An abstract graphic on the left side of the slide features a dark blue background with glowing blue molecular structures. These structures consist of small spheres connected by lines, resembling a network or a cluster of atoms. The structures are illuminated from the left, creating a bright blue glow that fades into the dark background. The overall aesthetic is scientific and modern.

# Understanding solvent-induced phase transformations driven by anomalous mass transfer

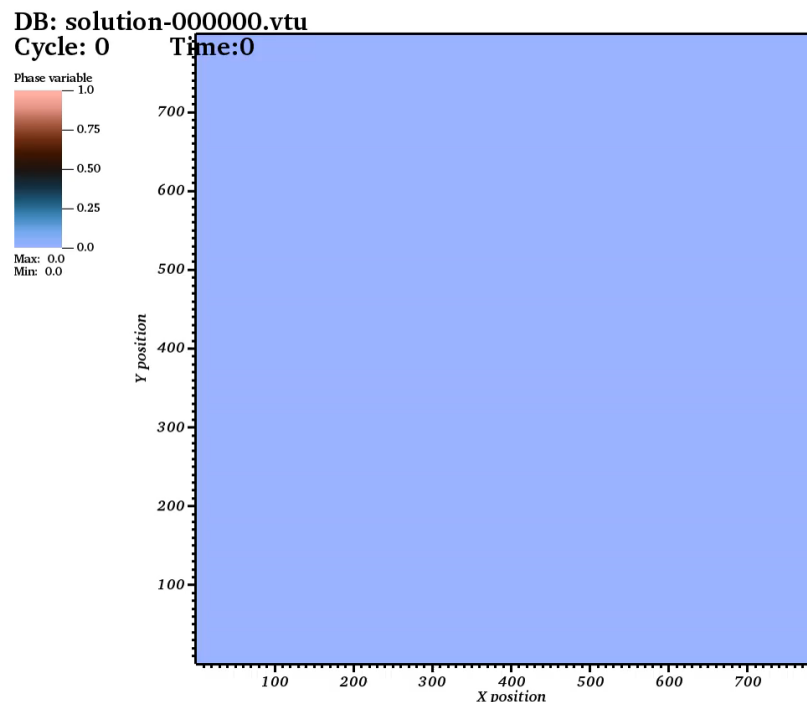
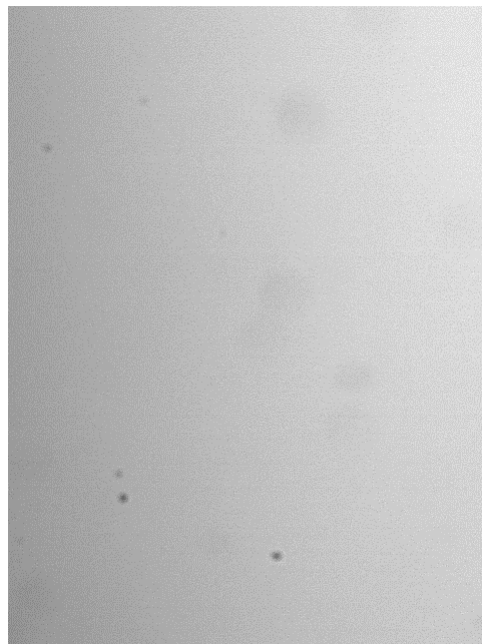
CMAC Open Days, 15/11/2023

Irene Moreno Flores

Supervisor: Dr Javier Cardona



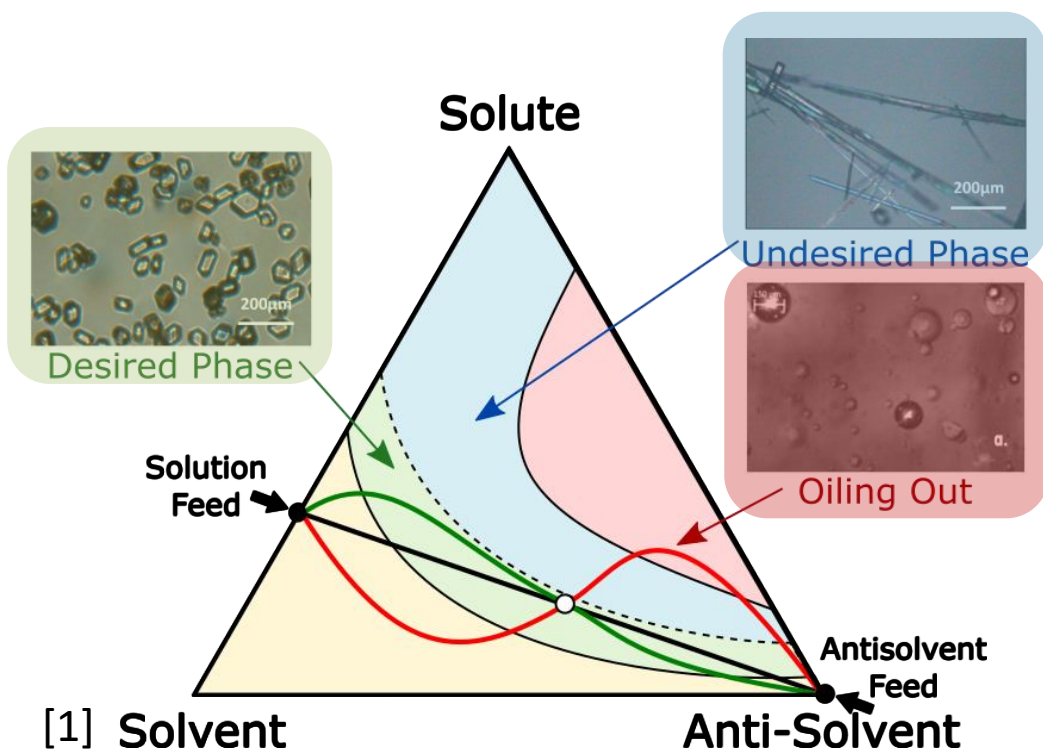
## Phase-field models to simulate mass transfer and phase transformations



