Mass Transfer in Emulsion Polymerization: high solids content latex and mixing effects

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ABSTRACT

The impact of different agitator configurations used during the emulsion polymerization of vinylidene fluoride (VDF) was studied with the goal of achieving a solids content of 55 wt % while minimizing particle coagulation and maintaining low levels of surfactant. The design and number of impellers, their spacing and the agitation speed were shown to have a strong influence on the transfer of gaseous monomer to the aqueous phase, and thus the rate of polymerization. Increasing the number of impellers on the central shaft, and decreasing the spacing of the impellers close to the latex surface had a strong influence on the ability to incorporate gaseous monomer, so the solids content and the latex level in the reactor increased. Furthermore, it was found that changes in the agitation rate during the reaction was necessary at high solids content to avoid destabilizing the particles in view of the low surfactant concentrations used.

KEYWORDS

Emulsion polymerization, gas-liquid mass transfer, agitation, vinylidene fluoride

1 INTRODUCTION

Unlike liquid-liquid systems, emulsion polymerization of vinylidene fluoride (VDF) to make polyvinylidene fluoride (PVDF) involves a supercritical gas-liquid system, at high temperature and pressure (i.e. ~80°C and ~90 bar), and with a surfactant concentration well below the critical micellar concentration (CMC). [1–3] The supercritical monomer is significantly less dense than water, so it needs to be drawn from the head space of reactor into the liquid phase. This implies that the polymerization rate may be limited by mass transfer between the phases.

Factors such as the agitation speed, type of impeller and setup configuration, can directly influence mass transfer. The amount of monomer available in the liquid phase is for instance directly related to the agitation speed [1,3]. When the speed is increased, more and finer bubbles can be created, thus increasing the surface area of contact between the gas-liquid phases. This can boost the concentration of monomer in the liquid phase, which enhances particle nucleation and growth. Also, the impeller type may affect mass transfer [4,5]. There exists a range of impellers. Radial flow impellers (e.g. Rushton Turbine) move the fluid parallel to its axis of rotation, and are effective for gas-liquid and liquid-liquid dispersion, but they often create high shear and poor axial pumping (i.e. poor gas entrainment from the head space). Axial flow impellers can be employed to direct the flow to the head (up-pumping) or

to the bottom (down-pumping) of the reactor and are thus are adapted to enhance the entrainment of gas from the head space into the continuous aqueous phase [6-11].

During the operations of gas-liquid unbaffled stirred reactors, a vortex can be created [12-14]. In many operations, it is usually aimed to eliminate vortices, however in gas-liquid systems, the vortex promotes gas dispersion via the formation of bubbles at its tip and increases the gas-liquid exchange surface area. Therefore, the ingestion of gas from the headspace by the vortex constitutes an interesting way of increasing gas hold-up in a stirred vessel. The vortex shape is again influenced by the impeller geometry, speed as well as the fluid viscosity [13,15–17].

For tanks with height to diameter ratios greater than the standard 1 – 1.5, multiple impellers are often required to improve the circulation and narrow the distribution of shear and energy dissipation. It becomes however important to tune the spacing between the impellers to ensure good pumping.[7,8] For instance Mendez-Ecoscia et al. [1] compared 2 agitation systems for VDF emulsion polymerization and their influence on the rate of polymerization. They compared an agitation setup (S1) with four 6-pitched blade (45°) down-pumping turbine and a second one (S2) where the bottom impeller was replaced by an A345 hydrofoil. This hydrofoil has a much higher pumping capacity than the smaller 6-pitched blade turbine. Using the same formulation, it was shown that the rate of polymerization with S2 was noticeably higher than with S1. This increase was attributed to a measured increase of mass transfer coefficient (k_La) with S2. In reactions where it is necessary to disperse a gas in a liquid, sometimes spargers are used to generate bubbles.[12] However, this is not an option here as the latex can deposit on the sparger and clog the pores, and there are safety issues regarding the risk of initiator being swept back into monomer reservoirs.

In the current paper we will use the reactor and basic polymerization recipe developed by Mendez-Ecoscia et al. [1], where latexes with a solids content of around 15 % w/w were produced in a semi-batch pilot reactor, to target solids content of 55 % w/w with a minimum of surfactant. Given that the density of PVDF is 1.8 g/cm^3, this corresponds to a polymer volume fraction of about 30 %, so below the level where considerable viscosity challenges may appear. So, the strategy of producing a latex with multiple particles sizes to increase the solids content while limiting the latex viscosity, as proposed by Boutti et al. [18] will not be considered. However, clearly the design of the agitation system is a key to maintain high polymerization rates. So, the main objective of the current paper is to understand the factors influencing the polymerization rate in order to obtain coagulum-free, high solid (>55 % w/w) latexes in a minimum amount of time. We will compare three configurations of impellers (Figure 1): (a) hydrofoils; (b) 6-pitched blade turbines (PBT); and (c) propellers or profiled agitators. Hydrofoil impellers are designed for applications in which an axial flow with a low shear are desired. [7] They are efficient for gas dispersion in a viscous system, liquid blending and solids suspension, and are able to pump a higher flow per unit power when compared to a PBT. PBT are often commercialized as “standard” equipment for lab scale reactors as they are inexpensive and non-proprietary. These are simple tools, typically made with an inclination of 45 °C, flat and have blades with right-angled corners. Propellers are similar, but are profiled to enhance pumping and reduce the shear, particularly at the blade tips.

