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Guiding mineralization process development with geochemical modelling

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Mineralization of CO_2

Mineralization in the international context

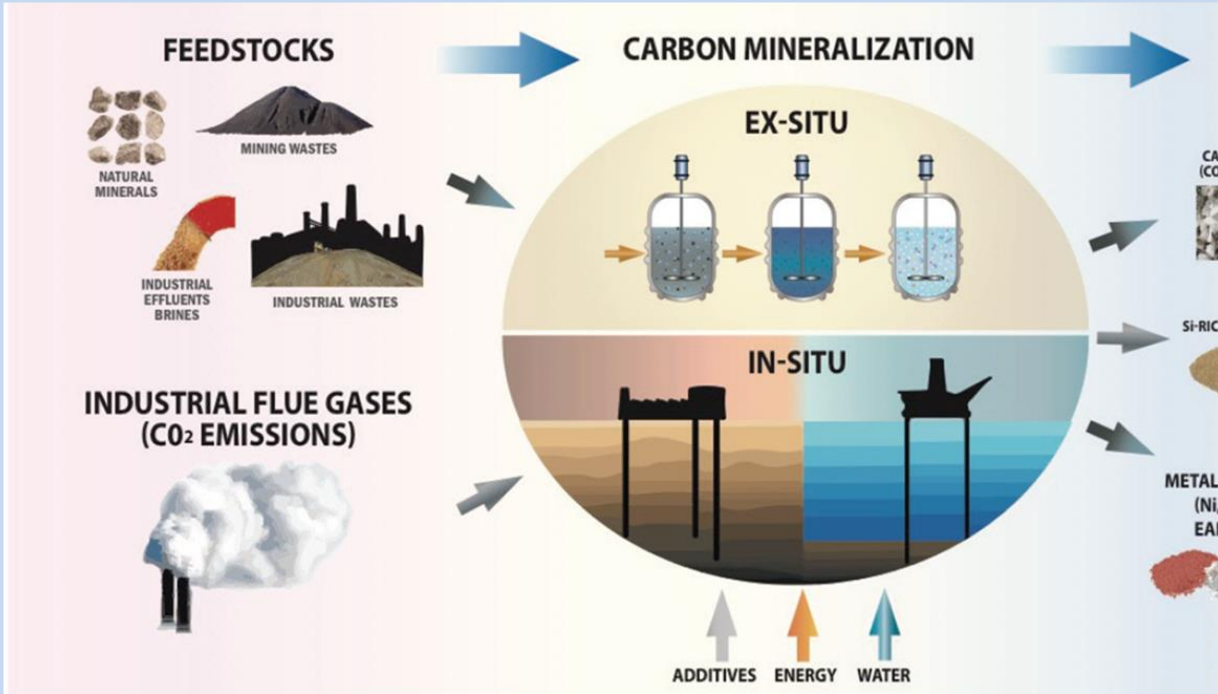
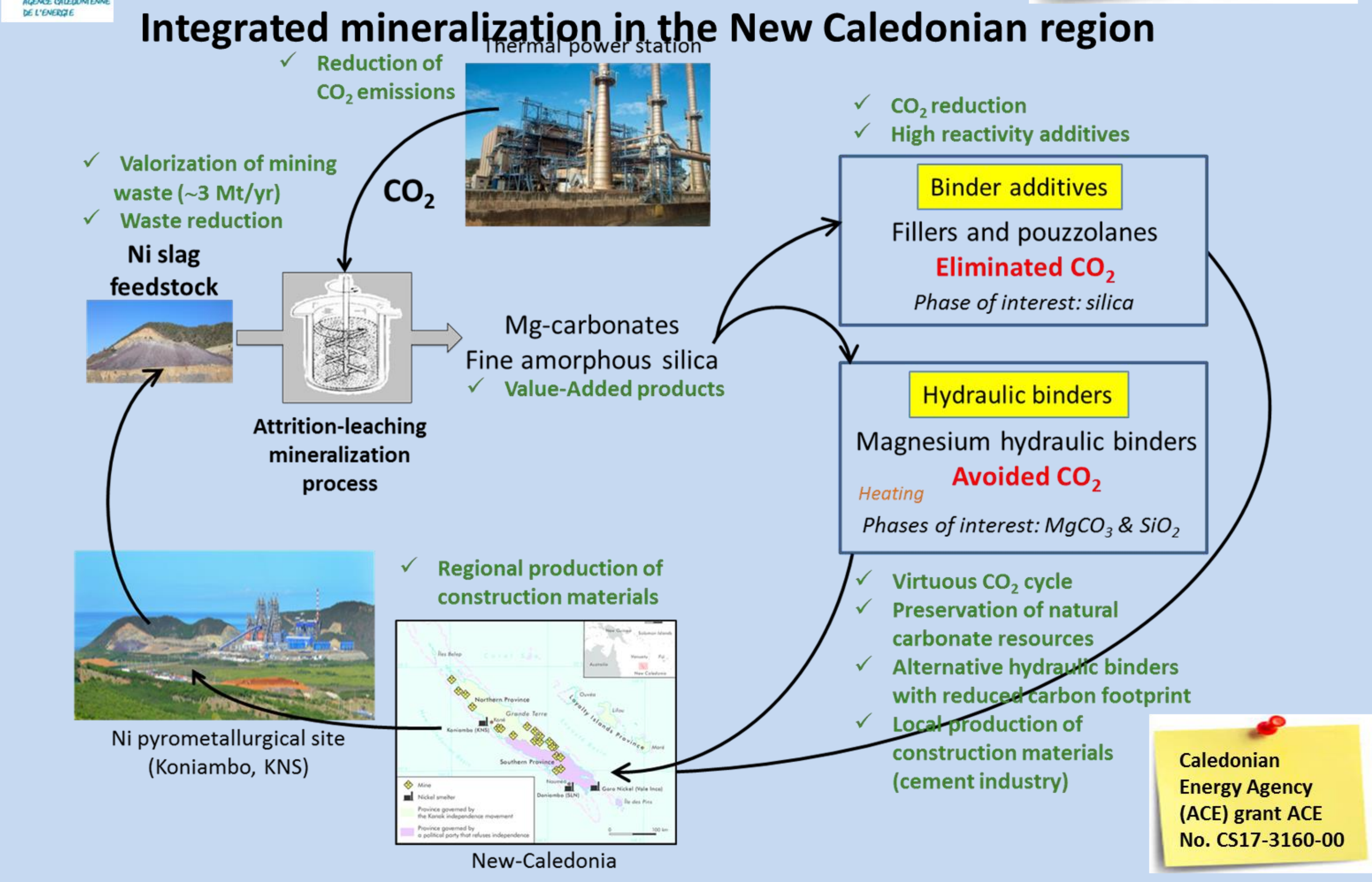


