Development, implementation and use of a generic nutrient recovery model (NRM) library

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Presentation outline

- Problem statement
- Objectives
- Model development methodology
- Model simulation & validation results
- Recommendations for research
- Conclusions & perspectives

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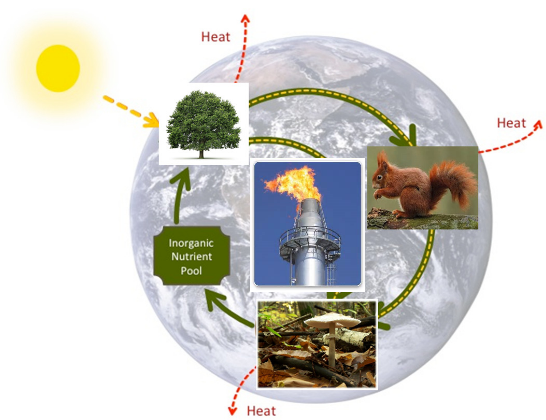
PROBLEM STATEMENT

Our nutrient world



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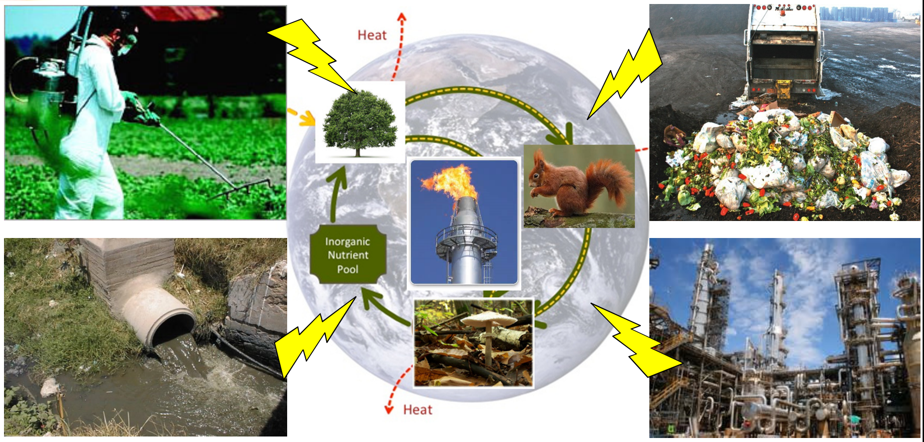

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Our nutrient world

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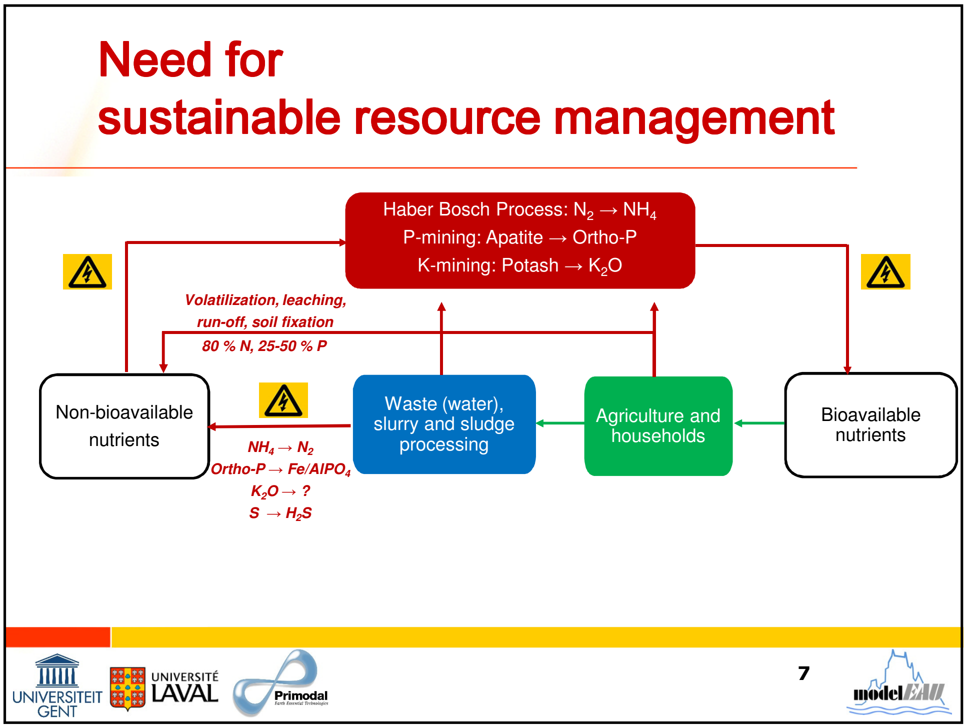
Need for
sustainable resource management
Haber Bosch Process: $N_2 \rightarrow NH_4$
P-mining: Apatite → Ortho-P
K-mining: Potash → K_2O
Volatilization, leaching,
run-off, soil fixation
80 % N, 25-50 % P
Non-bioavailable nutrients
Waste (water), slurry and sludge processing
Agriculture and households
Bioavailable nutrients
$NH_4 \rightarrow N_2$
Ortho-P → $Fe/AlPO_4$
$K_2O \rightarrow$?
$S \rightarrow H_2S$
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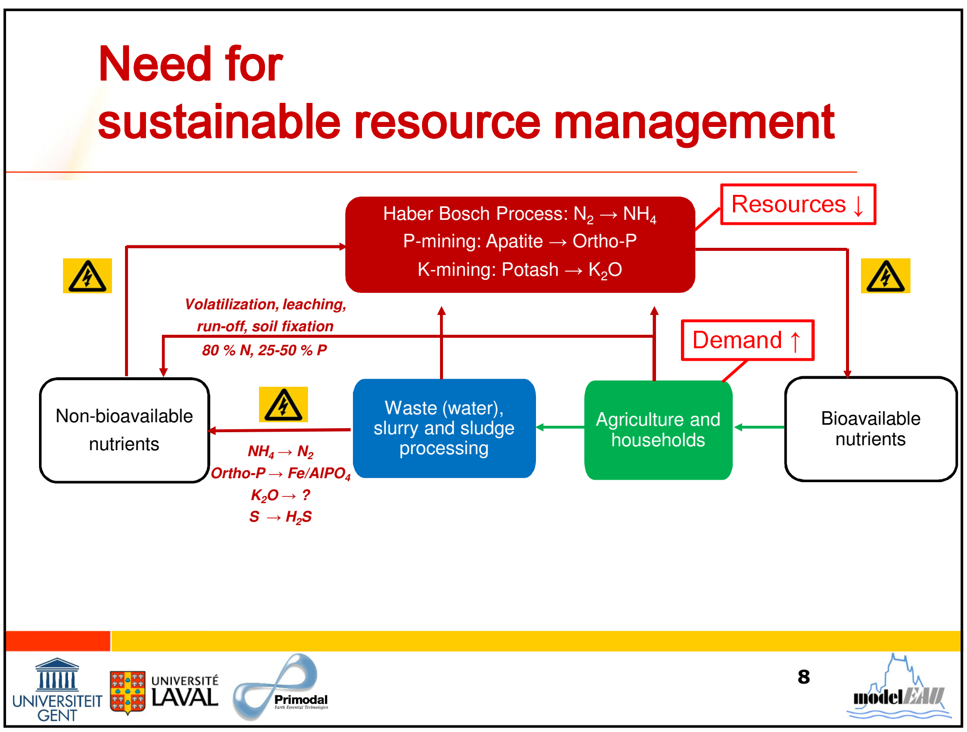
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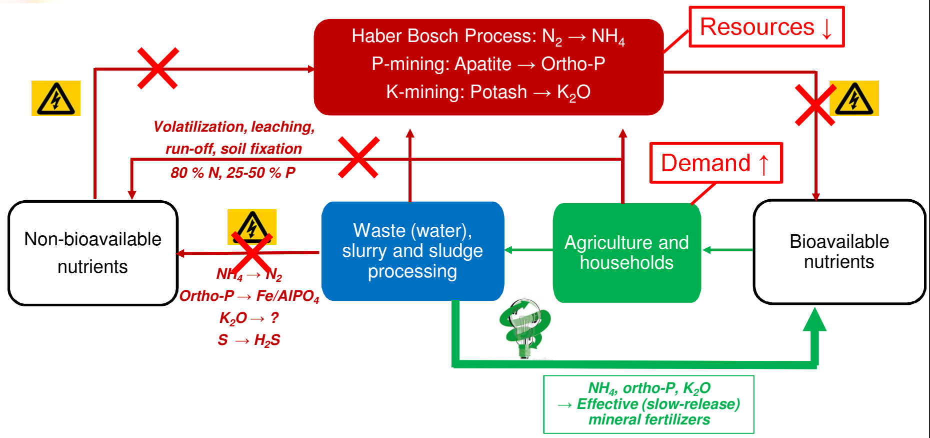
Need for sustainable resource management



