



# ALGEBRAIC AND GEOMETRIC METHODS OF ANALYSIS

MAY 25-28, 2026

INTERNATIONAL MATHEMATICAL CONFERENCE

**Title: HOL, CFD and AI as integrated methods of analysis**

**Author: Enzo Bonacci (The Natural Sciences Unit of ATINER)**

**Topic: Geometric and topological methods in natural sciences**

**Organizers: N. Konovenko – Y. Fedchenko – B. Feshchenko  
S. Maksymenko – O. Prishlyak**

**DOI: <https://doi.org/10.13140/RG.2.2.17837.45281>**

# INTRODUCTION

Since the mid-1990s, algebraic and geometric methods of analysis have been implemented in digital simulations with exponentially increasing efficacy in STEM applications [8].

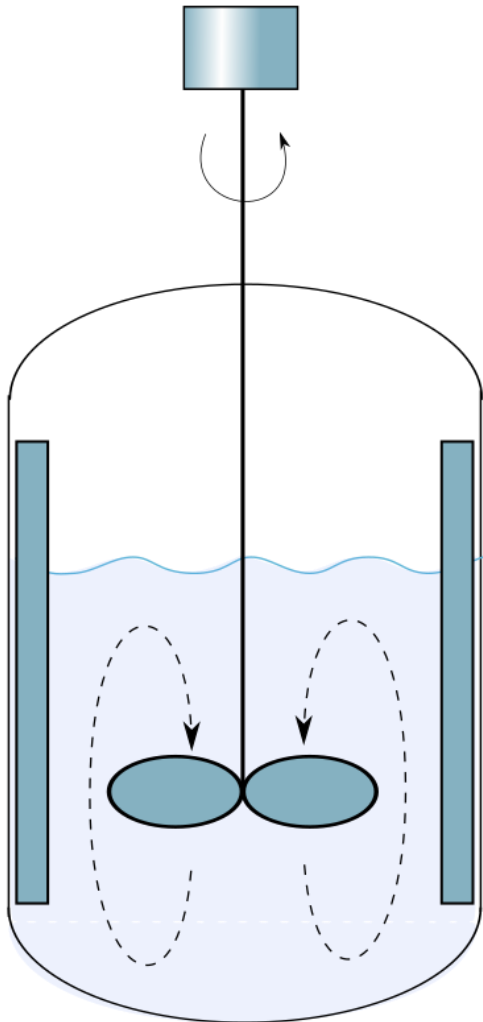
The outcomes are so accurate that many decisions about engineering questions like, e.g., selecting a three-blade marine impeller instead of a Rushton turbine as mixer in the batch crystallization of the citric acid monohydrate (CAM), could rely solely on Artificial Intelligence (AI) and Computer Fluid Dynamics (CFD).

Nevertheless, as a pivotal experience at La Sapienza's DICMALAB plainly showed [1–5], Hands-On Laboratory (HOL) enriches the comprehension of a process [7] revealing crucial issues about safety and sustainability [6].

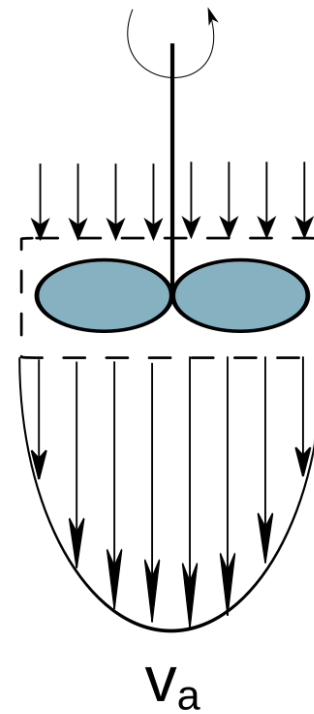
When possible, an *integrated* approach among AI, CFD, and HOL seems preferable to the choice between the alternative *virtual* and *traditional* laboratory [9] for solving science problems.

