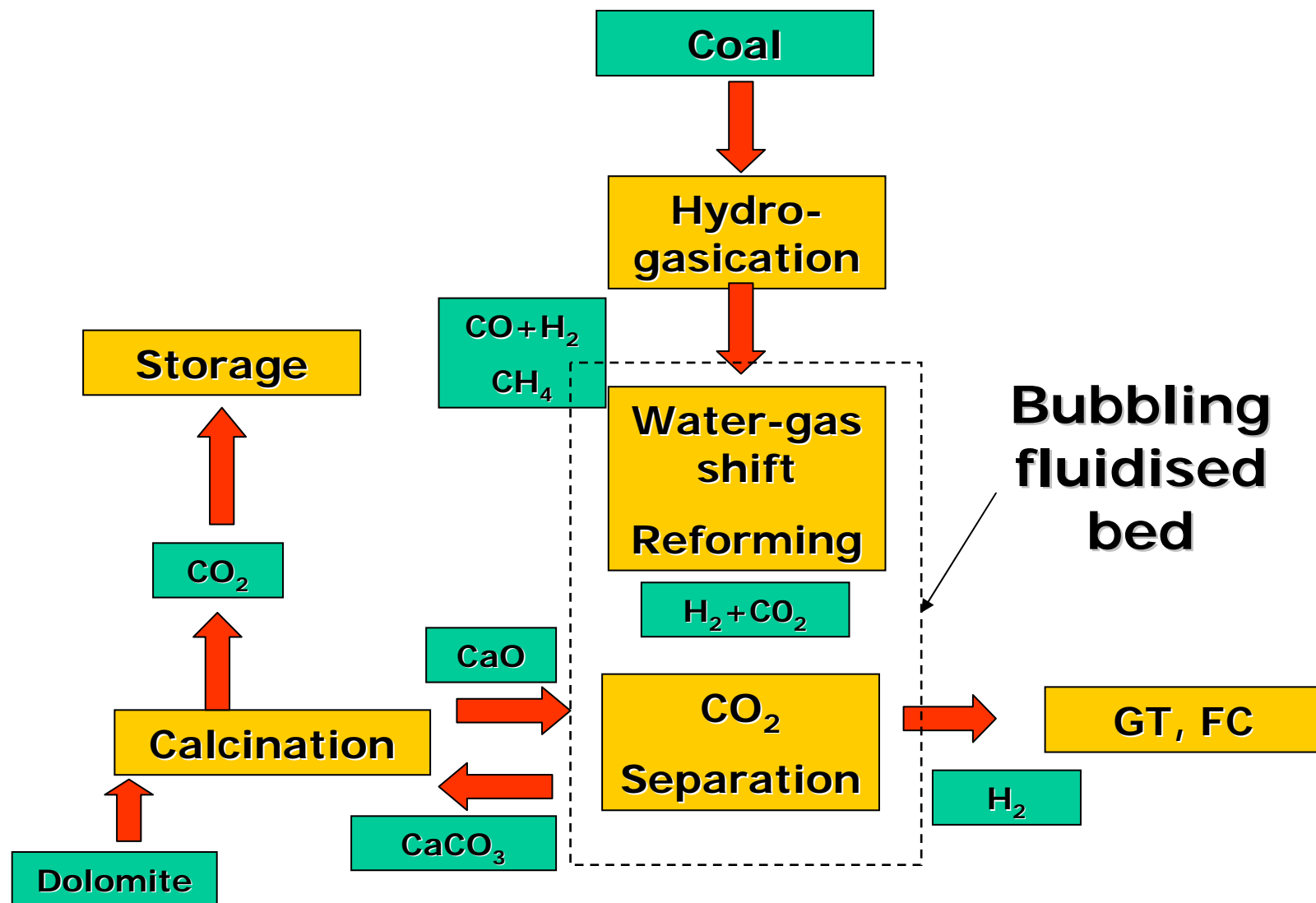


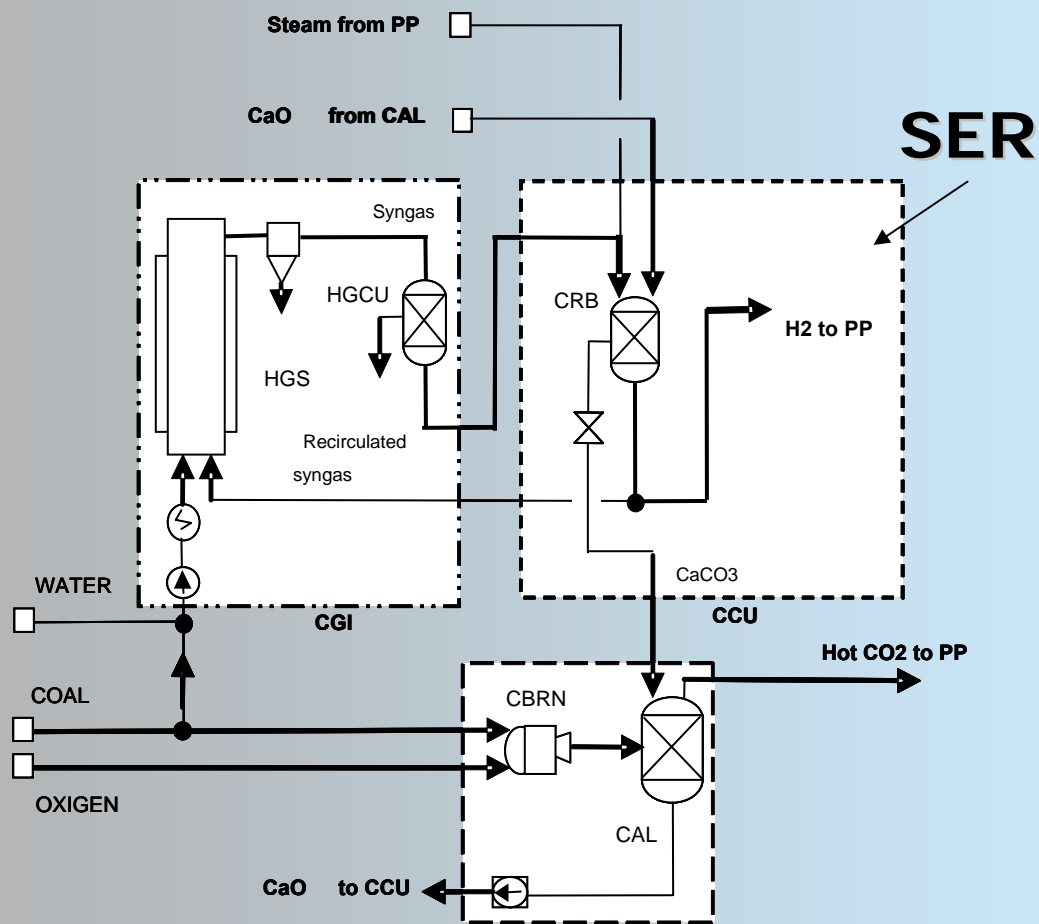
Experimental and numerical investigation on chemical
looping carbon capture based on solid particles

