Barracuda Modelling of Waste Plastic Recycling Systems, and their Validation using Positron Emission Particle Tracking

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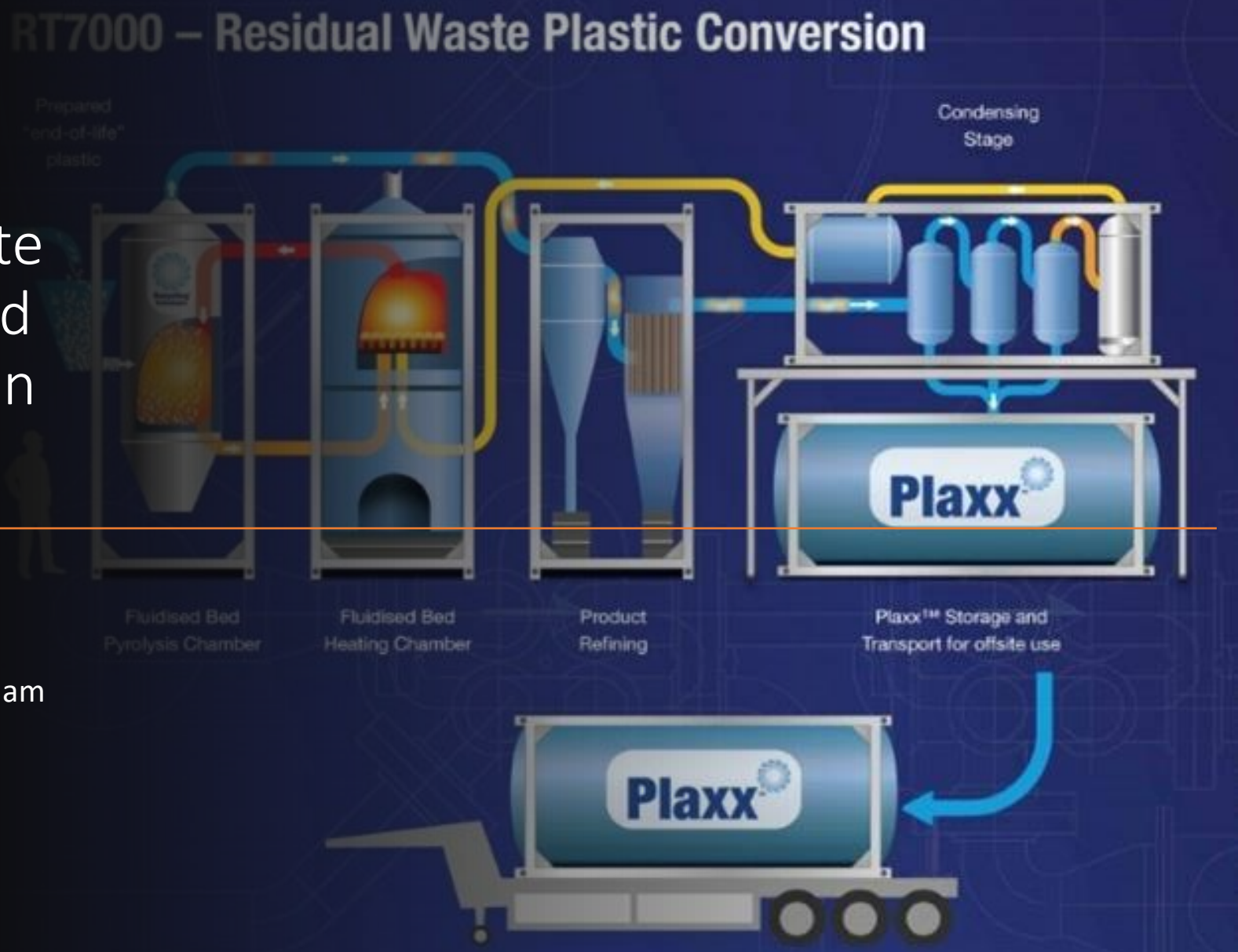

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Note

The simulations shown in these slides have been adapted in terms of their geometry and operating conditions, and certain quantitative experimental and numerical data rescaled or redacted to avoid the disclosure of IP and other sensitive information

Overview

1. The plastic waste crisis, and how best to address it
2. The importance of validation for numerical models → Barracuda + PEPT
3. Using PEPT-validated Barracuda models to help address the plastic waste crisis

Plastic Waste - A Global Challenge

- **~400 million tonnes** per annum produced.
- Equivalent to the mass the human population every 1.5 years
- 91% of plastic is **not recycled**
- Of the 9% that *is* nominally recycled, the majority forms **low-quality** second-life products.

Is plastic really the enemy?

- The idea of **eliminating** plastics is currently very vogue
- But is this an achievable goal?
- And even if achievable, is it a **sensible** goal?

Is plastic really the enemy?

- Lightweight, durable nature highly useful in many cases
- → irreplaceable without **some trade-off**
- Which in many cases can outweigh the benefit!

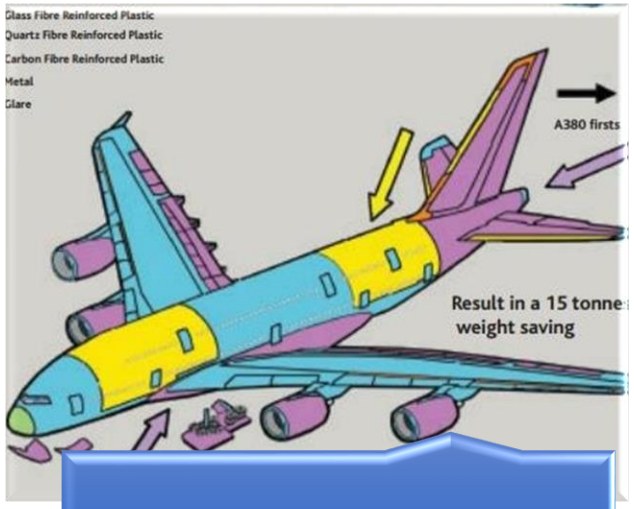
Is the **cure** worse than the **disease**?

Increased transport costs

Decreased functionality & reusability

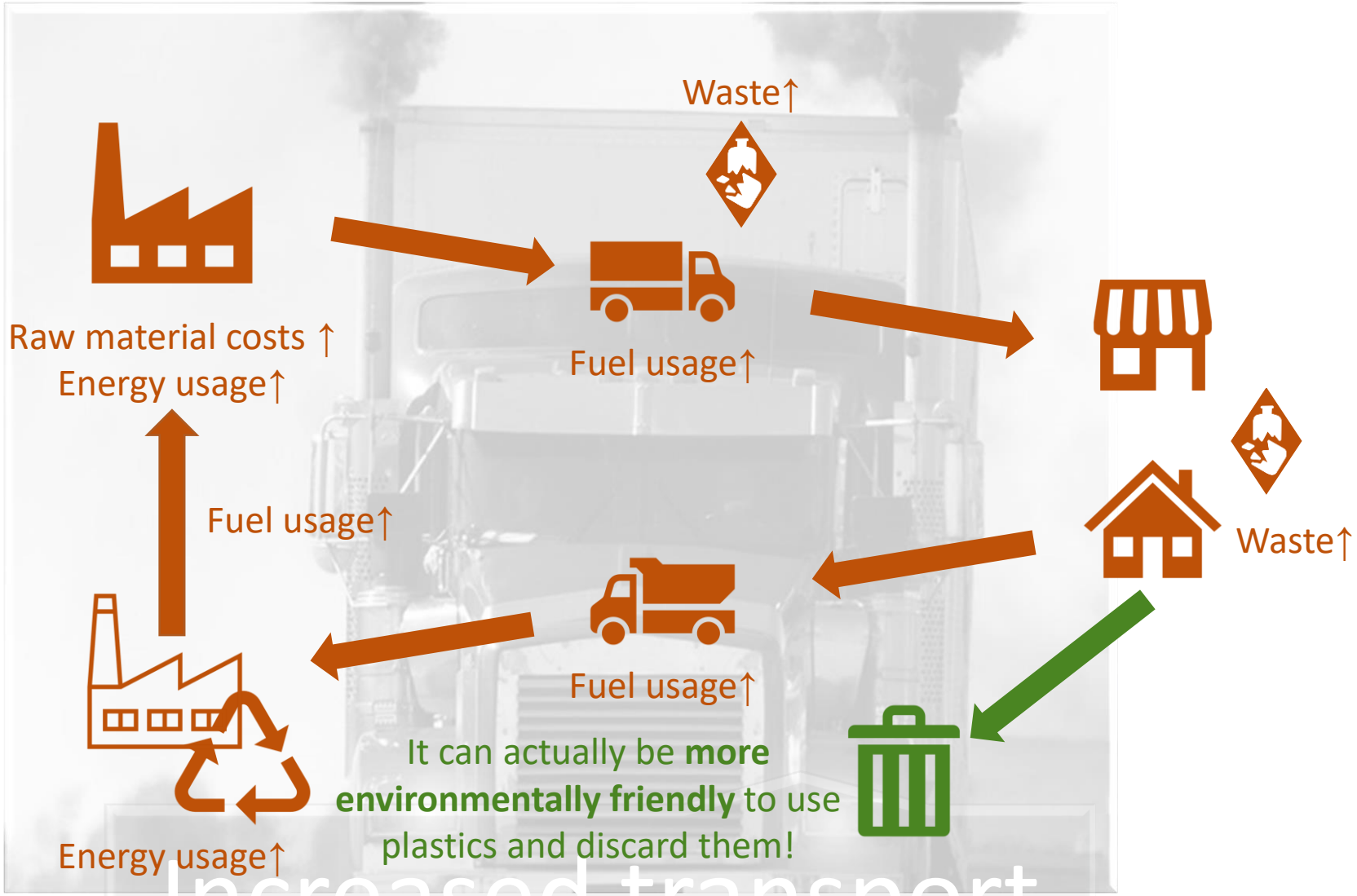
Increased food waste

Increased losses



Decreased efficiency

Example: Glass bottles vs plastic bottles



Increased transport costs

But what if we **didn't have to?**

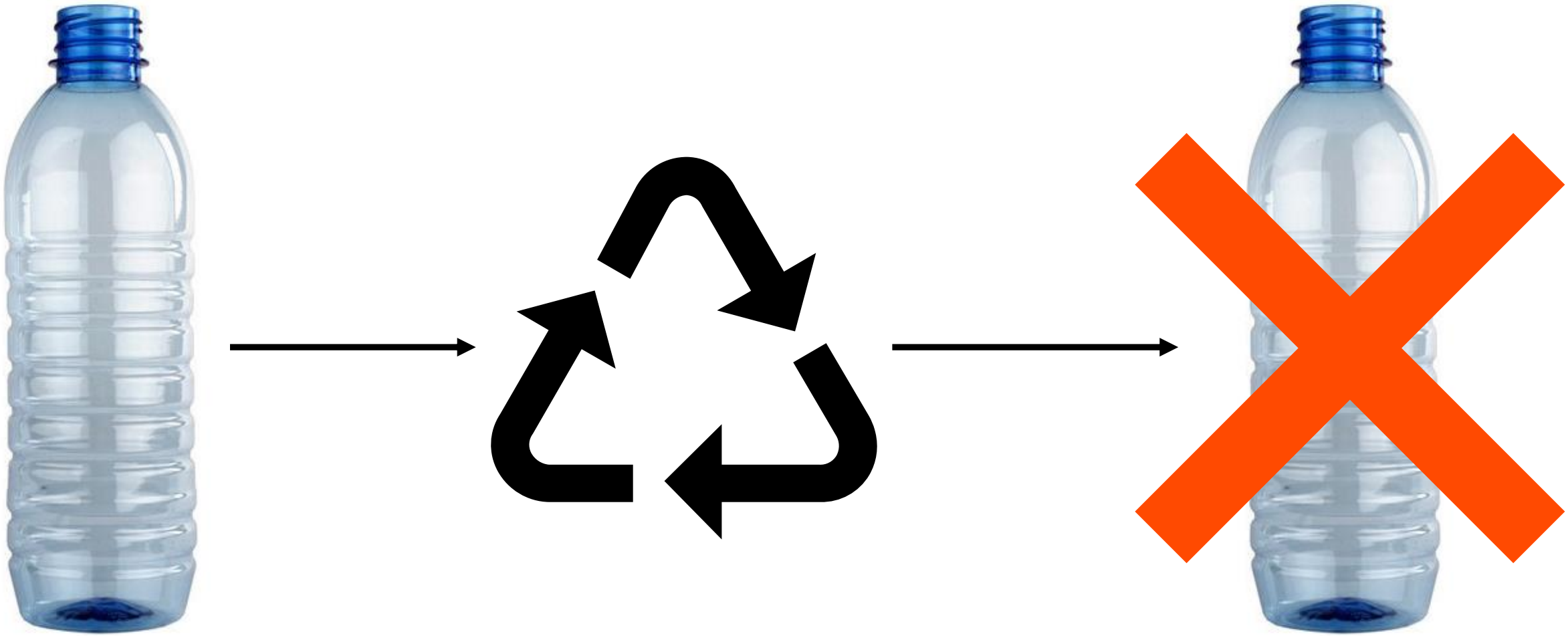
Is plastic really the enemy?

Removing plastic is not the solution

Is plastic really the enemy?