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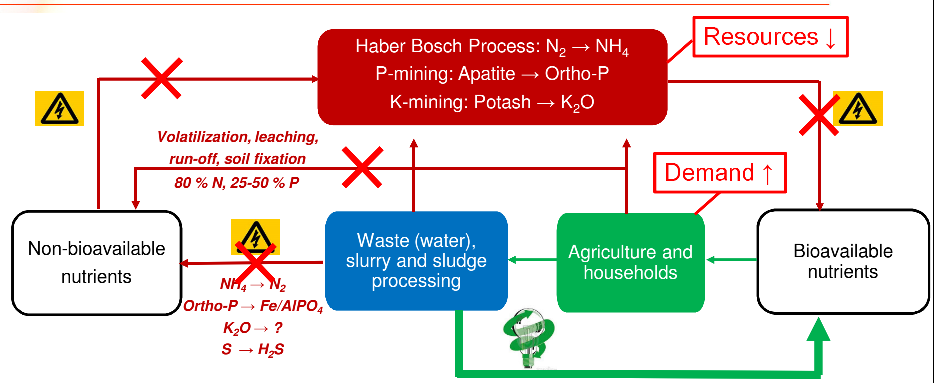
Need for sustainable resource management



Waste Water Treatment Plant (WWTP)
→ Water Resource Recovery Facility (WRRF)

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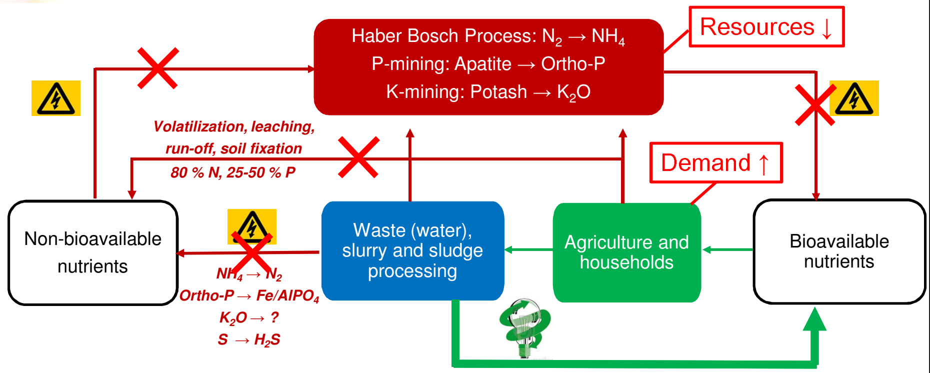
Need for sustainable resource management



Station d'épuration (STEP)
→ Station de récupération des ressources de l'eau (StaRRE)

Nutrient recovery processes

- Precipitation → struvite, calciumphosphates

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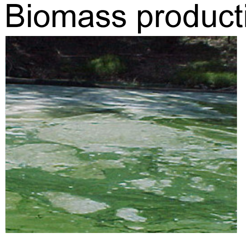
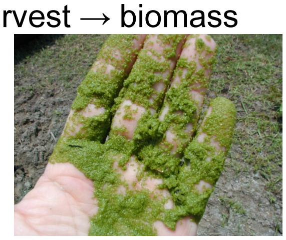
- Membrane filtration → H_2O, N-K concentrates
- Biomass production and harvest → biomass