Figure 3.15. Scheme of carbon mineralization and of the range of its products. | Image courtesy of Florent Bourgeois, Laboratoire de Génie Chimique; Au-Hung Park and Xiaozhou Sean Zhou, Columbia University

Source: Mission Innovation Report , 2018[2]

Mineralization can meet the 3 criteria set by the IEA [1]:
- ✓ CO_2 emissions reduction
- ✓ Economic self-sufficiency
- ✓ Scalability

Integrated mineralization in the New Caledonian region



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Geochemical modelling

Geochemical modelling an indispensable tool for development of mineralization processes

The challenge

Mineralization is a global niche market CO_2 mitigation solution. Its scope is territory dependent and combines feedstock selection, mineralization technology and product valorization through local materials supply chains. Development of mineralization pathways must integrate economic, environmental and technological assessment.

The proposed approach

Mineralization process metamodels are needed to provide input process data to a higher-level decision-making frameworks such as Life Cycle Analysis.

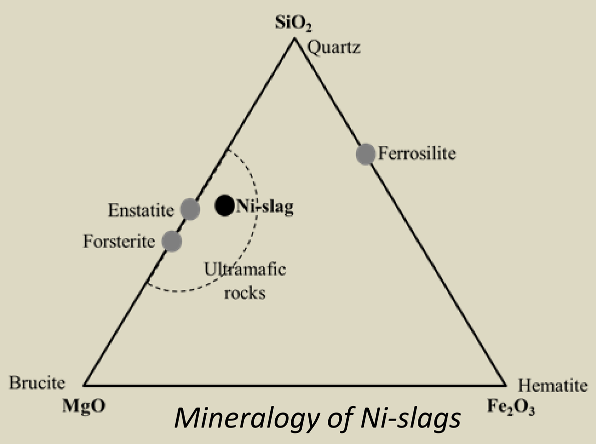
Geochemical modelling is a pivotal brick for mineralization modelling. Geochemical modelling is defined here as a modeling framework that predicts the evolution of the chemical composition of phases in the mineralization system, based on thermodynamic and kinetic models.

