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Mechanistic Role of Shear Rate on Transport-Controlled Crystal Growth in Antisolvent Crystallization

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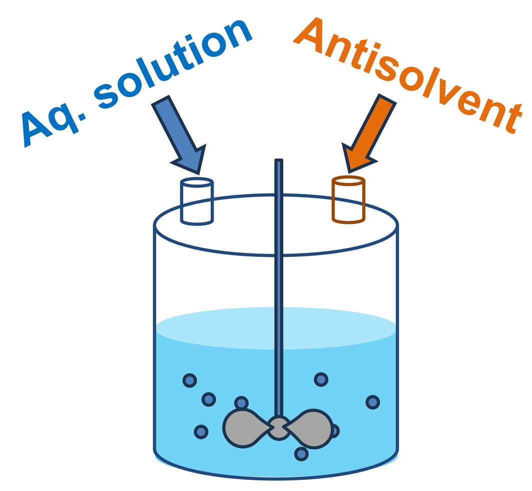
INTRODUCTION & AIM

- Hydrodynamics plays a central role in antisolvent crystallization by governing mixing and supersaturation, which in turn controls crystal growth [1].
- Antisolvent crystallization is widely used in:
  - Pharmaceutical manufacturing
  - Battery materials production
  - Metal salt crystallization
  - Fine chemicals



Knowledge Gap

Previous studies report:
- ✓ Flow fields
- ✓ Supersaturation distributions
- ✓ Crystal size distribution

However,
- ✗ The mechanistic pathway linking shear rate to crystal growth through transport phenomena remains less explored

Objective

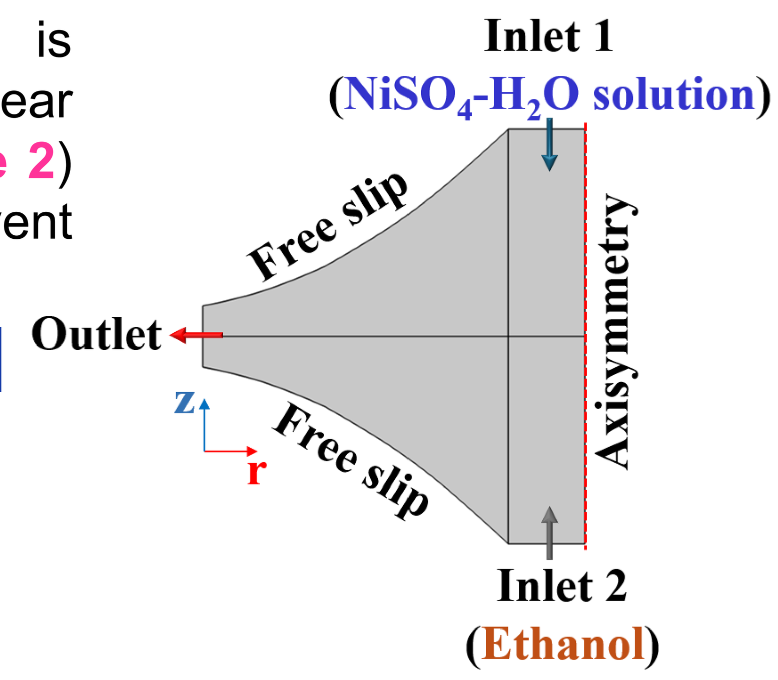
To establish how shear-mediated transport controls supersaturation distribution and consequently crystal growth in antisolvent crystallization

METHOD

COMPUTATIONAL FRAMEWORK

Coupled computational fluid dynamics–population balance model (CFD-PBM) is employed to investigate the influence of shear rate (***for two velocities***: Case 1 and Case 2) on crystal growth in an antisolvent crystallization system [2].