# THREE-BLADE MARINE IMPELLER

3-blade marine impeller

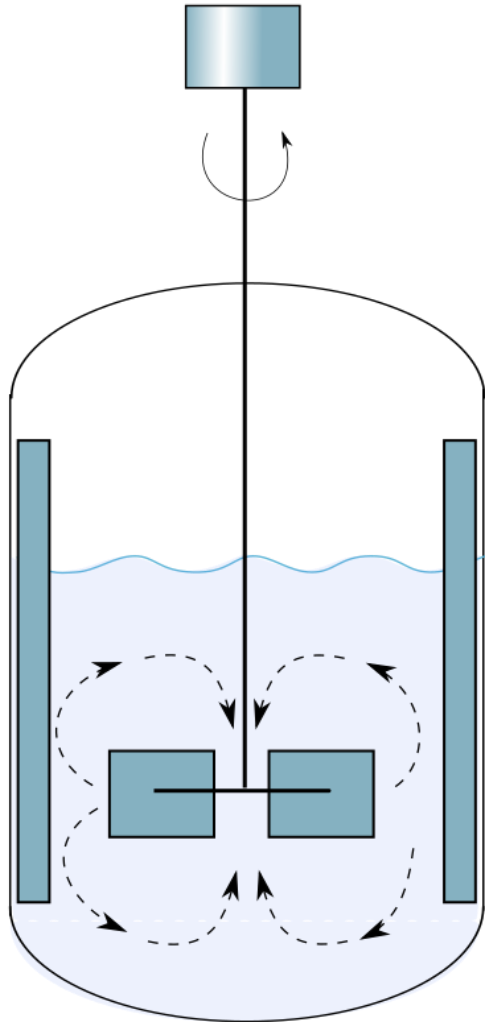


Axial flow

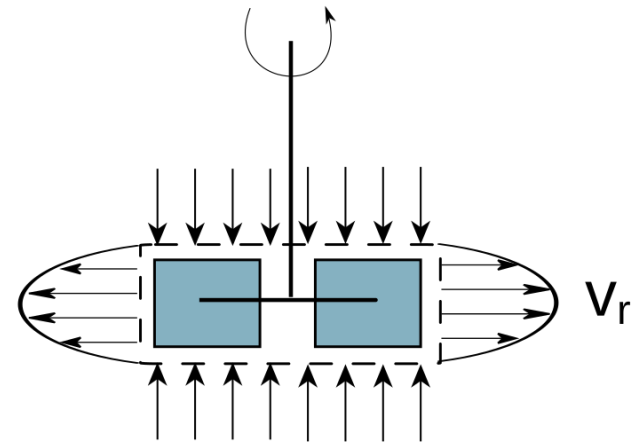


# RUSHTON TURBINE

Rushton turbine

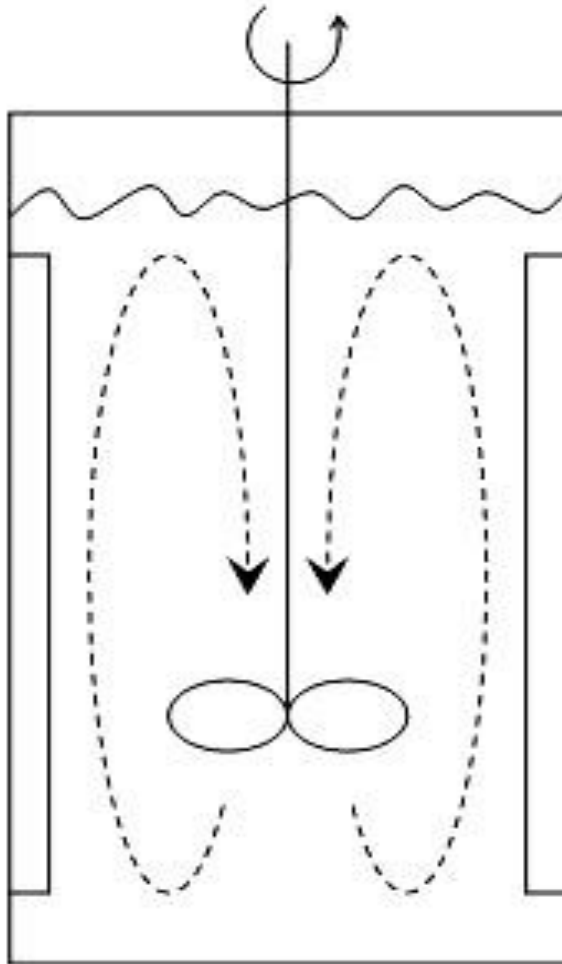


Radial flow



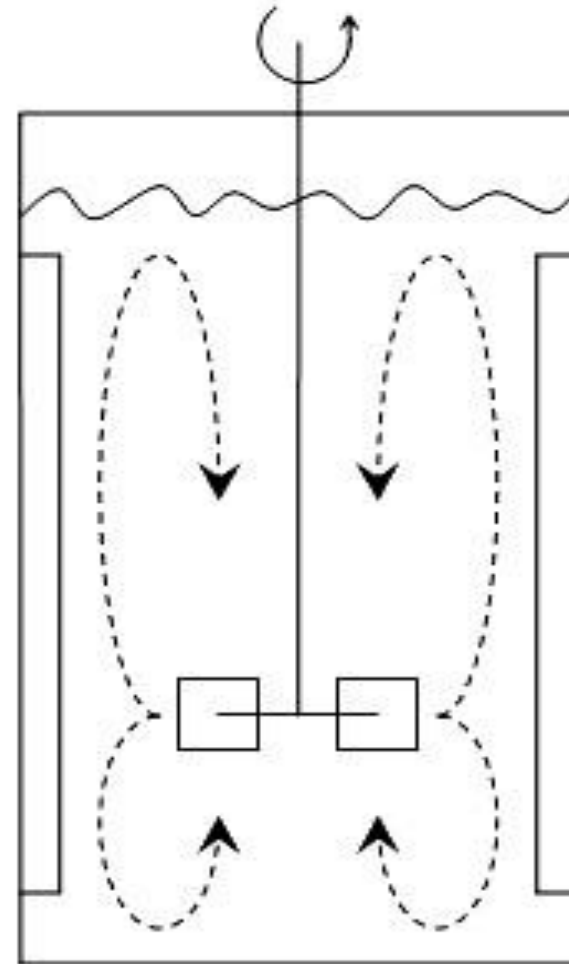
# WHICH IS THE BEST MIXER FOR CAM?

**3-blade marine impeller**



**Axial flow**

**Rushton turbine**



**Radial flow**

# INTEGRATED METHODS OF ANALYSIS

Which mixer is better for the batch crystallization of the citric acid monohydrate (CAM) between the Rushton turbine and the three-blade marine impeller?

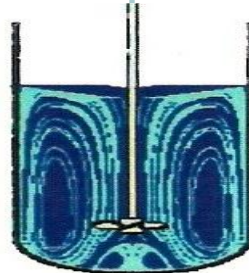
Artificial Intelligence

Ask ChatGPT



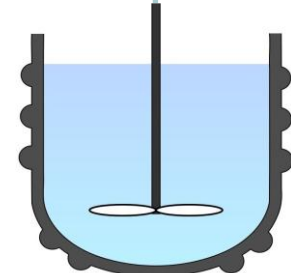
Computational Fluid Dynamics

CFD simulations



Hands-on Laboratory

DICMALAB's tests



# ASKING CHATGPT

**Question:** *Which mixer is better for the batch crystallization of the citric acid monohydrate (CAM) between the Rushton turbine and the three-blade marine impeller?*

**Answer:** For batch crystallization of citric acid monohydrate, a three-blade marine impeller is generally better due to:

- Its ability to provide low shear mixing.
- Better control over crystal growth and particle size distribution.
- Reduced risk of secondary nucleation and attrition.

