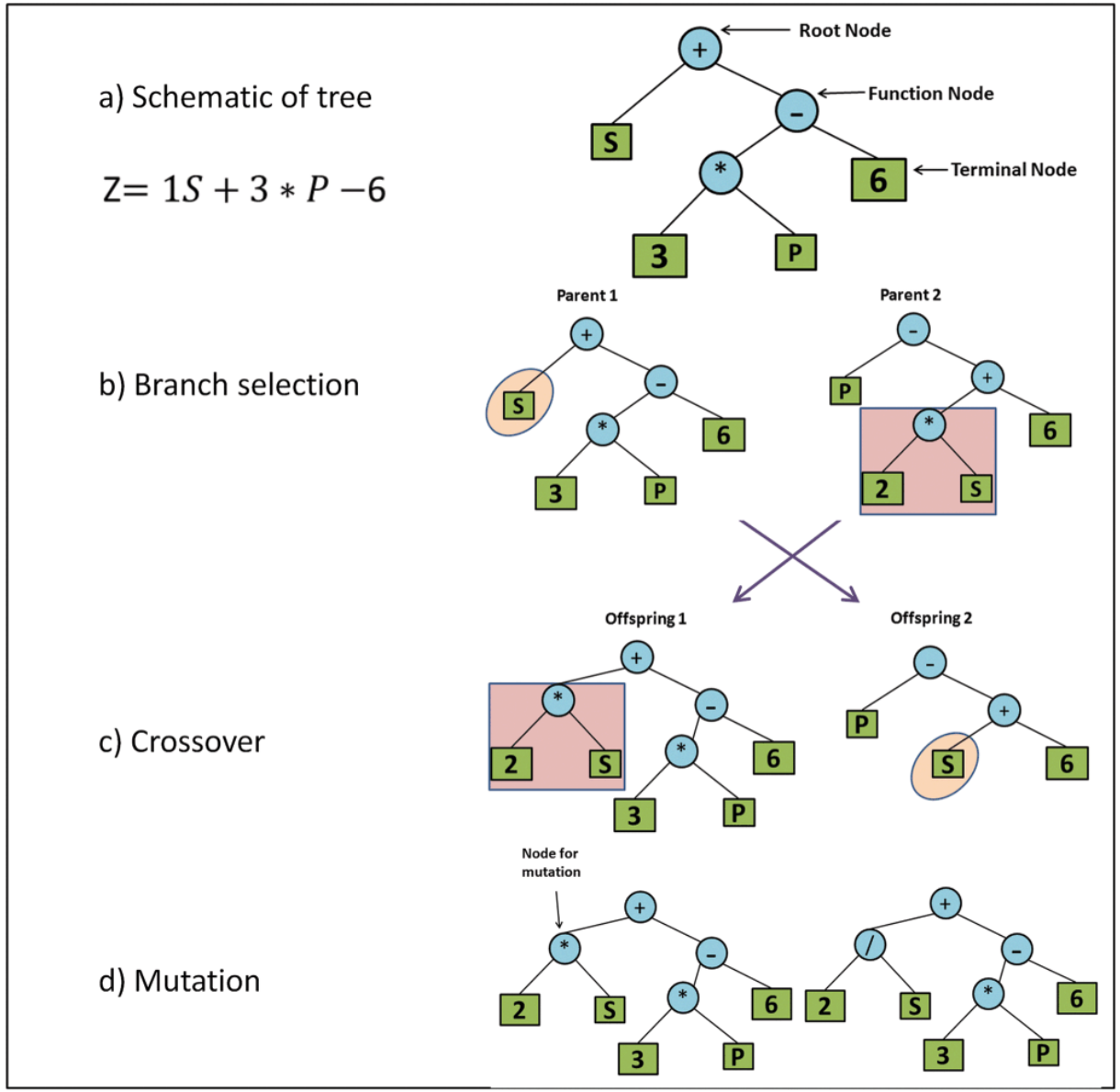
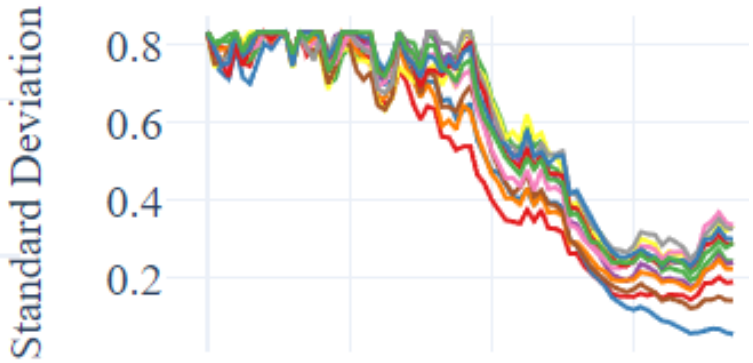
