# NEWSLETTER

## Optimizing Hydrogenation Scale-up with VisiMix: A Gas-Liquid Mixing Case study

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## Introduction

Hydrogenation is a vital process in fine chemical and pharmaceutical manufacturing, playing a key role in producing high-value intermediates and active ingredients. The efficiency of this reaction depends on how effectively hydrogen gas disperses and transfers into the liquid phase. When gas–liquid mixing is inadequate, it can lead to slower reactions, incomplete conversion, and higher energy consumption—issues that become more pronounced during scale-up. Achieving uniform hydrogen distribution and maximizing mass transfer are therefore essential for reliable performance.

**VisiMix** provides a powerful solution by offering deep insight into reactor hydrodynamics—enabling engineers to visualize and quantify mixing intensity, **gas dispersion**, **mass transfer coefficient** ($k_La$), **Gas hold up,** and the **specific mass transfer area** within seconds. With these insights, teams can fine-tune reactor design and operating conditions to achieve faster hydrogenation, improved yields, and smoother technology transfer from lab to plant scale.

## The Challenge

When the hydrogenation process was scaled up from a **10 L** laboratory reactor to a **100 L pilot** hydrogenator, the reaction time unexpectedly increased from **16 hours** to nearly **60 hours.** After 20 hours of reaction, an additional quantity of catalyst was added in an attempt to accelerate completion; however, the desired conversion was still not achieved, and the total reaction time extended to about 60 hours. Operating conditions such as temperature and hydrogen pressure were identical, yet the scale-up failed to deliver the same efficiency.

The primary concern was whether the extended reaction time was due to **poor catalyst suspension** (2.5% w/w of 20% Pd(OH)2 wet, impregnated on Carbon) or **limited gas–liquid interaction.**

**Key Challenges:**

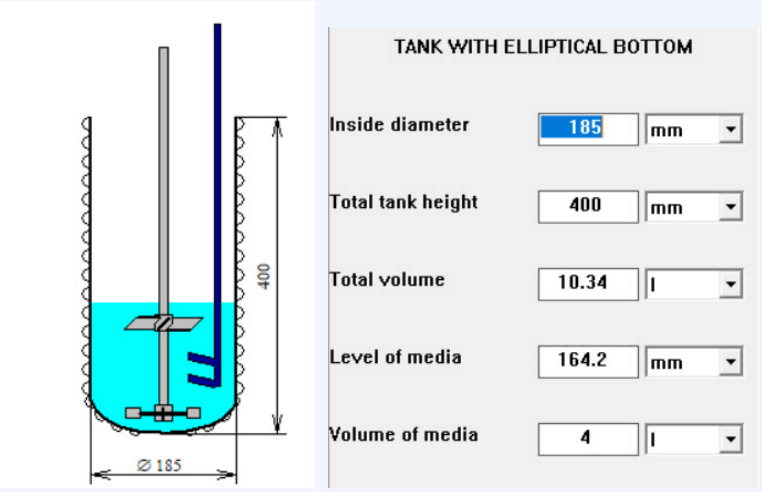
- Achieving uniform hydrogen gas dispersion at a larger scale.
- Maintaining effective catalyst suspension.
- Understanding how reactor geometry and impeller positioning influence gas–liquid mass transfer.
- Balancing mixing intensity and reaction efficiency to replicate lab-scale performance in the pilot setup.

## The Solution

The team utilized **VisiMix Turbulent** and conducted a detailed simulation to understand the mixing dynamics inside the pilot hydrogenator.

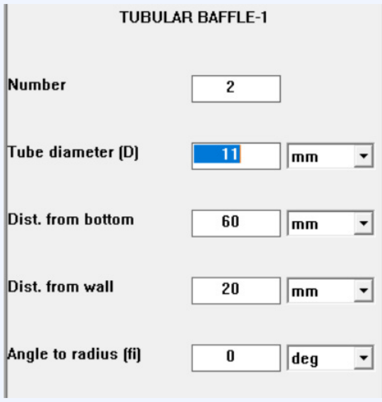
***Step-1: Laboratory simulation:***

The laboratory system was modeled in VisiMix, incorporating tank geometry, baffles, impeller design, reaction mass properties, and solid concentration and density to study catalyst suspension, along with gas characteristics and flow rate to accurately capture gas–liquid mixing dynamics.