However, specific process conditions (e.g., viscosity, scaling, vessel size) and desired crystal properties should guide the final choice.

Computational fluid dynamics (CFD) simulations or pilot studies can help confirm the optimal mixer.

# AI RESPONSE

**1<sup>st</sup>: 3-blade marine impeller**

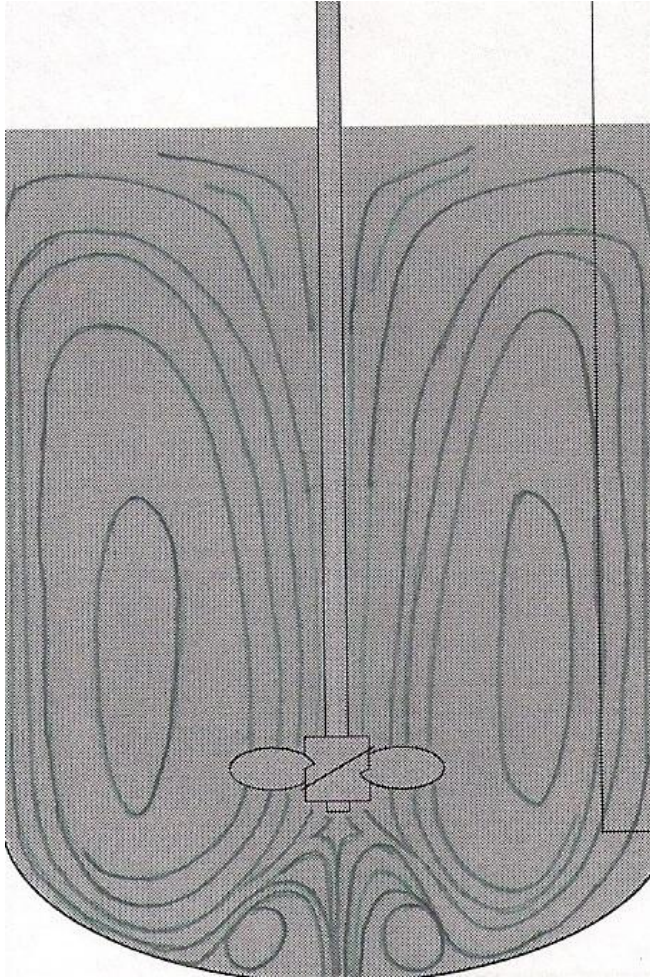


**2<sup>nd</sup>: Rushton turbine**



# COMPUTER FLUID DYNAMICS

**Manual calculation**

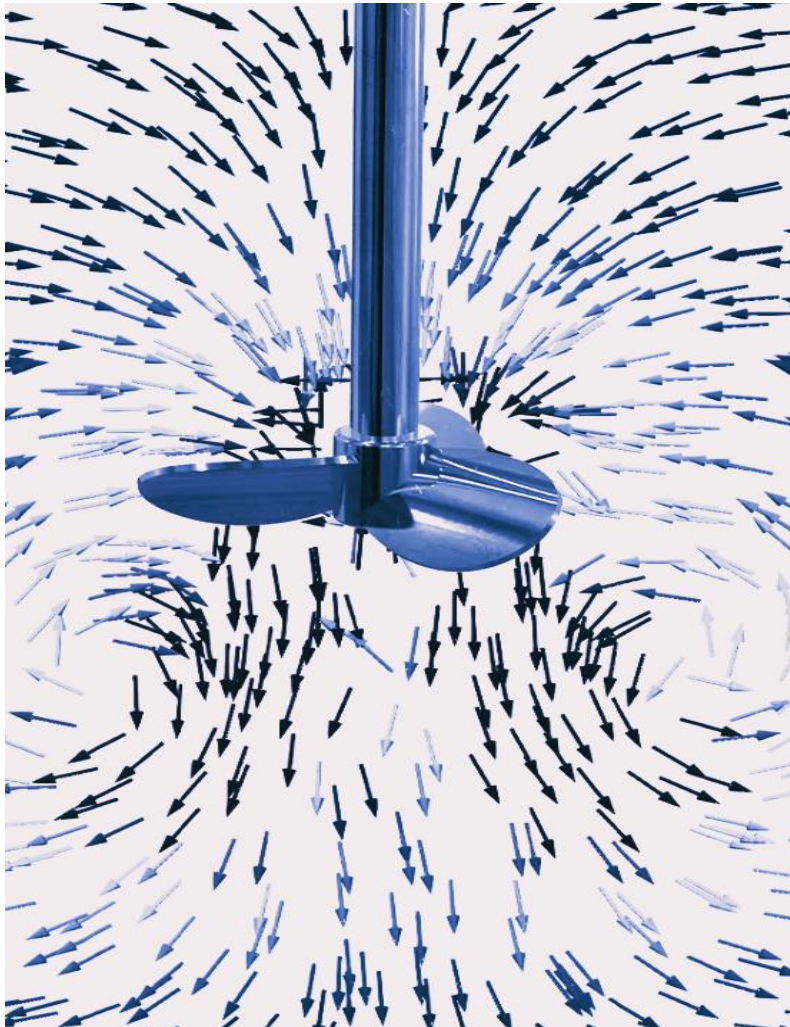