Nutrient recovery processes

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- Ammonia stripping → NH_3
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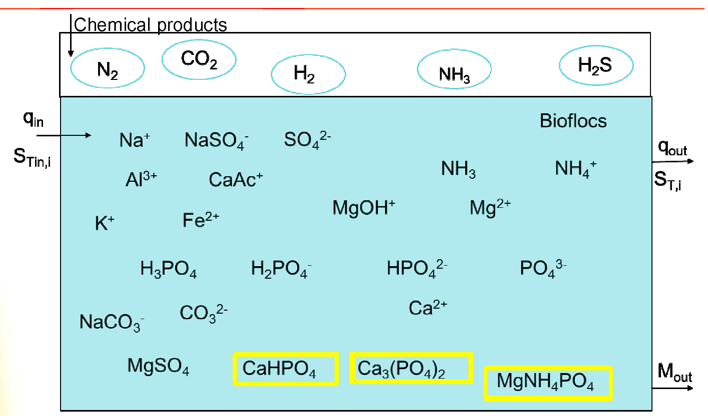
- …

⇒ Mainly physicochemical unit processes !

Prerequisite = marketable fertilizers



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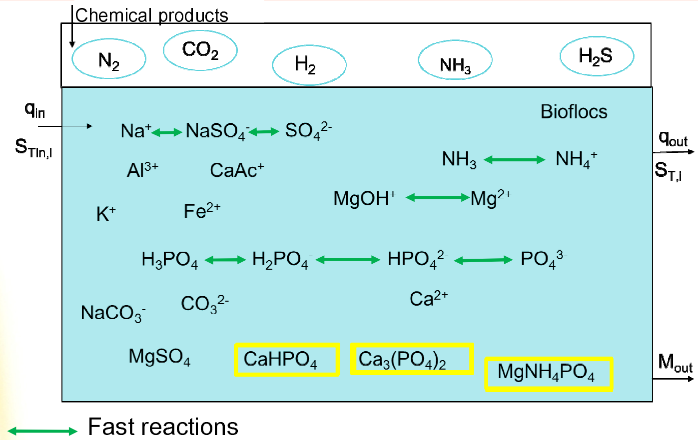

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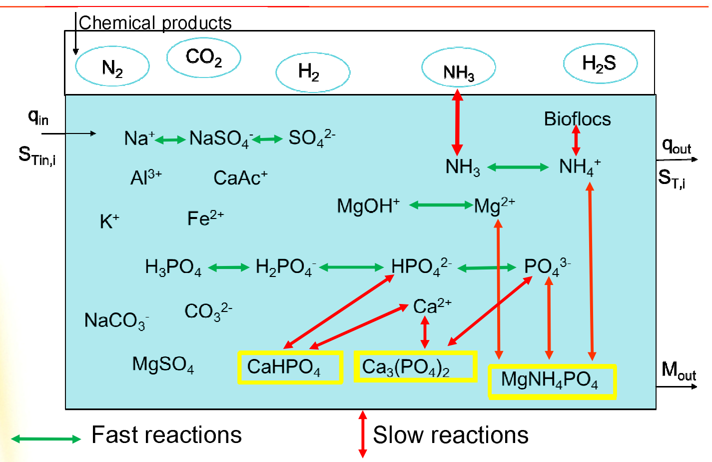

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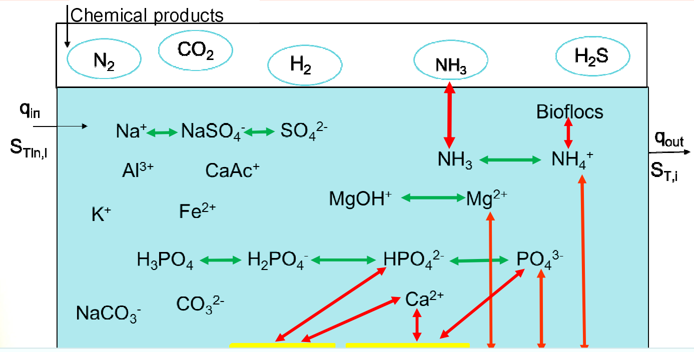
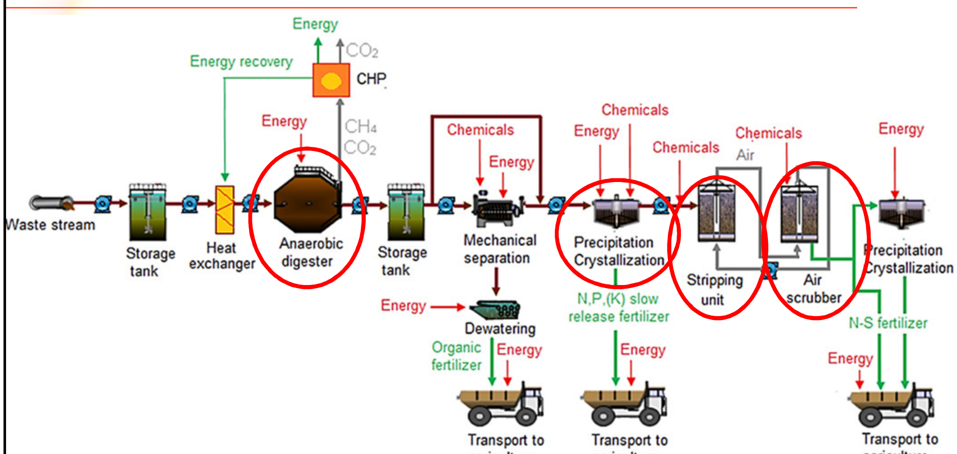


