

Validation of CFD models to predict hydrodynamics of stirred tank flows in the transitional flow regime.

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The aim of this study is to advance understanding of transitional flow in a stirred tank geometry equipped with an A320 hydrofoil impeller [1]. The suitability of a dynamic turbulence - stress blended eddy simulation (SBES) closure model for CFD has been assessed, alongside a generalised k- ω shear stress transport model (GEKO), by comparison with experimental data from Particle Image Velocimetry (PIV) and torque measurements [2]. Unsteady flows of water and Newtonian aqueous glycerol solutions (40 – 100 wt%) have been measured over a wide range of values of Reynolds number, Re, from 8 – 25,000, spanning laminar to turbulent flow via the transitional regime. Two flow scenarios using different fluids were investigated for each value of Re, which was scaled by changing tip speed according to fluid viscosity. PIV measurements were taken in a single vertical plane and time-averaged over all blade positions. ANSYS Fluent (version 2023R1) software was used to build transient CFD simulations for selected cases with a ~1.2M element mesh, given mesh independency.

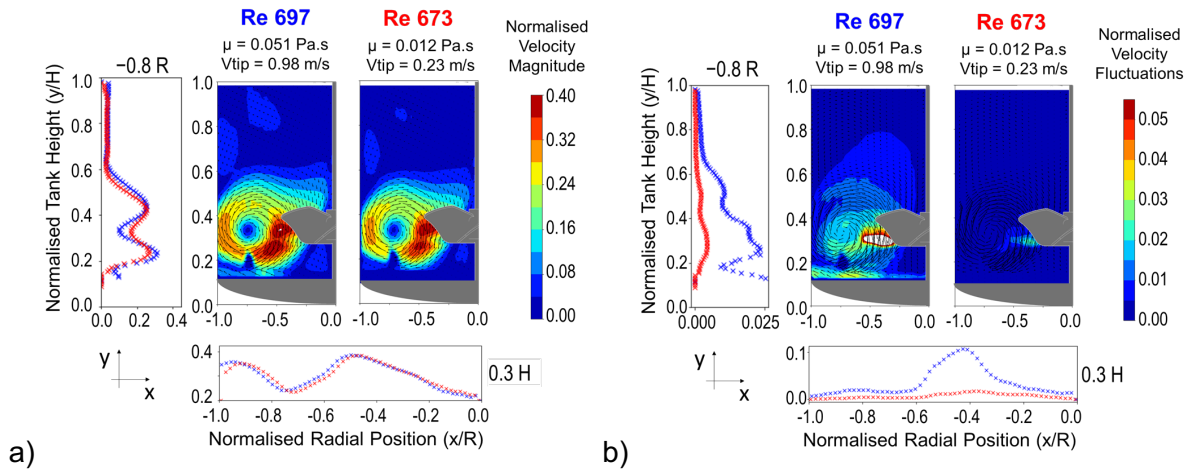


Fig 1: Contour plots of PIV data with radial and axial lines ($-0.8R$ from impeller and $0.3H$ from tank bottom, respectively) of a) normalised velocity magnitude and b) normalised velocity fluctuations for two cases at $Re \sim 680$ (left/blue - $V_{tip} = 0.98$ m s⁻¹, $\mu = 0.051$ Pa s, right/red - $V_{tip} = 0.23$ m s⁻¹, $\mu = 0.012$ Pa s).

The PIV results showed that, for constant viscosity, increasing Re always increases velocity magnitude and its fluctuations. However, the values of velocity magnitude normalised by tip speed (V_{tip}) initially decrease with increasing Re for laminar flows before increasing through the transitional flow regime until becoming independent of Re, signifying fully turbulent

flow. Normalised velocity fluctuations increase with Re for all flow regimes. In the transitional regime, two cases with the same transitional Re but different viscosity do not present self-similar hydrodynamics of flow. Though the normalised velocity magnitudes compared between flows of two glycerol solutions ($\mu = 0.051$ and 0.012 mPa s) at $Re = 680$ ($V_{tip} = 0.98$ and 0.23 m s⁻¹ respectively) are self-similar (Fig 1a), the normalised velocity fluctuations differ very significantly (Fig 1b). The flow with higher fluid viscosity and faster corresponding V_{tip} has a greater level of normalised velocity fluctuation in the down-pumping circulation loop.