Application and geochemical model set-up

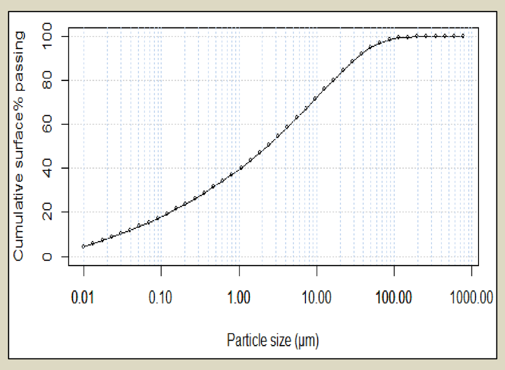
- Attrition-leaching mineralization process [1]
- Geochemical model inputs for feedstock of interest: Ni-slags

Geochemical modelling framework

- **Software: PhreeqC [5]**
- **Thermoddem version 2017 database**
- **R interface to PhreeqC [6,7]**



Mineralogy of Ni-slags



Particle size distribution

$$r = k_0 e^{-\frac{E_a}{RT}} a_{(H^+)}^{0.25} a_{(Mg^{2+})}^{-0.125}$$

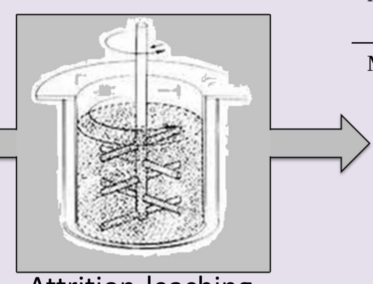
Surface leaching rate model [8]

Results

Geochemical modelling : a guiding tool for mineralization feedstock & product valorization assessment

First-hand prediction of mineralization system speciation

Ni-slag ~ enstatite ($MgSiO_3$)
SiO_2;MgO 0.824;
Fe_2O_3 0.104;Al_2O_3 0.022

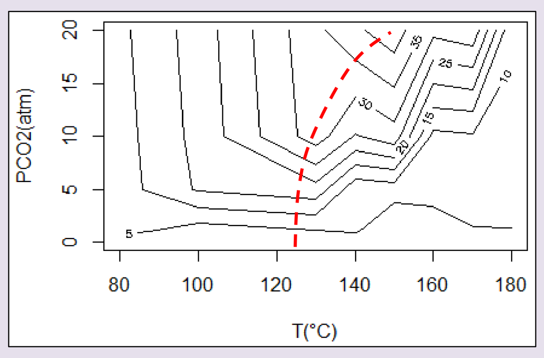


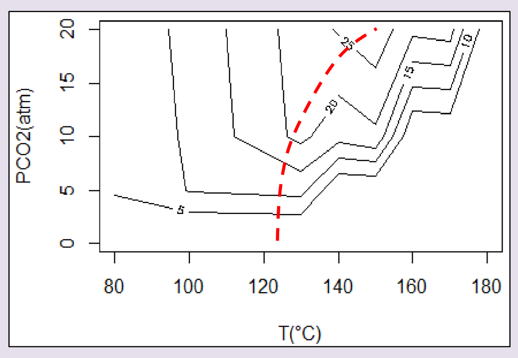
Attrition-leaching mineralization reactor