2D computational domain



SYSTEM STUDIED (*at Constant Temperature*)

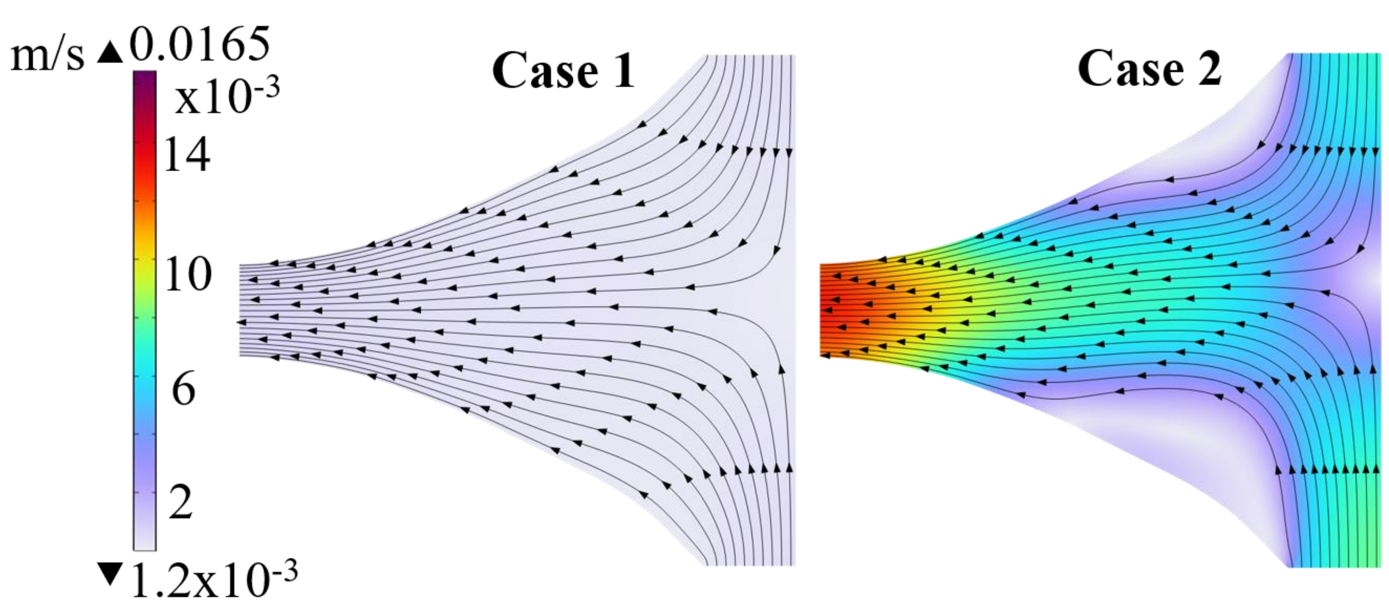
- Salt: $NiSO_4.6H_2O$
- Solvent: Water
- Antisolvent: Ethanol
- Geometry: 2D-axisymmetric
- Flow regime: Laminar

GOVERNING PHYSICS

- **Supersaturation (S):** Generated when Ethanol addition reduces solubility
- **Crystal Growth:** Size-independent growth rate as a function of local Supersaturation
- **Species Transport:** Mass transport by convection and diffusion