Insights in chemical speciation required for fertilizer quality optimization

Potential flow diagram of a WRRF



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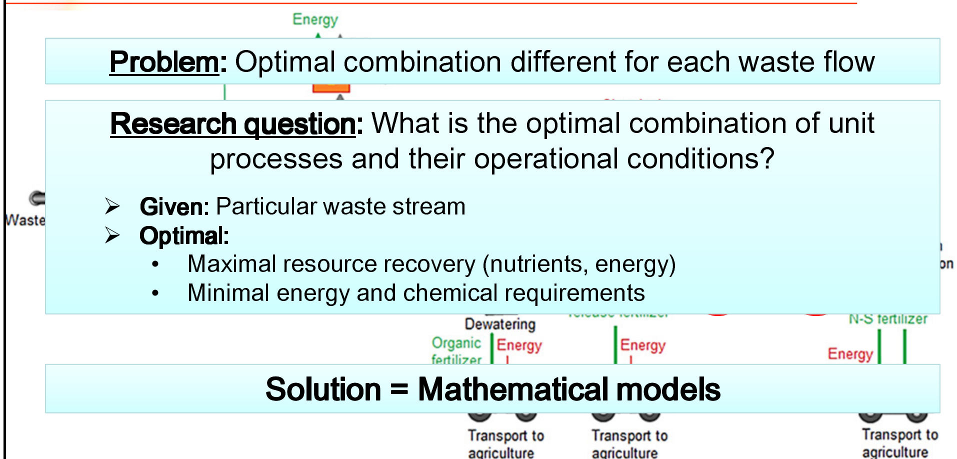

Problem: Optimal combination different for each waste flow

Research question: What is the optimal combination of unit processes and their operational conditions?

- **Given:** Particular waste stream
- **Optimal:**
  - Maximal resource recovery (nutrients, energy)
  - Minimal energy and chemical requirements

Solution = Mathematical models

Modelling challenges

Existing WWTP models

- Good description of biological principles for N & COD removal
- Lack of physicochemical reactions and speciation
- No models for nutrient recovery systems

Modelling challenges

Existing WWTP models → WRRF models

Existing WWTP models:
- Good description of biological principles for N & COD removal
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WRRF models:
- Physicochemical principles essential to describe nutrient recovery
  - pH ? Ion-pairing ? Precipitation ? Redox ? …
- Some progress made for an. digestion (CEIT, UCT, etc.)
- No models for selective nutrient recovery based on detailed speciation and reaction dynamics

Modelling challenges

Existing WWTP models → WRRF models

⇒ Lack of models to adequately put together optimal treatment trains and their operating conditions

OBJECTIVES

Specific research objectives

1. To develop generic models for the best available resource recovery systems including:
   - detailed chemical speciation
   - biological and physicochemical reaction kinetics
   - interactions between three phases (liquid-solid-gas)

2. To apply the models as a tool for optimization of single processes and treatment trains in order to:
   - maximize resource recovery (nutrients, energy)
   - minimize energy and chemical requirements

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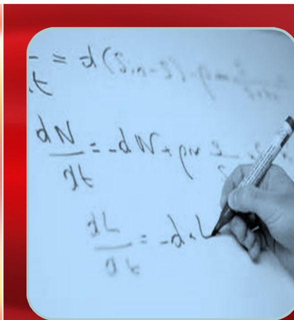
MODEL DEVELOPMENT METHODOLOGY



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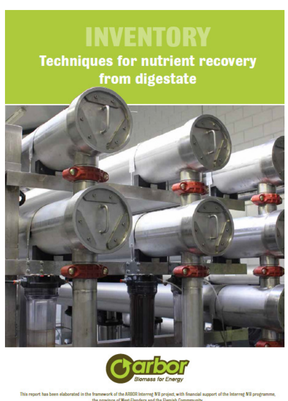
I. Selection of unit processes and input streams

- Selection of unit processes (Vaneeckhaute et al., submitted):



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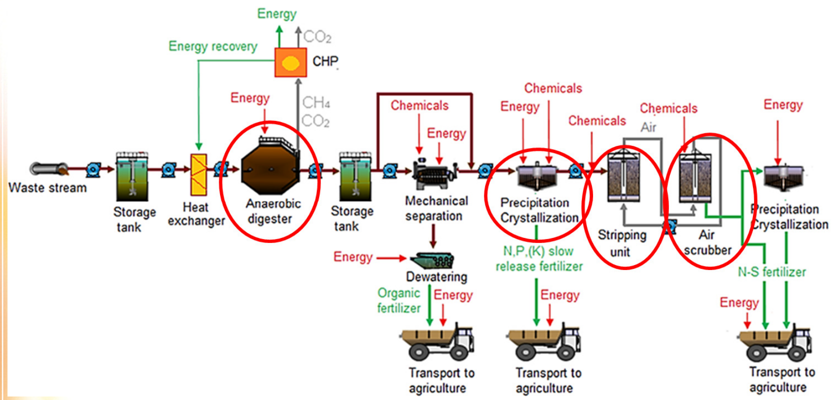


I. Selection of unit processes and input streams

- Selection of unit processes (Vaneeckhaute et al., submitted):

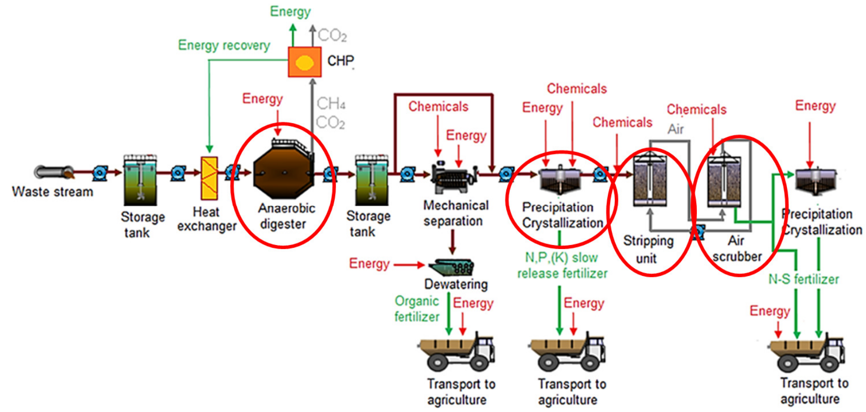
Type	Unit	Model name
Key units	1. Anaerobic digester	NRM-AD
	2. Precipitation/crystallization unit	NRM-Prec
	3. Stripping unit	NRM-Strip
	4. Air scrubber	NRM-Scrub
Ancillary units	1. Separation unit	NRM-Settle
	2. Storage tank	NRM-Store
	3. Chemical dosing unit	NRM-Chem
	4. Heat exchanger	NRM-Heat