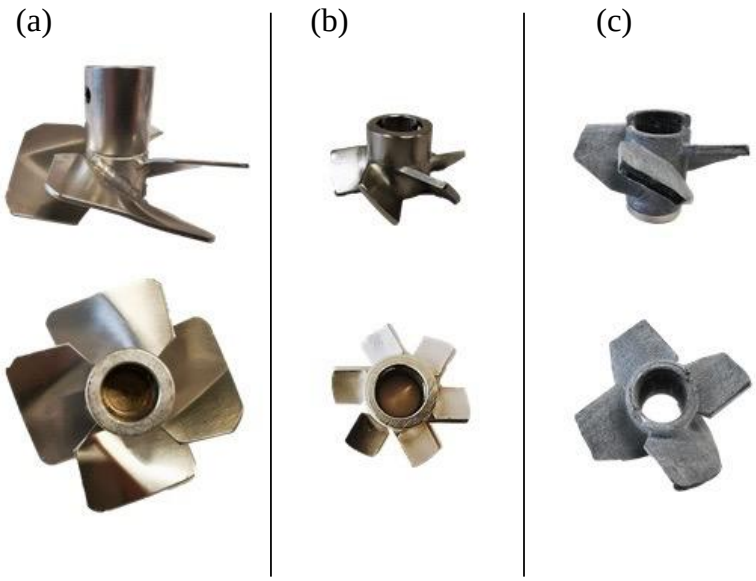

Figure 1. The three types of impellers to be compared in this paper: (a) Hydrofoil (9.1 cm diameter); (b) PBT (4 cm diameter); and (c) AX1 impellers (propeller, 8 cm diameter).

2 MATERIALS AND METHODS

2.1 Polymerization Reactor and Procedure

The reactor used for polymerization is a 3.8 L stainless steel 316 unbaffled jacketed reactor with a dip tube and a thermocouple located 5 mm from the reactor wall. The reactor is 46 cm deep with an ID of 10 cm. All polymerizations are performed in semi-batch mode, with a feed of liquefied VDF regulated to ensure a constant pressure in the reactor head space as described in reference [1]. The rate of polymerization is monitored by calorimetry. [22] The reference polymerization recipe is given in Table 1.

Agitation is ensured by a variable number of impellers mounted on a central shaft that descends from the motor at the top to 16 cm from the bottom of the reactor. The shaft is held in place by a guide that descends 15 cm from the top of the reactor. The different agitation setups considered can be composed of the three different types of impellers: (1) a 4 blade hydrofoil that is 9.1 cm in diameter and that can be configured as an A345 and an A315 (up-pumping or down-pumping respectively); (2) 6-pitched blade turbine (PBT) impellers with a 4 cm diameter; and (3) 4 bladed AX1 impellers that are 8 cm diameter.

The reference agitation system, Setup S2 [1], is shown in Figure 2 and consists of an up-pumping hydrofoil at the bottom of the shaft and three down-pumping PBT, the first one 10 cm above the hydrofoil, and the next two 8 cm above the previous impeller. These spacings, were chosen to be evenly distributed in the useful volume of the reactor. It is a common practice in gas liquid dispersion to have the lowest impeller being up-pumping and the others being down-pumping.

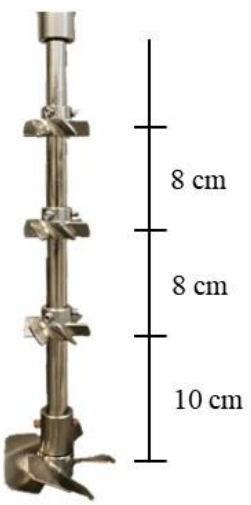

Figure 2. Reference agitation system Setup S2 (up-pumping hydrofoil at the bottom of the shaft + three 6-blade impellers at 10-8-8 cm distance).

Table 1 Reference recipe.

Surfactant	1.5 ($g \cdot \mathbf{L_w^{-1}}$)
Wax	3.4 ($g \cdot L_w^{-1}$)
Potassium persulfate (KPS)	0.09 ($g \cdot L_w^{-1}$)
DI water	1.6-2.2L
RPM	450 min^{-1}
Reactor Temperature	83°C
VDF Pressure	88 bars

The vinylidene fluoride (VDF) monomer and proprietary anionic surfactant with a critical micellar concentration (CMC) around 11 g/L (at 85 °C) and a parking area of a_s =25 $Å^2$ [23] were kindly provided by Arkema (Pierre Bénite, France). Potassium persulfate (KPS) (99 %, Acros Organics) was used as initiator, and ethyl acetate (99.5 %, Sigma Aldrich) as chain transfer agent (CTA). Deionized water is used in the reactor charge, for rinsing the tubes, and to prepare the different solutions (KPS, CTA). Commercial paraffin/wax is used as antifouling agent [24–26].

2.2 Characterization

The solids content of the latex was calculated by gravimetry. Three samples of latex were weighted, and placed in aluminum pans, and placed in an oven at 70 °C for 18 hours to evaporate the water. Once dried, the samples were weighted again to collect the mass of polymer.

The particle diameter D_p was measured using a Nano Zetasizer (Malvern Instruments®) with the default detection angle of 173º, and the measured diameter being the average of three different measurements. An indication of the polydispersity of the particle size distribution is provided, where values below 0.08 can be considered to correspond to monodisperse samples.

3 RESULTS

3.1 Reference polymerization and problem statement

A VDF emulsion polymerization was performed with the setup S2 (same as [1]), using the formulation of Table 1, a total water volume of 1.6 liters and at an agitation speed of 450 rpm. The rate of polymerization as a function of time for is shown in Figure 3.

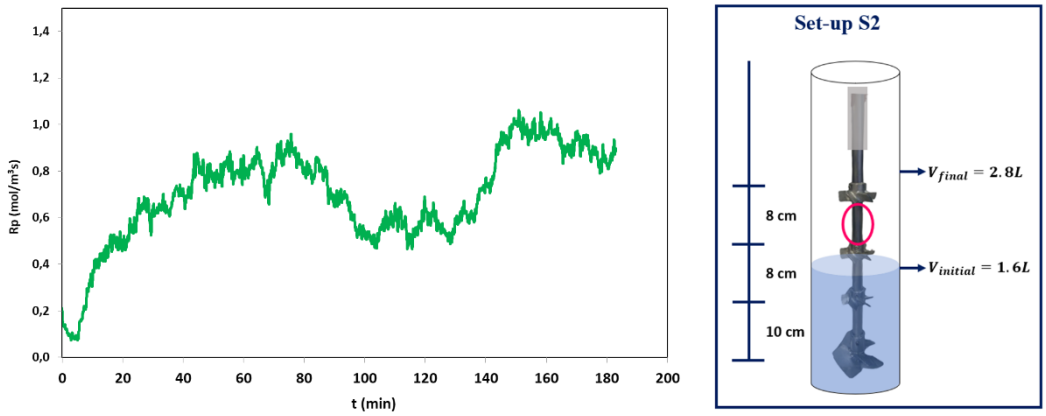

Figure 3. Polymerization rate for reference recipe and Setup S2 at 400 rpm (180 min).

