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1. Introduction

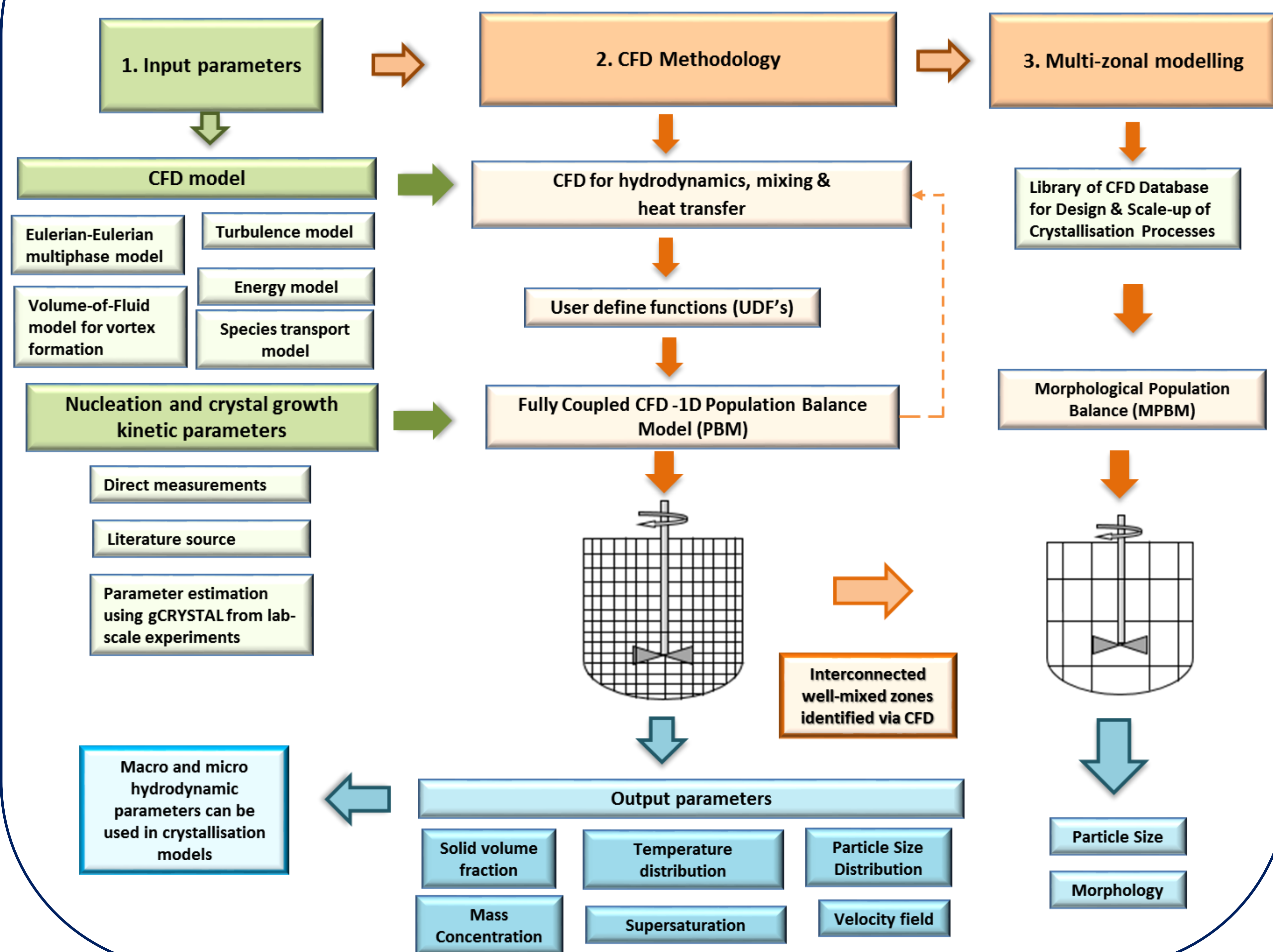
- Crystallisation process modelling methodology for accurate prediction of crystal size and shape distribution can facilitate process development and scale up
- Most modelling approaches designed to predict crystal size distribution (CSD) assume perfectly mixed conditions in the crystallizer leading to inaccurate predictions
- Computational fluid dynamics (CFD) coupled with PBM can provide detail insight of the hydrodynamics and effect of kinetic parameters on CSD in batch cooling crystallisation process.
- Multi-zonal modelling can be use to reduce extensive computational time required for CFD-PBM simulations