Nutrient recovery model

- *Full-scale application*
- *Economic feasibility*

I. Selection of unit processes and input streams

- Selection of input waste streams:



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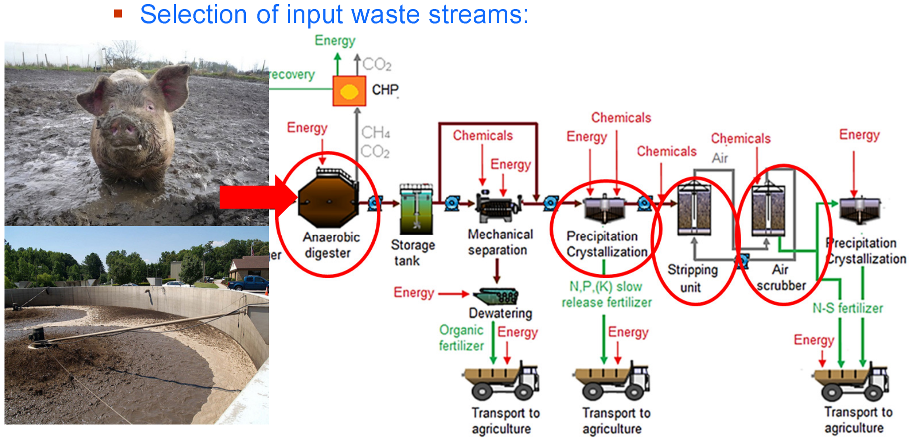

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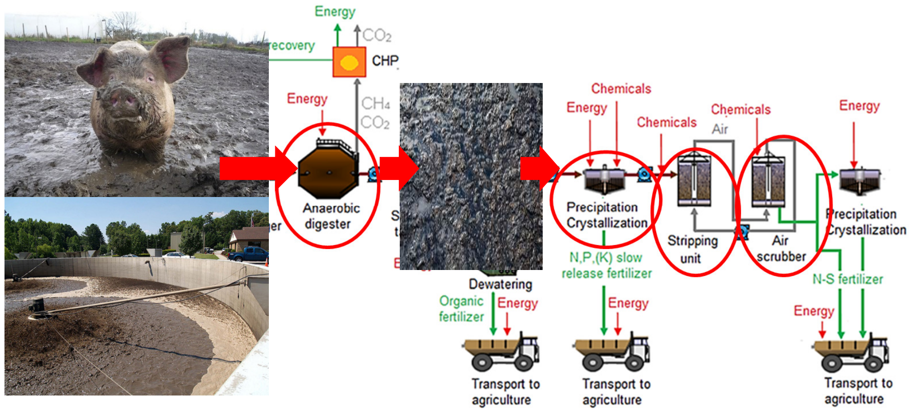

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I. Selection of unit processes and input streams

- Selection of input waste streams:

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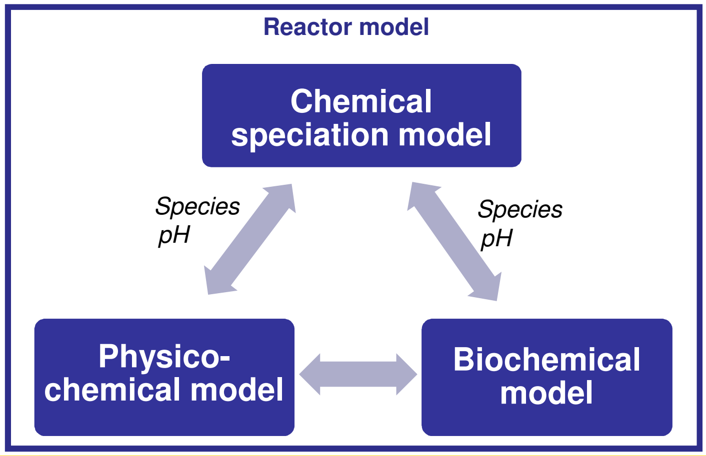
II. Model theory and implementation

Combined three-phase physicochemical-biological models



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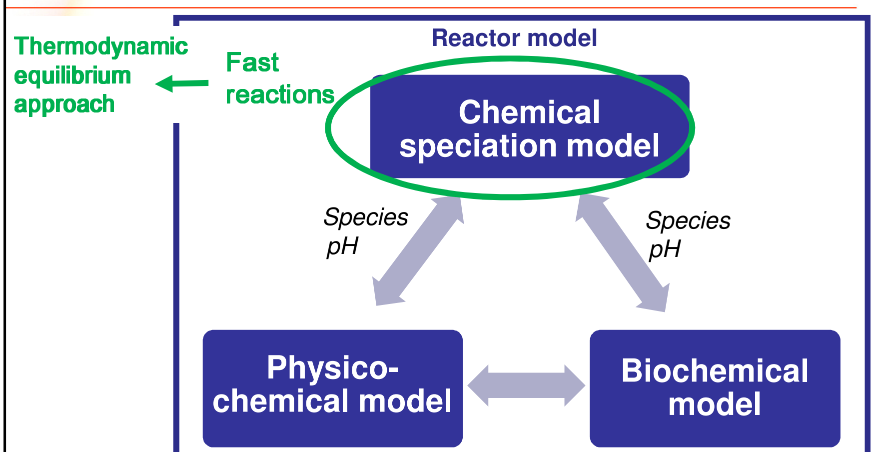
II. Model theory and implementation

Combined three-phase physicochemical-biological models



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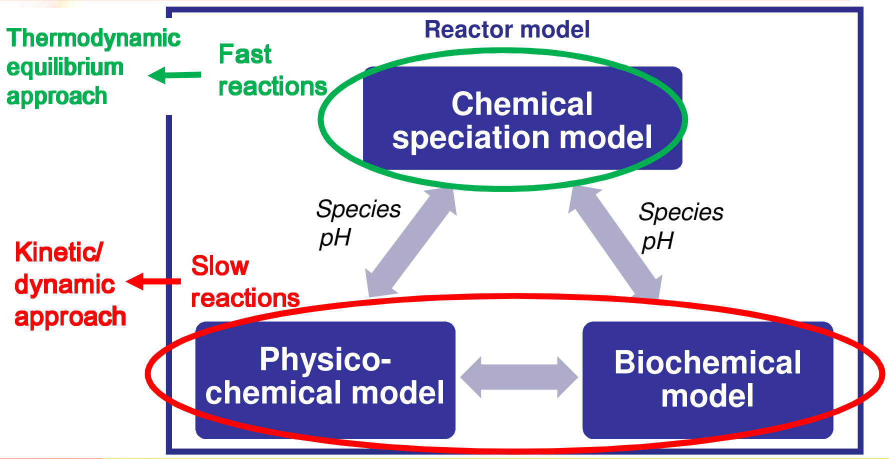
II. Model theory and implementation
Combined three-phase physicochemical-biological models