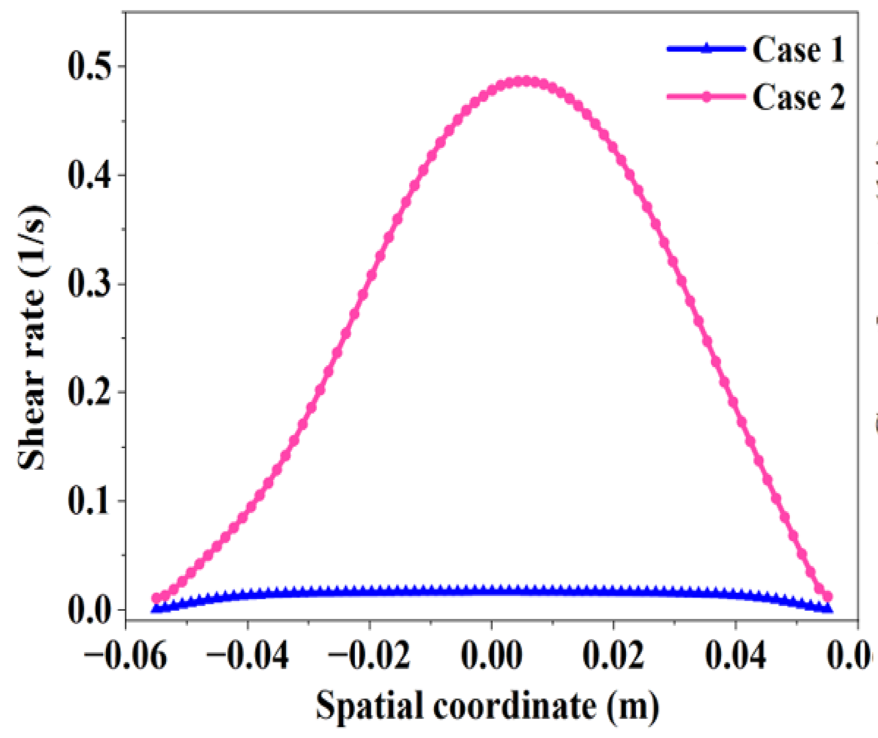
RESULTS & DISCUSSION

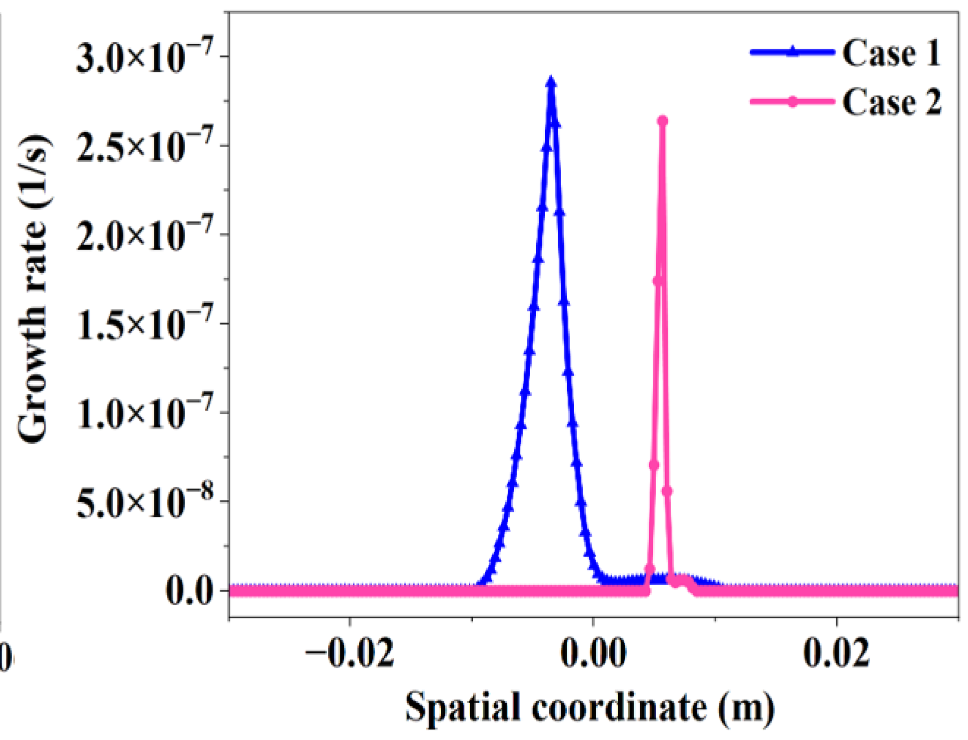
VELOCITY FIELD



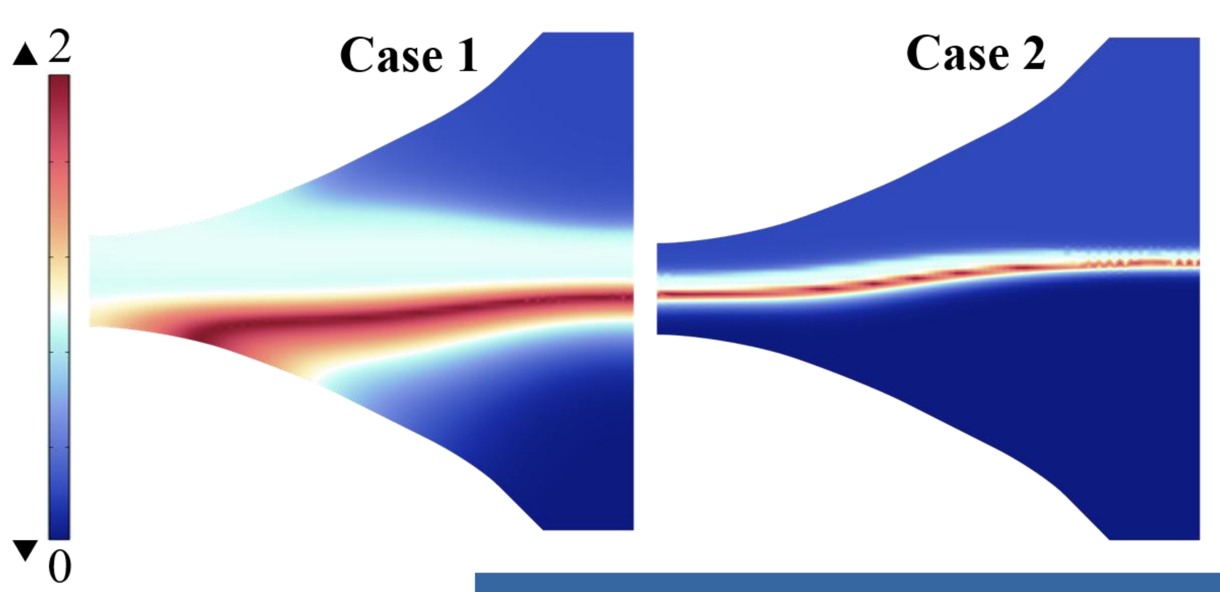
1) Smooth and symmetric convergence of solution and antisolvent streams
2) Increasing shear rate elevates local velocity gradients and momentum transport

