Optimization of parameters during phosphoric acid production using Response Surface Methodology: Toward a Biomimetic Process

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-SUPPLEMENTARY DATA-

Table S1 Model coefficients according to the factorial design

	Coefficient	Standard deviation	t.exp.	Signif.%
b_0	3.569	0.0126	134.26	<0.01***
b_1	-0.175	0.0325	-5.38	0.0666***
b_2	-0.225	0.0325	-6.91	<0.0123***
b_3	-0.627	0.0325	-19.27	<0.01***

Table S2 Analysis of variance according to the factorial design

Source of variation	Sum of squares	Degrees of freedom	Mean squares	F ratio	Signif.%
Regression	3.8000	3	1.2667	149.3694	<0.01***
Residues	0.0678	8	0.0085		
Validity	0.0196	5	0.0039	0.2432	91.9
Error	0.0483	3	0.0161		
Total	3.8679	11			

Table S3 Residual table according to the factorial design

	Yexp.	Ycalc.	Difference
1	4.590	4.597	-0.007
2	4.220	4.231	-0.027
3	4.120	4.131	-0.027
4	3.750	3.781	-0.047
5	3.310	3.326	-0.032
6	2.950	2.976	-0.042
7	2.850	2.876	-0.042
8	2.550	2.526	0.008
9	3.640	3.569	0.211
10	3.670	2.569	0.101
11	2.530	2.569	-0.039
12	3.510	3.569	-0.059

Table S4 Model coefficients according to the Box-Behnken plan

	Coefficient	Standard deviation	t.exp.	Signif.%
b0	3.543	0.058	60.98	<0.01***
b1	-0.129	0.035	-3.62	1.52*
b2	-0.203	0.035	-5.69	0.234**
b3	-0.609	0.035	-17.11	<0.01***
B1-1	-0.010	0.052	-0.20	85.0
B2-2	-0.013	0.052	-0.25	81.5
B3-3	0.015	0.052	0.28	79.2
B1-2	-0.005	0.050	-0.10	92.5
B1-3	-0.007	0.050	-0.15	88.7
B2-3	0	0.050	0	100

*significant at the 95% level (p<0.1); ** significant at the 99% level (p<0.05); *** significant at the 99.9% level (p<0.01)

Table S5 Analysis of variance (Box-Behnken plan)

Source of variation	Sum of squares	Degrees of freedom	Mean squares	F ratio	Signif.%
Regression	3.4275	9	0.3808	37.6011	0.0459***
Residues	0.0506	5	0.0101		
Validity	0.0472	3	0.0157	9.0721	10.1
Error	0.0035	2	0.0017		
Total	3.4782	14			

Table S6 Residual table according to the Box-Behnken plan

	Yexp.	Ycalc.	Difference
1	3.740	3.846	-0.106
2	3.580	3.599	-0.019
3	3.470	3.451	0.019
4	3.290	3.184	0.106
5	4.330	4.277	0.053
6	4.000	4.035	-0.035
7	3.110	3.075	0.035
8	2.750	2.802	-0.052
9	4.410	4.356	0.054
10	3.880	3.951	-0.071
11	3.210	3.139	-0.071
12	2.68	2.734	-0.054
13	3.590	3.543	0.047
14	3.530	3.543	-0.013
15	3.510	3.543	-0.033