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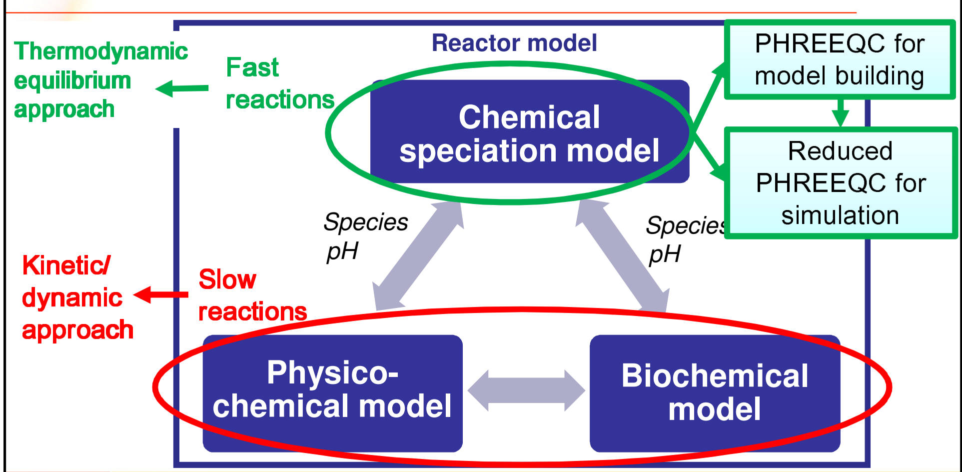
II. Model theory and implementation
Combined three-phase physicochemical-biological models



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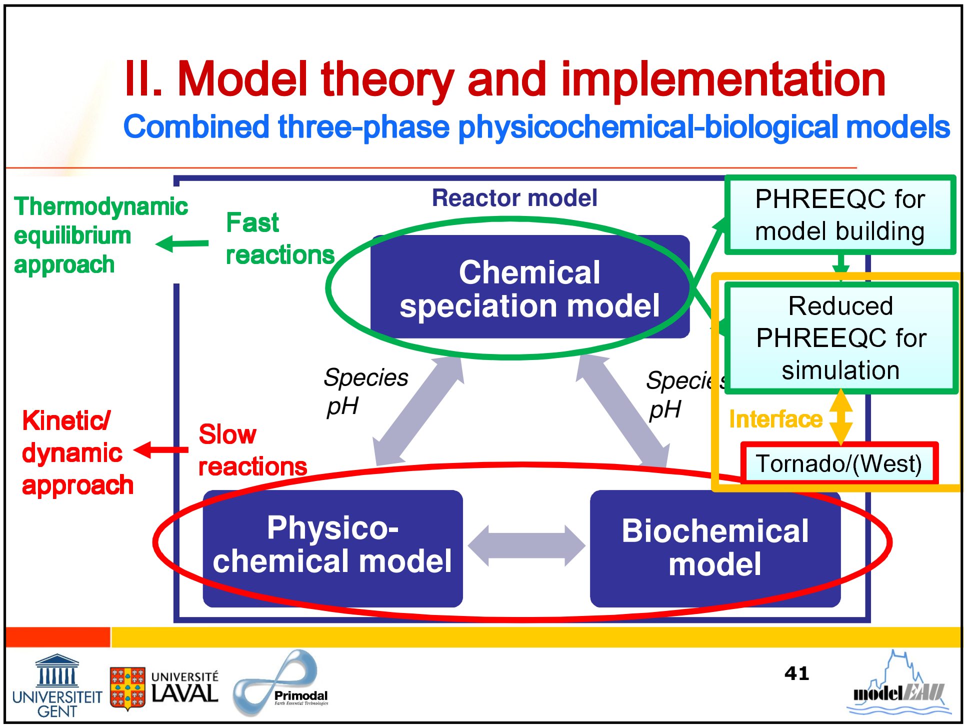
II. Model theory and implementation
Combined three-phase physicochemical-biological models
Reactor model
Thermodynamic equilibrium approach
Fast reactions
Chemical speciation model
PHREEQC for model building
Reduced PHREEQC for simulation
Species pH
Species pH
Interface
Tornado/(West)
Kinetic/ dynamic approach
Slow reactions
Physico-chemical model
Biochemical model
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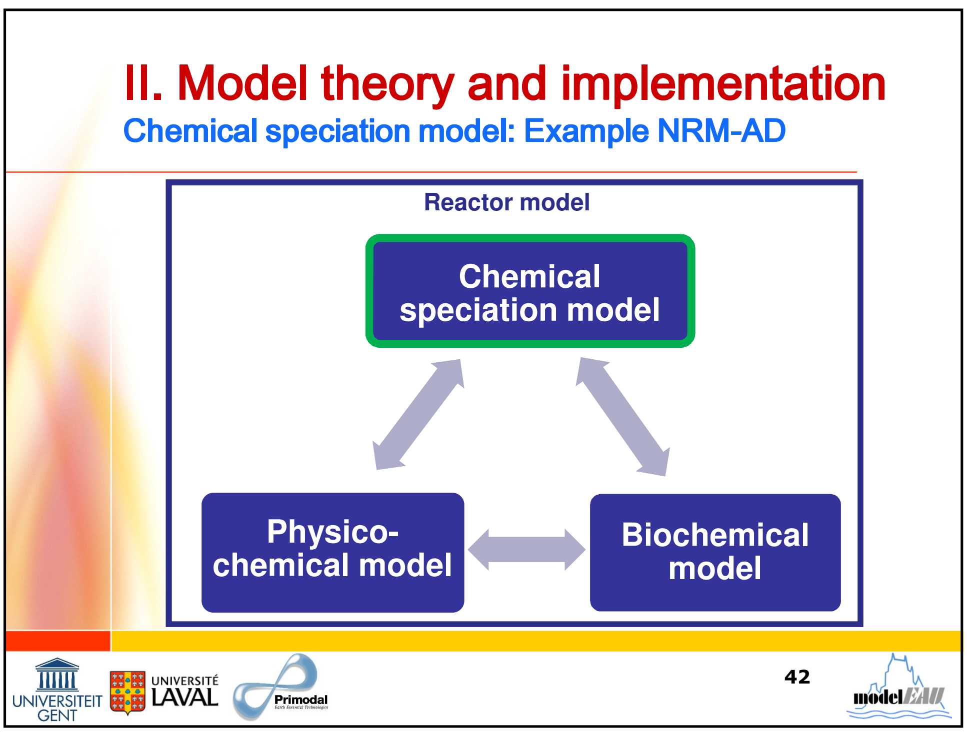
II. Model theory and implementation
Chemical speciation model: Example NRM-AD
Reactor model
Chemical speciation model
Physico-chemical model
Biochemical model
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II. Model theory and implementation