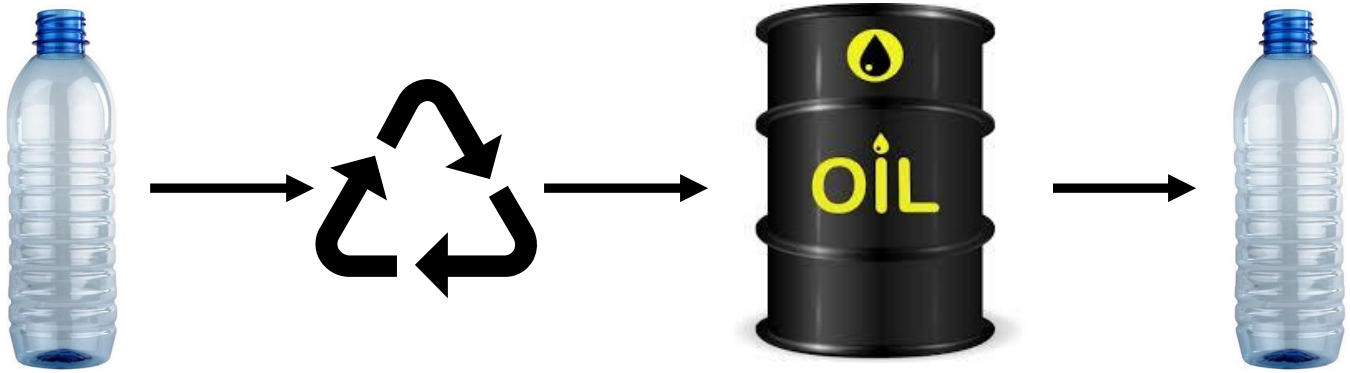
Recycling plastic is the solution

Downcycling is not recycling



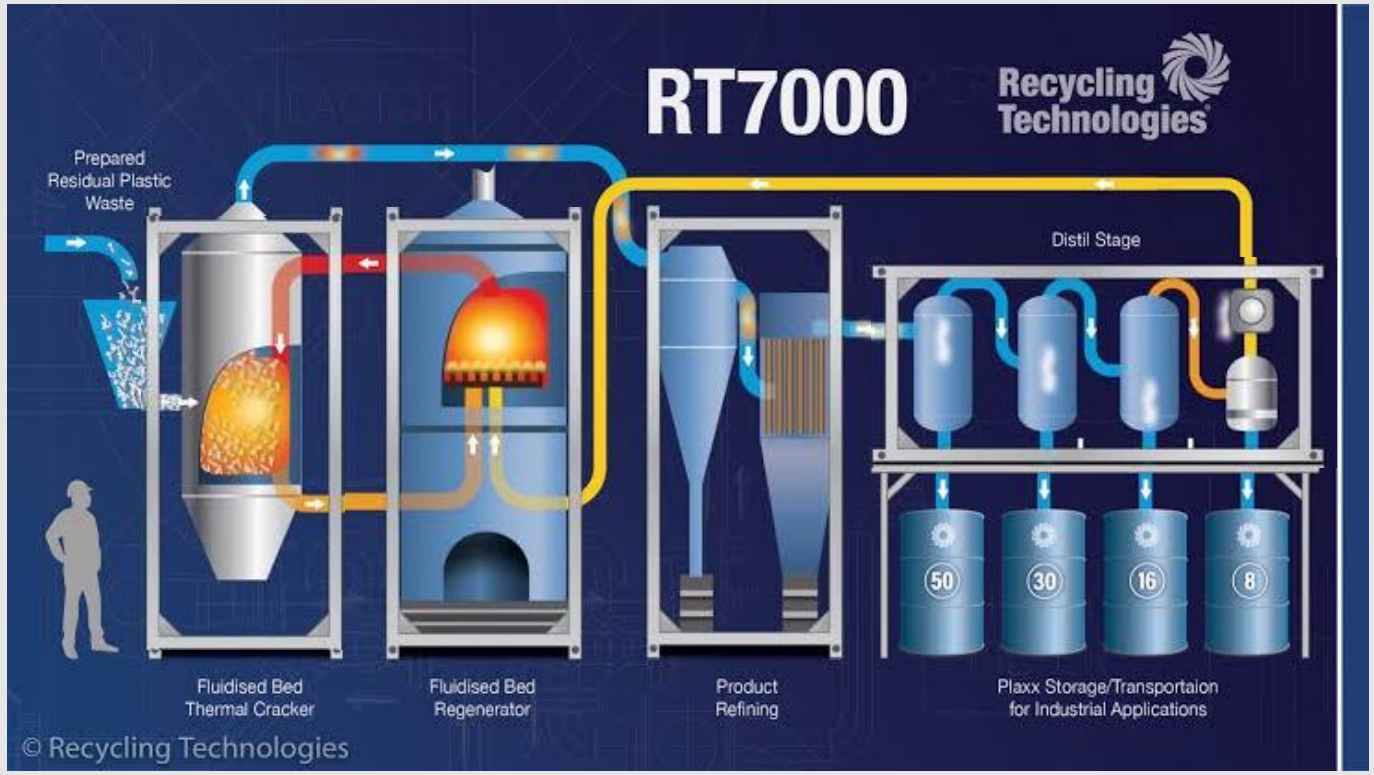
Downcycling is not recycling

Basically just **delaying landfill**! Is there a **better way**?



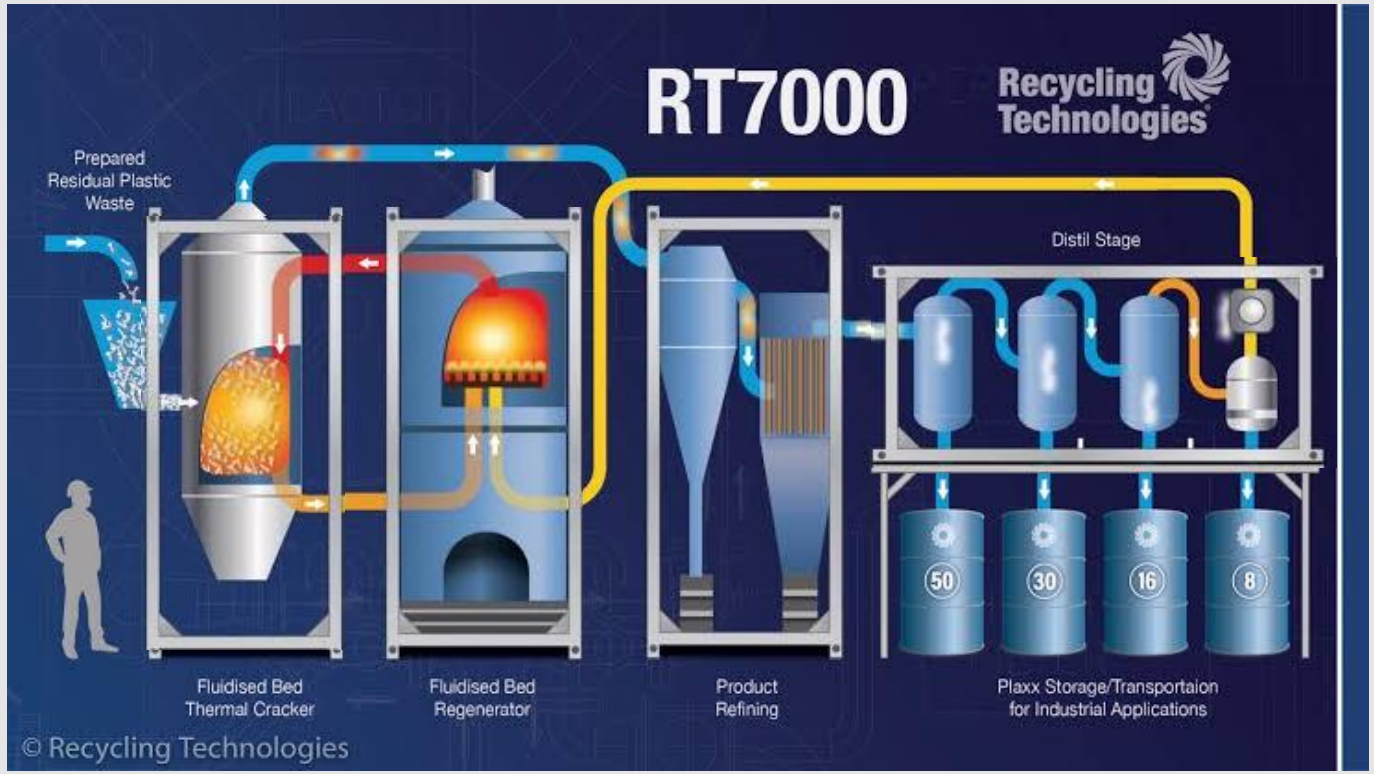
How can we (practically) achieve this?

Waste Plastic Pyrolysis



- Working with industrial partner Recycling Technologies Ltd.
- Efficiently convert plastic waste into **valuable petrochemical feedstocks and fuels**.
- Fluidised bed technology allows **large-scale processing**.

Waste Plastic Pyrolysis



Modular design minimises transport.

Waste Plastic Pyrolysis

Benefits of modular design:

Easy & efficient to set up new plants

→ network of local plants

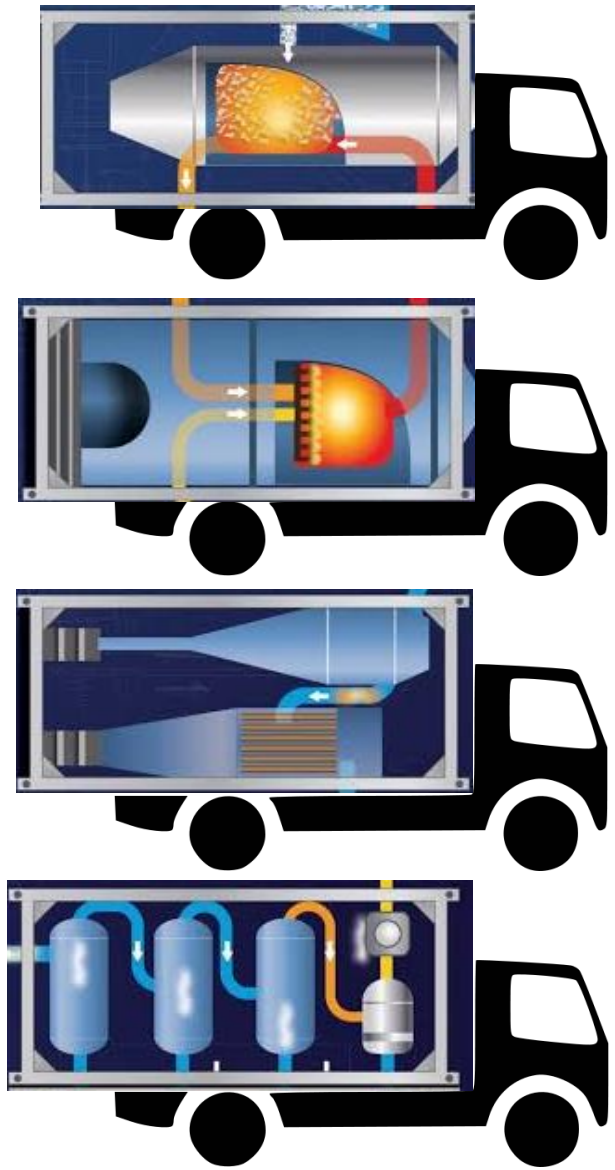
→ minimise transport costs

Affordable & accessible to developing countries

Implementable with little infrastructure

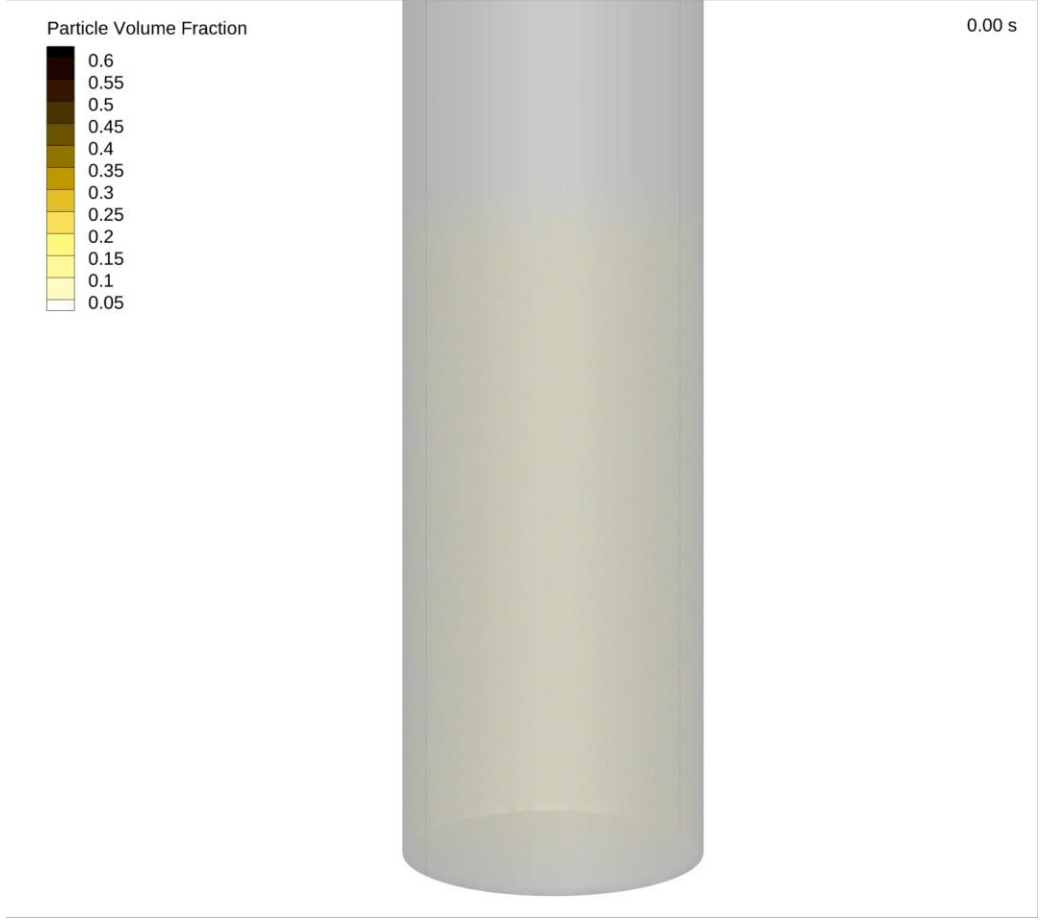
→ Address plastic waste crisis where need is most pressing

Modular design minimises transport.