S. Stendardo, A. Calabrò, P.U. Foscolo.

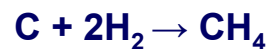
1. Description of the Zecomix concept



1. Schematic of chemical island



1. Chemical looping carbon capture



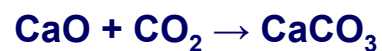
Hydrogasification



Water-Gas Shift



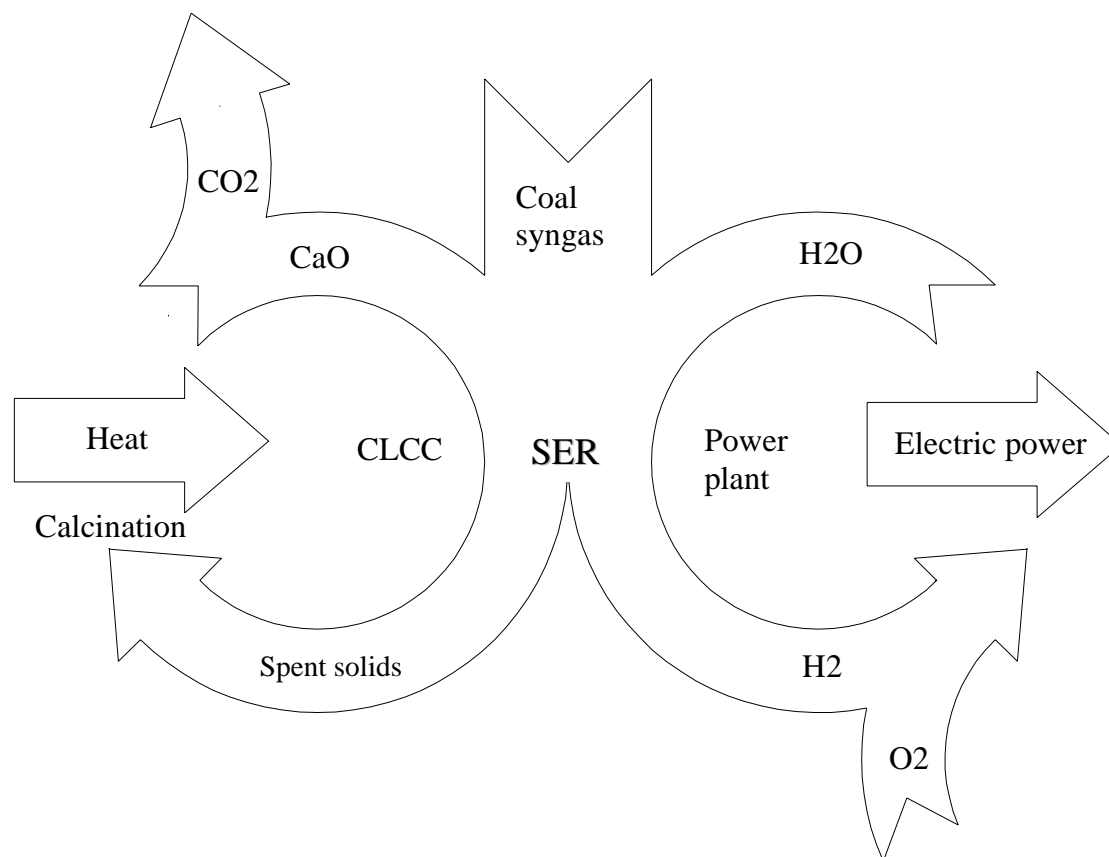
Steam Methane Reforming



Carbonation



Calcination



- Construct, test and evaluate the feasibility of SER
- Characterize the CO₂ sorbents under various conditions of temperature
- Evaluate thermal desorption characteristics of CO₂ from dolomite

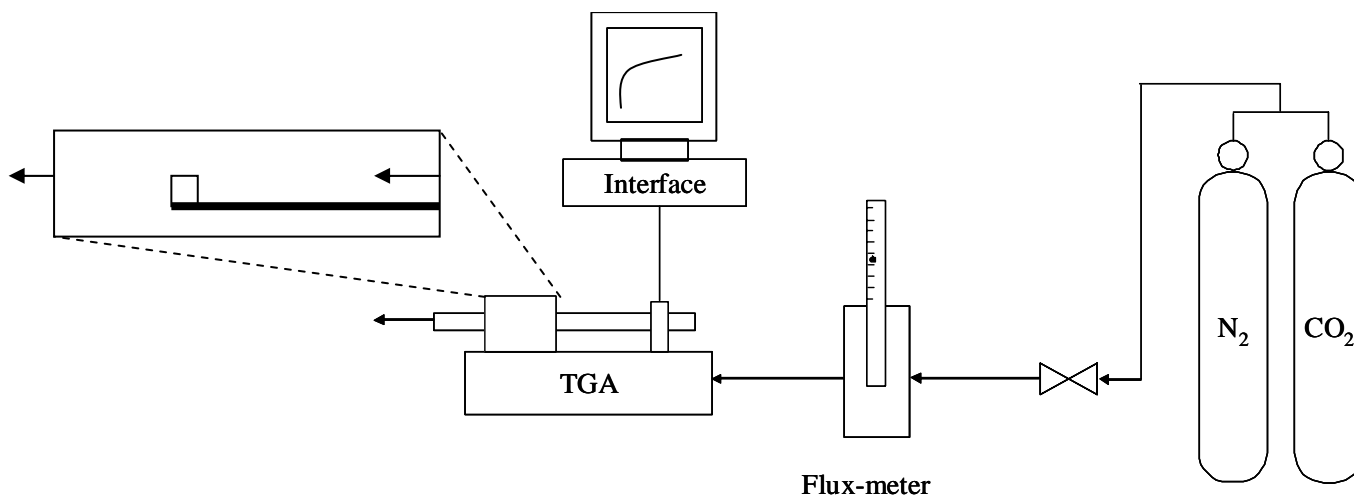
Evaluation of:

