Modelling of precipitation process by hybrid large eddy simulation - multizonal approach Application to uranium oxalate

M. Bertrand, E. Plasari, O. Lebaigue, . Lamarque N, F. Ducros, H. Muhr

To cite this version:

HAL Id: hal-02417727
https://hal.archives-ouvertes.fr/hal-02417727
Submitted on 18 Dec 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
**Introduction**

- Precipitation process modelling: coupling of chemistry and hydrodynamics
- Different methodologies in the literature from hybrid methods based on multizonal models to a fully coupling in which the population balance equations are directly implemented into a CFD code
- Hybrid modelling: multizonal model that comprises several perfectly mixed compartments parameterised using LES

**OBJECTIVES**

- Development of a multizonal approach with hydrodynamic information entirely extracted from LES
- Application to the simulation of the uranium oxalate precipitation performed in a vortex reactor

**CFD modelling**

**Vortex reactor:**
- Operating in the fuel reprocessing industry
- Unbaffled cylindrical glass vessel
- Stirred by a cylindrical magnetic rod

**LES Modelling [1]:**
- CFD code: Trio_U developed at CEA www-trio-u.cea.fr
- Using the Large Eddy Simulation approach
- Homogeneous unstructured grid with about 650,000 tetrahedral elements
- Free surface: Discontinuous Front Tracking method
- Magnetic rod: Immersed Boundary Condition model
- Under-grid model: WALE

**Micromixing phenomena**

Which micromixing time with LES simulation?

- Two models developed [3], based on the classical Eddy Dissipation Concept of Magnussen and Hjertager:
  - LES variance model
  - LES diffusive model

<table>
<thead>
<tr>
<th>Radius (mm)</th>
<th>U(0) [m/s]</th>
<th>z=180mm Theta=0° expe</th>
<th>z=180mm Theta=180° expe</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.10</td>
<td>0.20</td>
<td>0.30</td>
</tr>
<tr>
<td>0</td>
<td>0.40</td>
<td>0.50</td>
<td>0.60</td>
</tr>
<tr>
<td>100</td>
<td>0.70</td>
<td>0.80</td>
<td>0.90</td>
</tr>
</tbody>
</table>

**Precipitation modelling**

Experimental study of the uranium IV oxalate precipitation:

\[ \text{U(IV)O}_2 + 2 \text{H}_2\text{C}_2\text{O}_4 \rightarrow \text{U(C}_2\text{O}_4)_2\text{H}_2\text{O} + 4 \text{HNO}_3 \]

- Crystallite properties: \( L_{e2} \approx 0.9 \mu m \)
- Crystallite properties: \( L_{e2} \approx 8 \mu m \)

**Conclusion**

- One-way coupling between the multizonal and LES models used to study in a quantitative way the influence of different operating parameters, allowing a better control of process or design
- Hybrid approach allows both:
  - an accurate description of the flow field and relevant hydrodynamic data for the population balance resolution using LES,
  - a flexible and efficient precipitation process modelling using multizonal model.

**Results [2]:**

- In agreement with Nagata’s model: rotation of the fluid around the vessel symmetry axis
- Variation of the tangential velocity module in space and time with the rod position
- Good agreement with theoretical aspects and experimental measurements performed by Laser Doppler Velocimetry

**Application to uranium oxalate precipitation**

**Population balance and turbulence [3]**

Classical approach

- in chemical engineering science

Hybrid methods

- Fully coupling

工业化沉淀器

**Population balance resolution**