So what's the problem?

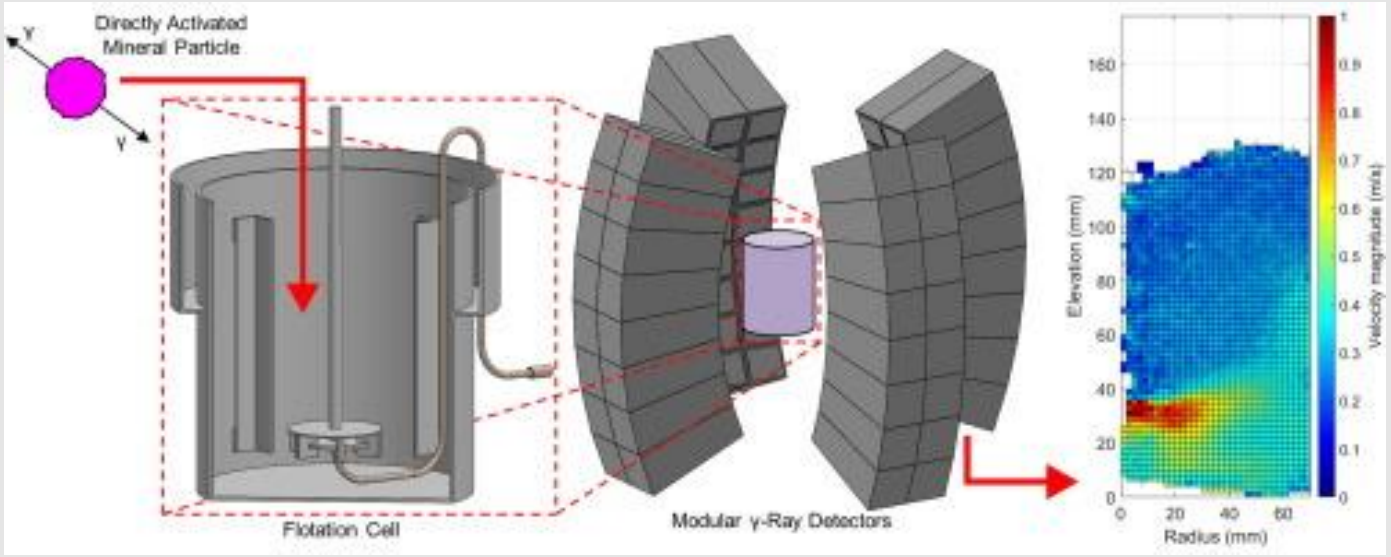
- Proven concept → commercial reality
- Reactor hydrodynamics **not fully understood**
- Improved knowledge needed for optimisation
- Large, opaque systems – how can we improve knowledge?



So what's the solution?

- A two-pronged approach: Numerical modelling + experimental imaging
- Positron emission particle tracking: an experimental technique that lets us "see inside" experimental systems
- MP-PIC (Barracuda): a numerical modelling technique capable of accurately predicting flow dynamics of large, multiphase systems

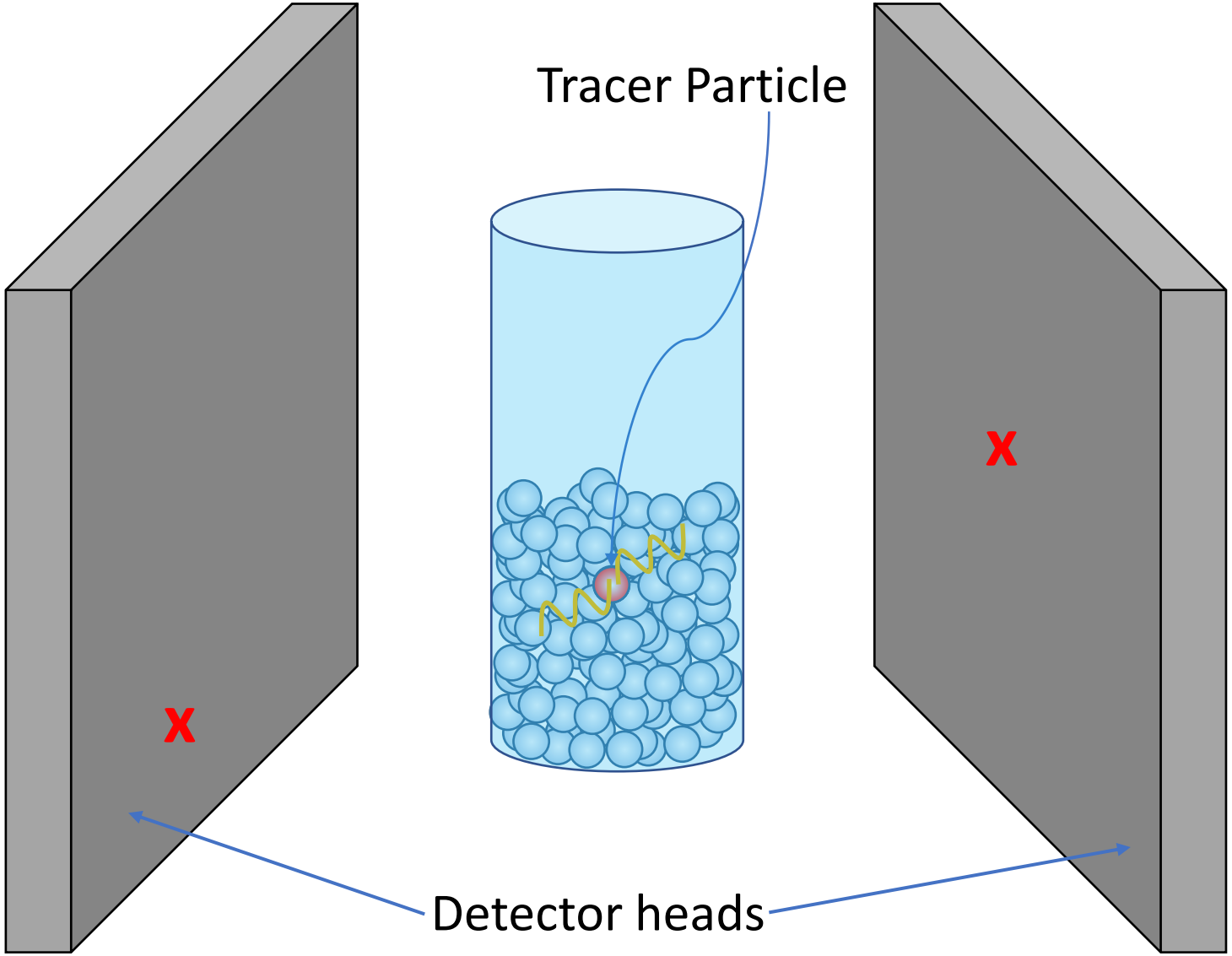
Positron Emission Particle Tracking



- Uses highly-penetrating gamma radiation to directly track the three-dimensional motion of particles through particulate, fluid and multiphase systems, with high temporal and spatial resolution.
- PEPT is **uniquely well suited** to validation of MP-PIC models
  - Detailed, 3D images of dynamics → direct, quantitative comparison with DEM data
  - Can “see inside” steel-walled industrial systems

Positron Emission Particle Tracking

Windows-Yule, C. R. K., Seville, J. P. K., Ingram, A., & Parker, D. J. (2020). Positron Emission Particle Tracking of Granular Flows. *Annual Review of Chemical and Biomolecular Engineering*, *11*.



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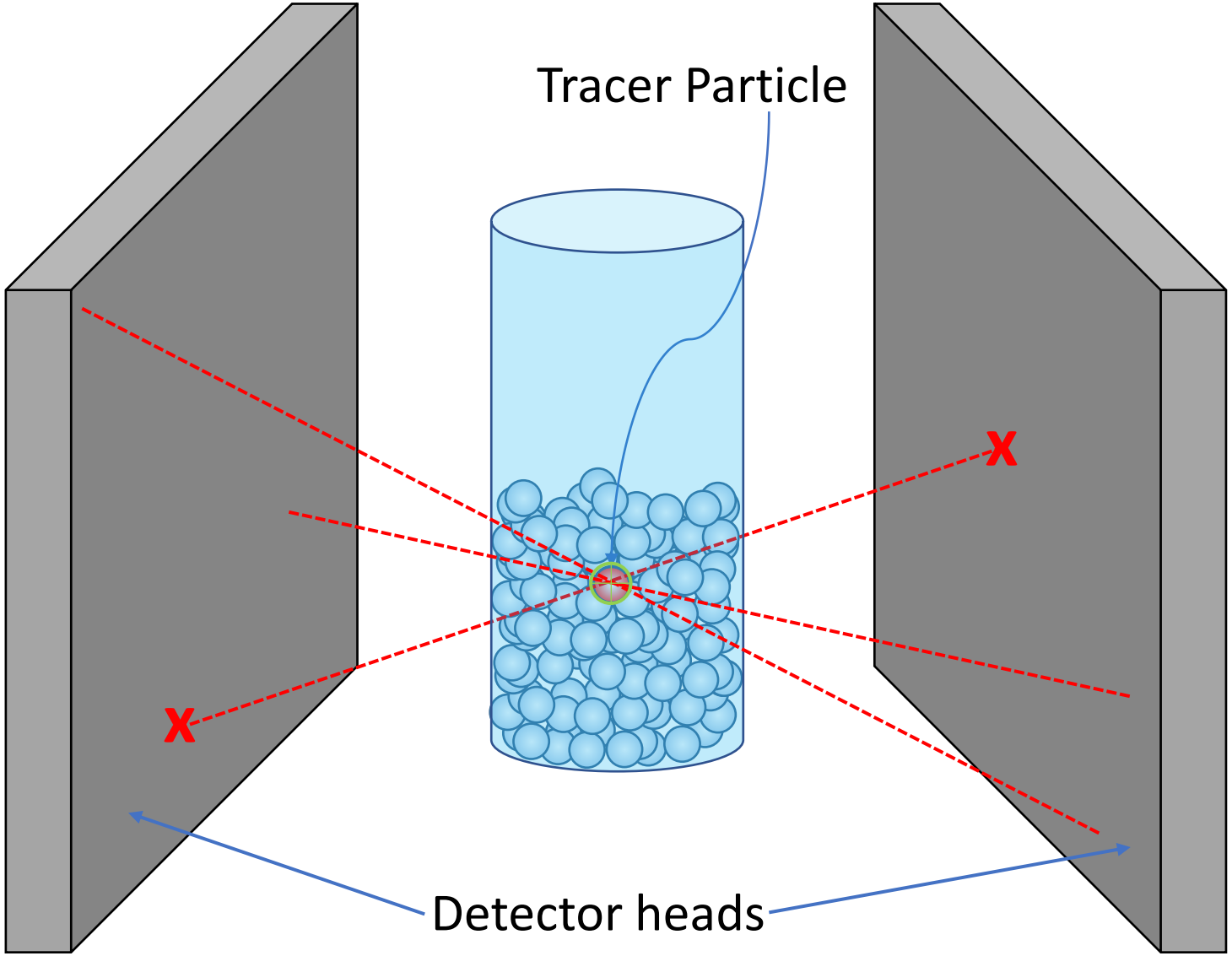
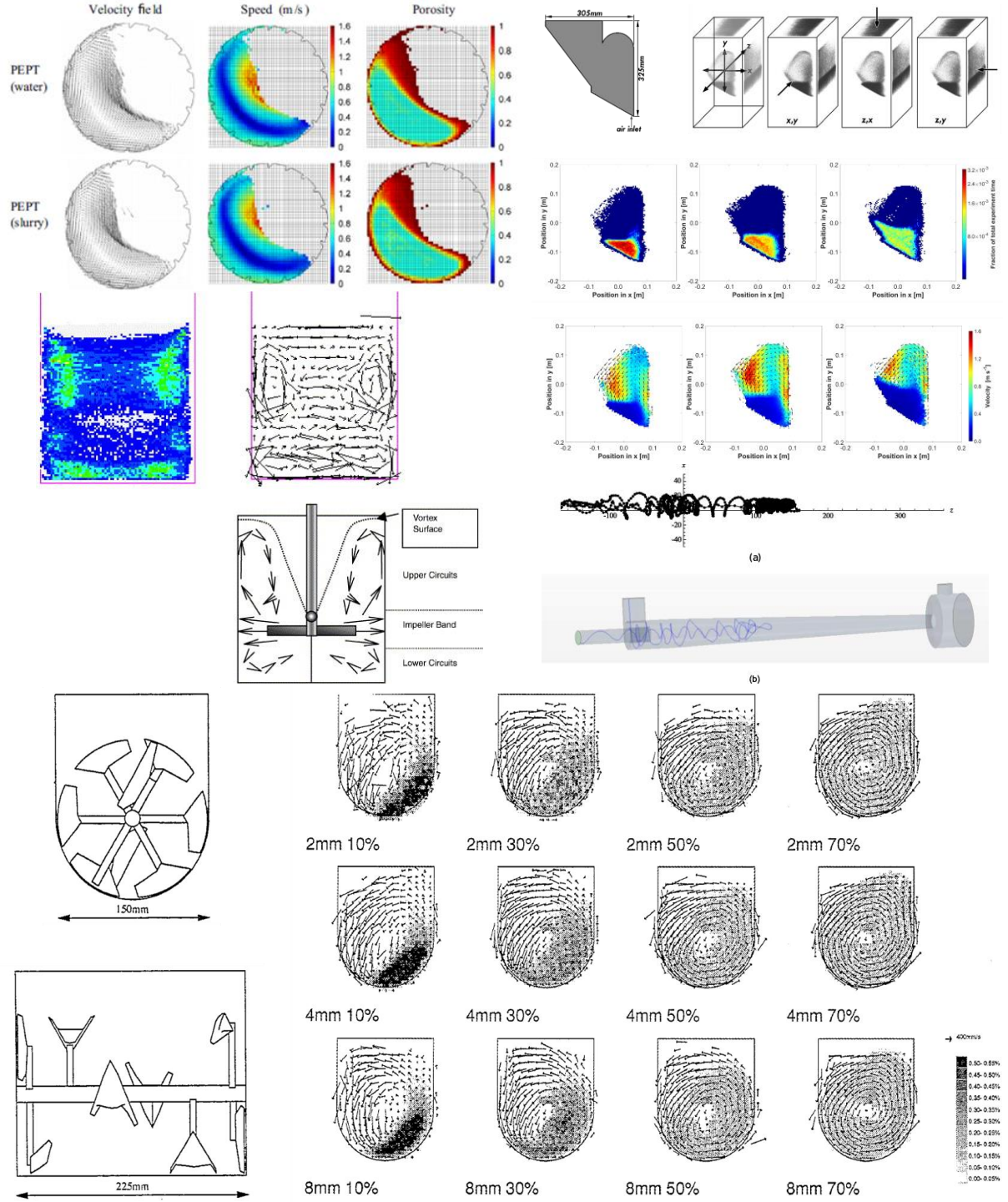