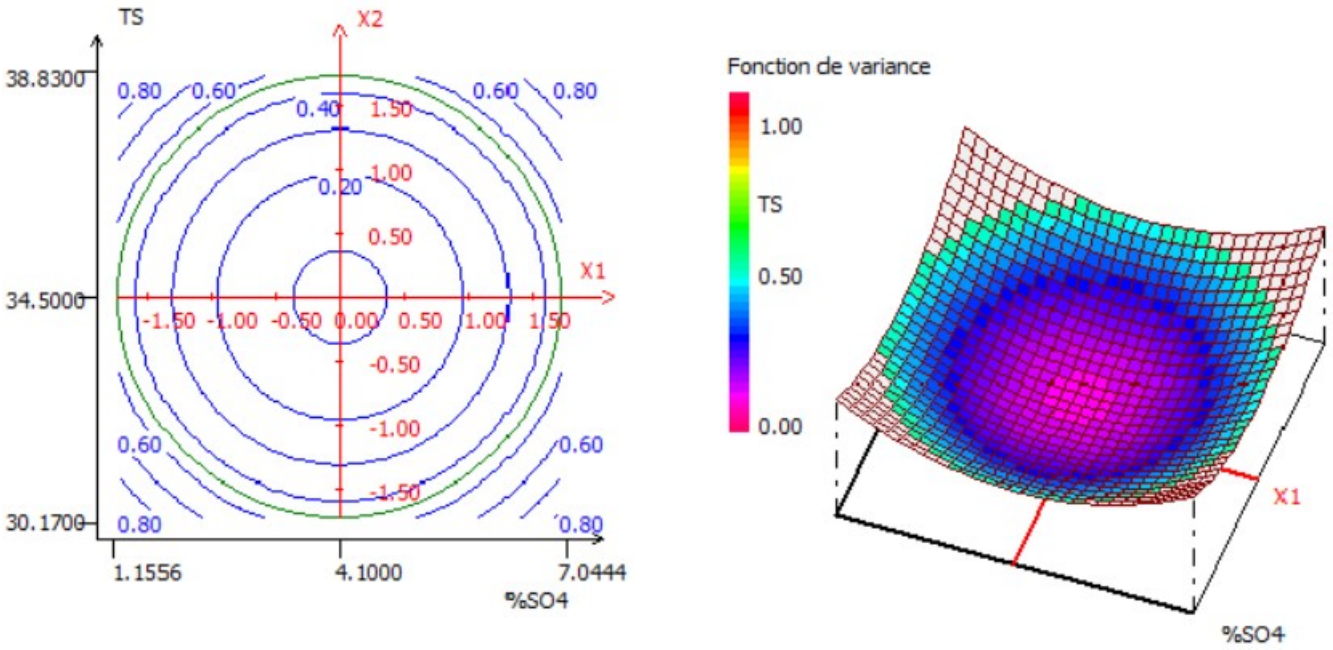


Figure S1 Variation of the variance function - in the plane: $\%SO_4$, TS - $\%P_2O_5$ = 30 % (fixed factor)