Chemical speciation model: Example NRM-AD

I. Physicochemical component selection (21)

Ac, Al, Bu, Ca, C(IV), Cl, C(-IV), Fe, H(0), H(I), K, Mg, Na, N(-III), N(0), N(IV), O(0), P, Pro, S(-II), S(+VI), Va

II. Speciation calculation

PHREEQC/ MINTEQC

Corrections:
- *Ion activity*
- *Temperature*

III+IV. Selection species/reactions ⟹ reduced model

77 species ↕ ± > 3000 species

12 acid-base reactions
43 ion-pairing reactions
23 precipitation reactions
7 gas-liquid reactions

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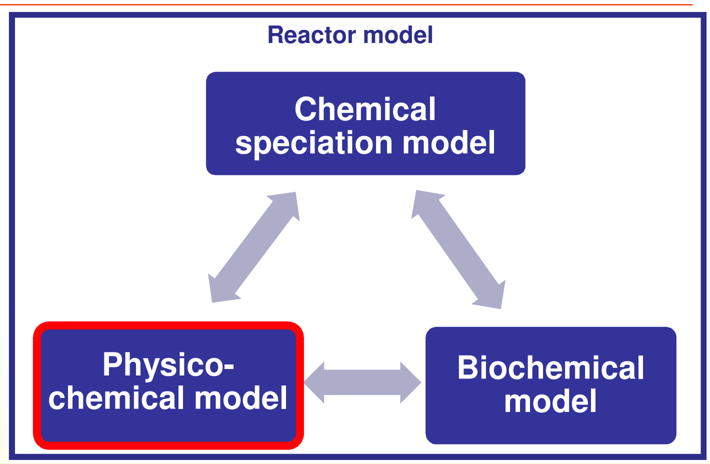
II. Model theory and implementation

Physicochemical transformation model



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II. Model theory and implementation

Physicochemical transformation model

- Liquid-gas transfer:
  - $\rho_{CO2,T} = k_L a_{CO2} * (S_{CO2,liq} - H_{CO2} * p_{CO2,gas})$

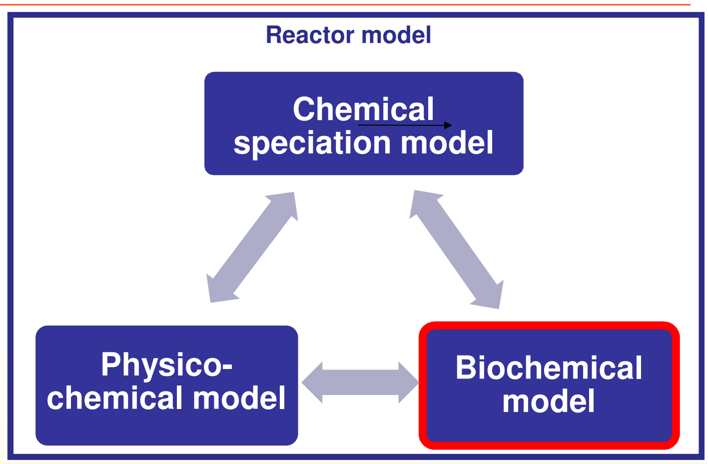
Calculated by PHREEQC at every time step

- Liquid-solid transfer:
  - $\rho_{struv} = k_{r,struv} * [S_{r,struv} - 1]^2$

Relative supersaturation
Calculated by PHREEQC at every time step

II. Model theory and implementation

Biochemical transformation model (NRM-AD)



II. Model theory and implementation

Biochemical transformation model (NRM-AD)

BIOCHEMICAL

- ADM 1 (19): Disintegration, hydrolysis, acidogenesis, acetogenesis, methanogenesis *Batstone et al. (2002)*

→ COD-conversions
N-release/uptake

II. Model theory and implementation

Biochemical transformation model (NRM-AD)

BIOCHEMICAL ⟷ **PHYSICOCHEMICAL**

BIOCHEMICAL:

- ADM 1 (19): Disintegration, hydrolysis, acidogenesis, acetogenesis, methanogenesis *Batstone et al. (2002)*

PHYSICOCHEMICAL:

- Acid-base systems (9)
- Ion-pairing (43)
- Precipitation-dissolution (23)
- Gas-liquid exchange (7)

II. Model theory and implementation

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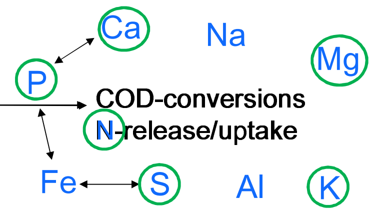

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Biochemical transformation model (NRM-AD)

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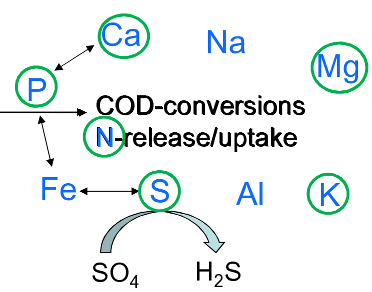
- Extension 1 (8): Sulfurgenesis *Knobel & Lewis (2002)*