TANK WITH ELLIPTICAL BOTTOM

| | | |
|---|---|---|
| Inside diameter | 185 | mm |
| Total tank height | 400 | mm |
| Total volume | 10.34 | l |
| Level of media | 164.2 | mm |
| Volume of media | 4 | l |



TUBULAR BAFFLE-1

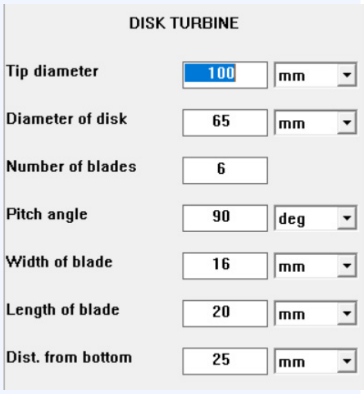
Number 2

Tube diameter (D) 11 mm

Dist. from bottom 60 mm

Dist. from wall 20 mm

Angle to radius (fi) 0 deg



DISK TURBINE

Tip diameter 100 mm

Diameter of disk 65 mm

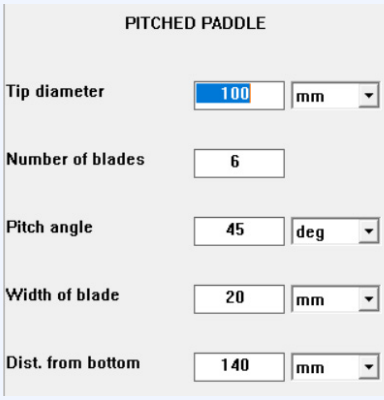
Number of blades 6

Pitch angle 90 deg

Width of blade 16 mm

Length of blade 20 mm

Dist. from bottom 25 mm



PITCHED PADDLE

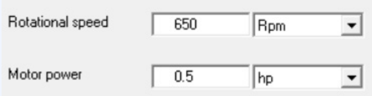
Tip diameter 100 mm

Number of blades 6

Pitch angle 45 deg

Width of blade 20 mm

Dist. from bottom 140 mm

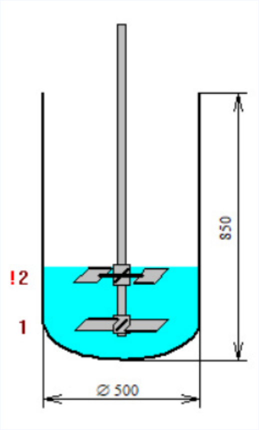


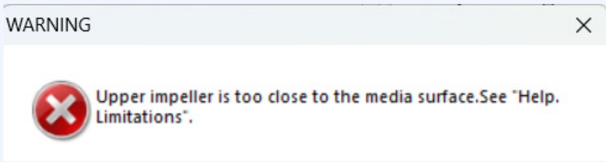
Rotational speed 650 Rpm

Motor power 0.5 hp

***Step-2: Pilot Plant Simulation:***

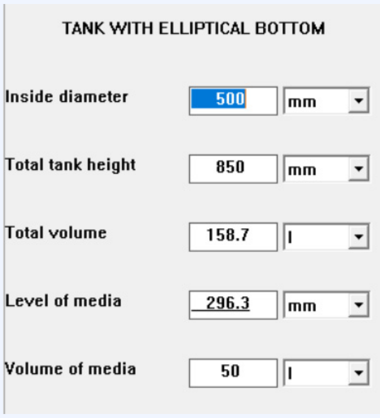
Similarly, the 100 L pilot plant hydrogenator was modeled in VisiMix, including its geometry, baffles, impeller design, reaction mass and solid properties, and gas characteristics and flow rate, to evaluate scale-up of mixing dynamics from laboratory to pilot scale.