SHEAR RATE and GROWTH RATE DISTRIBUTION



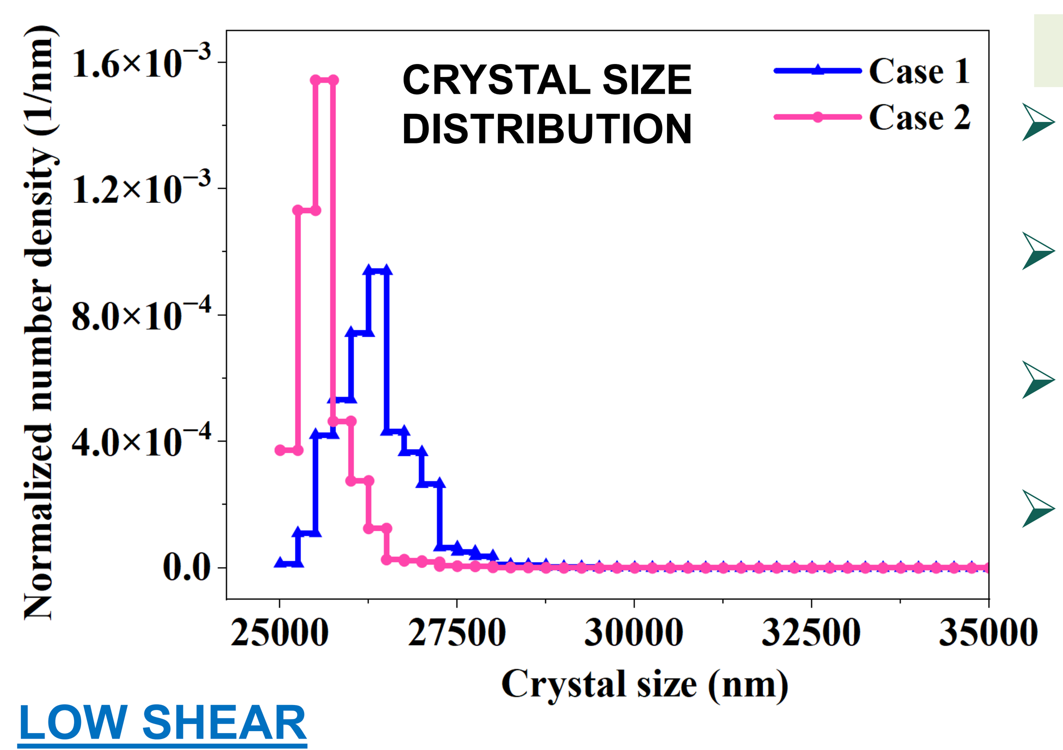


SUPERSATURATION DISTRIBUTION



1) Supersaturation is generated at the solution–antisolvent interface
2) Higher shear rates produce sharper supersaturation gradients and greater spatial confinement