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Biochemical transformation model (NRM-AD)

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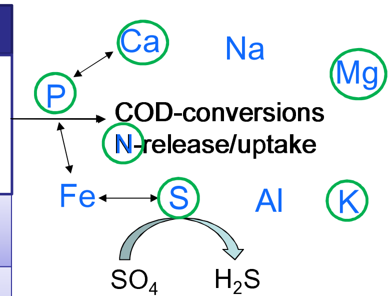
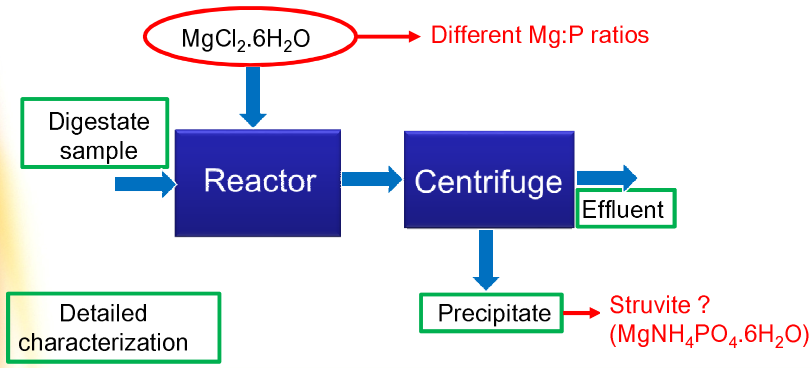
• Extension 1 (8): Sulfurgenesis *Knobel & Lewis (2002)*
• Extension 2: Inclusion new components in stoich. matrix ADM 1 (P, K, S)
• Optional extension 3 (4): EBPR sludge (*Ikumi, 2011)*



MODEL SIMULATION & VALIDATION RESULTS

NRM-Prec: Validation

- Lab-scale experiments P-precipitation



NRM-Prec: Validation

- Simulation vs. experimental results (after 12h)

Mg:P	Digestate 1 % P-recovery			Digestate 2 % P-recovery	
	Exp.	Model without NaH_2PO_4	Model with NaH_2PO_4	Exp.	Model with NaH_2PO_4
1:1	41	95.60	41.32	28	27.76
2:1	44	97.91	43.62	29	29.29

⇒ Importance of a detailed solution speciation and input characterization !

NRM-Prec: Scenario analyses and process optimization

- Main precipitates: struvite, Ca- and Mg-phosphates, Ca- and Mg-carbonates, $AlPO_4$, Fe- and Al-carbonates
  ⇒ No pure struvite fertilizer !
- Practical recommendations (if struvite is target):
  - Removal of $CaCO_3$ prior to precipitation (Huchzermeier et al., 2012)
  - Perform struvite precipitation upstream of Fe/Al dosing

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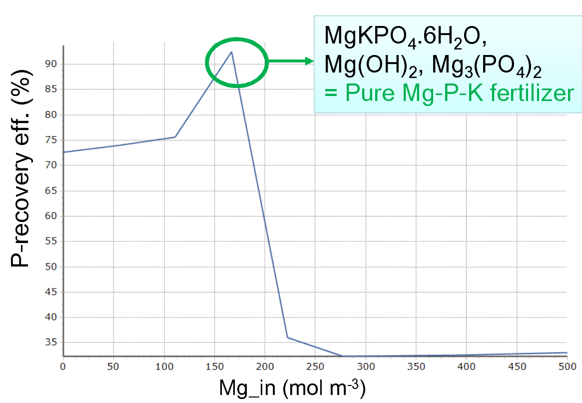
NRM-Prec: Scenario analyses and process optimization



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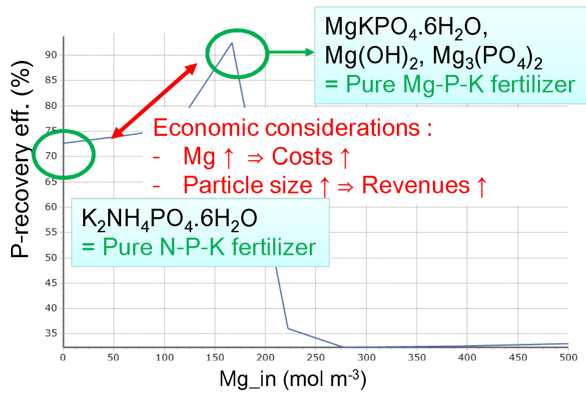
NRM-Prec: Scenario analyses and process optimization



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RECOMMENDATIONS FOR RESEARCH

Recommendations for further experimental research

- Detailed characterisation input composition
  → Essential for process optimization
- Determination kinetic rates in real matrix ↔ pure solutions
  → Better prediction of fertilizer quality in time
- Development generic chemical analysis procedure for precipitate identification

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CONCLUSIONS & PERSPECTIVES

Conclusions

- Generic nutrient recovery model (NRM) library created
- PHREEQC-Tornado/West interface developed & verified
- Default parameters + proper input characterization
  ⇒ Good agreement with steady state experimental results (to be confirmed)
- Opportunities for better process understanding and optimization

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Perspectives

- Further dynamic data collection (on-going):
  - NRM-AD: Full-scale Greenwatt (BE)
  - NRM-Prec: Pilot-scale St. Hyacinthe (QC)
  - NRM-Strip/NRM-Scrub: Pilot-scale Waterleau (BE)

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Perspectives

- Further dynamic data collection (on-going):
  - NRM-AD: Full-scale Greenwatt (BE)
  - NRM-Prec: Pilot-scale St. Hyacinthe (QC)
  - NRM-Strip/NRM-Scrub: Pilot-scale Waterleau (BE)
- Selection most important parameters for process optimization: Global sensitivity analysis (on-going)
- Process optimization (on-going): Single units + treatment train

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Acknowledgements

Ecochem UGent
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mip Supporting the green economy
Fonds de recherche Nature et technologies Québec
CRSNG NSERC

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QUESTIONS ?

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