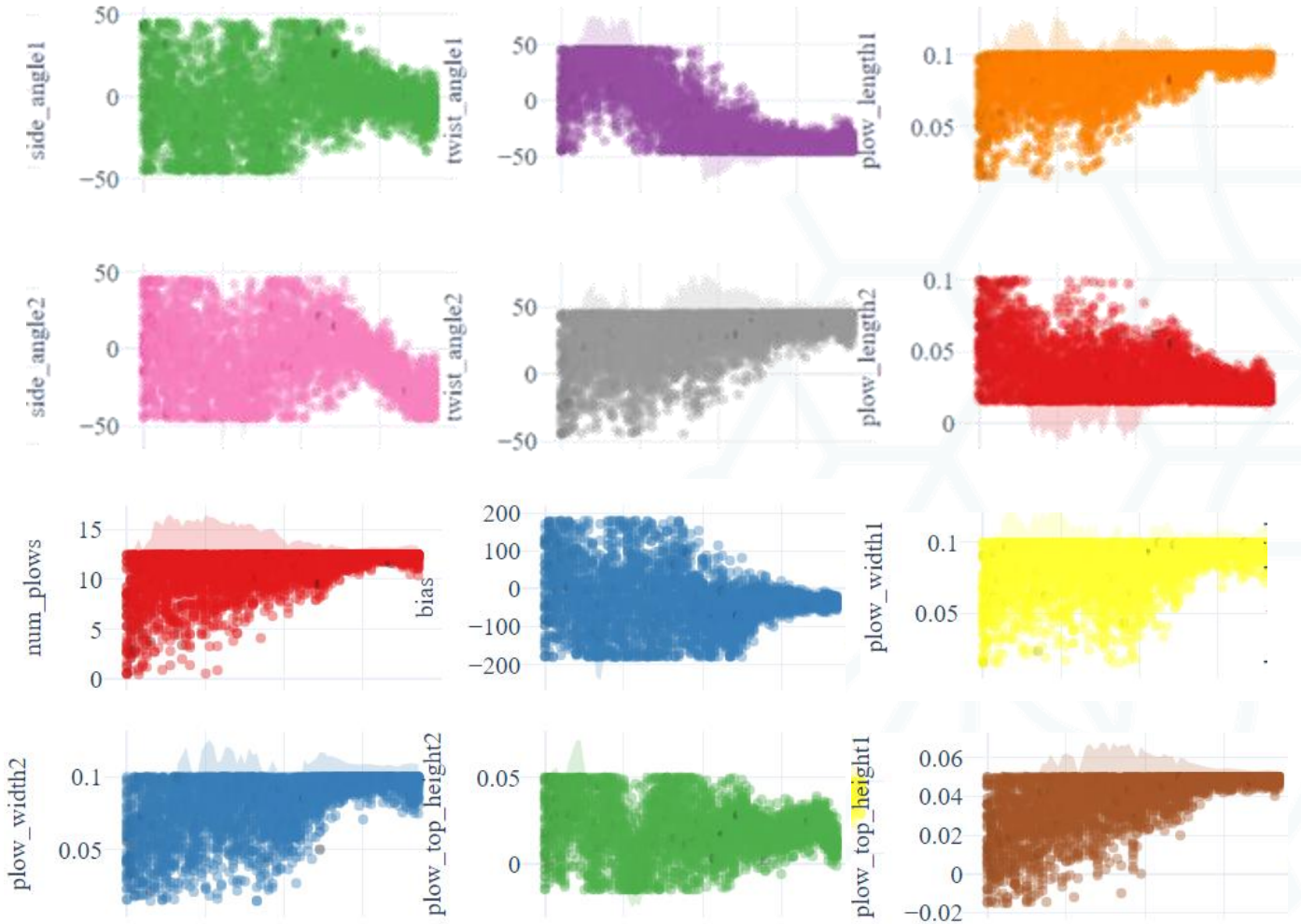
Symbolic regression