Note that the polymerizations presented here are all semi-batch reactions where VDF is fed to maintain a constant pressure. The polymerization rate (R_p) initially increases as new particles are formed, begins to reach a plateau at around 60 minutes and then unexpectedly decreases at about 75 min of polymerization (corresponding to the cumulative injection of approximately 600 g of monomer since the beginning). The reaction rate remains stable between 100 and 140 min, then rises during 10 minutes, then decreases once again. The final solids content was 36.7 wt %. No significant coagulum was seen upon visual inspection of the final latex.

The oscillations in the rate of polymerization are unlikely due to a shortage of radicals. An attempt to eliminate the initial decrease in the polymerization rate by adding a shot of initiator led to the coagulation of the latex (likely due to the renucleation of particles). Similarly, the free surfactant concentration is not at the origin of these oscillations. The reaction curves shown in Figure 4 tell us that adding additional surfactant can help to boost the rate of polymerization slightly, but sooner or later the rate slows down. While we cannot eliminate the oscillations, Table 2 indicates that the additional surfactant allowed us to increase the solids content with respect to the reference recipe, perhaps due to the stabilisation of a slightly higher number of particles.

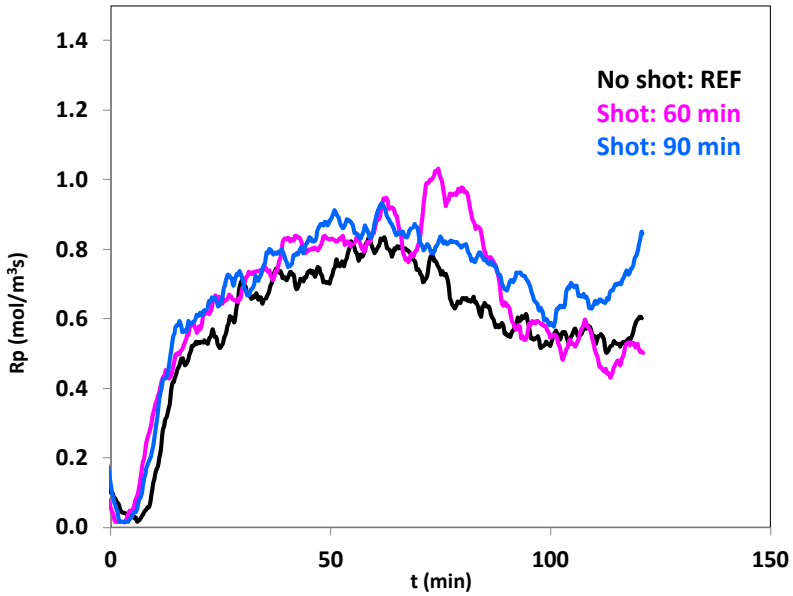

Figure 4. Polymerization rates of experiments performed with a shot of surfactant. Initial surfactant concentration = 1.5 g/L, with a shot of 0.4 g/L at 60 and 90 minutes.

Table 2 Effect of surfactant shots (of 0.4 g/L) on the latex properties.

Surfactant reinjection time (min)	**SC (wt %)**	**D_p (nm)**	**$N_p \times 10^{-19}$ ($1/m^3$)**
-	26.6	205	4.1
60	29.2	204	4.4
90	30.8	206	4.5

3.2 Cold flow experiments showing vortex formation as a function of the liquid height.

The nature of the agitation in the reactor seems to be the origin of the oscillations in the reaction rate. A glass version of the reactor with the same diameter and height was used to observe the mixing profile in the reactor. The only difference between them is that the glass container has a flat bottom and the reactor a conical one. Tests were performed with water in the glass container, to study the mixing at different agitation speeds and volumes.

The setup S2 agitation system was used to look at the influence of the volume of liquid in the reactor. The Figure 5 shows that the size and shape of the liquid vortex change with the water height.