Phase type	Phase name	Formula
Carbonates	Magnesite (Synthetic)*	$MgCO_3$
	Siderite*	$FeCO_3$
Metal (hydr)oxides	Amorphous Silica	SiO_2
	Goethite	FeO(OH)
Magnesium silicates	Talc	$Mg_3Si_4O_{10}(OH)_2$
	Antigorite	$Mg_{48}Si_{34}O_{85}(OH)_2$
	Montmorillonite(HcMg)	$Mg_{0.3}Mg_{0.6}Al_{1.4}Si_4O_{10}(OH)_2$
	Sudoite	$Mg_2Al_4Si_3O_{10}(OH)_8$
	Chlinochlore	$Mg_5Al(AlSi_3)O_{10}(OH)_8$
	Beidellite(Mg)	$Mg_{0.17}Al_{2.34}Si_{3.66}O_{10}(OH)_2$
	Saponite(Mg)	$Mg_{3.17}Al_{0.34}Si_{3.66}O_{10}(OH)_2$
	Saponite(FeMg)	$Mg_{.217}FeAl_{0.34}Si_{3.66}O_{10}(OH)_2$
Other silicates	Minnesotaite	$Fe_3Si_4O_{10}(OH)_2$
	Chamosite.Daphnite	$Fe_5Al(AlSi_3)O_{10}(OH)_8$
	Pyrophyllite	$Al_2Si_4O_{10}(OH)_2$

Desirable products

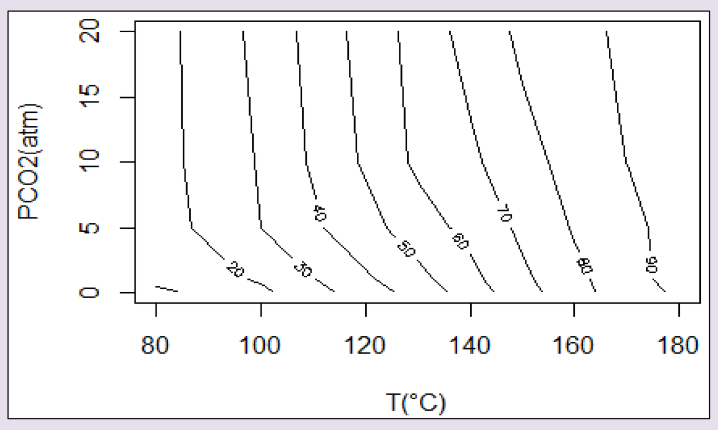
- Attrition-leaching mineralization process
- **Water + Ni-slag**
- **T = [100-180°C]**
- **P_{CO2} = [0.1-20 atm.]**





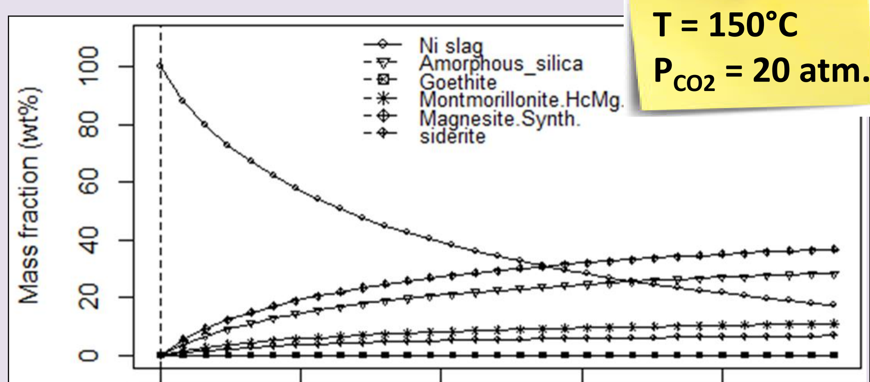
Predicted mass percent of carbonates (left) and amorphous silica (right) in mineralization product. Dotted lines indicate the best [T;P_{CO2}] set points.