Convergence





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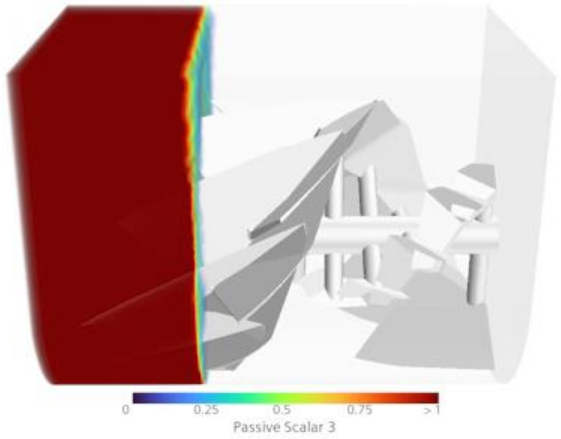
Passive scalar vs Particles



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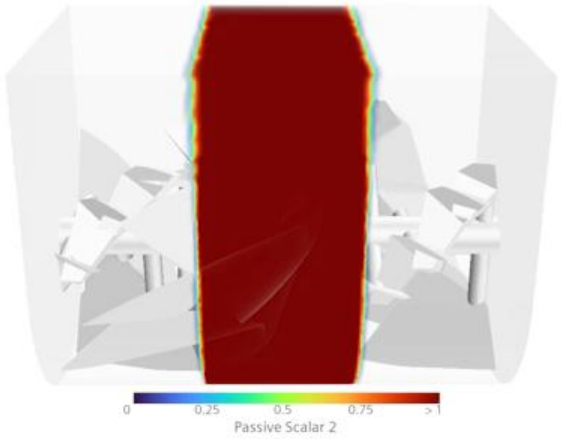

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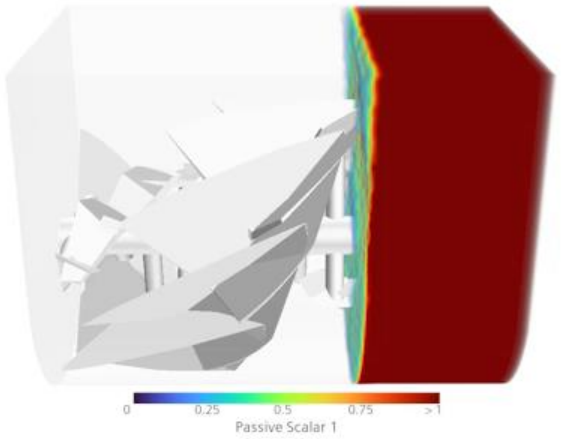

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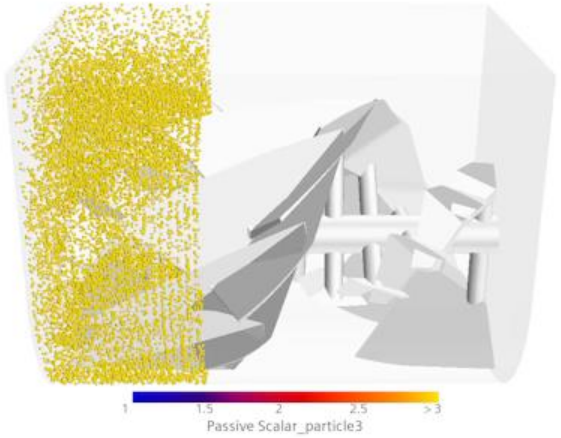

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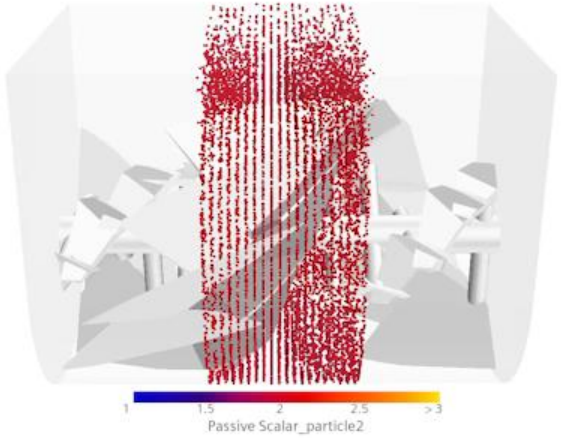

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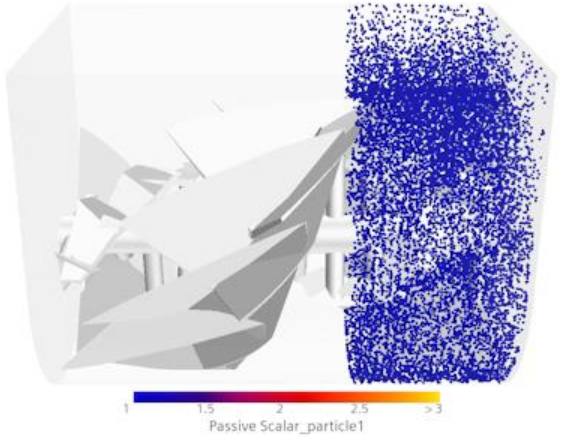

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