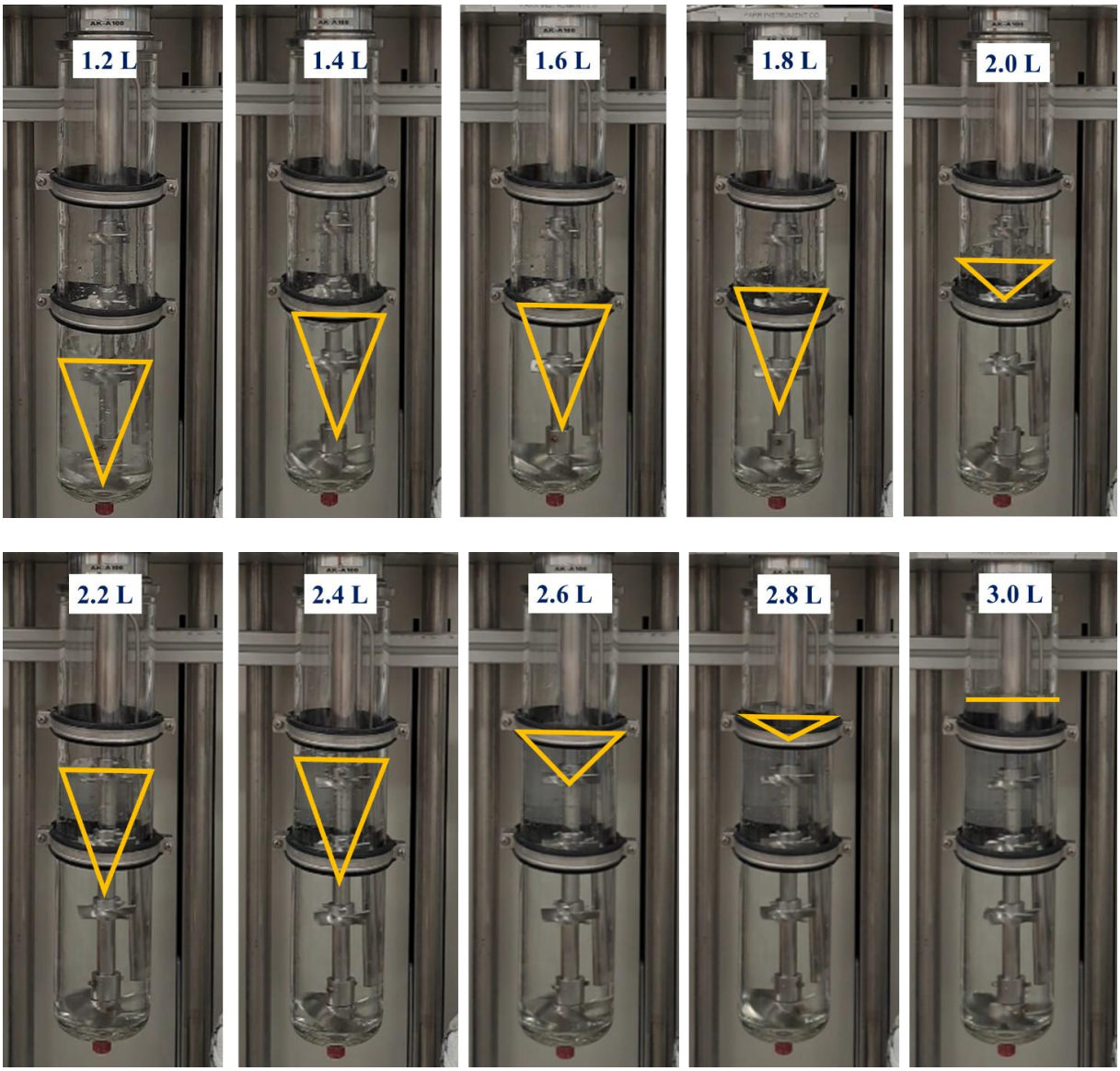

Figure 5. Vortex evolution for setup S2 at 500 rpm for volumes of water from 1.2 to 3.0 L.

The images in Figure 5 show that the vortex size and shape change significantly depending on the volume of liquid in the reactor, and the distance of the impellers from the water level. At low water volumes, the liquid level is not far above the hydrofoil (or bottom) impeller. This generates a conical vortex with a relatively large surface area that can enhance mass transfer between the head space and the liquid [13,15–17]. The size and shape of the vortex remain constant until 1.8 L. After this, the vortex to shrinks noticeably and its apex moves above the second lowest impeller. As the liquid level continues to rise, the vortex gets bigger, because it gets close to another impeller; approximately the same size and shape as seen for smaller volumes. Then, once the liquid level passes the last impeller at around 2.6 L, the vortex begins to shrink again, until at 3.0 L where there is no vortex at all. Note that the guide installed to prevent wobbling of the agitator shaft has a bigger diameter on the top and it is not possible to install impellers there. This makes it difficult to mix the reactor above this level, meaning that the useful volume of the reactor is 2.6-2.8 liters.

From this, it is possible to calculate the maximum amount of water to be used in the recipe to produce a latex with a solids content of 50 wt % at a latex volume of 2.6 L (where the vortex

intensity remains interesting). Using the density of the polymer phase (1.8 g/cm^3), the volume of water will be equal to 1.67 L, which corresponds to the maximum allowable amount of water at the desired solids content and latex volume.

3.3 Effect of the liquid level on the polymerization rate

To validate the hypothesis that the size and shape of the vortex are correlated with mass transfer, 2 polymerizations were done with the same concentrations as the reference recipe but using initial volumes of water of 1.6 and 2.2 L, so reaching final volumes of 2.1 and 2.7 respectively. The solids content for the 1.6 L experiment was 39 % (w/w), and that of the 2.2 L experiment was 32 %. Figure 6 shows the polymerization rates as a function of the mass of PVDF formed. First, note that the size and shape of the vortex appear to be similar between 1.6 and 2.1 L as well as between 2.2 and 2.7 L, where it decreases when increasing the height (c.f. Figure 5). Consequently, in the polymerization starting with a volume of 1.6 L of water (Figure 6) as the volume of the emulsion increases to approximately 2.1 L, the rate of mass transfer decreases. A similar observation can be done for the experiment starting at 2.2 Second, note that the rate at 1.6 L, although very similar in shape to the that of the 2.2 L experiment, is measurably higher. This is possibly due to fact that the hydrofoil impeller at the bottom has a high pumping capacity [1], enhancing the rate of mass transfer with the lower volume of water, although the initial vortex height appeared to be similar in both experiments. This can be inferred from Figure 5 if we compare the volumes of 2.2 and 1.6 L. In the case of the lower volume, the vortex practically touches the bottom of the reactor, meaning that a greater fraction of the liquid phase will be aerated than in the case with the higher volume.