- CO₂ sorption capacity of calcined dolomite
- performance in multi-cycling CO₂ capture

Development of:

- mathematical model of gas-solid reaction to predict solid sorbent conversion in a multi-cycling carbonation

2. Experimental apparatus

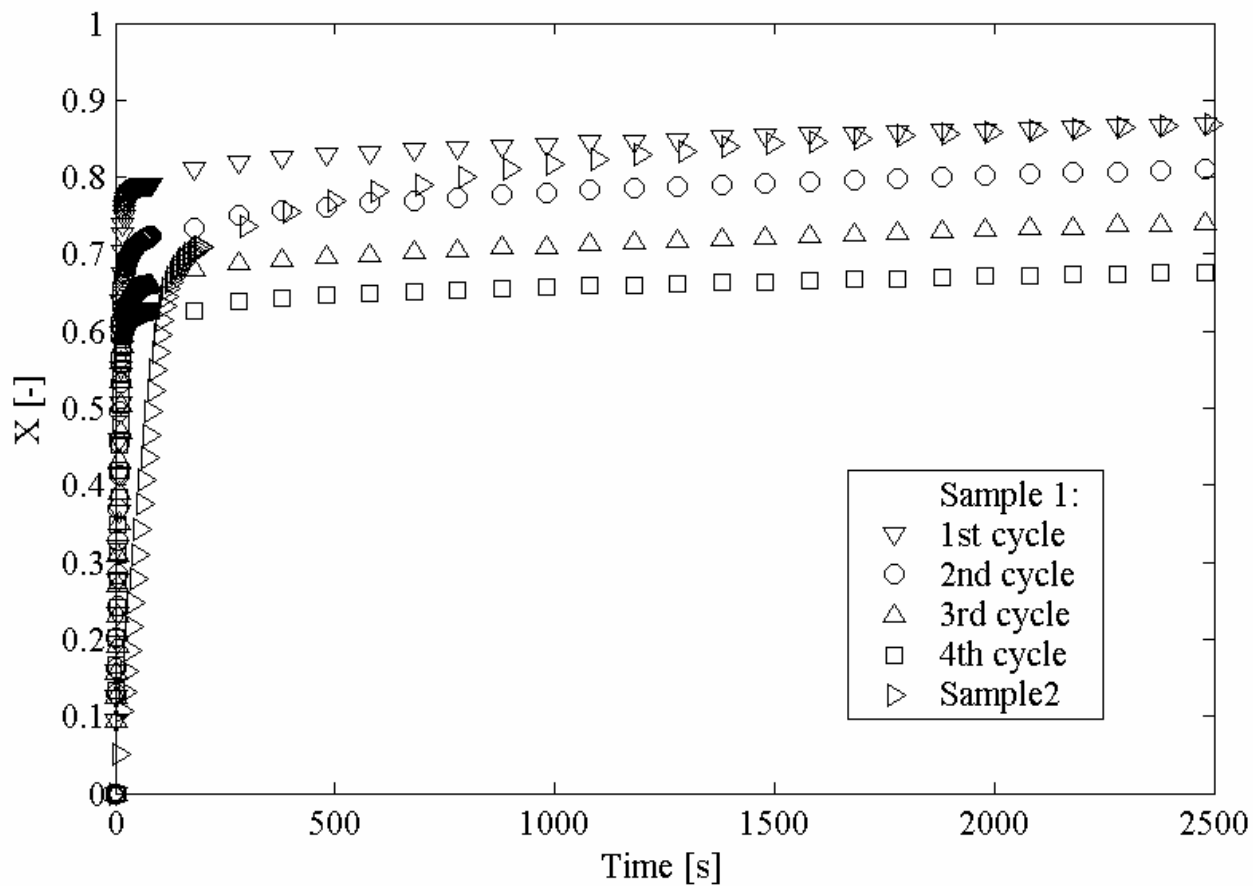


Parameters	Values
Maximum temperature	1000 °C
Calcination	N_2 atmosphere
Heat rate	10 °C/min
Carbonation	CO_2 atmosphere