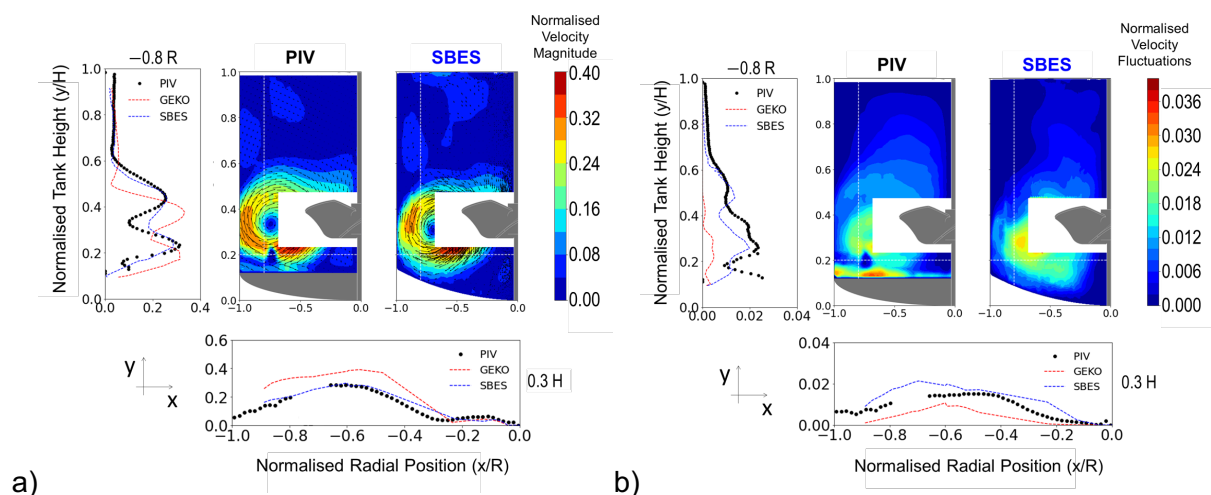


Fig 2: Contour plots comparing PIV (left/black) data with SBES (right/blue) and GEKO (red) predictions with radial and axial lines ($-0.8R$ from impeller and $0.3H$ from tank bottom, respectively) of a) normalised velocity magnitude and b) normalised velocity fluctuations for a single case ($Re = 680$, $V_{tip} = 0.98$ m s⁻¹, $\mu = 0.051$ Pa s).

When comparing the results from CFD, SBES outperforms GEKO (Fig 2), at the cost of additional computational requirement. Proper orthogonal decomposition (POD) of PIV data and periodic averaging of CFD results are used to further explore the impact of pseudo-turbulence arising from the periodicity of the impeller blades and baffles.

References

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Acknowledgments

GW is supported by the EPSRC Centre for Doctoral Training in Formulation Engineering (EP/S023070/1) at the University of Birmingham and Unilever Port Sunlight, UK.

Doubling Yield in Friedel-Crafts Process with Intensified Continuous Reactor

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1. Introduction

Fragrances and flavourings are high-value chemicals and their synthesis yield is essential. The current batch reactor technology has a slow mass transfer rate, resulting in 24-hour reaction times and only 40% yields. The reaction is for a gas-liquid acylation using liquid reactant acyl chloride and gaseous alkene. Furthermore, the high exotherm of the reaction means that temperatures must be controlled below 10°C to inhibit thermal degradation (Figure 1).



Figure 1 - Reaction Scheme

We have developed a continuous process using a continuous stirred tank reactor (CSTR) cascade, the SABRe reactor, and investigated the effect of mixing, temperature, and concentration on the product yield.

2. Experiment

The SABRe system is an integrated cascade of 10 CSTRs. The liquid reactant solution was introduced into the reactor via a diaphragm pump, the gaseous alkene was fed with a mass flow controller pump. Figure 2 shows the experimental set up.

The products were analysed by gas chromatography following a quench using an internal standard.

3. Results & Discussion

The variables assessed during process development have been mixing, concentration, catalyst amount and residence time. Each parameter is important for successful scale up of reaction.

To improve conversion, we investigated effect of mixing we varied mixing intensity for the SABRe and showed that the conversion could increase from 40% to 100% upon increasing mixing intensity from 150 rpm to 1500 rpm. Figure 3 evidences these changes.