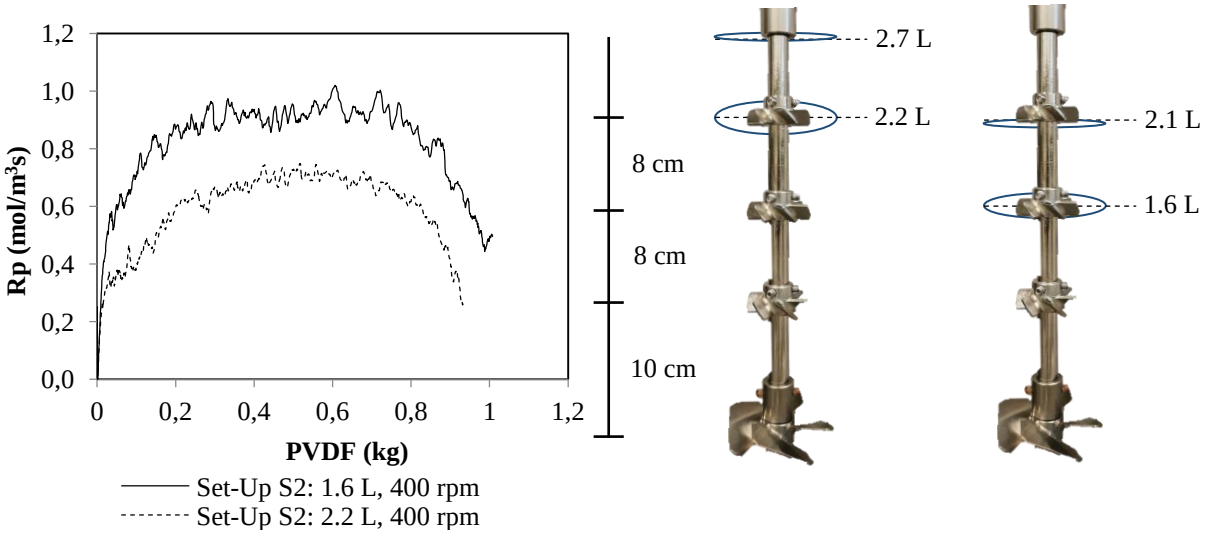

Figure 6. Effect of different volumes of water in the polymerization rate for reference recipe and Setup S2 at 400 rpm (180 min).

3.4 Improvement of the agitation configuration: down-pumping, closer impellers

The impact of the hydrofoil was also noticed in reference [3]. Here the authors noted that changing the hydrofoil from an “up-pumping” configuration (A345) to a “down-pumping” (A315) configuration led to an increase in the polymerization rate, due to an increase in the mass transfer flux from the gas to the liquid phases. Received wisdom tells us that gas

dispersion in vessels with a high height to diameter ratio is enhanced by using an up-pumping impeller at the bottom of the shaft, and a down-pumping impeller at the top. However, the results from reference [3] seem to suggest that this is not the case. Therefore, in an attempt to improve the agitation system, we switched the hydrofoil from an up-pumping configuration to a down-pumping.To avoid the decrease in the vortex between impellers, we added an extra 6-blade pitched turbine to the shaft. In this new configuration, referred to as Setup 2+D, the bottom 6-blade impeller remained at 10 cm above the hydrofoil, and the remaining 3 impellers are spaced 6 rather than 8 cm apart. Before performing polymerizations, a flow visualization experiment was carried out in the glass vessel. The Figure 7 shows that for a volume of 2.8 L, Setup 2+D generates significantly more bubbles in the liquid phase. It is therefore reasonable to assume that the down-pumping impeller at the bottom has a positive impact on gas-liquid mass transfer with respect to the up-pumping configuration.

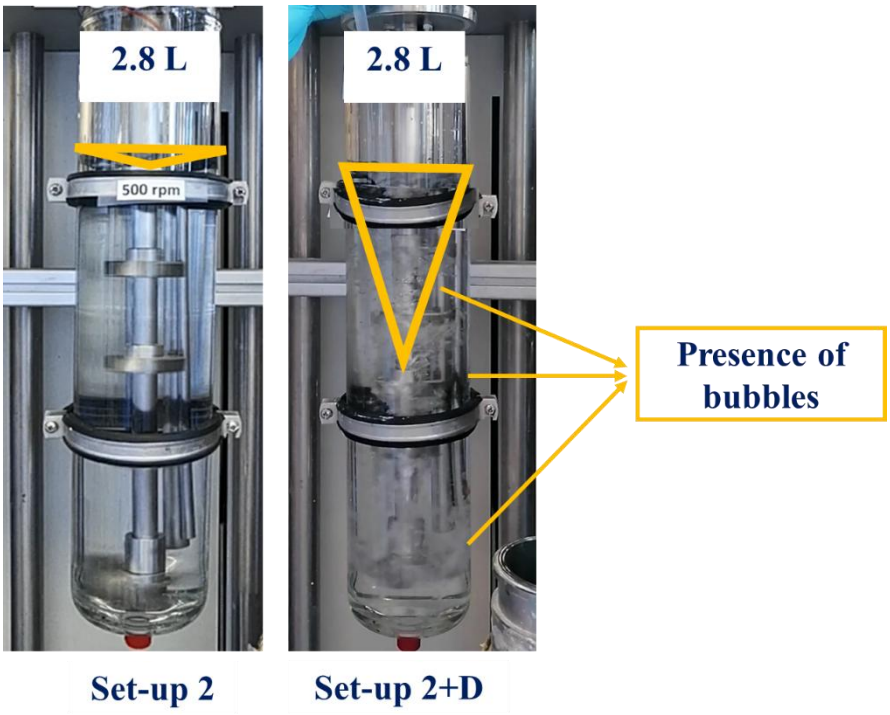

Figure 7. Vortex formation with Setup 2 (up-pumping hydrofoil + three 6-blade impellers at 10-8-8 cm distance each) and Setup 2+D (down-pumping hydrofoil plus four 6-blade impellers at 10-6-6-6 cm distance) at 2.8 L and 500 rpm.

Using the reference recipe and an initial volume of water of 1.6 L, 2 experiments were run to compare the rates of polymerization with Setups S2 and 2+D. Figure 8 shows that for low latex volumes, the rates of polymerization are similar during the initial stages of polymerization until 70 min. This suggests that both agitation configurations are sufficient to compensate the consumption of monomer from the polymerizing particles, leading to approximately a constant reaction rate. After 70 min, the rate of polymerization obtained with Setup 2+D remains higher (and constant) compared to Setup S2. The final number of particles per liter was similar for both experiments, N_p=4.1 × 10^{19} m^{-3} and 4.3 × 10^{19} m^{-3} for Setups S2 and 2+D, respectively. Indeed, the number of particles is determined during the

nucleation period, which was similar in both experiments. The polymerization with Setup S2 becomes mass transfer limited only after 70 min.