2. Aims and Objectives

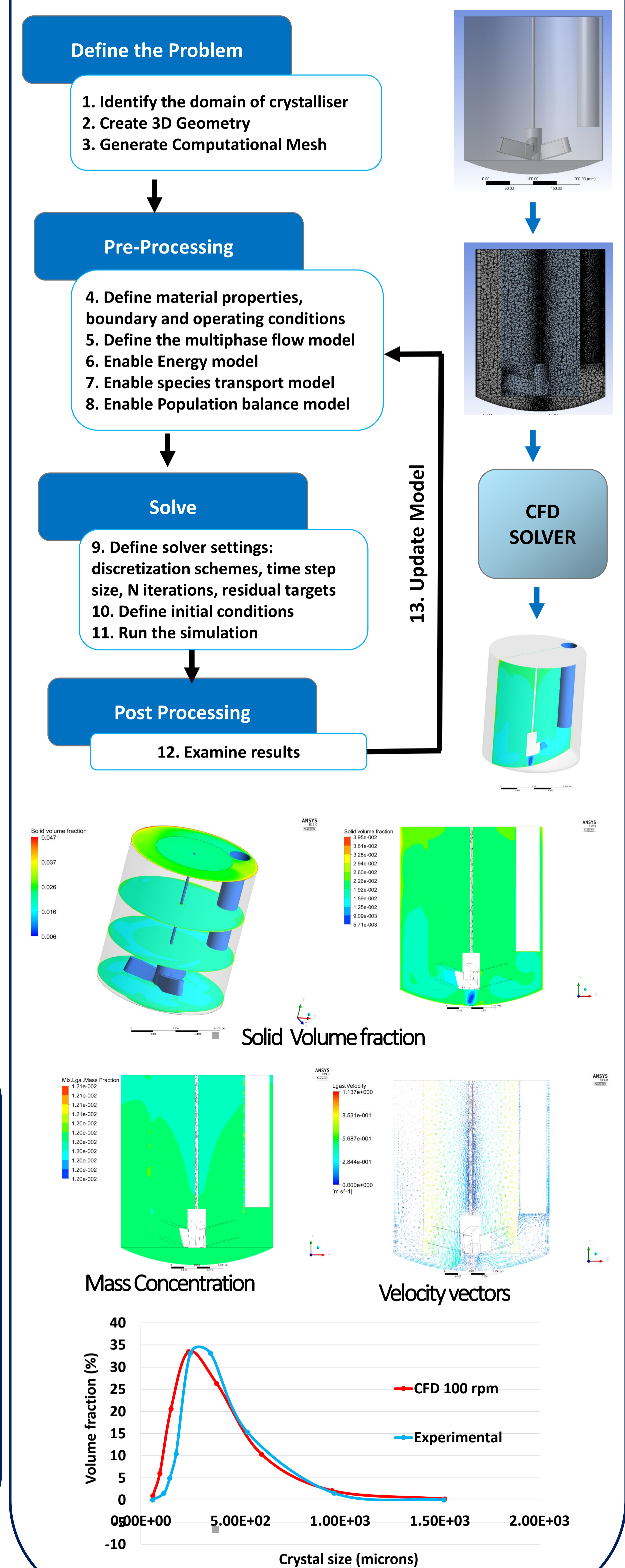
- Develop CFD coupled with a population balance model (PBM) methodology for batch cooling crystallisation processes
- Develop a computationally efficient multi-zonal modelling approach informed by CFD-PBM simulations in gFormulatedProduct
- Implement the digital design tools for the design and scale up/down of different crystallizers configuration and operating conditions

3. Work Flow for Digital Design of Crystallisation Processes

Case Study: Batch cooling crystallisation of L-glutamic acid (LGA) from aqueous solutions in a 20 L crystalliser



