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**THEME:** (please keep one item)

- Solution methods of PBM, stochastic PBM
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## **A COMPARTMENTAL-BASED APPROACH FOR THE MODELLING OF A VORTEX PRECIPITATION REACTOR FOR NUCLEAR ENERGY APPLICATIONS**

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### **1. CONTEXT**

Due to the manipulation of radioactive material, nuclear industry has to achieve very strict productivity and purity specifications. Thus, the chemical unit operations may involve specific designs. Traditional mixing technics are then adapted to set environmental and process specifications. In the case of actinide precipitation, the operation is conducted in a vortex reactor, which consists in an un-baffled tank reactor stirred by a magnetic rod located at the bottom of the vessel [1]. The reactor is fed by the two reactant solutions and the suspension flows out at the top of the reactor. The resulting internal flow pattern produces a vortex-shaped free surface and two macro mixing zones in the liquid phase: forced and free vortices (see Figure 1). The forced vortex, located in the center around the reactor axis, is characterized by poor axial mixing, while the free vortex zone, corresponding to the annular zone between the forced vortex and the reactor wall, can be described as a well-mixed compartment.

The concentration of both reagents and thus the supersaturation strongly depends on the spatial position in the vessel. The particle size distribution is not uniform spatially either. As a consequence, the quality of the produced crystals is directly linked to the local supersaturation, which itself directly depends on the reactor hydrodynamic behaviour.

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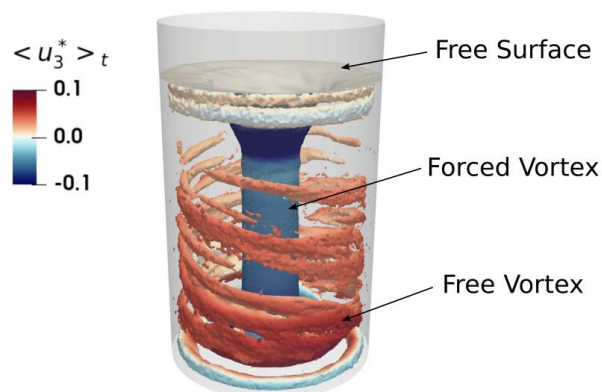


Figure 1 : Visualization of the free surface and the forced/free vortices from a well resolved LES study [1]. Iso-surfaces of the Q-criterion coloured by the time-averaged axial velocity are presented.

## 2. CFD SIMULATIONS AND POPULATION BALANCE

The main aim of this work is to develop a model for the simulation of a steady state vortex precipitator. To do so, three approaches are combined: mass balances, population balances and hydrodynamic simulations. Coupling these principles needs the independent study of (i) mixing and (ii) precipitation:

- Firstly, CFD simulations were performed at the macro scales [2] to study the local mixing conditions and to reproduce the flow behaviour, in agreement with the Rankine's combined vortex and the theory of Nagata [3]. Due to a strongly anisotropic turbulence originating from the dominance of the tangential velocity, a Large Eddy Simulation (LES) approach was adopted. The wall-adapting local eddy-viscosity (WALE) sub-grid scale model was employed to estimate the modelled viscosity. A mesh sensitivity study was carried out where a mesh at the same order of the turbulent micro-scales of Taylor was identified [1]. The open source TrioCFD was employed with a discontinuous front tracking method that captures accurately the free-surface vortex that separates the liquid/gas phases in the reactor. Very fast-irreversible reactions of type  $A+B \Rightarrow P$  were modelled and different configurations depending on the reactants feeding positions were examined. This procedure allowed the flow of the non-ideal vortex reactor to be schematically represented in a first approximation as a combination of five well-mixed zones (see Figure 2) [4]. The volumes and exchange flow rates between these zones were determined as well [5]. Reaction models based on an Eddy Dissipation Concept (EDC) were used as they showed to reproduce correctly the micro-mixing in the zones where the turbulent dissipation is significant [6].
- Crystallization mechanisms were studied separately in order to determine supersaturation expressions and nucleation, growth and agglomeration kinetics [7,8].

This work focuses on the solution of the population balance equation by combining hydrodynamic and crystallization kinetics in order to predict the characteristics of both solid and liquid phases leaving the vortex reactor.

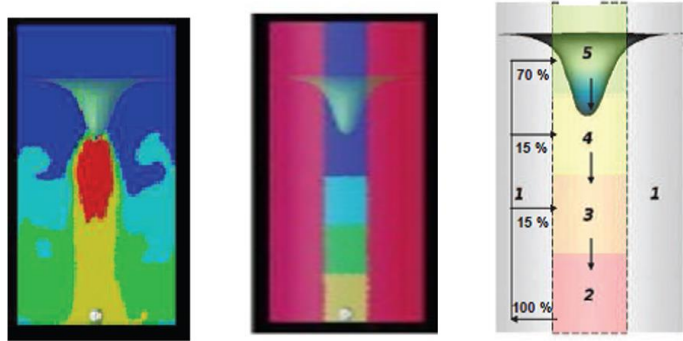


Figure 2 : Compartmental-based approach for vortex reactor simulation [5].

### 3. NUMÉRIQUE APPROACH FOR STEADY-STATE POPULATION BALANCE

Firstly, a tool to model the steady-state behaviour of a single compartment is developed, fixed point algorithms and discretisation methods are coupled in order to determine supersaturation and complete information about the population leaving the volume. The nucleation, growth and agglomeration kinetics are included in the same model to verify their coherence. After convergence analysis, a vector acceleration algorithm based on the  $\Delta 2$  of Aitken method [9] is included to ensure model robustness.

Later, the structure describing two reactors with recycle is studied. The solution algorithm, critical variables and convergence criteria are identified. An acceleration method is also performed to properly track the population evolution through the recycle stream.

Finally, the global vortex reactor is modelled by considering the 5 well-mixed zones (see Figure 3). Future works will be focused on the transient simulations of the vortex reactor in order to describe particle evolution in real time.

### ACKNOWLEDGMENTS

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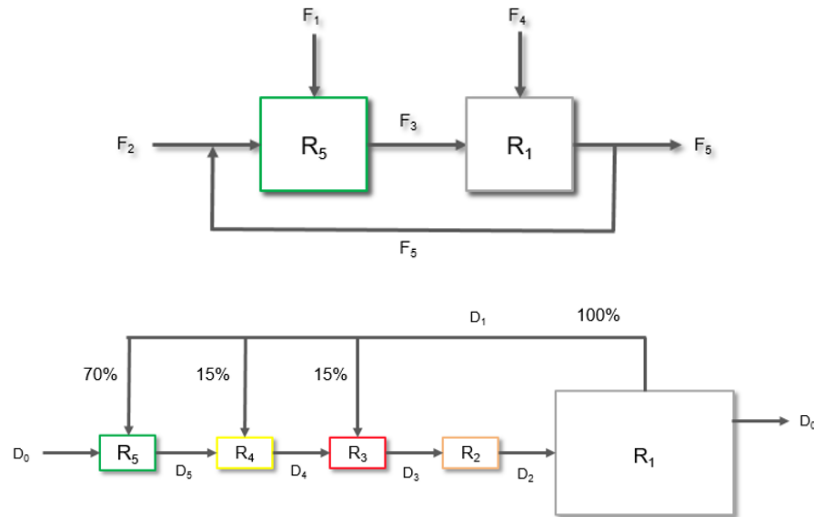


Figure 3 : Approach to develop the vortex reactor model: reactor network.

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