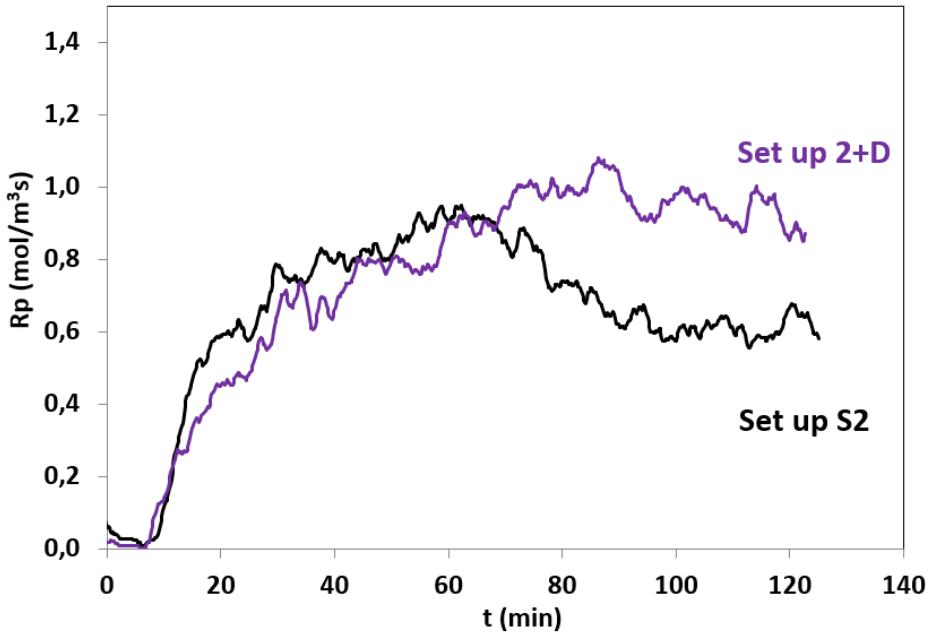

Figure 8. Rates of polymerization using the reference recipe, a stirring rate of 450 rpm, and an initial volume of water of 1.6 L with Setups S2 and S2+D

3.5 Effect of the agitation speed on the reaction rate

Figure 9 shows the impact of the rate of agitation on the rate of polymerization using Setup 2+D and the reference recipe. The initial rate increases in a very similar manner for all 4 experiments, regardless of the rate of agitation. During this period, particles are formed by homogeneous nucleation and the polymerization rate increases as the number of particles increases. During this time, the level of the latex is low, and the hydrofoil ensures good mass transfer with the different reactions rates. After a certain time, the 350 rpm experiment starts to slow down, followed by the experiment at 450 rpm that slows down at 90 min. It appears that 550 rpm is sufficient to ensure good mass transfer, at least until 120 minutes. Furthermore, Table 3 shows that the particle size increases (for a similar number of particles), as well as the polymer molecular weight when the agitation rate is increased from 350 to 550 rpm. This indicates that the monomer concentration in the particles increases over this range of agitation rates. Regarding the difference between the particle sizes and the molecular weights of the experiments at 550 and 650 rpm, they are small and attributable to experimental error. This indicates that the monomer concentration in the polymer in both experiments is the same, and thus the polymerization is not mass transfer limited at 550 rpm with this agitator setup and polymerization recipe. During these experiments, we never observed coagulation because reactions only last for 2 hours and the solid contents where close to 35%. However above 40% solids, agitation at 550 rpm can rapidly induce coagulation as we will see below.

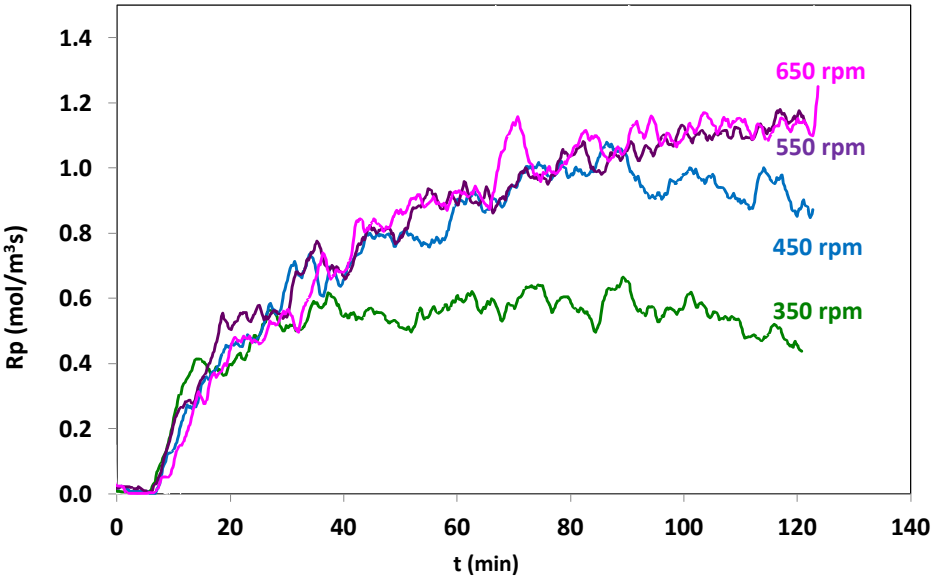

Figure 9. Polymerization rate for different agitation speeds (setup S2+D).

Table 3 Effects of the agitation speed.

Speed (rpm)	SC (wt%)	D_p (nm)	$N_p x10^{-19}$ (1/m^3)	Mw (kDa)	PD
350	25	157	4.3	392	2.3
450	28	183	4.3	559	2.7
550	32	210	4.7	571	2.2
650	32	207	4.9	577	1.8

3.6 Optimized configuration to increase the solids content

Two experiments were run with the objective of obtaining a solids content greater than 50 % w/w. The reference recipe was used, with Setup 2+D and different agitation speeds. The results are shown in Figure 10. In the first experiment, the agitation rate was set at 550 rpm since this appears to be the optimal speed based on the results of Figure 9. The first 3 hours of the experiment progressed well, but after approximately 190 minutes, the reactor began to vibrate noisily, and after opening the reactor, it was found that it was full of coagulum (Figure 11). Different attempts to overcome this showed that at first, we get a wet coagulum (i.e. it can be wiped away and/or washed off with water), then coagulation that becomes solid and hard.

A lack of stabilization by the surfactant was probably the reason for coagulation. Furthermore, an earlier modelling study from our group [21] showed that shear rates at the tips of the pitched blade agitators could be on the order of several hundred reciprocal seconds, meaning that orthokinetic coagulation could be an issue, in particular as the surface coverage of the latex particles by surfactant decreases.