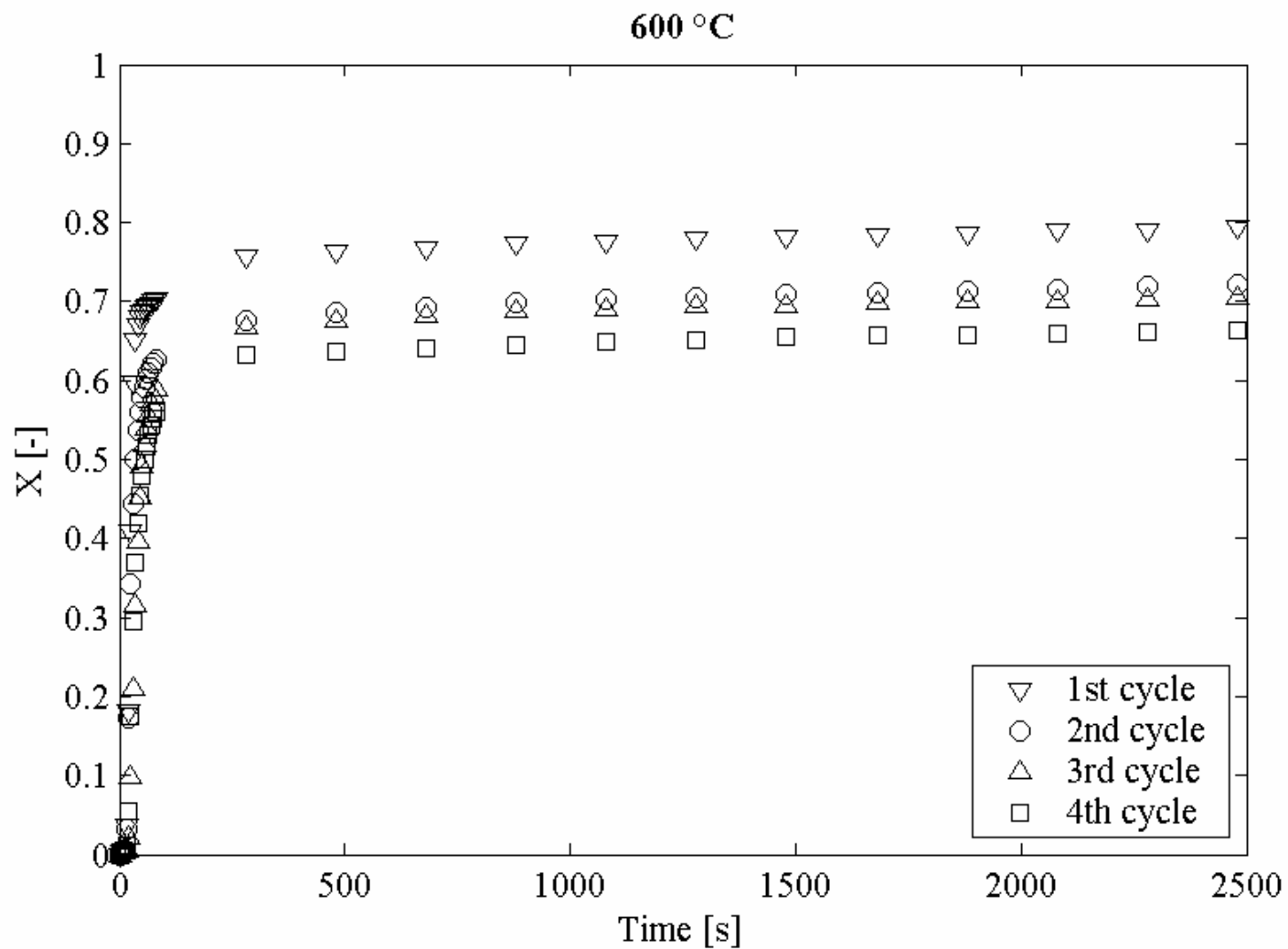
2. Used parameters

Parameters	sample 1	sample 2
f_{CaO} [-]	0.215	0.274
f_{MgO} [-]	0.164	0.155
ε_0 [-]	0.620	0.571
dp [m]	1.95E-04	1.64E-04
V_{CaO} [m ³ /kmol]	1.69E-02	
V_{CaCO_3} [m ³ /kmol]	3.69E-02	
V_{MgO} [m ³ /kmol]	1.11E-02	
V_{MgCO_3} [m ³ /kmol]	2.75E-02	
Z [-]	2.18	

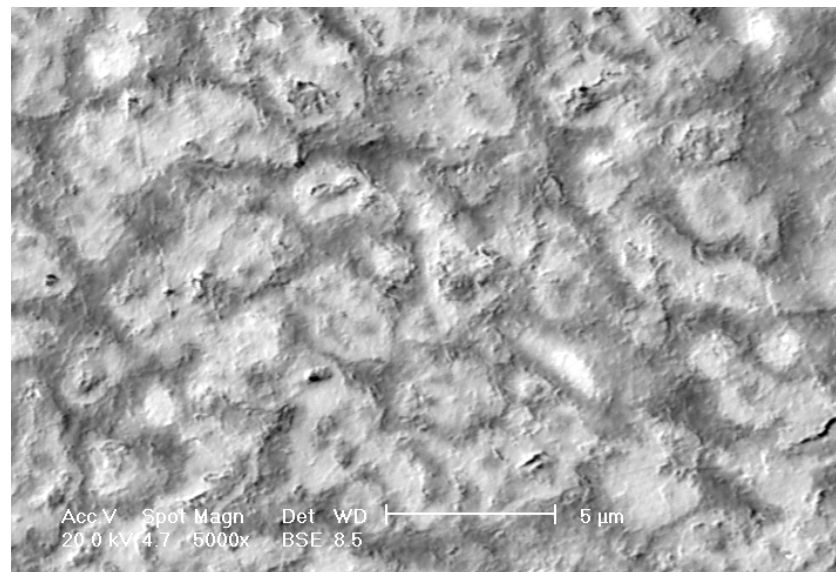
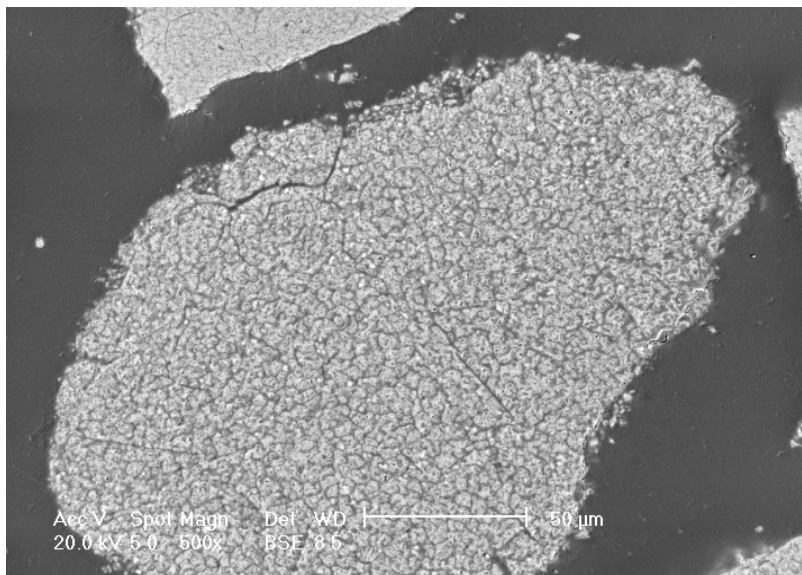
2. Experimental curves at 700 °C