**Visimix simulation**

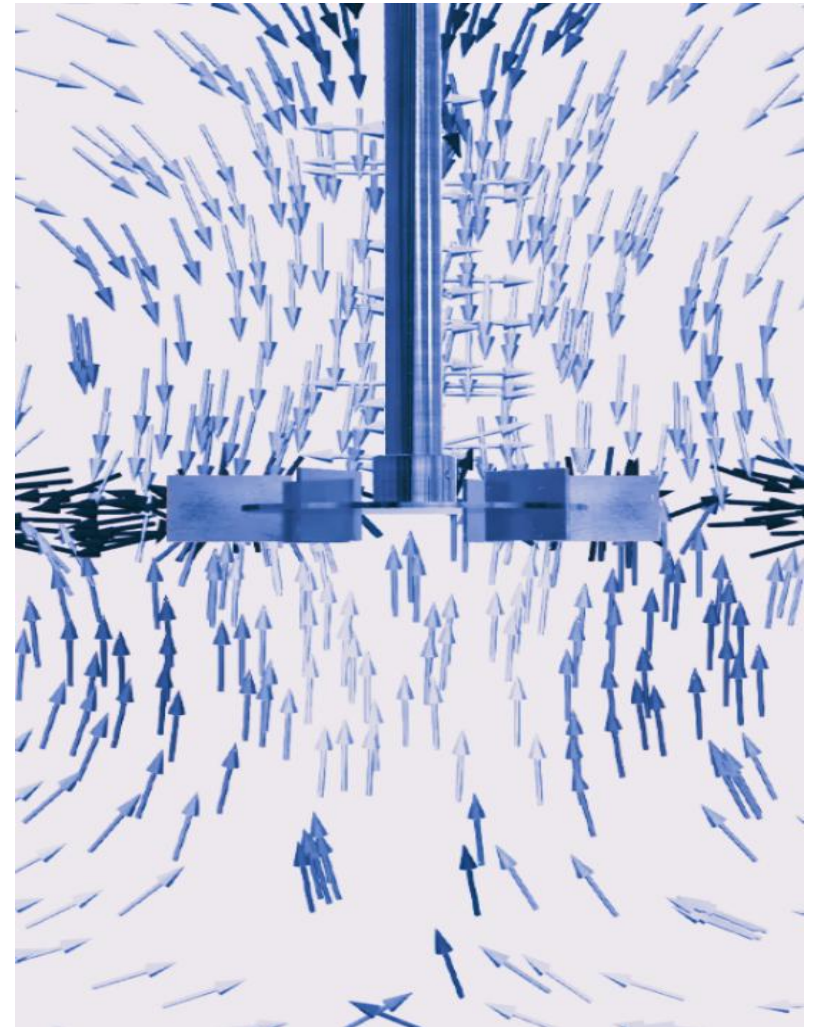


# CFD RESPONSE

**1<sup>st</sup>: 3-blade marine impeller**



**2<sup>nd</sup>: Rushton turbine**

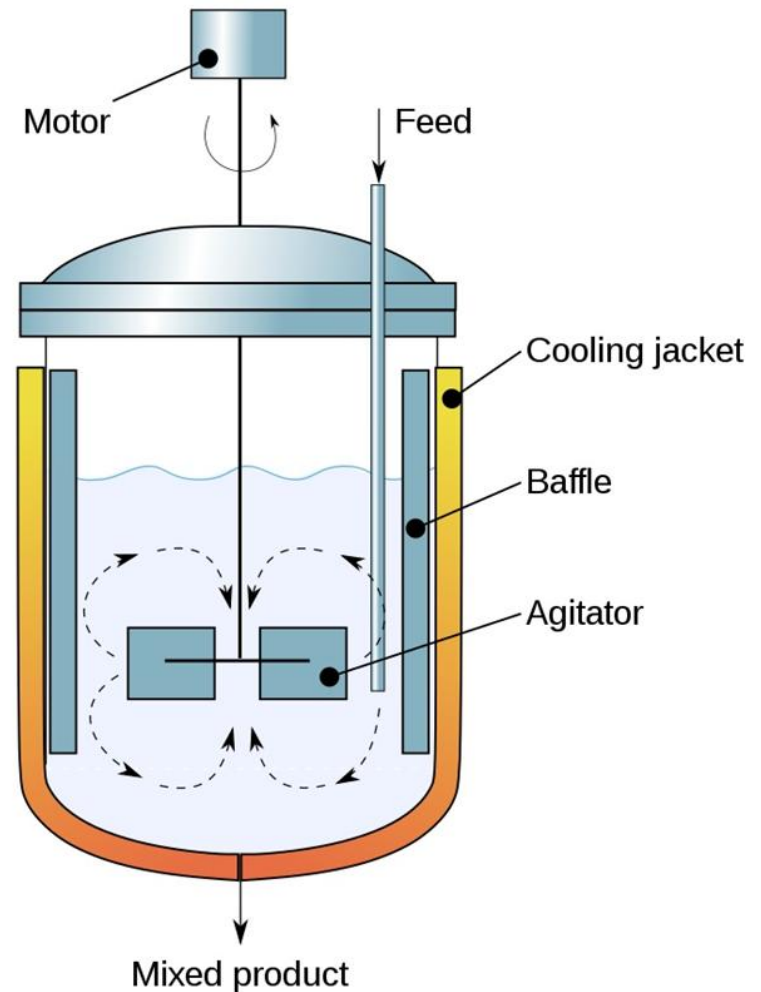


# BATCH CRYSTALLIZATION OF CAM

In the traditional laboratories of “La Sapienza” of Rome (San Pietro in Vincoli), in the 90s, the Department of Chemical Engineering Materials Environment (DICMA) tested a Rushton turbine and a three-bladed marine impeller inside a round-bottomed crystallizer for Citric Acid Monohydrate (CAM) at temperature  $T=19-22\text{ }^{\circ}\text{C}$  and at speed  $N_C=755\text{ rpm}$  [1–5].

The two stainless steel mixers available at DICMALAB had cylindrical rods ( $H=50\text{ cm}$ ,  $D=1\text{ cm}$ ) and were equally resistant to corrosion and mechanical stress.