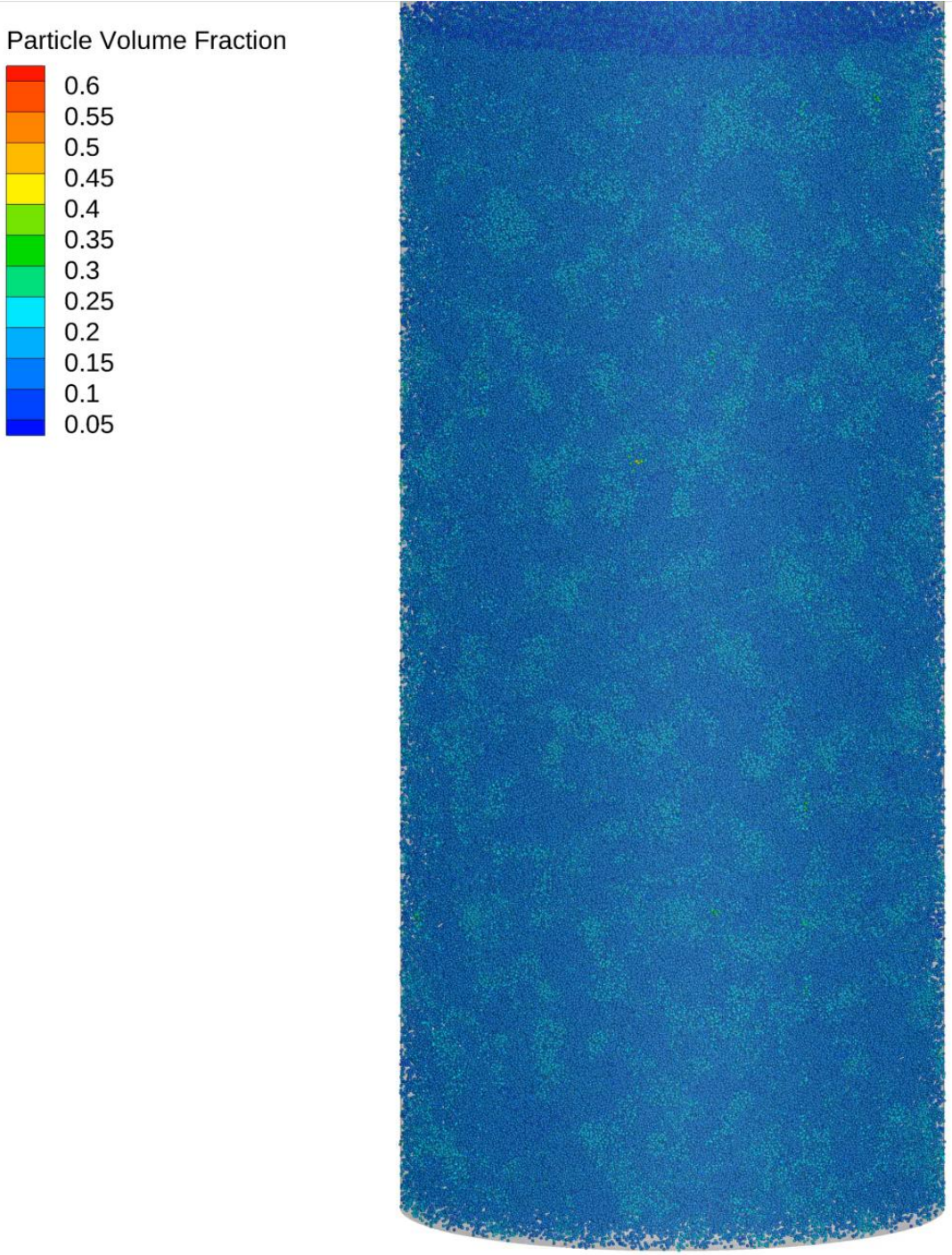


PEPT

- **Full, three-dimensional data** regarding system dynamics
- Capable of **penetrating steel-walled systems** and opaque beds
- Difficult to image **transient motion**
- No direct information regarding **stresses or chemical kinetics**

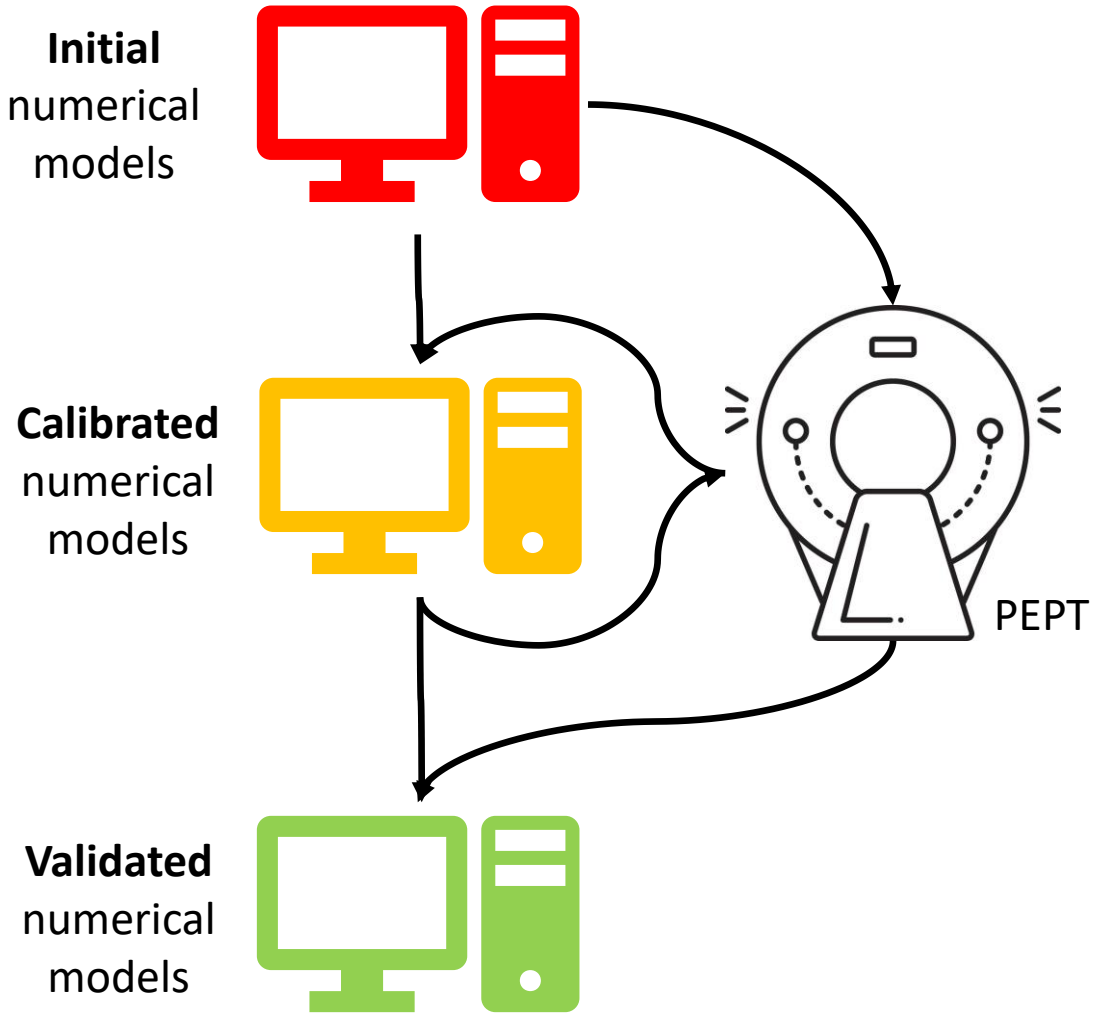
Barracuda

- **Full, three-dimensional data** regarding system dynamics
- Information regarding **transient motion**
- Full information regarding **stresses and chemical kinetics**
- **Can we trust output** without experimental validation?



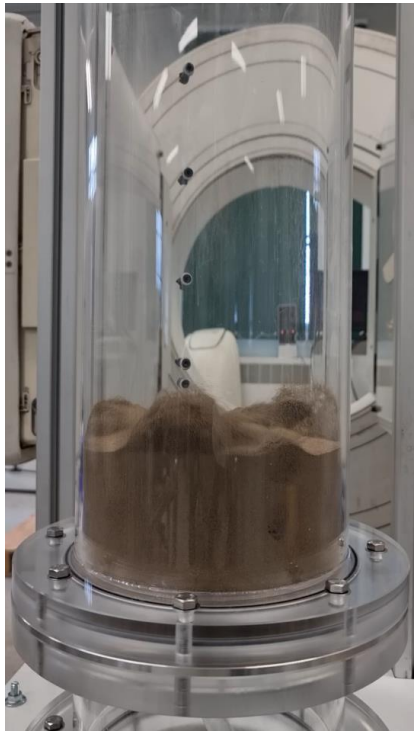
PEPT + Barracuda

- **Full, three-dimensional data** regarding system dynamics
- Information regarding **transient motion**
- **Full information** regarding stresses and chemical kinetics
- **Rigorously, quantitatively validated** outputs



Take-Home Point:

without strong validation, even the best simulations can be **inaccurate**, or even **unphysical**



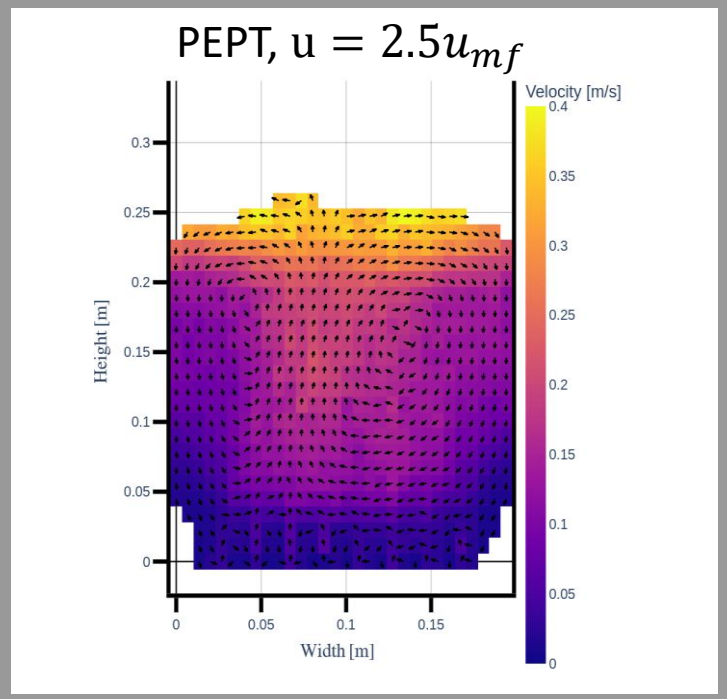
Validation

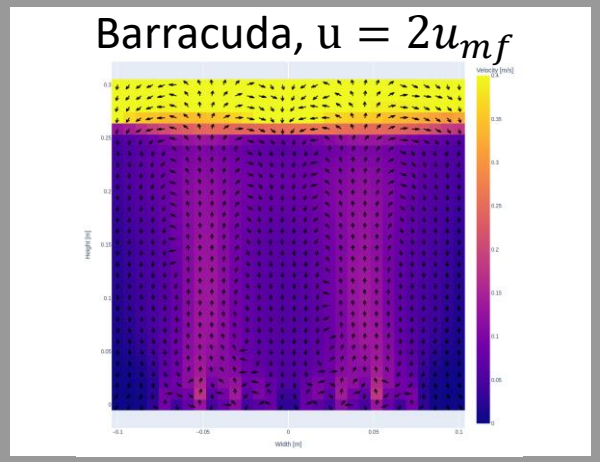
- Visually similar
- But how can we check validity **more rigorously**?