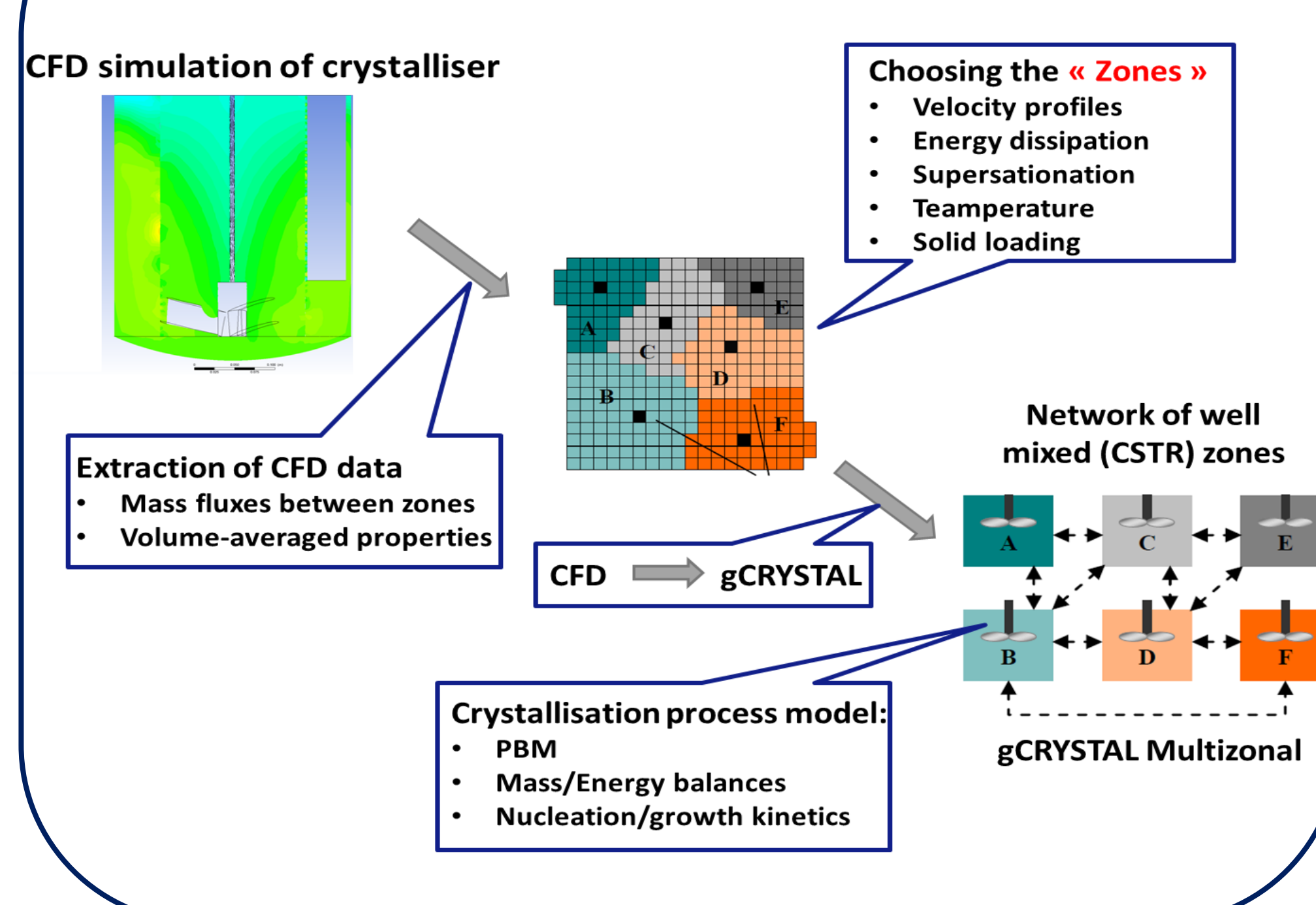
4. CFD modelling platform for batch cooling crystallisation in ANSYS Fluent



Highlights

- A transient 3D CFD-PBM model was developed to predict (CSD) in batch cooling crystallisation
- Predicted CSD's in a 20 L crystalliser are in good agreement with measurements
- The 3D- CFD-PBM model will aid efficient process optimisation for production of desire crystal sizes
- A multi-zonal modelling platform embedded in gCRYSTAL software can be use to reduce extensive computational time and scale up/ down of the process

5. Multi-zonal modelling approach



References

[1] K. Liang, PhD thesis, Department of Chemical Engineering, Heriot-Watt University, Edinburgh, 2002

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