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Introduction

Modeling approach

Main results



Conclusions

• Phosphoric acid is the key element in the phosphate industry where it is used in the production of fertilizers, in the food industry and even in the pharmaceutical industry [1].

• Design, operation and control of phosphoric acid manufacturing process still pose several problems due to :

(i) the lack of knowledge on many complex phenomena involved in the process,

(ii) the lack of accurate (thermodynamic, kinetic, hydrodynamic...) data.

• Need of the performance optimization of the phosphoric acid manufacturing process, especially the digestion tank which constitutes the heart of the process.

### Assumptions

- The digestion tank is considered as a perfectly stirred reactor.
- Isothermal conditions are assumed in the system.
- Particles are well dispersed in the liquid phase. They are spherical and shrink uniformly during the leaching process.
- The reaction involved is irreversible and takes place only at the surface of the particles.

#### Aim of the work

Analyze the effect of the particle size distribution (PSD) on the leaching process by developing a first-principles model for mono-sized particles first, and then incorporating a PSD to take into account the actual operating conditions in the digestion tank.



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Conclusions

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Introduction

### **Modeling Approach**

- Main results
- Leaching is a kinetic process characterized by a heterogeneous and non-catalytic reaction.
- Phosphoric acid is used to transform tri-calcium phosphate (TCP) into mono-calcium phosphate (MCP) through the following reaction :  $Ca_3(PO_4)_2 + H_3PO_4 \rightarrow 3CaHPO_4$
- The model equations are based on transient mass balance in the phases considered, i.e., solid phase, liquid bulk and liquid film surrounding the particles.



Schematic illustration of the SCM in the leaching mechanism



Example of granulometric analysis of phosphate ore

- Shrinking core model is used to describe the variation of the particle size of phosphate ore.
- Thickness of liquid film ( $\delta$ ) surrounding the phosphate particles decreases over time [2].
- The effect of the type of PSD is evaluated by using different distributions, i.e. Rosin– Rammler-Bennett (RRB), Gamma, Gaudin–Schuhmann (GGS) distributions.
- The variation coefficient (CV) is used to quantify the influence of particles' shape on the leaching model predictions, at different temperatures, acid concentrations, stirring speeds.



Diagram of the phenomenological modeling approach

XXIV International Conference on Chemical Reactors CHEMREACTOR-24, September 12 - 17, 2021





Conclusions

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Introduction

**Modeling Approach** 

Main results

- By increasing CV, the concentration of phosphoric acid decreases rapidly, and the conversion rate increases due to the increase of the fraction of the smaller particles compared to the average size.
- The particle size distribution is an important variable which influences the progress of the leaching process within the digestion tank.



Temporal profiles of the conversion rate (left) and phosphoric acid concentration (right) for different CV values of the Gamma distribution

- A very good agreement between the model predictions of the conversion rate and the measurements carried out at three values of temperature [4].
- By considering the PSD of phosphate ore particles, the activation energy and the CV are the potentially identifiable parameters.



Comparison of the model predictions and measured values of the conversion rate using GGS [4]

Identified values of the CV using different distribution functions

Distribution	Ea	95 % C.I	CV	95 % C.I
GGS			0.131	0.005
Gamma	7656.02	592.446	0.304	0.002
RRB			0.0455	0.017

• The Arrhenius equation characterizes the leaching behavior of phosphate ore particles in phosphoric acid solutions with a low activation energy which indicates that the diffusion step is the rate-limiting step of the leaching process.

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Introduction

**Modeling Approach** 

Main results



Conclusions

### Conclusions

- Development of a first-principles model to understand some of the complex mechanisms of the leaching of phosphate ore particles in phosphoric acid solutions.
- Shrinking core model describes well the leaching phenomenon of phosphate ore particles.
- Predicted results using the identified parameters of the model with incorporated PSD are more consistent with the collected experimental data.
- Development of appropriate methods and tools for industrial data processing.

#### **Outlooks**

- Identification of the unknown model parameters from the available experiments and validation of the model with additional measurements.
- Determination of the optimal operating conditions of the digestion tank.

#### References

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