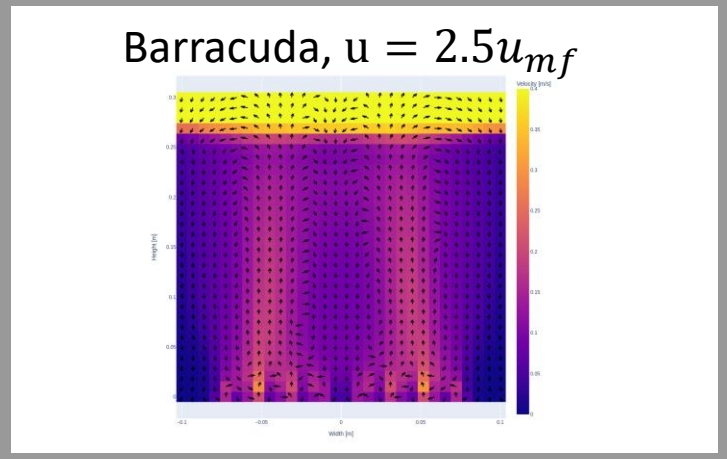
Validating Barracuda Results

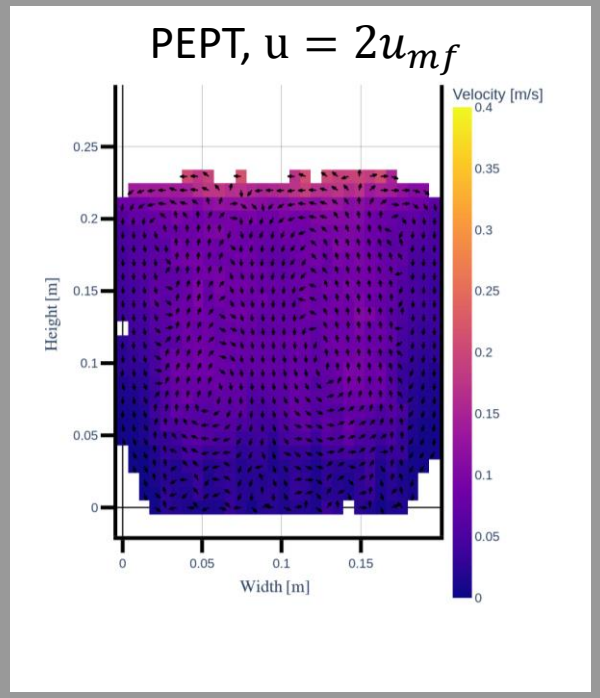
- As both PEPT and Barracuda provide full, three-dimensional dynamic information, can **directly compare** key fields and quantities
- For the systems of interest, we compared:
  - Flow patterns
  - Velocity distributions
  - Circulation (turnover) rates