2. Experimental curves at 600 °C

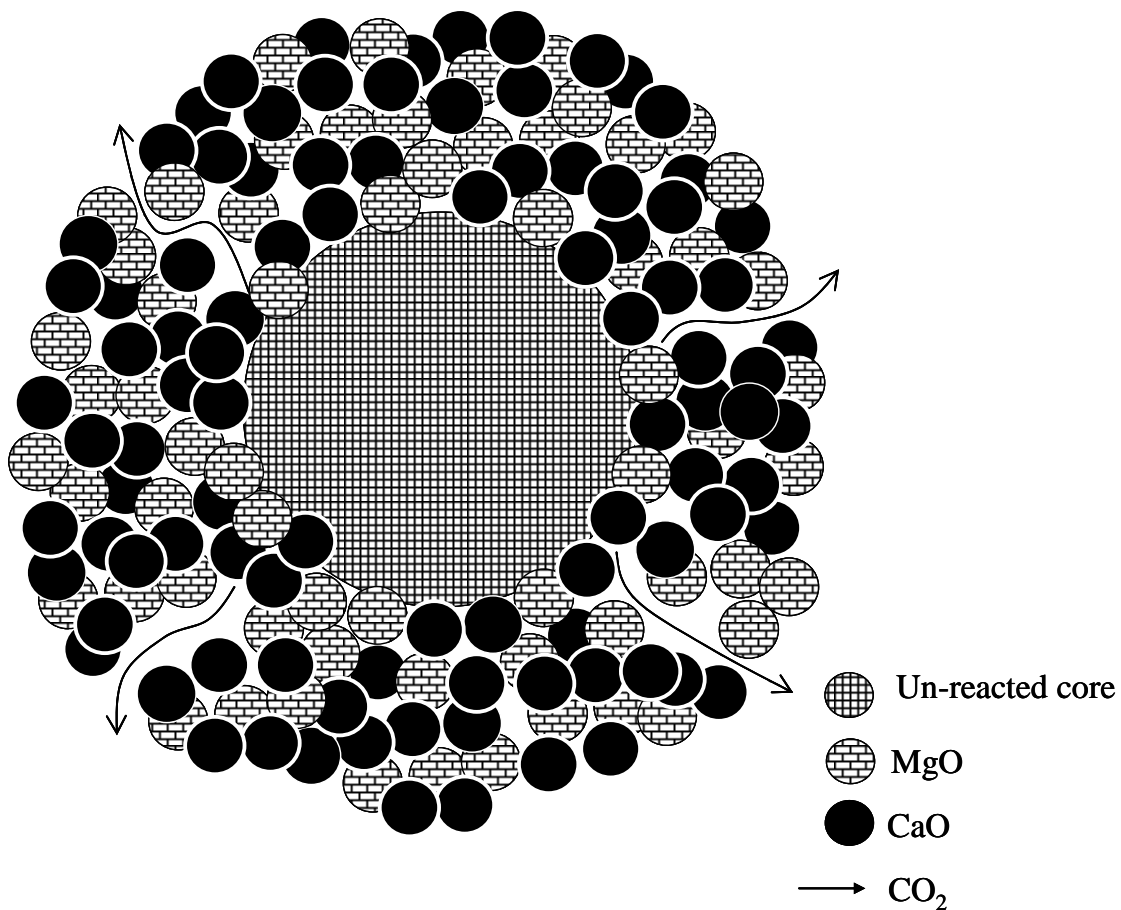


2. SEM micrographs

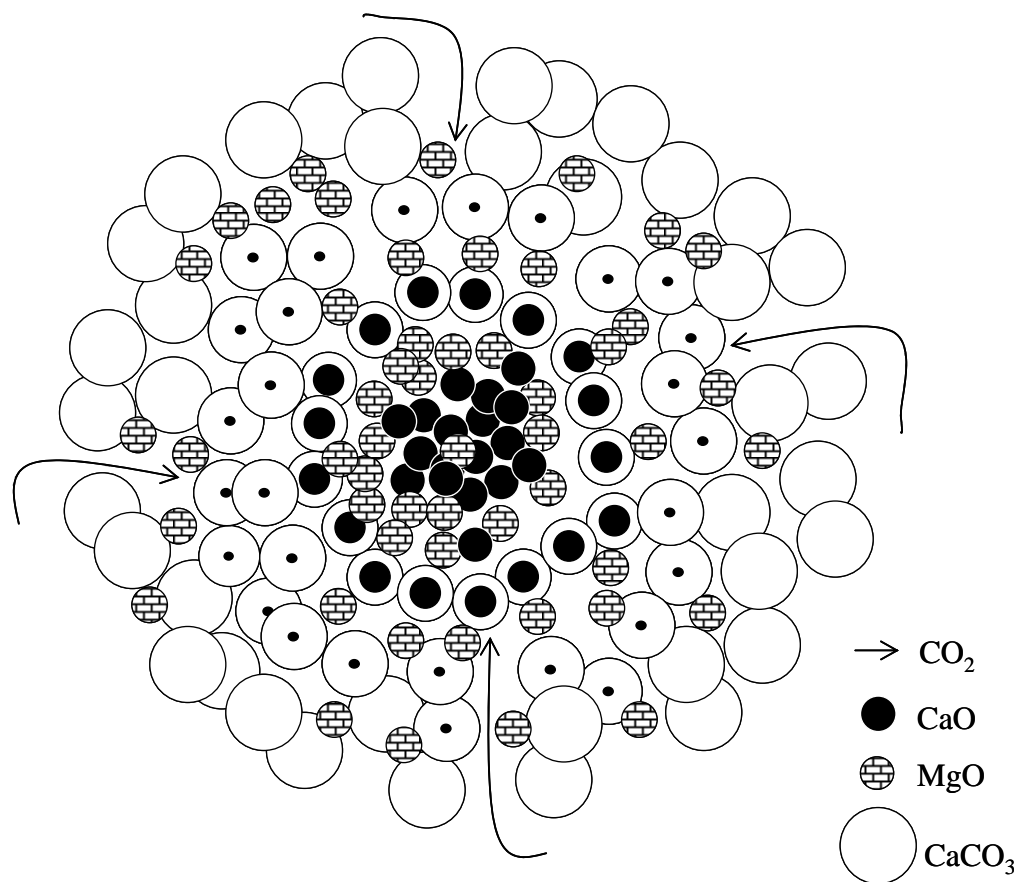


source: **Gallucci et al. 2008**

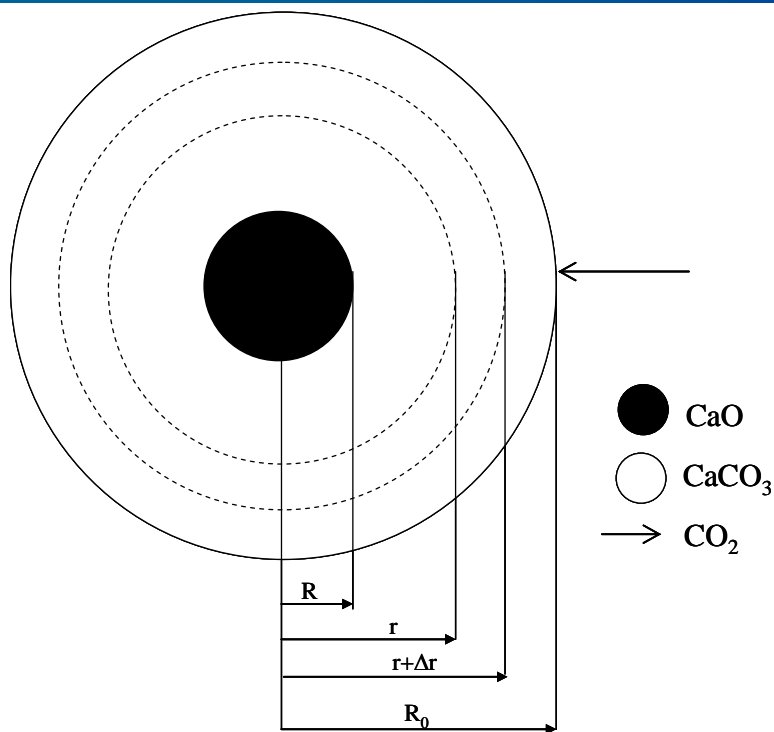
Non-porous spherical CaO and MgO grains



2. Carbonation process and product layer formation



2. Shrinking core grain

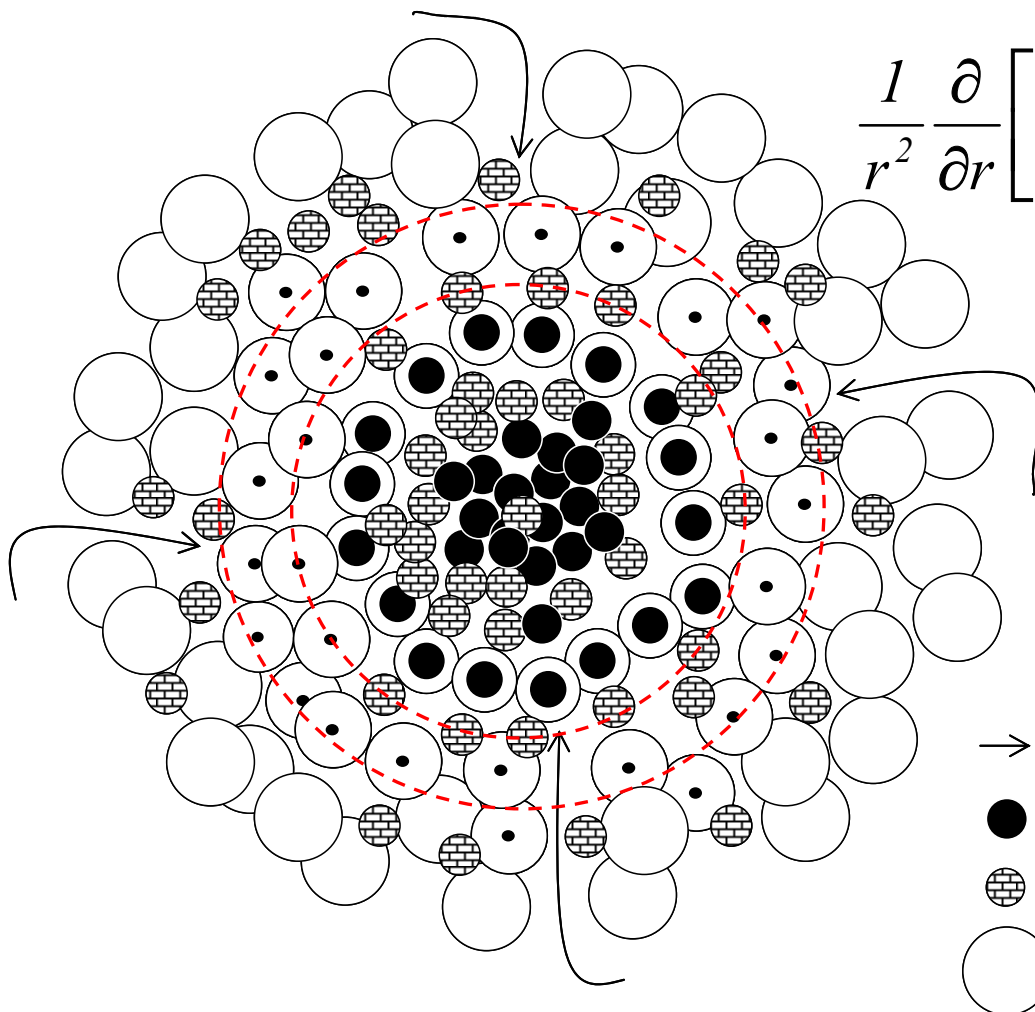


**Shrinking
core grain**