For this reason, the agitation rate in the second experiment was set at 550 rpm for 120 minutes, and then decreased to 450 rpm. This modification in the agitation condition allowed us to avoid shear-induced coagulation, but obviously decreased the mass transfer rate. It is worth noting that at an added mass of 0.6 kg, which corresponds to a time of around 140 minute, the rate starts to increase slightly as the liquid level increases and begins to touch the

4th 6-pitched blade turbine, thus increasing the mass transfer rate slightly. Even though changing the agitation rate slows down the polymerization, it appears to be important as the solids content increases to maintain the stability of the emulsion.

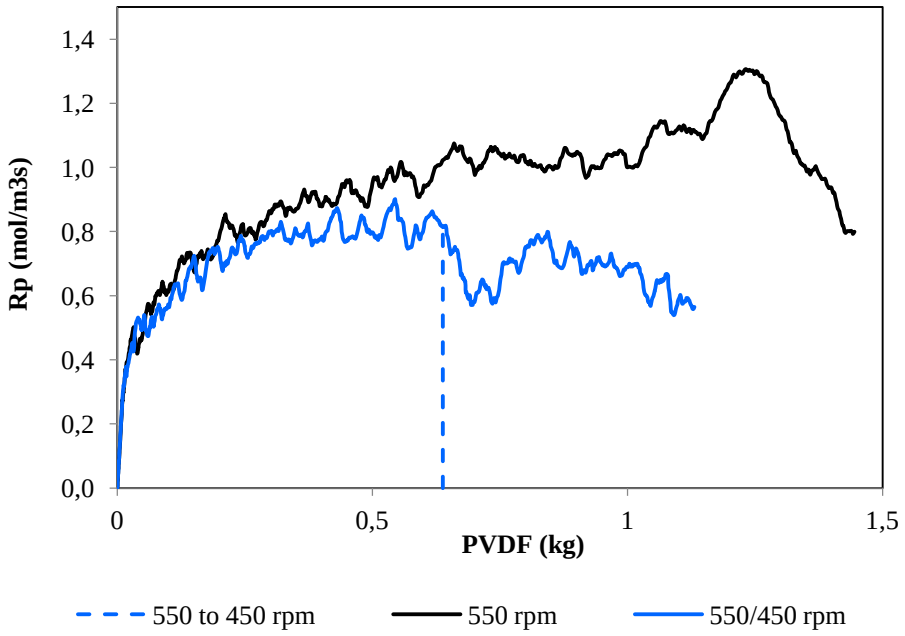

Figure 10. Effect of changing the agitation speed.

Figure 11. Coagulation in the reactor at a stirring speed of 550 rpm Setup S2+D.

To push the solids content above 40 % obtained previously, it is necessary to reduce the intitial volume of water. The calculation shows that reducing the intial volume to 1.3 L should allow us to ensure good mixing of the latex to get 55 % w/w of solids content (before

reaching the shaft guide free of impellers). However, an attempt to polymerize the mixture of 1.3 L led to significant coagulation early during the polymerization. The visualization of the cold flow in Figure 5 at 1.3 L shows that the vortex is quit important (apex of the vortex below the hydrofoil, in up-pumping configuration). Here, as the hydrofoil is in a down-pumping configuration, so this will intensify the mixing around the hydrofoil. The shear rate is probably very high around the hydrofoil with an initial volume of 1.3 L, causing coagulation and fouling.

For this reason, we made 2 changes (Setup 3). First, the hydrofoil was replaced by a 3-blade AX-1 profiled mixer that is designed to provide decent pumping at much lower shear than the hydrofoil. Second, the spacing between the impellers was reduced to 5 cm. The new configuration and the rate of polymerization are shown in Figure 12. The agitation rate was kept at 450 rpm. The final solids content was 53 % w/w, with an average particle diameter of 233 nm, and N_p=6.0×10^{19} per cubic metre. However, approximately 30 g of coagulum was found in the final product. Furthermore, while the decreased spacing between impellers helped to reduce the oscillations of the rate of polymerization, when the liquid level passed the last impeller at approximately 210 minute, we observe a steep decrease in the rate that cannot be recovered.

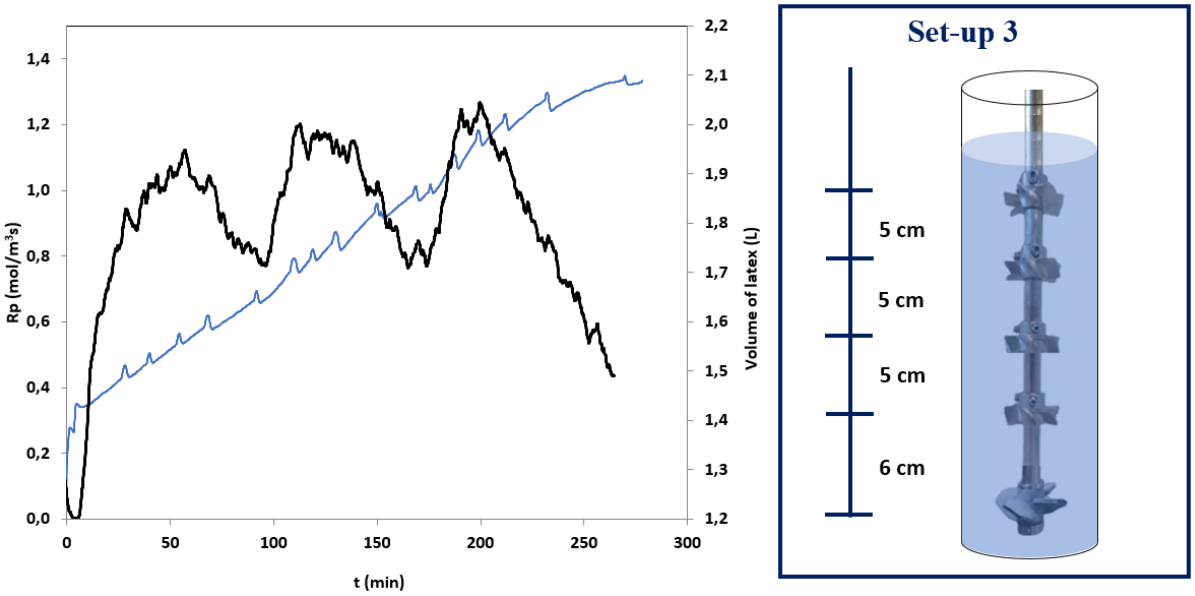

Figure 12. Rate of polymerization (Setup 3) and volume profile throughout polymerization. Rotation rate 450 rpm, surfactant concentration 1.5 g/L.