Flow Patterns & Velocity Fields

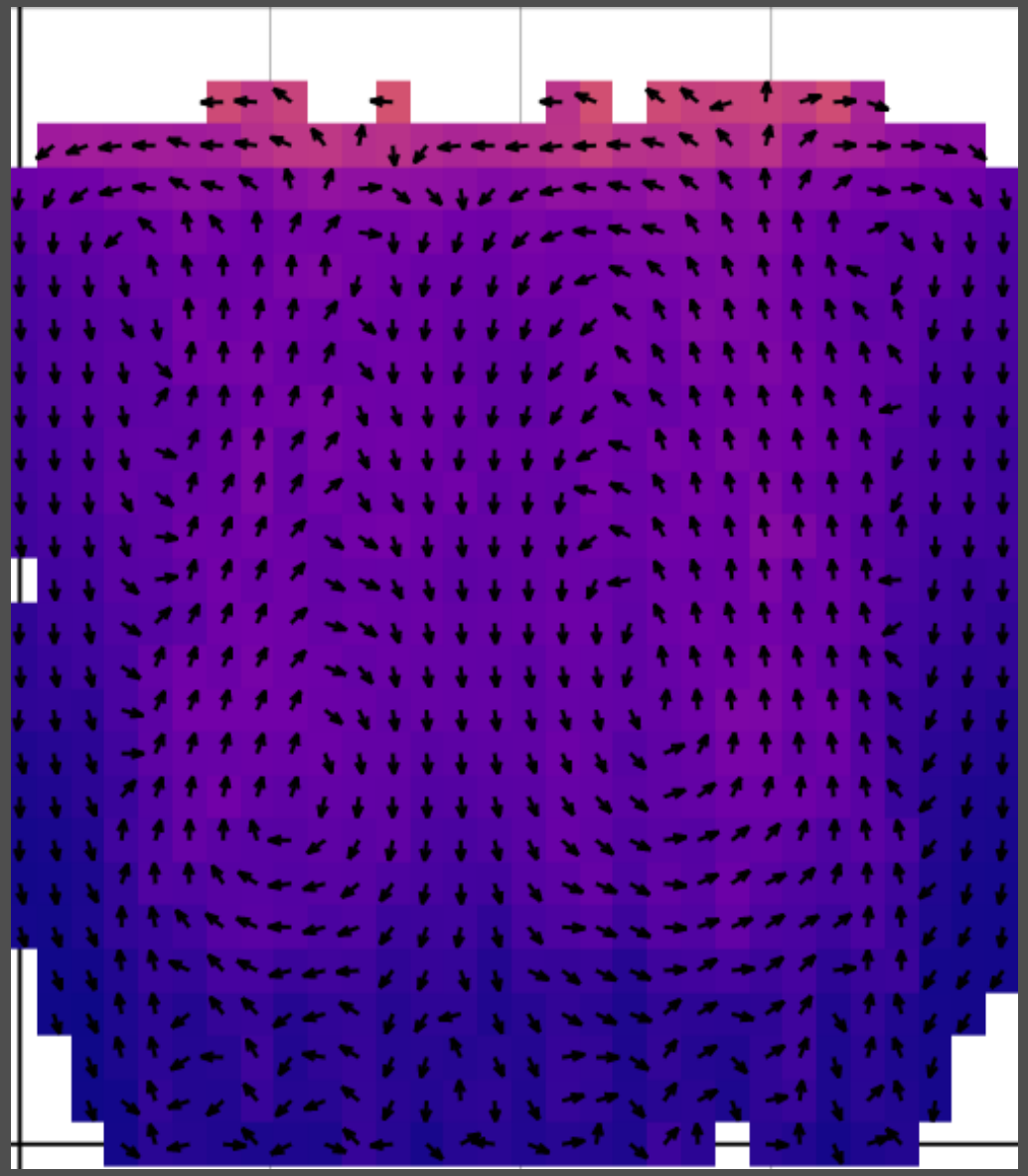


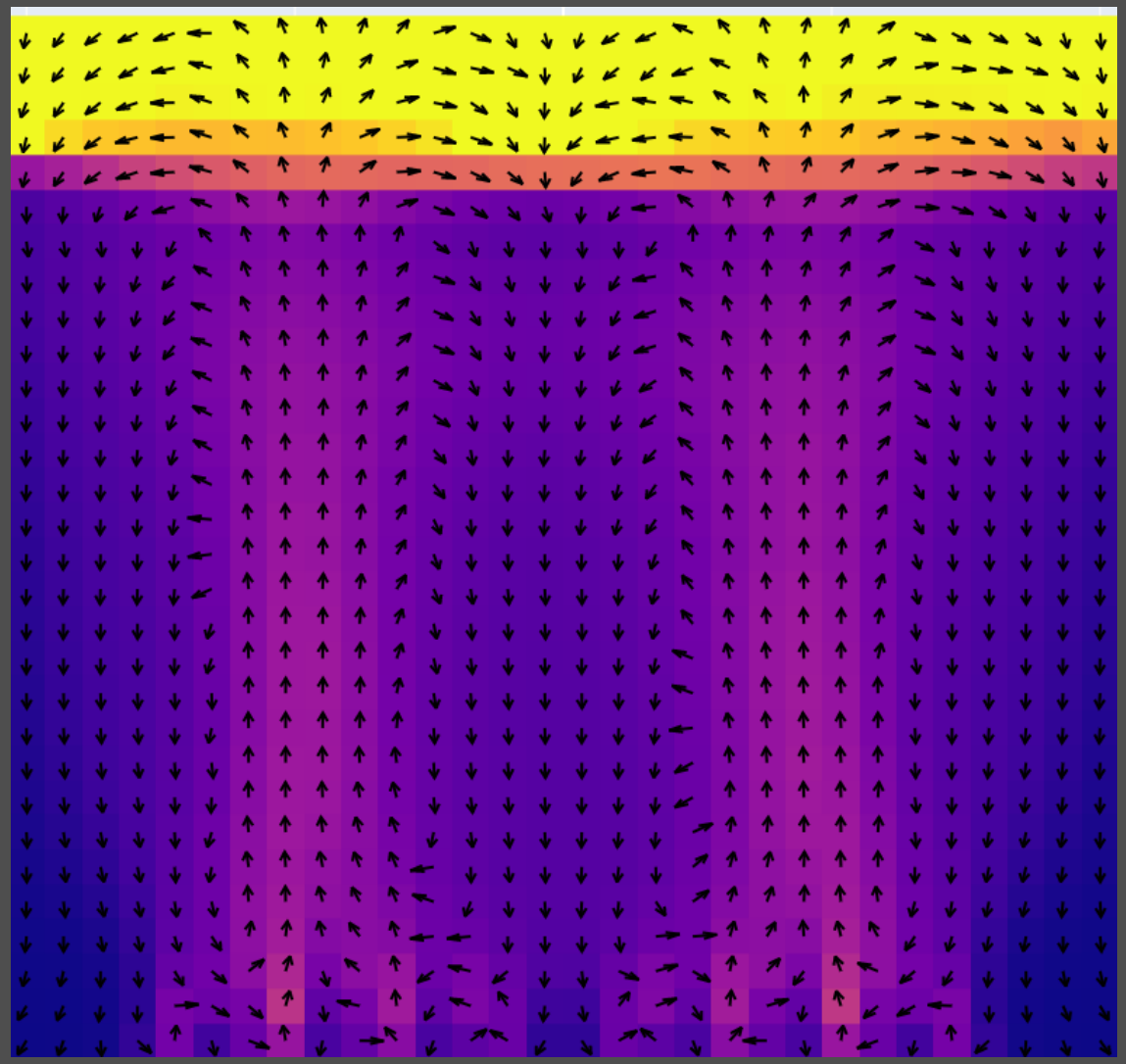


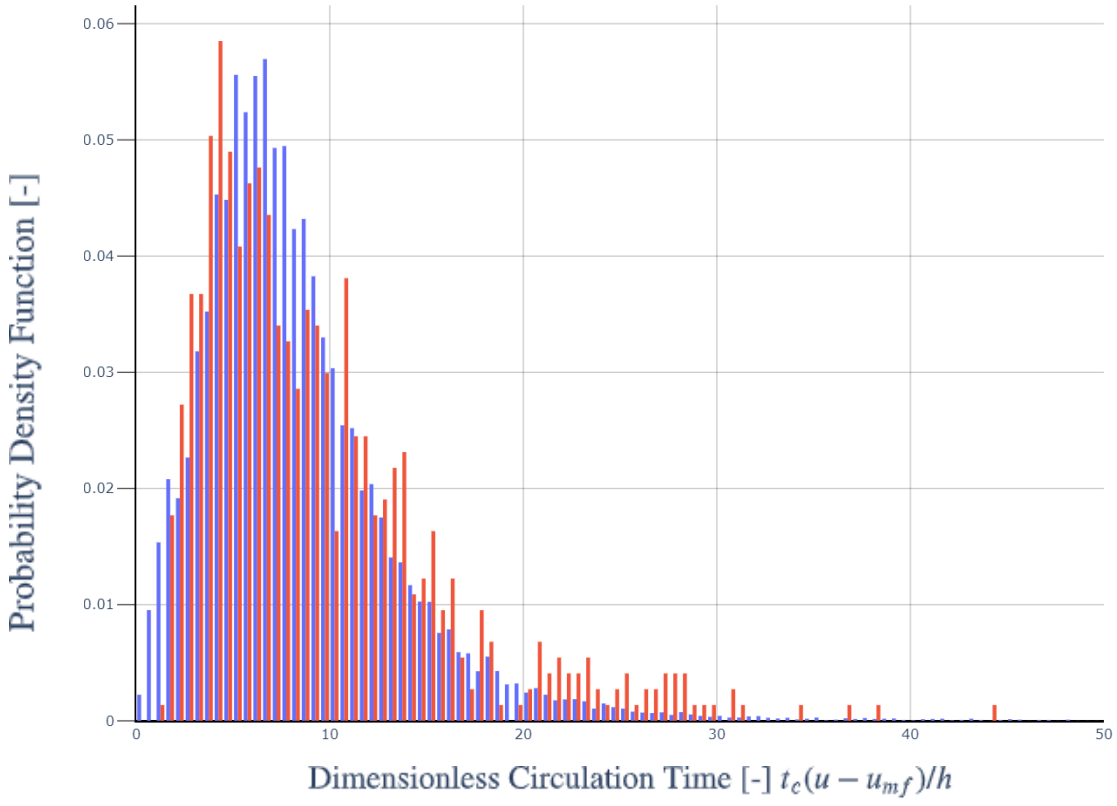


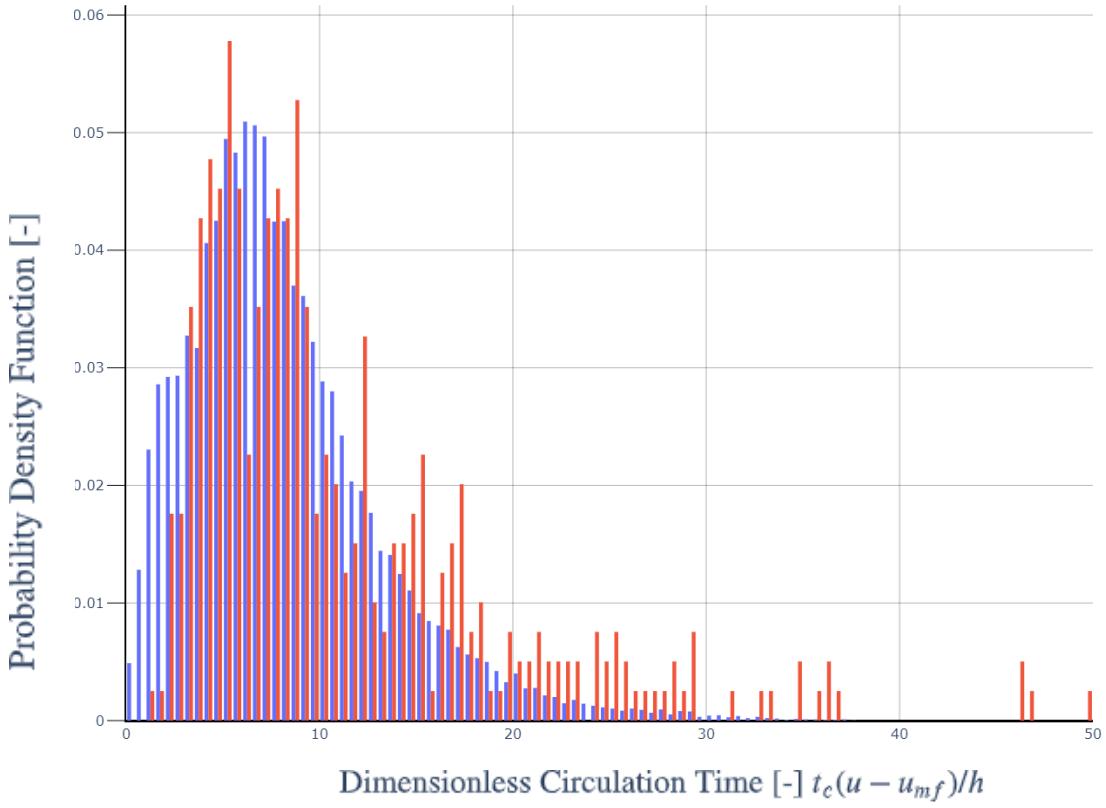


- Reasonable agreement between measured and predicted expanded bed heights
- Similar ranges of velocities between experiment and simulation
- Qualitatively matching flow patterns for lower u, some deviation at higher u





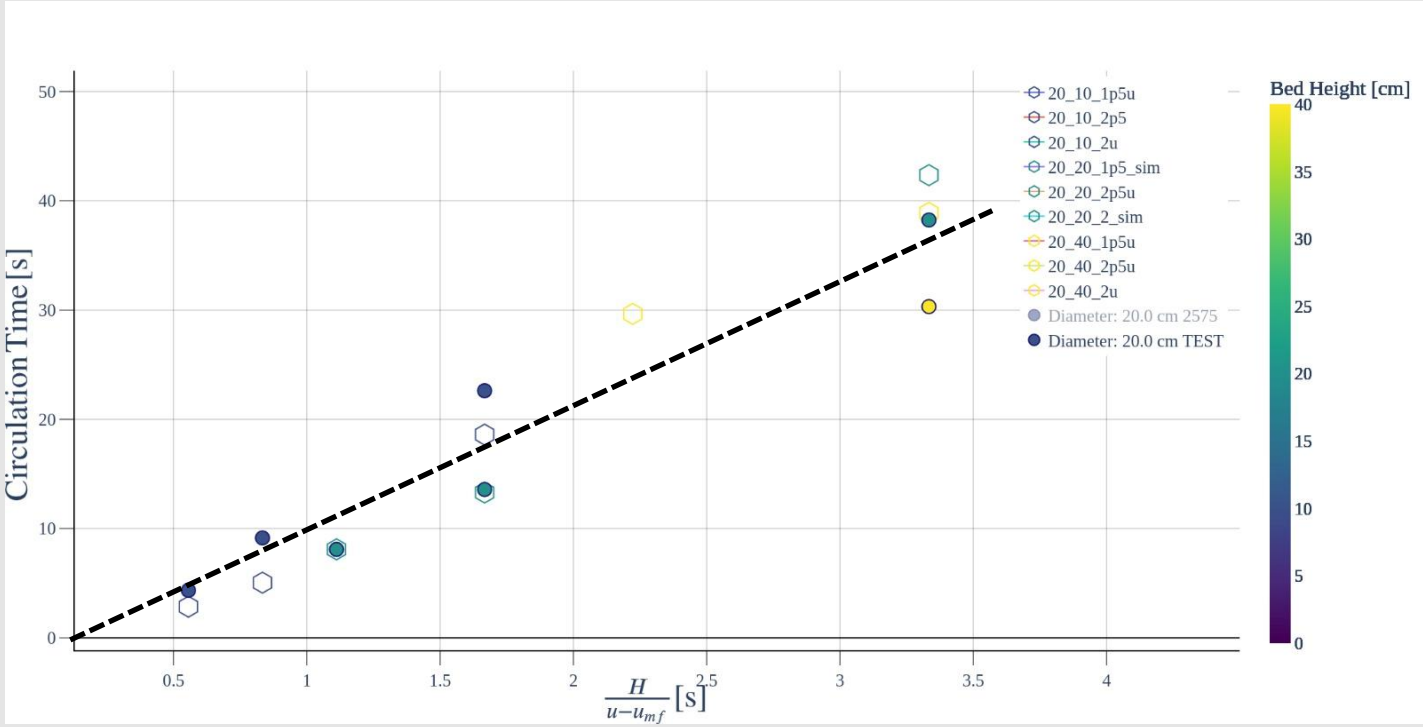




Circulation Rate

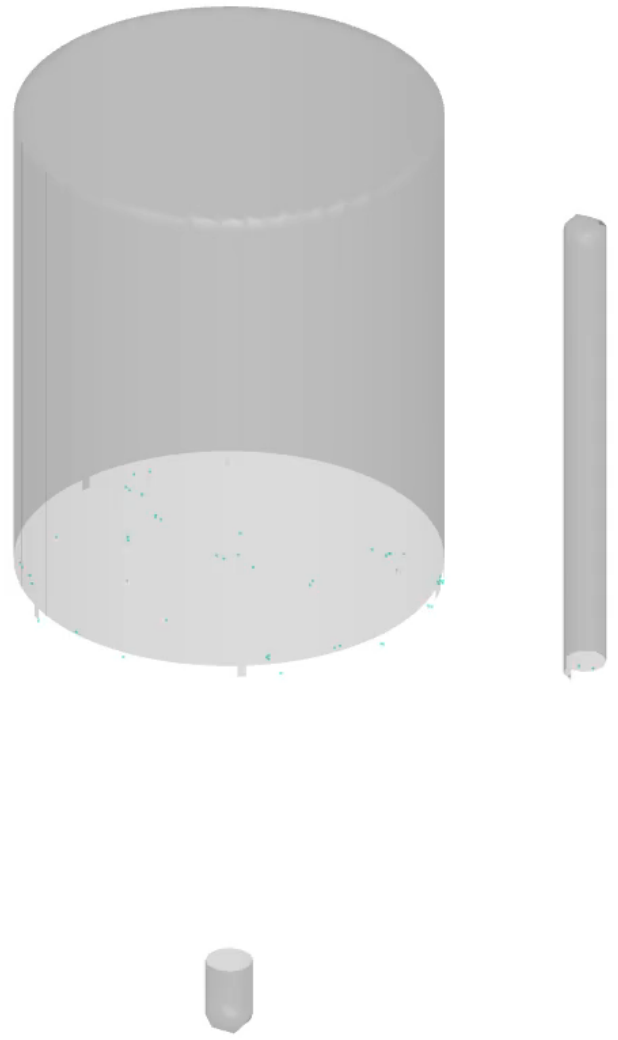
PEPT || MP-PIC

Circulation Rate



- Barracuda data scales with $\frac{H}{u-u_{mf}}$ as expected from the literature
  - → Results are **physical**
- Close correspondence between PEPT and Barracuda
  - → Results are **accurate**
- Disagreement largely due to **lack of statistics from experimental data**