WARNING

Upper impeller is too close to the media surface.See "Help. Limitations".



TANK WITH ELLIPTICAL BOTTOM

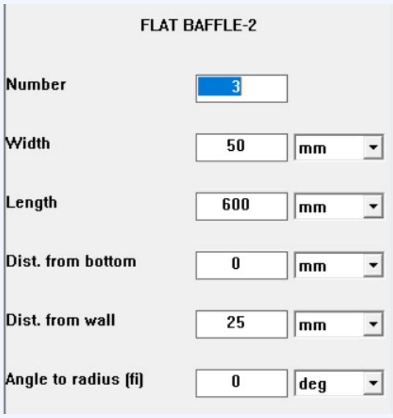
Inside diameter 500 mm

Total tank height 850 mm

Total volume 158.7 l

Level of media 296.3 mm

Volume of media 50 l



FLAT BAFFLE-2

Number 3

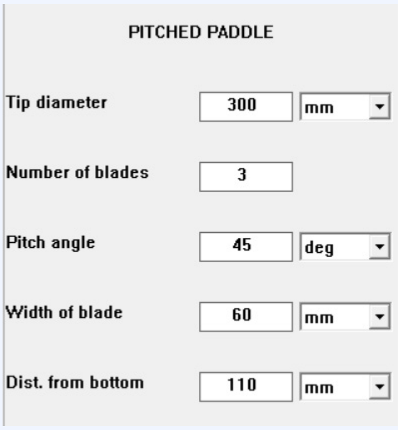
Width 50 mm

Length 600 mm

Dist. from bottom 0 mm

Dist. from wall 25 mm

Angle to radius (fi) 0 deg



PITCHED PADDLE

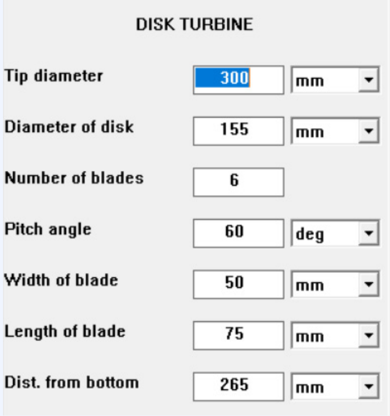
Tip diameter 300 mm

Number of blades 3

Pitch angle 45 deg

Width of blade 60 mm

Dist. from bottom 110 mm



DISK TURBINE

Tip diameter 300 mm

Diameter of disk 155 mm

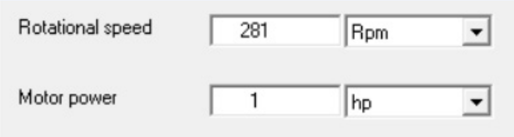
Number of blades 6

Pitch angle 60 deg

Width of blade 50 mm

Length of blade 75 mm

Dist. from bottom 265 mm



Rotational speed 281 Rpm

Motor power 1 hp

## SIMULATION RESULTS

## KEY SCALING UP PARAMETERS:

| **Parameter** | **Unit** | **Existing Lab (10 L)<br>2 baffles<br>650 RPM** | **Existing Pilot plant<br>V= 50 L<br>281 RPM** | **Proposed<br>V= 60 L<br>Distance from the bottom – 75 mm** |
|---|---|---|---|---|
| Energy dissipation in the bulk volume | W/kg | 4.76 | 6.21 | 5.69 |
| Microscale of turbulence in the bulk of volume | m | 1.59e-05 | 2.2e-05 | 2.2e-05 |
| Characteristic time of micro-mixing | S | 0.555 | 0.486 | 0.508 |
| Mixing power | W | 36 | 533 | 604 |
| **Liquid-Solid Mixing (for catalyst)** | | | | |
| Complete/ incomplete Suspension | | Complete Suspension | Complete Suspension | Complete Suspension |
| Maximum degree of non-uniformity – axial% | | 3.89 | 2.13 | 3.92 |
| Maximum degree of non-uniformity – radial% | | 2.65 | 5.97 | 1.89 |