$$N_{Ca} \frac{dX}{dt} = \frac{\sigma_{0CaO} k (1-X)^{2/3} (C_{AS} - C_{Ae})}{1 + \frac{k}{2D_{PL}} \delta_{CaO} \sqrt[3]{1-X} \left(1 - \sqrt[3]{\frac{1-X}{1-X+XZ}} \right)}$$

moles of CaO converted into CaCO₃ per unit time and particle volume

2. Gaseous reactant mole balance



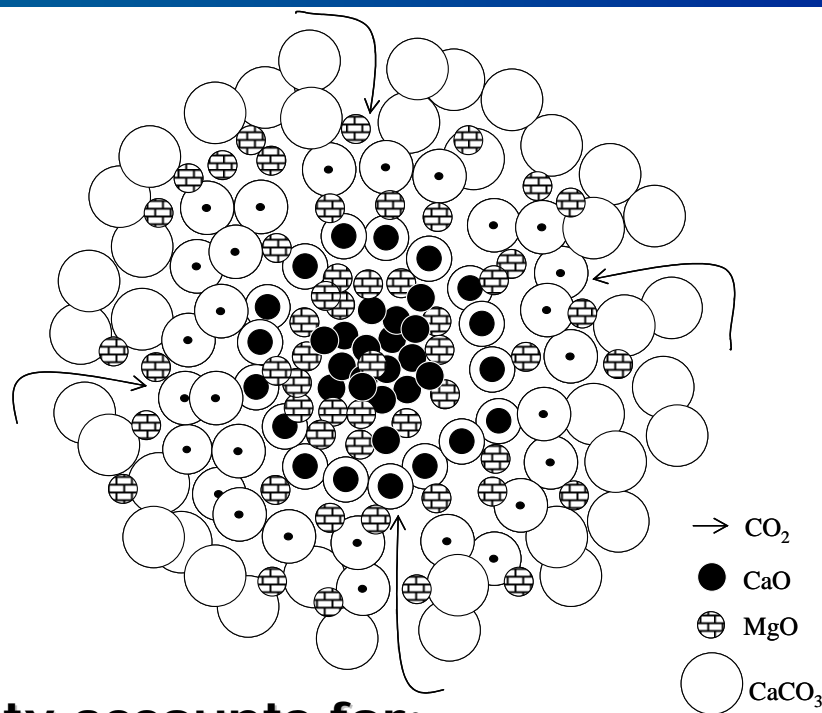
$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[D_e r^2 \frac{\partial C_A}{\partial r} \right] - N_{Ca} \frac{dX}{dt} = \frac{\partial(\varepsilon C_A)}{\partial t}$$