Applying the Calibrated model



3 main applications

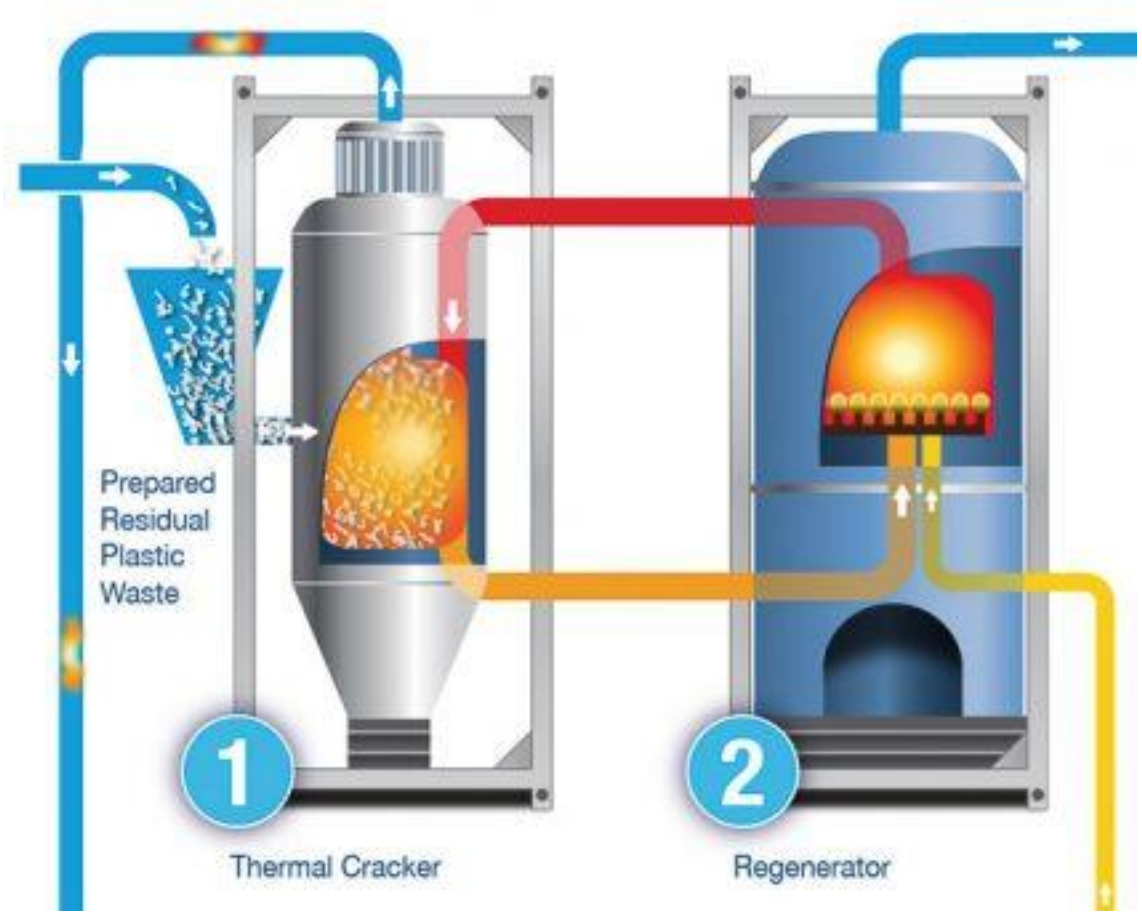
Troubleshooting

Optimisation

Designing new systems

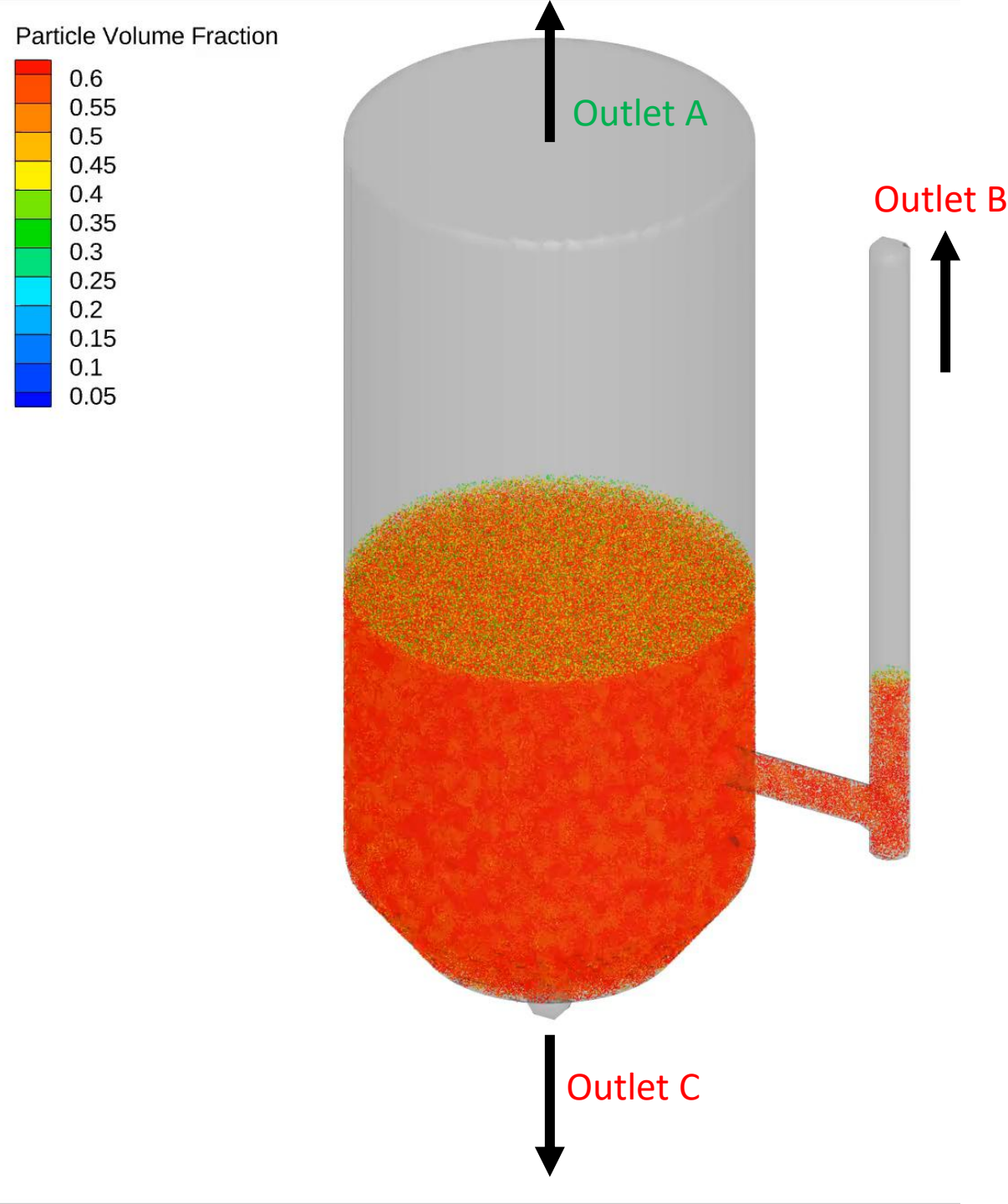
Example:
Troubleshooting

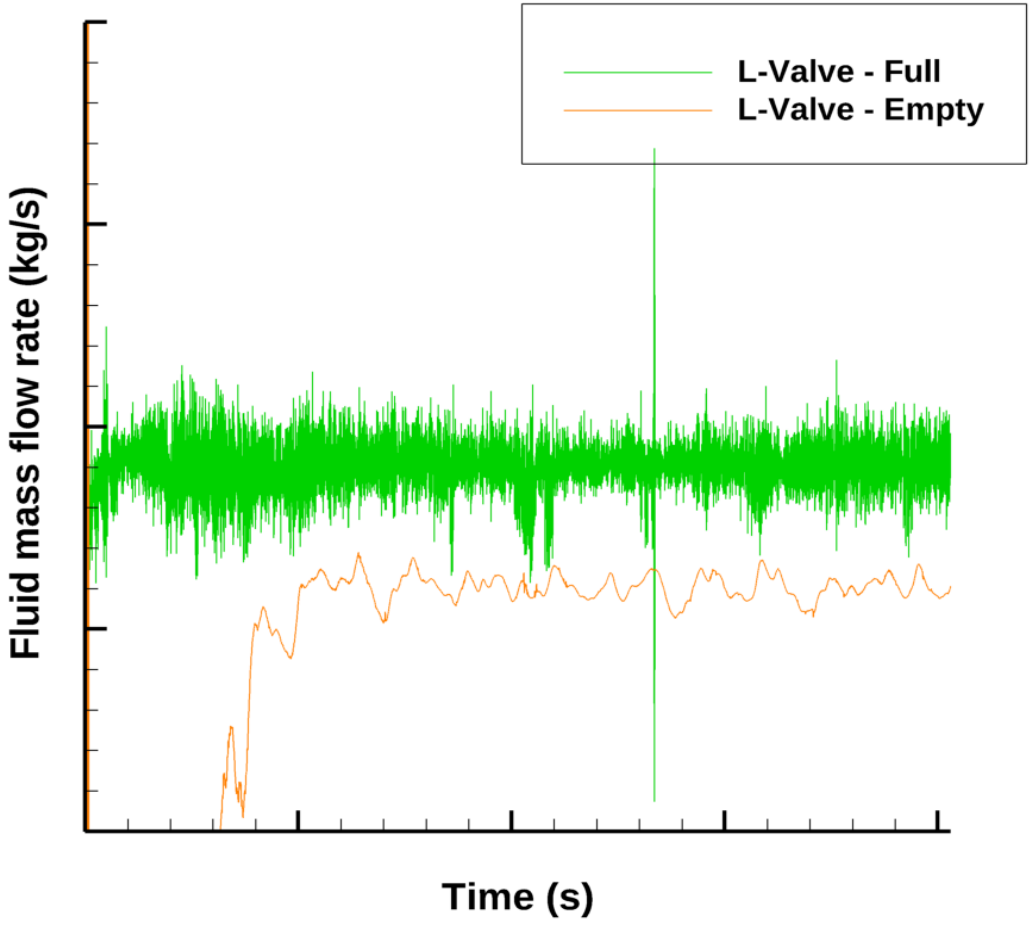
- Novel 2-reactor design
- One oxygen-free “thermal cracker” (pyrolysis)
- One “regenerator” unit with oxygen (reheating particles)
- **Do we need to worry about “slippage” of oxygen into cracker unit, or combustible gases into regenerator?**
- **How can this be minimised?**

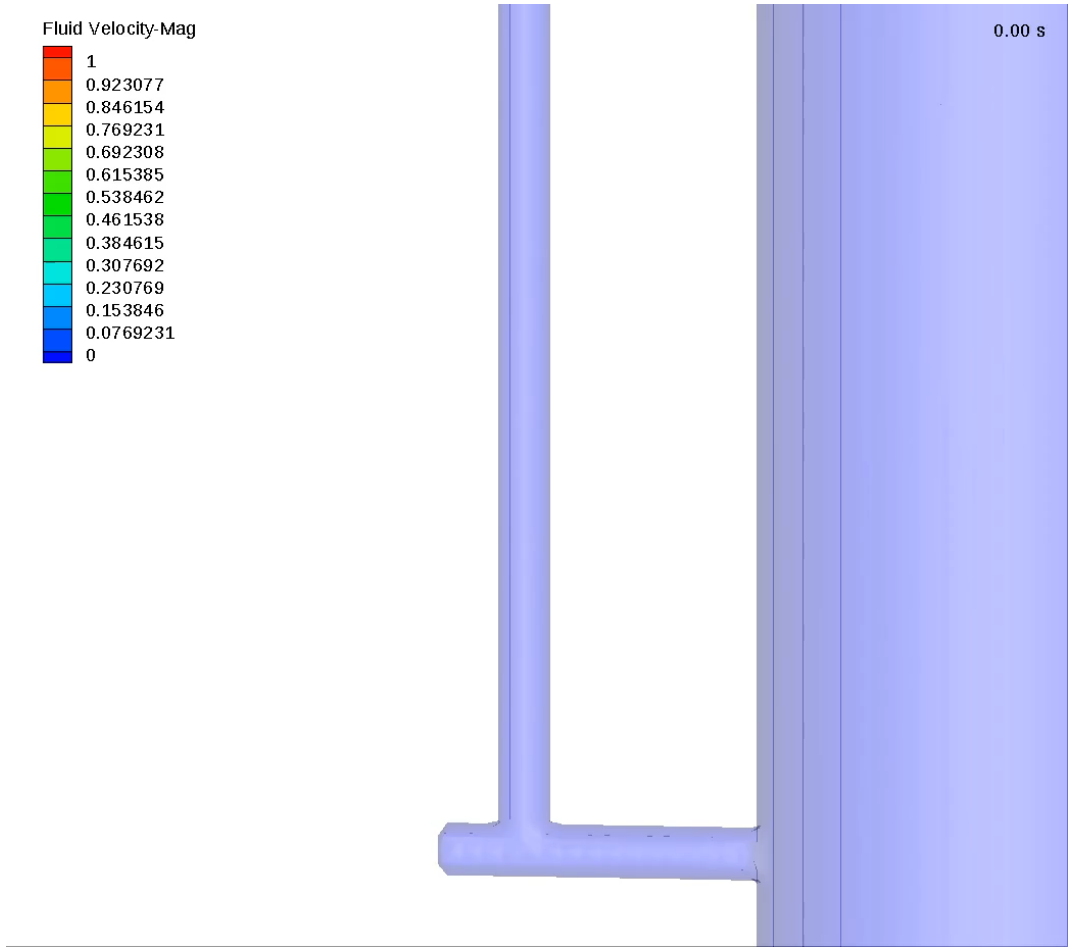


Example:
Troubleshooting

- **Full scale** model of thermal cracker*
- Hydrocarbon gases *should* escape through outlet A
- Escape through outlet B would be **highly problematic**