## Stirred-tank reactor

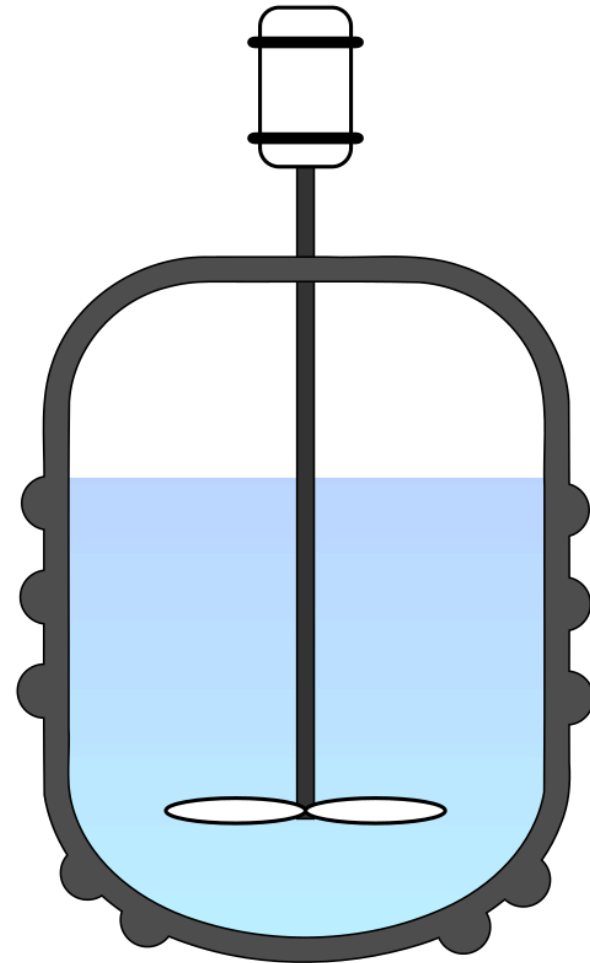


# DICMALAB RESPONSE

The DICMALAB's experiments confirmed the optimal crystal size distribution (i.e., a homogeneous distribution of large CAM crystals), generated by the three-bladed marine impeller at a speed  $\sim 2\%$  above the minimum value for solid suspension [10].

Those HOL tests established also the hazard of the Rushton turbine in terms of system stability, power consumption, and noise pollution; such mixer was therefore ruled out as dangerous (not just as a low-performing agitator) a decision not predictable via software [6].

**Safe, sustainable, prime mixing**



# CONCLUSIONS

Hands-on laboratories (HOL) may integrate the results provided by digital simulations (AI & CFD) in the investigation of STEM problems, even trivial.

When asked to choose between a three-blade marine impeller and a Rushton turbine for crystallizing citric acid, both AI and CFD showed the marine impeller as better; though correct, this outcome is incomplete and may create a false perception of a good vs. low-performing agitator.

In the nineties, at La Sapienza's traditional DICMALAB (Rome) each mixer was tested in terms of agitation efficiency, system stability, power consumption, and noise pollution.

It was thus observed that the Rushton turbine posed significant hazards in the crystallization process, a determination hardly predictable through software analysis.

# REFERENCES

- 1) **E. Bonacci.** *Experimental Survey on the Batch Crystallization of CAM.* In: Proceedings of the 96th National Congress of the Italian Physical Society, University of Bologna (Sept. 20-24, 2010), Atticon5594.
- 2) **E. Bonacci.** *Studio sperimentale sulla cristallizzazione dell'acido citrico* (Italian). Vol. 40 of *Diritto di Stampa*. Rome, Aracne Editrice, 2013 (ISBN 9788854857674).
- 3) **E. Bonacci.** A Pioneering Experimental Study on the Batch Crystallization of the Citric Acid Monohydrate. *Journal of Chemistry and Chemical Engineering* Vol. 8 No. 6 (2014) 611–620.
- 4) **E. Bonacci.** The Agitation Effects on the Batch Crystallization of the CAM. *International Journal of Mathematical Sciences & Applications* Vol. 7 No. 1 (2017) 65–71.
- 5) **E. Bonacci.** *Mixing optimization in the batch crystallization of CAM.* In: Proceedings of 8th the international scientific online conference “Algebraic and geometric methods of analysis” (AGMA 2024) – ONTU, Ukraine (May 27–30, 2024). DOI: 10.13140/RG.2.2.31891.49443.