- CO₂
- CaO
- ▨ MgO
- CaCO₃

$$D_e \frac{\partial C_A}{\partial r} = h_m (C_{A0} - C_A) \text{ at } r = R_0 \text{ and } t \geq 0; \quad \frac{\partial C_A}{\partial r} = 0 \text{ at } r = 0 \text{ and } t \geq 0$$

D_e = Effective diffusion coefficient

2. Effective diffusivity

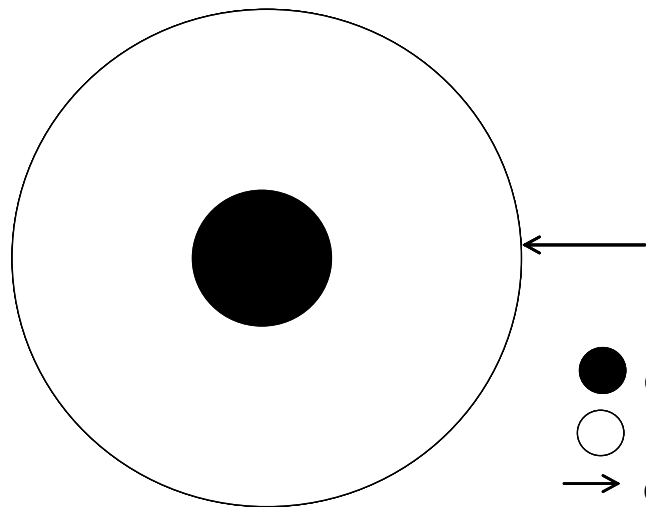


The effective diffusivity accounts for:

- Not all area available for diffusion
- Paths are tortuous
- Pores changing cross-sectional area

$$\text{Effective diffusivity } D_e = \frac{D\varepsilon\sigma}{\tau}$$

2. Product layer diffusion coefficient.



● CaO
 ○ Product layer
 → CO₂

$$D_{PL}(X) = D_{PL0} \exp(-aX^b)$$

**Partially
converted
grain**

Reference literature:

Haul and Stain, 1955

Anderson, 1969

Szekely and Evans, 1971

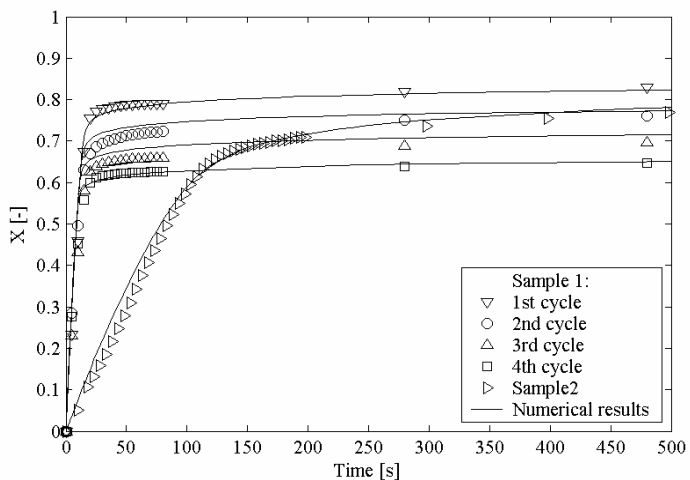
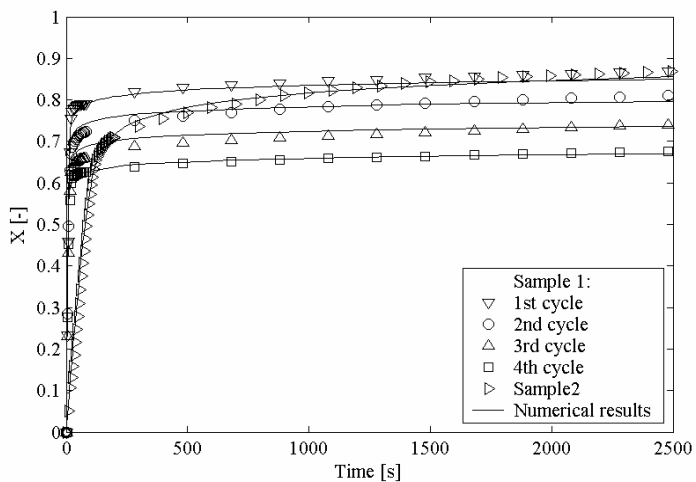
$$\lambda = \frac{r}{R_{in}}; \quad t^* = k\sigma_{0CaO}t; \quad C_A^* = \frac{C_A}{C_{A0}}$$