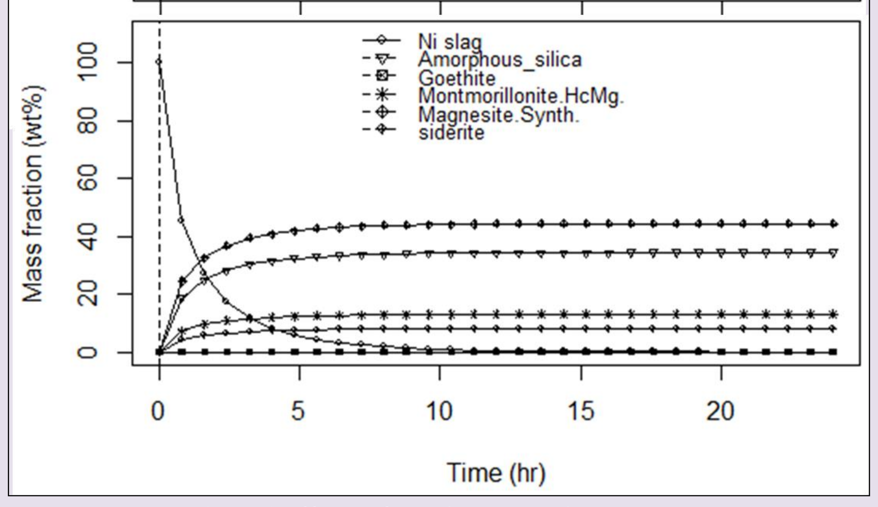
Geochemical modelling : a guiding tool for mineralization process design



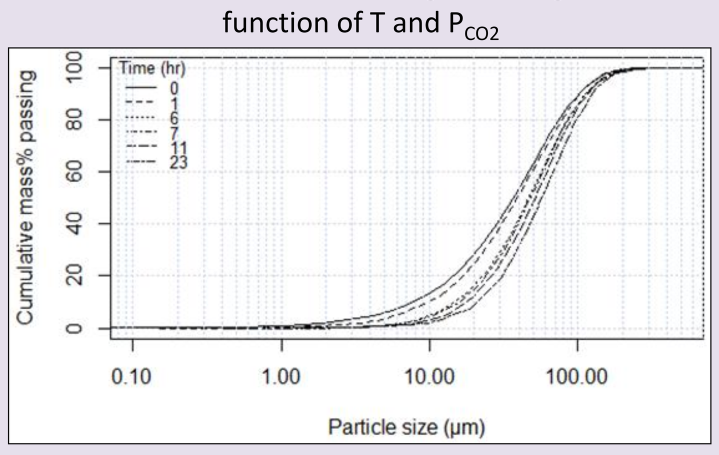
Predicted extent of leaching of Ni-slags as a function of T and P_{CO2}

T = 150°C
P_{CO2} = 20 atm.





Predicted effect of Ni-slag particle top size on product speciation as a function of process time
Top figure: 100 µm; Bottom figure: 10 µm



Predicted rate of change of Ni-slag PSD as a function of attrition-leaching processing time

Conclusions

- Mineralization is a promising CO_2 utilization solution that can meet all three criteria set by the IEA: CO_2 emissions reduction, economic self-sufficiency and scalability.
- Mineralization process development is challenging as its scope is territory dependent and combines feedstock selection, mineralization technology and valorization of mineralization products through local materials supply chains.
- The challenge with developing mineralization processes starts with the complexity and variety of mineralization systems' geochemistry.
- It is claimed that geochemical modelling is a pivotal building block for developing and modelling any mineralization process.
- Application to the attrition-leaching mineralization process for valorization of Ni-slags is used to exemplify the capacity of geochemical modelling as a mineralization process development guide. It is ideally suited for the attrition-leaching mineralization process as this process is unimpeded by surface leached layers and hence operates at the thermodynamic and kinetic limits of the feedstock.
- Geochemical modelling provides first-hand information critical to evaluation of both feedstock and product valorization potential. From an technological standpoint, geochemical modelling also provides insightful information about the effect of many operating variables on process performance.

Perspectives

- To harvest its full potential for mineralization process design, geochemical modelling must be embedded into a supervisory framework that converts geochemical model predictions into environmental and economic units, using regionalized impact and value assessment methods.
- The authors see significant potential in integrating geochemical modelling using PhreeqC into an LCA programming environment such as openLCA [9].
- A word of caution. If the potential of geochemical modelling for mineralization process design is indisputable, its depends strongly on user's expertise and critical thinking. It is no substitute for dedicated experiments, which are indispensable for fine tuning geochemical model settings. In the context of mineralization of Ni-slags by attrition-leaching, additional product characterization is underway to confirm the predicted speciation, with respect to Al content in particular, and coupling geochemical modelling with a validated attrition model is required for further process development and optimization.

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SCIENCE AT THE CORE OF INDUSTRIAL PROCESSES