Concentration was an important factor to optimise since downstream processes utilise distillation. If the concentration is higher less energy per kg of product is used. Yield for a 10% solution and a 20% solution was 75% and 79% respectively. Doubling concentration is halves distillation energy usage.

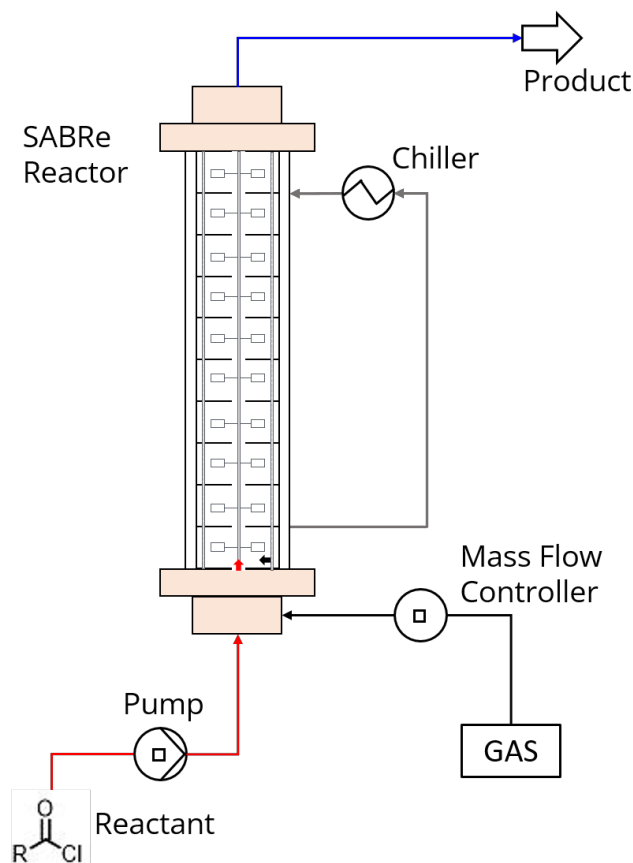


Figure 2 – Experimental Setup

Catalyst amount is critical for performance McQuade and co-workers showed that aluminium chloride Lewis-acid is efficient for a similar reaction type and Gambacorta and co suggests that high stoichiometry amounts typical for reaction. Increasing catalyst amount to a stoichiometric amount yielded a further 20% to conversion (1,2).

Oh and Co-workers developed a AlCl_3 catalysed reaction for acyl chlorides they found that reducing reaction times improved reaction selectivity (3). Therefore, we tested reducing residence time. Reducing reaction time from 24 hours in batch to 10 minutes in the SABRe enhanced yields from 40% to 82%. This is because the enabled fast reaction cycles limited the overreaction of the product. This is only possible by fast heat transfer and mass transfer capabilities of the mixing technology. The high heat transfer limits exotherm generation below 10°C so reaction can progress safely and mass transfer exploits fast reaction kinetics. We verified this by gassing performance in a lab scale batch and saw that over time by-product formation increased proportionally.

Ultimately, following the lab scale optimisation the measured yield of the process increases to 82%, this is shown in Figure 4.