The final steps in the improvement of the agitation system to achieve the goal of a minimum of 55 % w/w solids content were straightforward at this point: (1) the surfactant concentration was doubled from 1.5 to 3.0 g/L and a second shot of surfactant (bringing the total concentration to 4.5 g/L) is added after 150 minutes; (2) a sixth impeller was added at the bottom of the shaft (a second AX1 3 blade propeller) to increase the total mixed height of the agitated zone (referred to as Setup 4); (3) the agitation rate was dropped from 450 rpm to 350 rpm after 170 minutes to reduce shear induced coagulation seen at high solids content. The results of this final polymerization are shown in Figure 13.

We still see oscillations in the rate of polymerization, but the amplitude of the variations is less than in the previous experiments, and at the end, the polymerization rate is clearly improved by the presence of the upper impeller. The final solids content after 220 minutes

was 55 % w/w, the average particle size as 223 nm, with N_p=7.5×10^{10} particles per cubic metre and, with no measurable coagulation. The improved stability and uniformity of the agitation conditions allowed us to reach the desired solid content of 55 % w/w in less time than in the previous experiment because of the more uniform agitation which maintained an acceptable level of mass transfer throughout the polymerization.

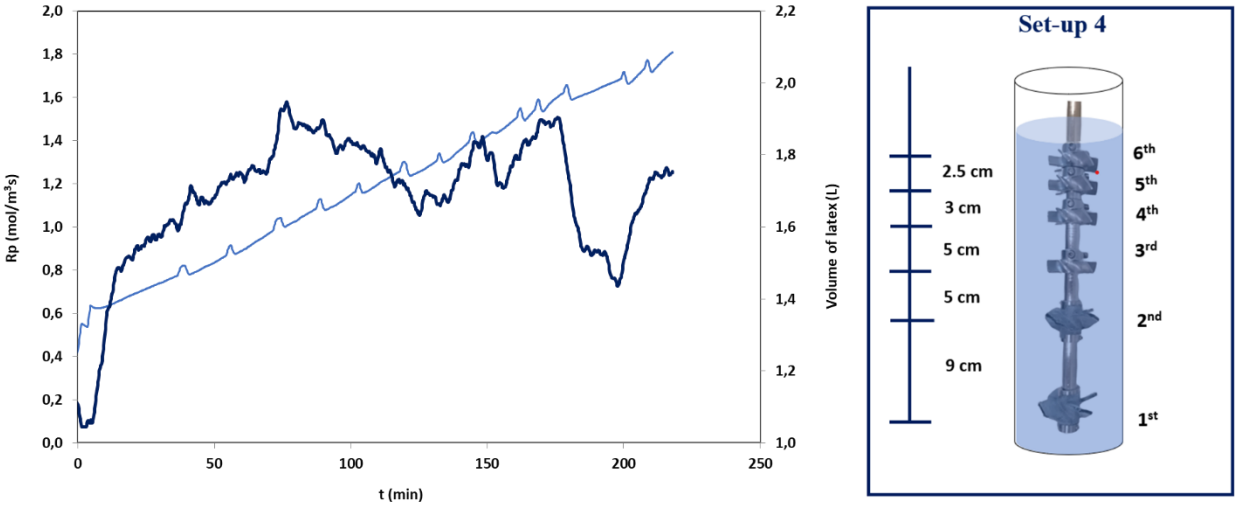

Figure 13 Polymerization rate for Setup 4 and volume profile throughout polymerization. Agitation rate 450 rpm then 350 rpm after 170 min and 3 g/L of surfactant plus a shot at 150 min.

4 CONCLUSIONS

The importance of the agitation setup, and consequently, the importance of mass transfer in the emulsion polymerization of VDF has been presented. It was observed that there were mass transfer limitations on the reactor due to a poor design of the agitation system from the start.

The rate of polymerization and the variations in the rate as a function of time appear to be strongly influenced by the design of the agitation system. The profile is strongly influenced by the number and type of impellers, but also by their spacing. Furthermore, as solid content increases (and thus the viscosity of the latex also increases), it appears necessary to reduce the spacing between the blades.

Furthermore, the design of the reactor and of agitation system limits the initial volume of water that can be used when we wish to get to high solid contents. The problem stems from the fact that: (a) when the apex of the vortex is between two impeller levels, the mass transfer rate from the head space to the emulsion is limited; and (b) when the liquid level reaches the level of the shaft guide the vortex completely disappears, essentially reducing the same rate of mass transfer to zero. It was found that with the initial conditions, although it was theoretically possible to begin with 2.2L of water, the maximum solid content produced was around 32 wt % for this reason.

Trial and error modification of the agitation system (and initial volumes) allowed us to avoid poor mixing when the liquid level is between two impellers by increasing the number of

impellers. The replacement of the hydrofoil by the AX1 impellers enabled also a decrease in the shearing that causes the coagulation of the latex specially when the solids content is higher than 40 wt%.

It was shown that the solids content of 55 wt % was produced by optimizing the agitation setup, and slightly increasing the surfactant concentration. The improved agitation system allowed us to significantly reduce the mass transfer limitations, and the additional surfactant increased the stability of the emulsion.

In closing, one could imagine that using tools like computational fluid dynamics (CFD) to optimize the mixing in the reactor, and to predict how different agitation systems impact the gas-liquid mass transfer rates. It would be quite desirable if this were realizable with realistic computational times. However, experience with these tools, especially in cases where one has a free liquid surface and bubbles need to be generated, and when a certain number of agitators with different sizes and shapes could be used makes such an approach unrealistic at the current time. Truth be told, occasionally thoughtful trial-and-error experiments can still be cheaper and faster!

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