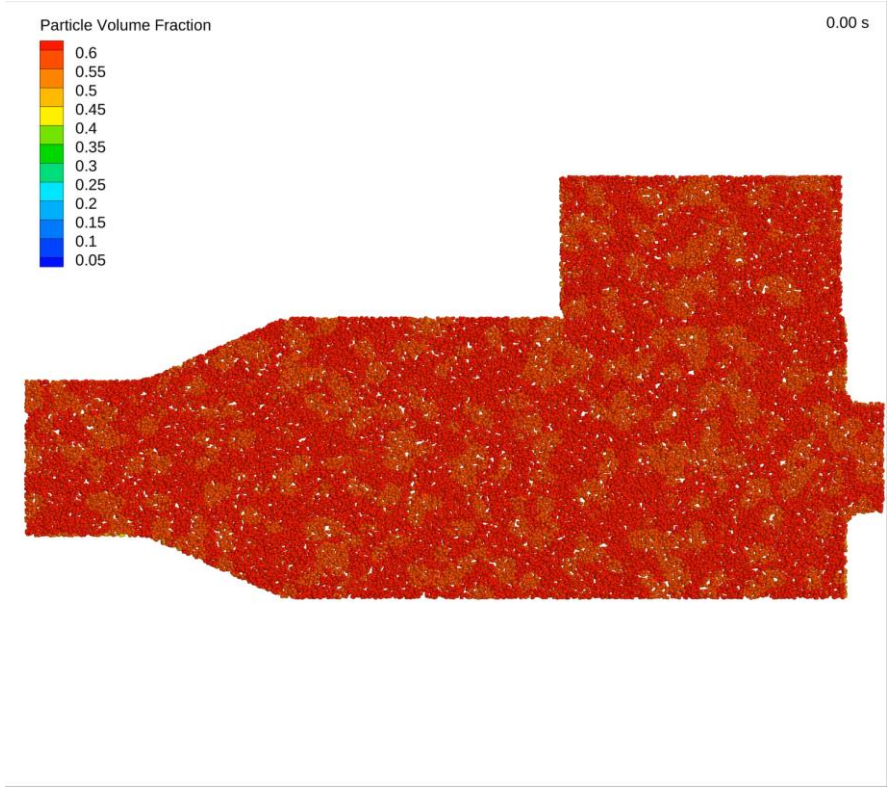


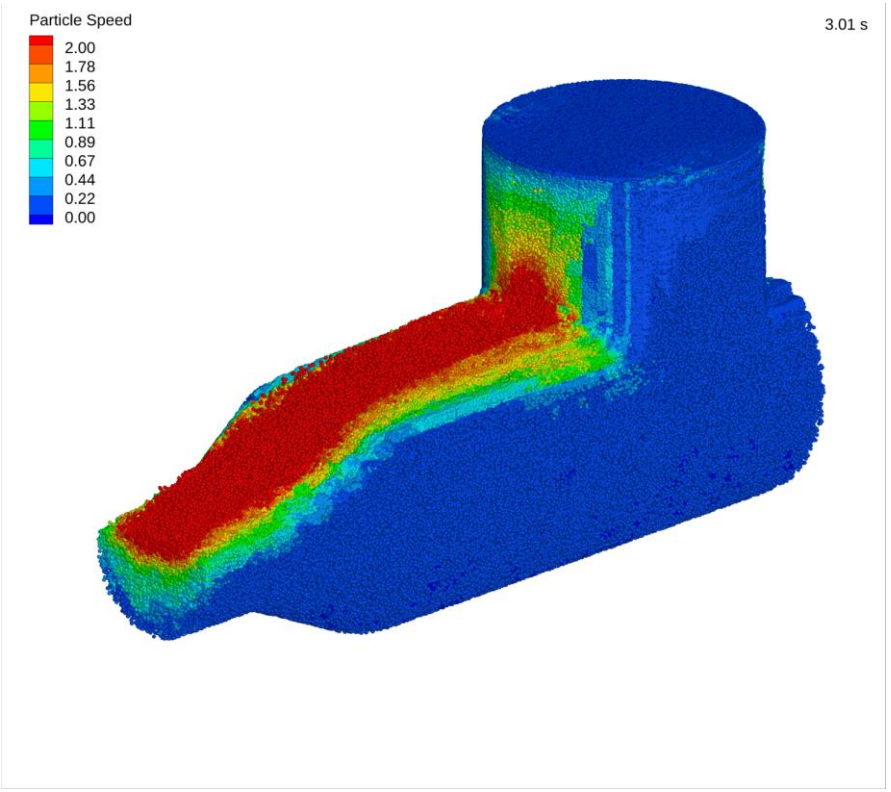


Example:
Troubleshooting

- Left: Empty standpipe
- Right: Full standpipe

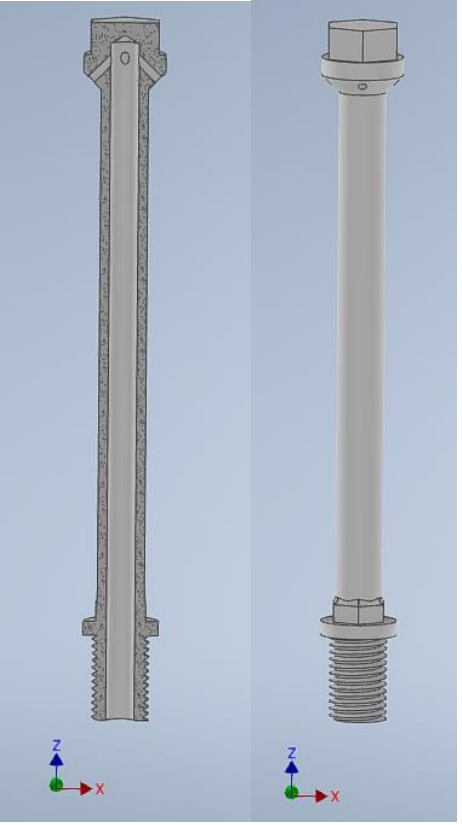
Conclusion: simply ensuring the standpipe is filled can notably **enhance safety and efficiciency**



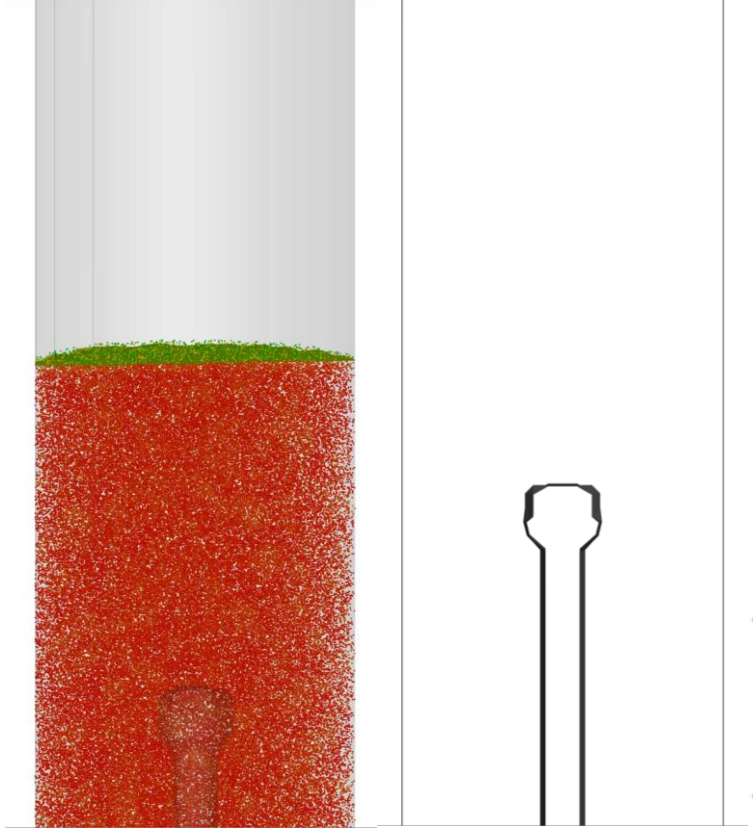


Example: **Optimisation**

- **Question:** is an L-valve more efficient when flow is *continuous* or *pulsed*?
- The answer is [REDACTED]

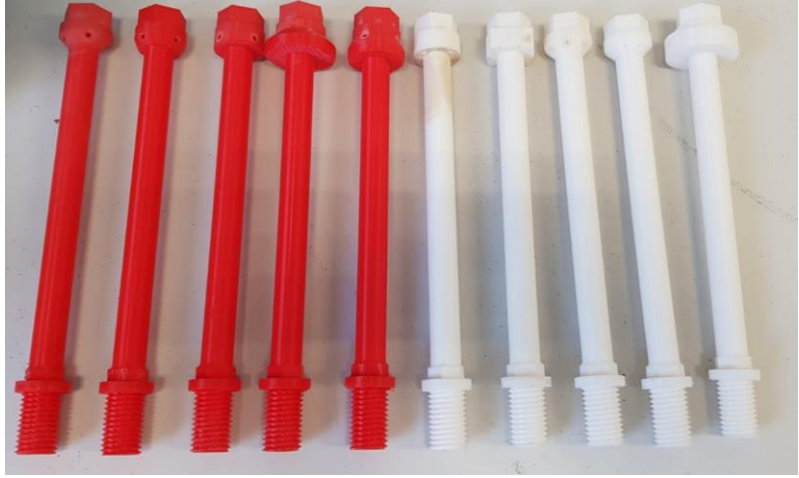


CAD Design

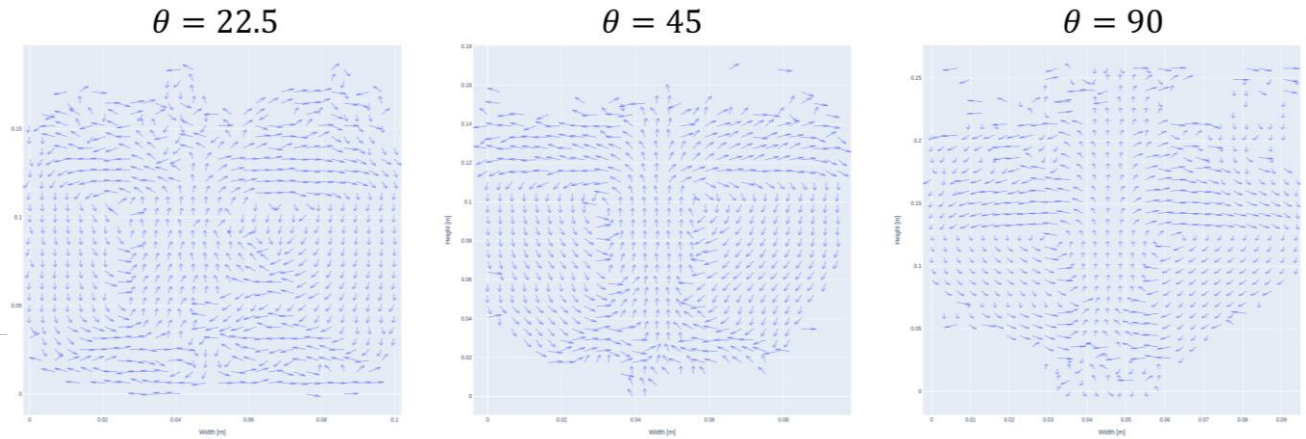


Barracuda Modelling

3D Printing



PEPT imaging



Example: **Design**

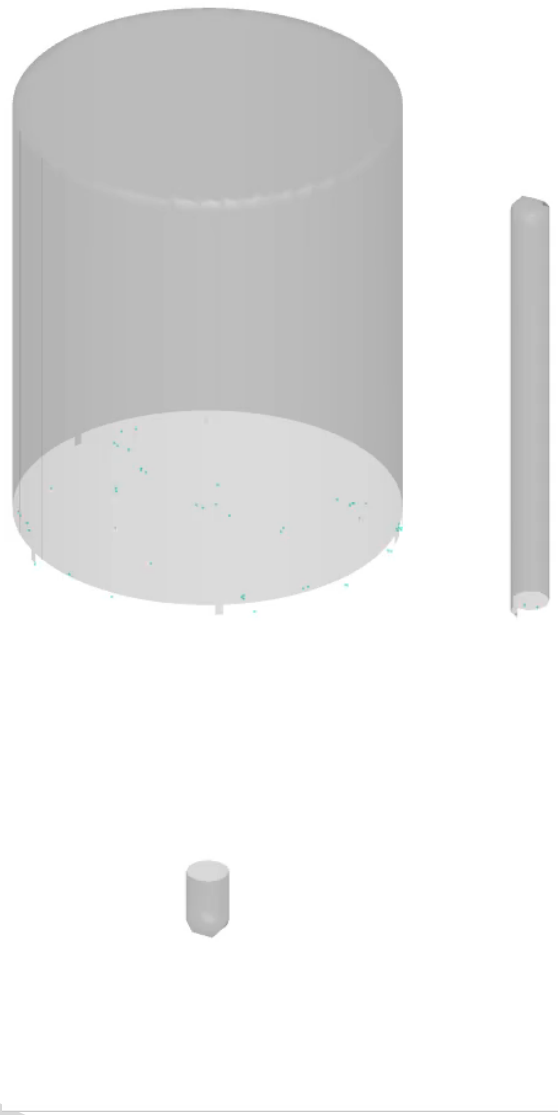
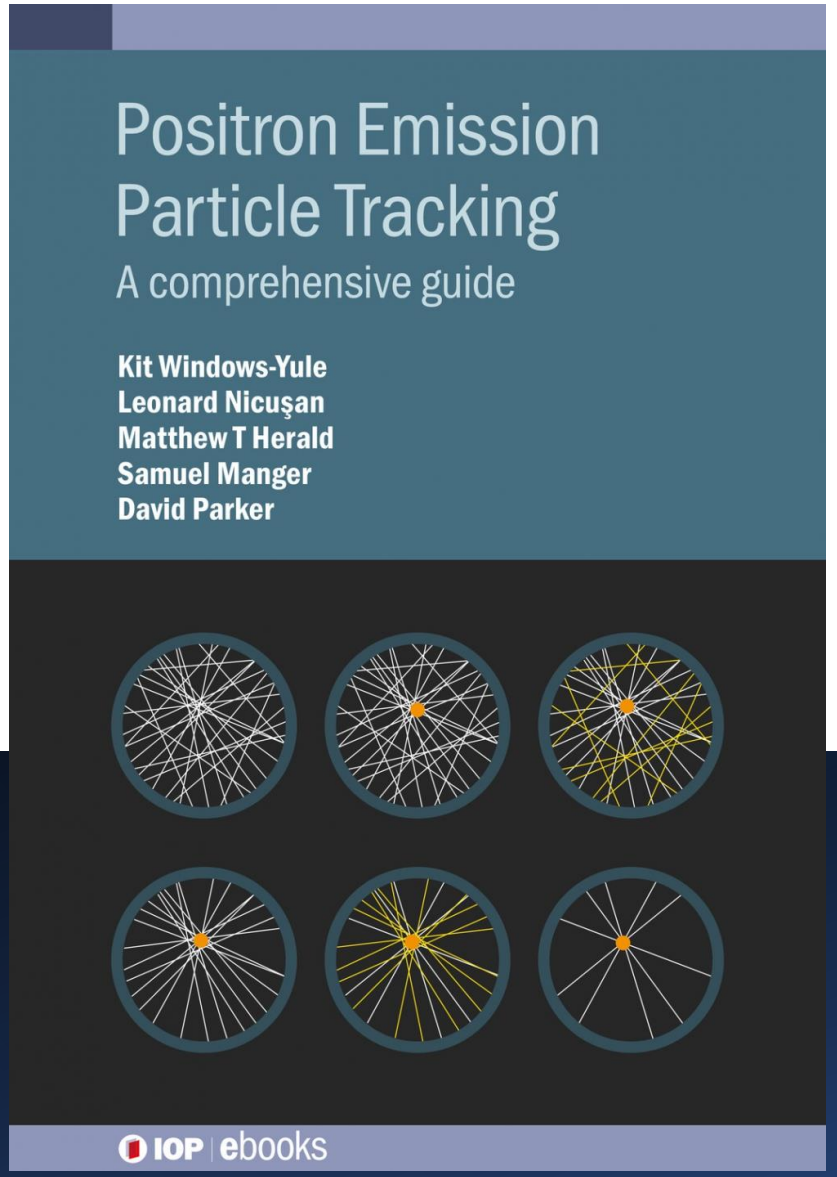
- Barracuda + PEPT + 3D printing = **Advanced Rapid Prototyping**
- Novel distributor designs can be tested in Barracuda, 3D printed using the **same STL file**, and validated in PEPT

The theory of marginal gains

- Individually, these examples may not be groundbreaking
- However, together (alongside other examples not shown!) these small improvements can add up to make a **significant difference**
- In this, and many other, novel systems, the sum of these marginal gains can potentially be the difference between commercial viability or… not

Summary

- Plastic waste is one of the great environmental challenges of our age
- …but eliminating plastics may be more costly than keeping them!
- Working with Recycling Technologies to develop an alternative solution
- Validation against high-resolution PEPT data shows Barracuda is capable of **quantitatively predicting** key system features such as turnover rate
- The validated code is being used in a variety of ways, from troubleshooting to rapid prototyping, to optimise, piece by piece, RT's paradigm-shifting systems.



Any and all questions are very welcome