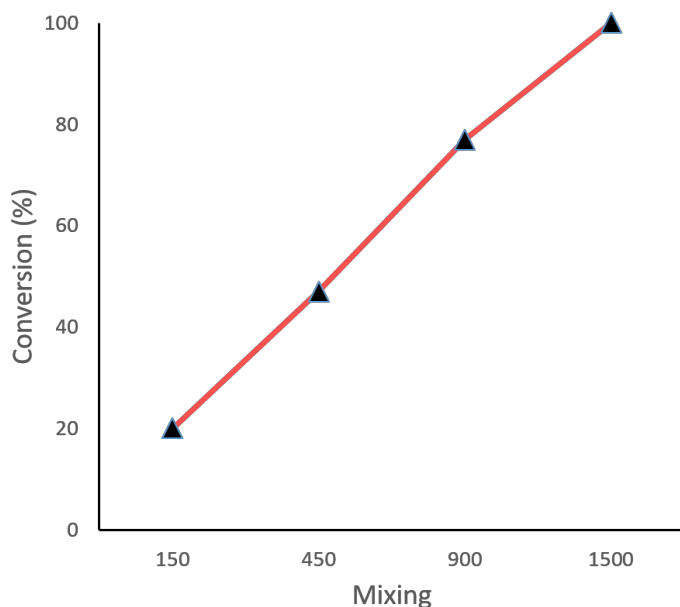


Figure 3 – Mixing intensity results

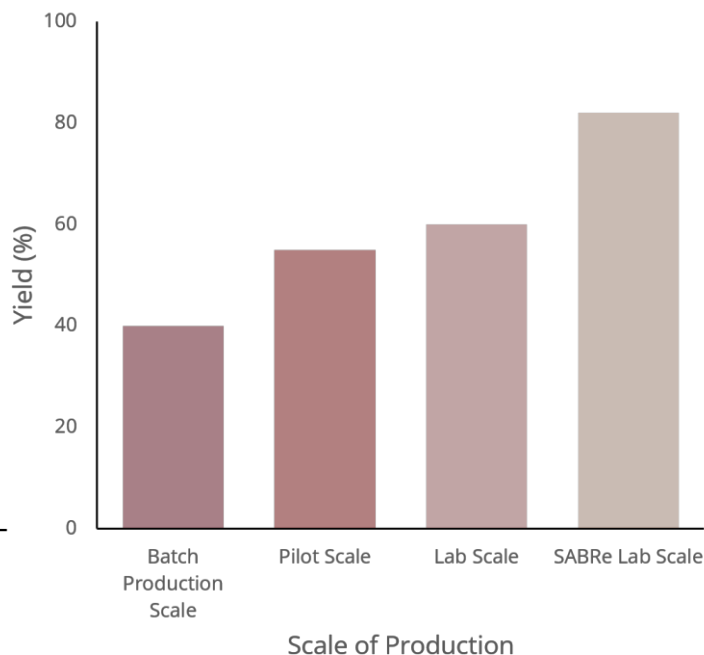


Figure 4 – Scale of Production Results

4. Conclusion

- Using the SABRe system has doubled the yield to 82% from the industrial scale 40%
- Mixing is key to increase interfacial area of biphasic mixture to exploit fast kinetic reaction
- Enhanced residence time distribution and heat transfer capabilities enable fast reaction cycles that limit overreaction, improve selectivity and thus increase yield
- A 50% energy saving during distillation is made since half the amount of solvent is used by kg of reactant
- Process scale-up and piloting activities will begin early January

5. References

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Investigation of high gas flow rates on hydrodynamics in two-phase gas-liquid stirred tanks using Positron Emission Particle Tracking (PEPT)

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Two-phase gas-liquid stirred tanks are used in a variety of industrial sectors which involve aspects of broth fermentation and cell cultivation processes. However, despite their ubiquity, understanding of these systems is significantly limited in comparison to single-phase systems. Optical-based imaging techniques such as Particle Image Velocimetry (PIV) present significant challenges when being applied to two-phase systems, due to the opacity of the two-phase fluid at industrially relevant gas hold-ups. Most experimental investigations focusing on the hydrodynamic flow patterns within two-phase vessels have thus been limited to systems at very low gassing rates (<1 VVM), which are unrealistic when compared to typical pilot scale production facilities.

In this investigation, Positron Emission Particle Tracking (PEPT), a non-invasive measurement technique, has been used to study the fluid dynamics of a 200mm diameter gas-liquid stirred vessel, agitated by a standard Rushton turbine, under a range of different operating conditions at industrially relevant gas hold-ups and superficial velocities. Because PEPT relies upon highly penetrating gamma radiation emitted from a tracer particle instead of the optical properties of the media or the vessel, translucent and opaque fluids can be successfully imaged. The flow dynamics have been studied in both the flooded ($Re = 500$) and dispersed ($Re \approx 1400$) flow regimes for a viscous Newtonian aqueous glycerol solution (70% Glycerol v/v) of dynamic viscosity $\nu = 2.81 \times 10^{-5} \text{ m}^2\text{s}^{-1}$. Additionally, experiments involving a shear-thinning non-Newtonian solution of 1% concentration CMC ($K = 0.9772 \pm 0.0143 \text{ Nsm}^{-2}$ and $n = 0.7070 \pm 0.0025$) at $Re = 500$ have also been performed. Gas flow rates have been varied between 1.6, 3.0 and 5.0 VVM for all flow cases, corresponding to superficial gas velocities of 0.0053, 0.01 and 0.0167 ms^{-1} , representing more typical gas velocities seen in pilot scale reactors. For all the cases, a single-phase measurement has been performed as a control experiment.