**DataFactory:**

Isoniazid in cyclohexane

# Background and motivation



**Gap in fundamental understanding** of how mixing processes occur (LLPS, Ouzo effect, uphill diffusion)

**Current understanding:** mixing process evolves through black line (ideal)

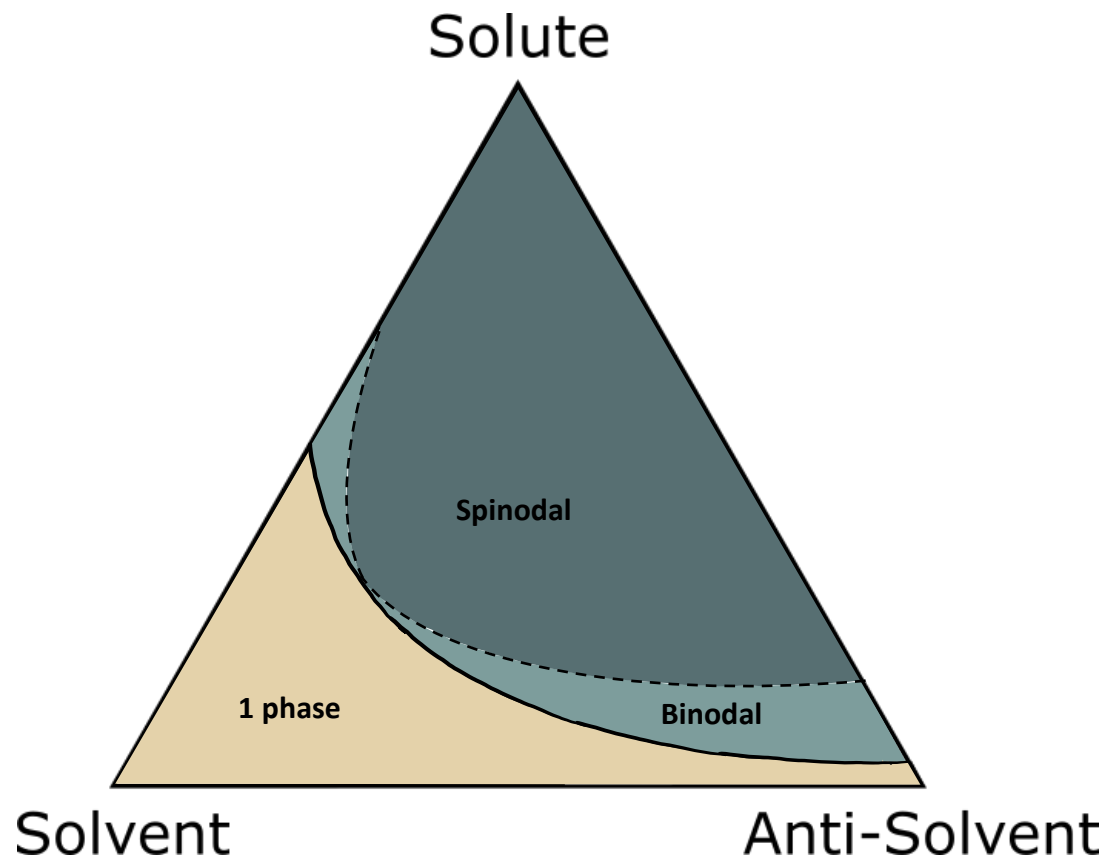
**Green line:** Desired outcome still achieved

**Blue area:** Appearance of undesired crystal phase

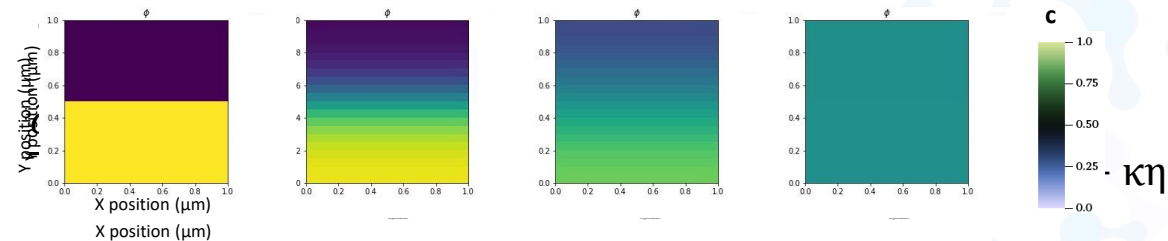
**Red line:** The system liquid-liquid phase splits

**Aim** Accurate modelling of antisolvent/cooling, seeded/unseeded crystallisation

# Model comparison



Diffusion coefficient  $D$  [m<sup>2</sup>/s]



**Come to my poster**

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