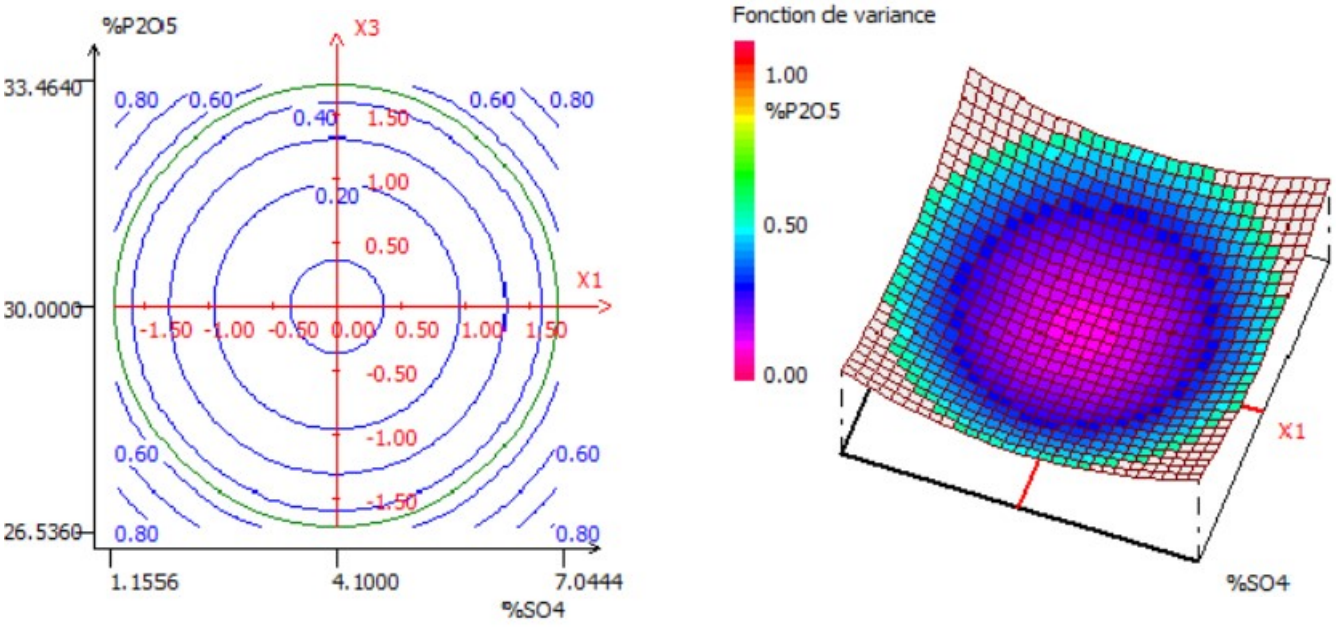
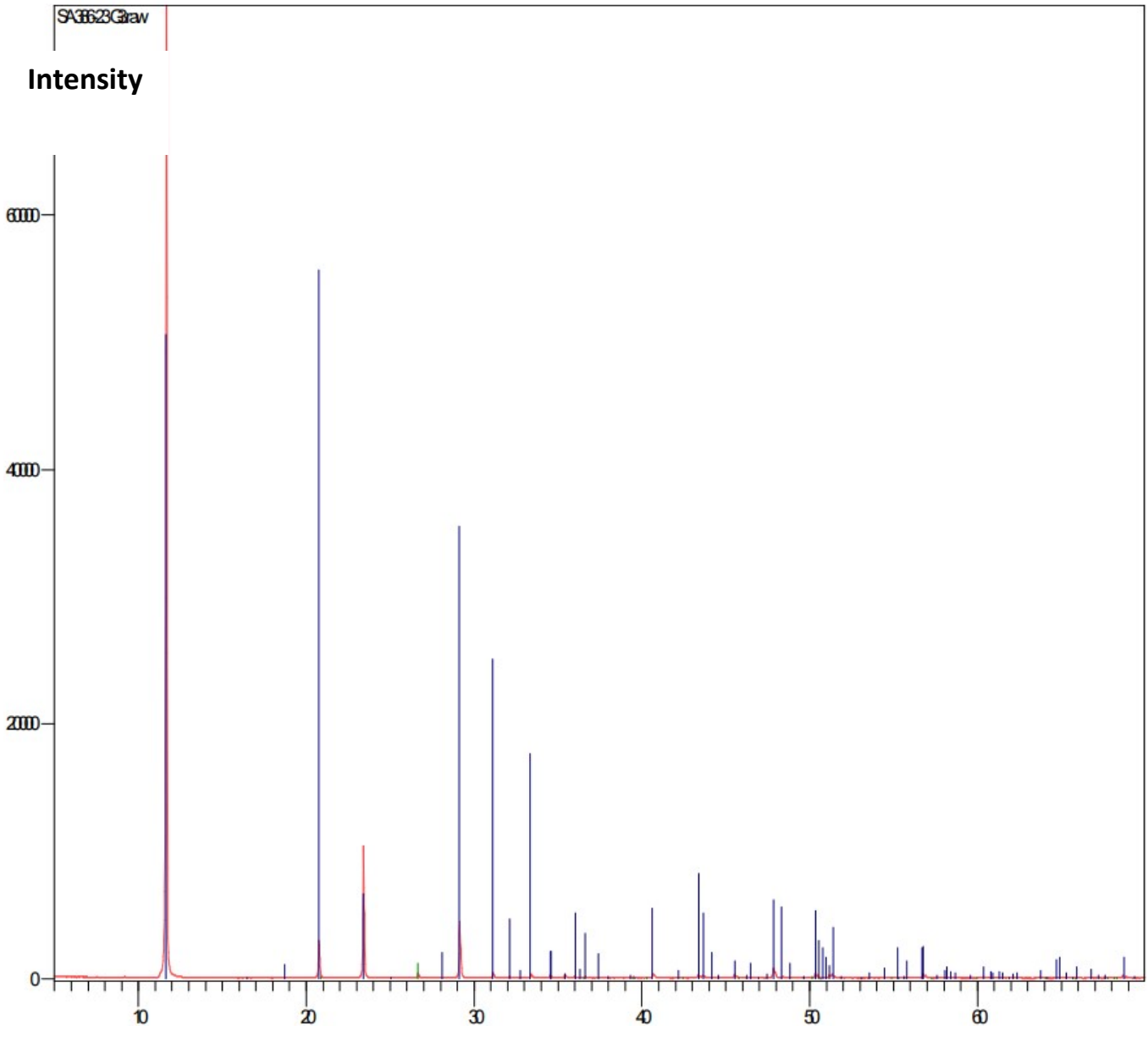
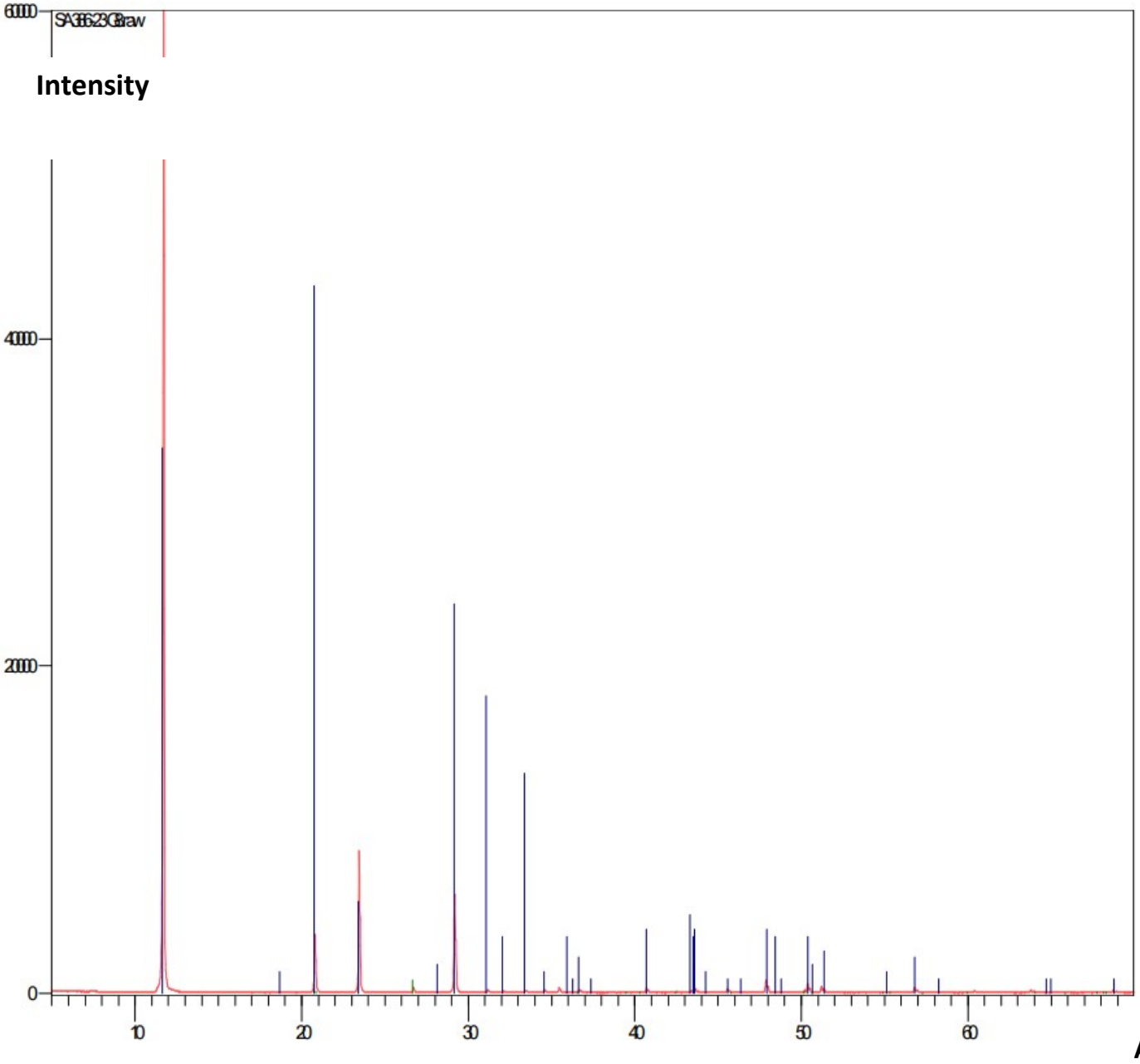


Figure S2 Variation of the variance function - in the plane: $\%SO_4$, $\%P_2O_5$ - TS = 34.5% (fixed factor)



Visible	Ref. Code	Compound Name	Chemical Formula
++++	70-0984	Gypsum	Ca (S O4) (H2 O)2
++++	46-1045	Quartz, syn	Si O2

Figure S3 XRD Pattern for the phosphogypsum LF



Visible	Ref. Code	Compound Name	Chemical Formula
++++	36-0432	Gypsum	Ca S O4 !2 H2 O
++++	46-1045	Quartz, syn	Si O2

Figure S4 XRD Pattern for the phosphogypsum HF