# REFERENCES

- 6) **E. Bonacci.** *The importance of hands-on laboratories in the Virtual Era: a case of study at La Sapienza's DICMALAB.* In: Proceedings of the 111th National Congress of the Italian Physical Society, University of Palermo (Sept. 22-26, 2025), Atticon16456.
- 7) **R.K. Scheckler.** Virtual labs: a substitute for traditional labs? *International Journal of Developmental Biology* Vol. 47 No. 2–3 (2003) 231–236.
- 8) **Science Direct.** *Virtual Laboratories* (in subject area: *Computer Science*). URL (2026): [www.sciencedirect.com/topics/computer-science/virtual-laboratories](http://www.sciencedirect.com/topics/computer-science/virtual-laboratories)
- 9) **Science Interactive.** *Virtual Labs vs Hands-on Labs: How to Know Which is Right for Your Online Science Lab.* URL (2023): [www.scienceinteractive.com/blog/2023/virtual-labs-vs-hands-on-labs-how-to-know-which-is-right-for-your-online-science-lab/](http://www.scienceinteractive.com/blog/2023/virtual-labs-vs-hands-on-labs-how-to-know-which-is-right-for-your-online-science-lab/)
- 10) **T.N. Zwietering.** Suspending of Solid Particles in Liquid by Agitators. *Chemical Engineering Science* Vol. 8 No. 3–4 (1958) 244–253.

# IMAGE CREDITS

## Slide 1.

[www.imath.kiev.ua/~topology/conf/agma2026/assets/images/agma\\_bg.jpg](http://www.imath.kiev.ua/~topology/conf/agma2026/assets/images/agma_bg.jpg)

## Slide 3.

[https://it.m.wikipedia.org/wiki/File:Axial\\_flow\\_agitated\\_vessel.svg](https://it.m.wikipedia.org/wiki/File:Axial_flow_agitated_vessel.svg)

[https://it.m.wikipedia.org/wiki/File:Axial\\_flow\\_agitated\\_vessel\\_flow\\_velocity.svg](https://it.m.wikipedia.org/wiki/File:Axial_flow_agitated_vessel_flow_velocity.svg)

## Slide 4.

[https://it.m.wikipedia.org/wiki/File:Radial\\_flow\\_agitated\\_vessel.svg](https://it.m.wikipedia.org/wiki/File:Radial_flow_agitated_vessel.svg)

[https://it.m.wikipedia.org/wiki/File:Radial\\_flow\\_agitated\\_vessel\\_flow\\_velocity.svg](https://it.m.wikipedia.org/wiki/File:Radial_flow_agitated_vessel_flow_velocity.svg)

## Slide 5.

[https://en.wikipedia.org/wiki/Impeller#/media/File:Mixing\\_flusso\\_assiale\\_e\\_radiale.jpg](https://en.wikipedia.org/wiki/Impeller#/media/File:Mixing_flusso_assiale_e_radiale.jpg)

## Slide 8.

[DALL·E 2024-12-24 17.38.25](#)

[DALL·E 2024-12-24 17.36.14](#)

<https://chatgpt.com/share/6772e18d-9ce8-800f-83c0-6f9bfca4edd7>

## Slide 11.

[https://en.wikipedia.org/wiki/Baffle\\_\(heat\\_transfer\)#/media/File:Agitated\\_vessel.svg](https://en.wikipedia.org/wiki/Baffle_(heat_transfer)#/media/File:Agitated_vessel.svg)

## Slide 12.

[https://en.m.wikipedia.org/wiki/Batch\\_reactor#/media/File%3ABatch\\_reactor\\_STR.svg](https://en.m.wikipedia.org/wiki/Batch_reactor#/media/File%3ABatch_reactor_STR.svg)