From the PEPT measurements, velocity scalar and vector fields have been determined alongside calculation of the degree of dispersion in the system, providing an alternative quantitative measure of mixing time and mixing performance. The flooded experiments ($Re = 500$) quantitatively identified a high-velocity bubble plume along the vessel axis dominating the flow, matching previous qualitative observations, as shown by Figure 1.

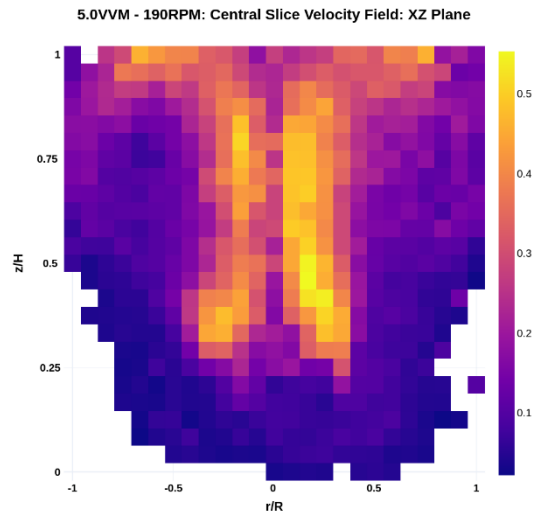


Figure 1: Central Slice Velocity Field - 5 VVM, 190RPM

The Newtonian and non-Newtonian CMC dispersed experiments have highlighted a strong impact of the gas flow rate on the hydrodynamics, with the direction of the high velocity out jet becoming more vertical as the gas flow rate increased, an example of such is shown by Figure 2. In addition, the velocity vector fields illustrate a change in the overall flow pattern, with more compressed vortices between the impeller and the fluid free surface.

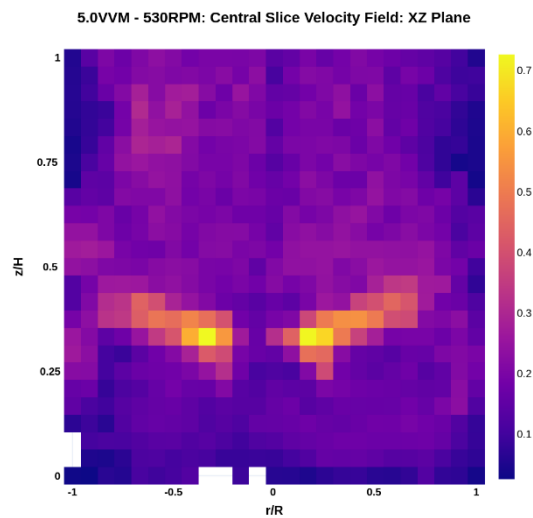


Figure 2: Central Slice Velocity Field - 5VVM, 530RPM

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

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Viscous mixing in stirred tanks is a process employed in a wide range of industries and requires a thorough understanding of the material properties and the hydrodynamics within the system. Using Computational Fluid Dynamics (CFD), mixing environments can be fully simulated to highlight regions of poor mixing and predict the influence of parameters such as impeller shape or material properties. This study applies a novel AI-driven technique to improve axial mixing in a poorly performing lab-scale ploughshare mixer. In laminar flow, the rate of mixing is a function of the rotation rate and the mixer geometry [1]. Therefore, mixing can be improved by either increasing the rate of impeller rotation or by instead modifying the impeller geometry such that the mechanism responsible for axial mixing is promoted.

Using HARPPP, the AI-driven tool from EvoPhase, the components of the ploughshare shape were generalised and an optimisation strategy using evolutionary algorithms was applied to morph the geometry shape for maximum axial mixing. In each epoch, 48 simulations are run in parallel, each running for approximately 20 hours. Illustrated in Figure 1, each simulation possesses three passive scalars initially occupying a third of the available volume along the shaft axis (left, middle, right of tank). The material properties ($\mu = 1.17 Pa s$, $\rho = 1260 kg m^{-3}$) and the rotation rate ($N = 33 rpm$) are constant between simulations. After 10 seconds of rotation, the uniformity of each passive scalar is evaluated, and a measure of mixing error is input to HARPPP which then applies multi-objective optimisation to minimise each mixing error (i.e. maximise the mixing rate).