MECHANISTIC INTERPENETRATION



Engineering Applications

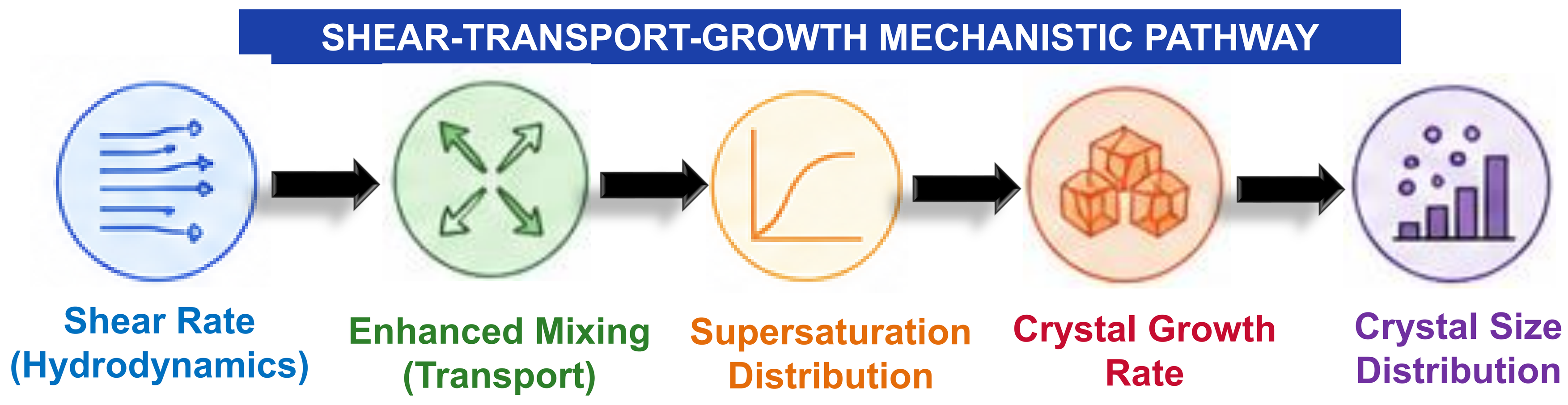
- Enables rational design of antisolvent systems.
- Provides guidance for scale-up of crystallizers.
- Improves control of crystal size distribution.
- Applicable to battery-material and pharmaceutical crystallization.

LOW SHEAR
- Weak mixing
- Broad supersaturation fields
- Distributed growth zone
- Broader crystal size distribution

With Increasing Shear Rate →

HIGH SHEAR
- Intense mixing
- Sharp supersaturation gradient
- Localized growth zone
- Narrower crystal size distribution

SHEAR-TRANSPORT-GROWTH MECHANISTIC PATHWAY



KEY FINDINGS

- ✓ Velocity gradients increase with velocity, enhancing momentum transport
- ✓ Growth zone becomes increasingly localized
- ✓ Shear rate peaks in the mixing region and increases with inlet velocity
- ✓ Higher shear creates sharper supersaturation gradients
- ✓ Increased flow rate narrows the supersaturation zone

CONCLUSIONS

1. A mechanistic framework for understanding shear-mediated transport effects in growth-dominated antisolvent crystallization systems is provided.
2. Hydrodynamic shear to crystal growth and CSD is connected.
3. Shear is observed to modify the mixing of aqueous and organic phases and transport dynamics within the system.
4. Crystal growth follows the local supersaturation distribution.

FUTURE WORK/ REFERENCES/ACKNOWLEDGMENT

- Extension to transient and turbulent conditions
- Investigation of scale-up implications

[1] Marchisio et al., Effect of fluid dynamics on particle size distribution in particulate processes, Chem. Eng. Technol. 29 (2006) 191–199.
[2] Jha et al., Metal recovery from spent batteries through antisolvent crystallization in a T-mixer using a coupled CFD-PBE approach, in: Centre for Evaluation in Education and Science (CEON/CEES), 2025: pp. 407–412.