$$\Phi = R_0 \sqrt{\frac{k\sigma_{0,CaO}}{D_{e0}}}$$

$$\beta = \frac{k\delta_{CaO}}{2D_{PL0}}$$

$$Sh_e = \frac{Sh}{2} \left(\frac{D_{AB}}{D_{e0}} \right)$$

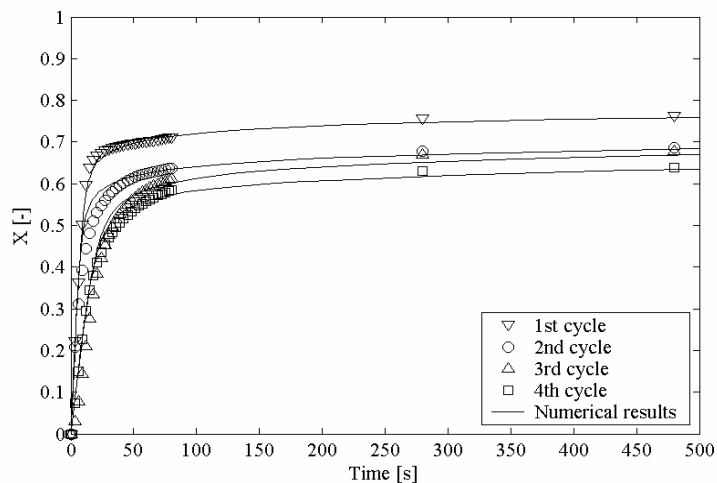
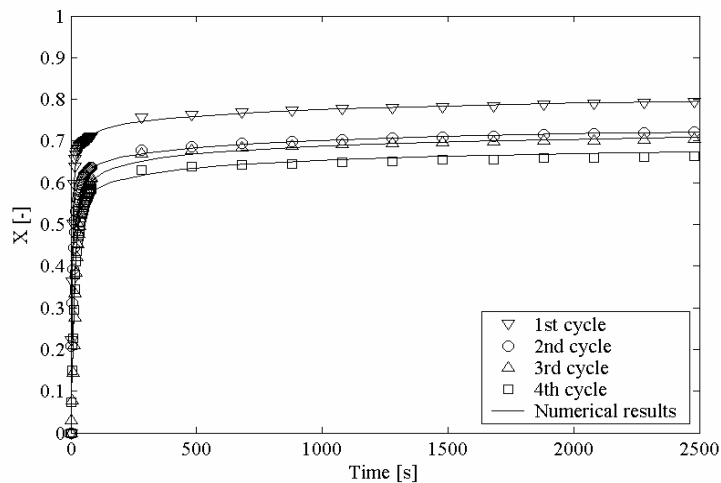
2. Comparison between numerical and experimental results: 700 °C carbonation process



Parameters	sample 1	sample 2
Sh_e [-]	15.14	5.771
Φ [-]	0.237	0.048
β [-]	0.0014	0.017

	a	b	X_N	D_{PL}	
	[-]	[-]	[-]	$[m^2/s]$	
sample 2	12.1	0.9	0.868	1.33E-14	
sample 1					
number cycle	1st	36.8	2	0.868	1.82E-17
	2nd	42.3	2	0.810	1.77E-17
	3rd	50.8	2	0.739	1.79E-17
	4th	60.9	2	0.675	1.78E-17

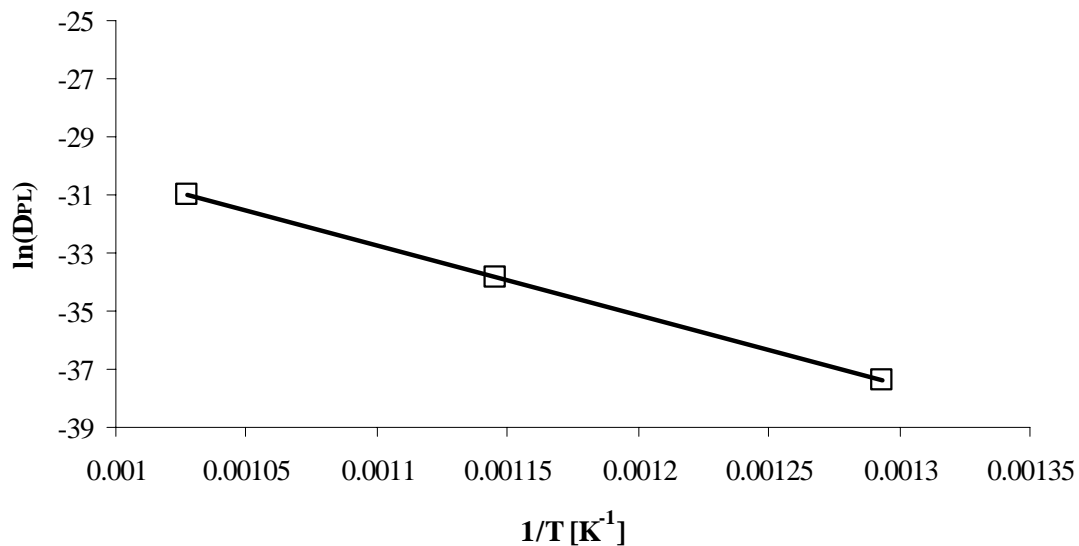
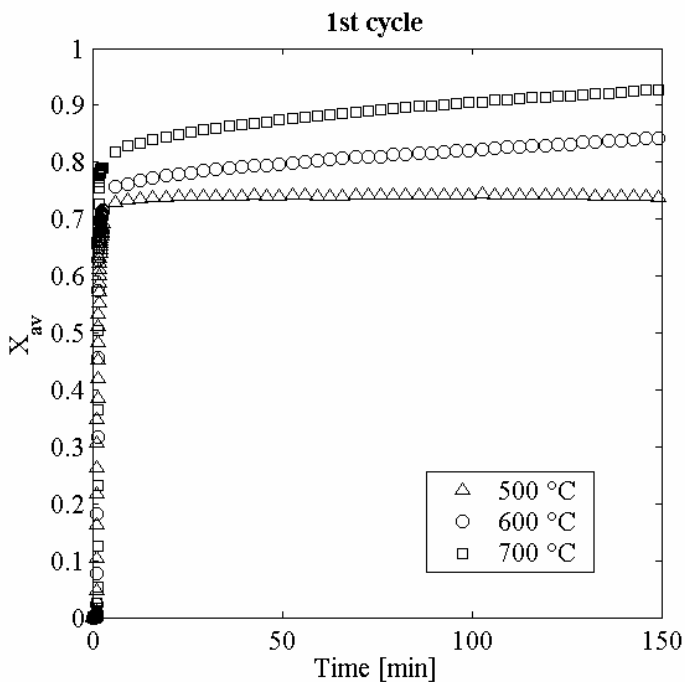
2. Comparison between numerical and experimental results: 600 °C carbonation process



	<i>a</i>	<i>b</i>	X_N	D_{PL}	
number cycle	1st	44.0	2	0.790	1.82E-17
	2nd	53.3	2	0.722	1.77E-17
	3rd	55.8	2	0.700	1.79E-17
	4th	63.0	2	0.664	1.78E-17

2. Activation energy of the product layer diffusion

	Temperature [°C]	D_{PL} [m ² /s]
sample 1 first cycle	500	1.01e-16
	600	1.99e-15
	700	3.45e-14



$$D_{PL}(T) = 1.01 \cdot 10^{-16} \exp \left[\frac{181,620}{R} \left(\frac{1}{773} - \frac{1}{T} \right) \right]$$

Bhatia and Perlmutter, 1981 (179.2 KJ/mol)

- A spherical grain model has been proposed to study the CO₂ uptake;**
- The model can be used to predict the conversion during single-step and multi-cycling carbonation;**
- The activation energy of product layer diffusion was evaluated;**