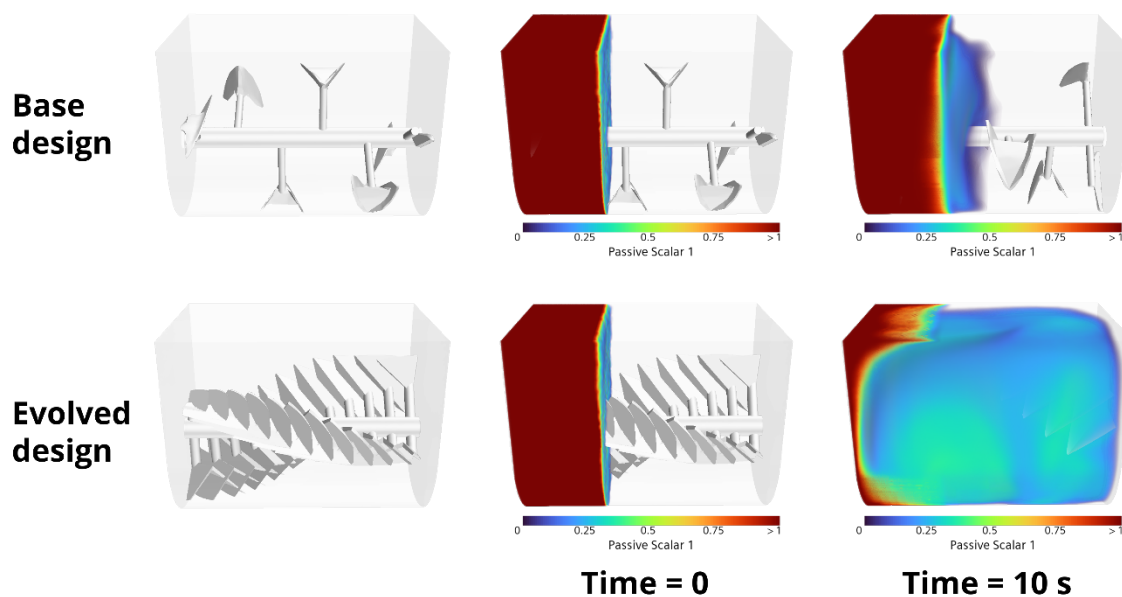


Figure 1. A comparison between the performance of the base design (Top) and an evolved design (Bottom). In the second column, a single scalar tracer is depicted initially occupying the left-most third of the tank. The third column reveals the concentration of the tracer after 10 seconds of simulation.

Upon exploring a wide range of impeller shapes, the algorithm discovered that a double-helix design was able to promote axial mixing far more efficiently than any other design. The mechanism operates similarly to a helical ribbon in that one side of the impeller shifts material along one axis while the other side promotes the opposite effect. Illustrated in Figure 2, the evolved designs achieved a 1000x mixing improvement over the base design for the same power requirement. The generality of this technique allows for future application on a wide variety of unit processes unrelated to mixing.

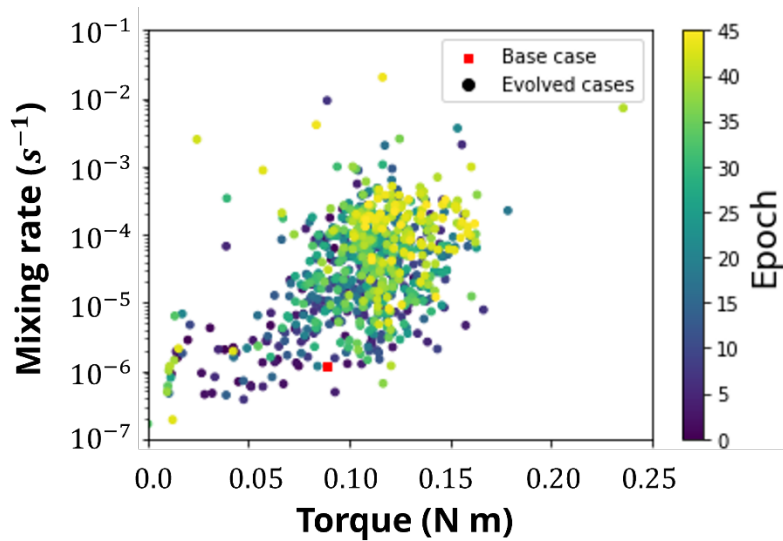


Figure 2. Scatterplot of mixing rate versus torque for simulations coloured by epoch. The red square indicates the base design.

References

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