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Comparison of the method of classes and the quadrature of moment for the modelling of Neodymium Oxalate Precipitation

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Introduction

- Oxalic precipitation:
  - To deal with radioactive waste and recover the actinides lanthanides
  - To facilitate the development of experimental methods

- Modelling approach:
  - Experimentation \(\rightarrow\) Thermodynamics + kinetics & numerical methods

Thermodynamics et kinetic laws

- Supersaturation ratio (S) \(\rightarrow\) The driving force of the precipitation process
- Kinetic laws of nucleation, crystal growth and agglomeration = f (S)

Homogeneous primary nucleation

\[ R = 3 \times 10^{10} \exp \left( \frac{67000}{RT} \right) \exp \left( \frac{-187}{(LT)^2} \right) \]
\[ S > 50 \]

Crystal growth

\[ G = 2.91 \times 10^{-4} \exp \left( \frac{-14000}{RT} \right) \left( p_{O_2} \right)^{0.5} (S-1) \]
\[ 293K < T < 333K \]

Agglomeration

\[ \gamma = \frac{55.1 \times 10^{-2}}{V} \exp \left( \frac{-40900}{RT} \right) \]
\[ S > 61 \]
\[ 293K < T < 333K \]

Continuous experiments

- Short mean residence time = 1 min \(\rightarrow\) high S
- Constant agglomeration kernel: \(\beta\)
- Scanning Electron Microscopy \(\rightarrow\) crystal size distributions

Experimental Study

MSMPR

- Continuous precipitation until steady state
- \(V = 200 \text{ ml}\)
- Temperature = 20\(^\circ\) C
- four stainless steel baffles
- stainless steel four 45\(^\circ\) pitched blade turbine \(\rightarrow N_p = 1.5\)

Two population balances

Method of classes

\[ \frac{dN_p}{dt} = \frac{V}{\tau} \left( R_p - \frac{1}{\nu} \frac{dG}{d\nu} \right) \]

Main results

- Comparison of volume fractions at 5 \(\tau\)

Conclusions

- Kinetic laws (\(R_p, G, \) et \(\beta\)) and loose agglomerates from experimental runs
- Two population balance models: solved by the Method of classes and QMOM
- Both methods compared well with experimental data during transient and at steady state
- QMOM required much less computational effort and is preferentially used with the reconstruction method detailed in [10]

Références


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