| **Parameter** | **Unit** | **Existing Lab (10 L) 2 baffles 650 RPM** | **Existing Pilot plant V= 50 L 281 RPM** | **Proposed V= 60 L Distance from the bottom – 75 mm** |
|---|---|---|---|---|
| **Gas-Liquid Mixing** | | | | |
| **Check distribution** | | **Satisfactory distribution of gas in the tank is expected** | **No satisfactory gas distribution.**<br>Upper impeller is too close to the surface for gas distribution | **Satisfactory distribution of gas in the tank is expected** |
| Gas hold-up | | **0.206** | | **0.251** |
| Sauter mean bubble diameter | m | 0.00149 | | 0.00154 |
| Specific mass transfer area | sq.m/ cub.m | 828 | | 976 |
| **Specific mass transfer coefficient ($k_La$)** | **1/s** | **1.08** | | **1.32** |
| Estimated surface aeration rate | m/s | 0.0291 | | 0.068 |

## Key Observations:

- The **energy dissipation** in the bulk volume was better in the pilot plant compared to the lab (4.76 W/kg), enhancing turbulence and mixing intensity to support improved suspension and catalyst dispersion at a larger scale.
- The microscale of turbulence in the pilot plant (~2.2e-05 m) is larger than that in the lab (~1.59e-05 m), but still sufficient for maintaining efficient micro-mixing, as confirmed by the characteristic micro-mixing times (~0.486 – 0.5 s).

### CATALYST SUSPENSION

- The lab reactor (10 L, 2 baffles, 650 RPM) achieved complete suspension with acceptable non-uniformity (axial 3.89%, radial 2.65%), supported by higher energy dissipation and turbulence despite the smaller scale.
- In the **pilot plant**, with a reaction mass volume of 50 L operating at 281 RPM in a baffled configuration, complete suspension was achieved. Axial uniformity improved to 2.13%, while radial non-uniformity was slightly higher at 5.97%, which is attributed to scale-related effects.
- The longer reaction time observed in the pilot plant is **not due to poor catalyst suspension**, as uniform suspension with low non-uniformity values was achieved at the pilot scale.

### Gas-Liquid Mixing

- In the **existing case** where the reaction mass volume is **50 L,** the distance from the bottom is **110 mm,** and the distance between two impellers is **135 mm, gas distribution was poor,** as the **upper impeller is too close to the liquid surface**, restricting gas dispersion and reducing mass transfer efficiency.
- **Satisfactory gas distribution is observed when the reaction mass volume is 60 L, the distance from the bottom of the first impeller is decreased to 75 mm, and the distance between the impellers is increased to 150 mm,** where improved geometry enables better gas dispersion and overall mixing.
- The specific mass transfer coefficient (kla) improved from **1.08 1/s in the lab to 1.32 1/s** in the pilot plant, indicating enhanced gas-liquid interactions, though further improvements are needed to match lab reaction rates.
- The observations confirm that while **complete suspension** is achievable at pilot scale, **geometrical constraints, mass transfer limitations, and inadequate gas-liquid interaction** hinder reaction efficiency, leading to longer reaction times and incomplete hydrogenation unless further optimizations are implemented.

## Conclusion

Simulation of the 100 L hydrogenator revealed that gas dispersion was limited due to the upper impeller being too close to the liquid surface, causing incomplete hydrogenation despite proper catalyst suspension. VisiMix confirmed that catalyst mixing was uniform, indicating the issue was insufficient gas–liquid interaction rather than poor catalyst dispersion. By adjusting the reaction mass volume to 60 L, setting the first impeller 75 mm from the bottom, and maintaining at least 150 mm between impellers, gas distribution and mass transfer were optimized.

**By optimizing the reactor geometry and impeller positioning, the hydrogenation time dropped from 60 hours to just 8 hours — nearly eight times faster — outperforming the lab results, achieving successful hydrogenation, and saving millions of rupees while eliminating the need for excess costly catalyst.**

**Try VisiMix for Free – Start Today**

**Want to model your own process and avoid costly mistakes?**

**Click here to download your free trial of VisiMix**