

**Supporting information for:  
Improving the cellulose enzymatic digestibility of  
sugarcane bagasse by atmospheric acetic acid  
pretreatment and peracetic acid post-treatment**

**Yuchen Bai<sup>1,2</sup>, Mingke Tian<sup>1,2</sup>, Zhiwei Dai<sup>3,4</sup> and Xuebing Zhao<sup>3,4,\*</sup>**

<sup>1</sup> China Food Flavor and Nutrition Health Innovation Center, Beijing Technology and Business University, Beijing 100048, China; baiyuchen@btbu.edu.cn (Y.B.)

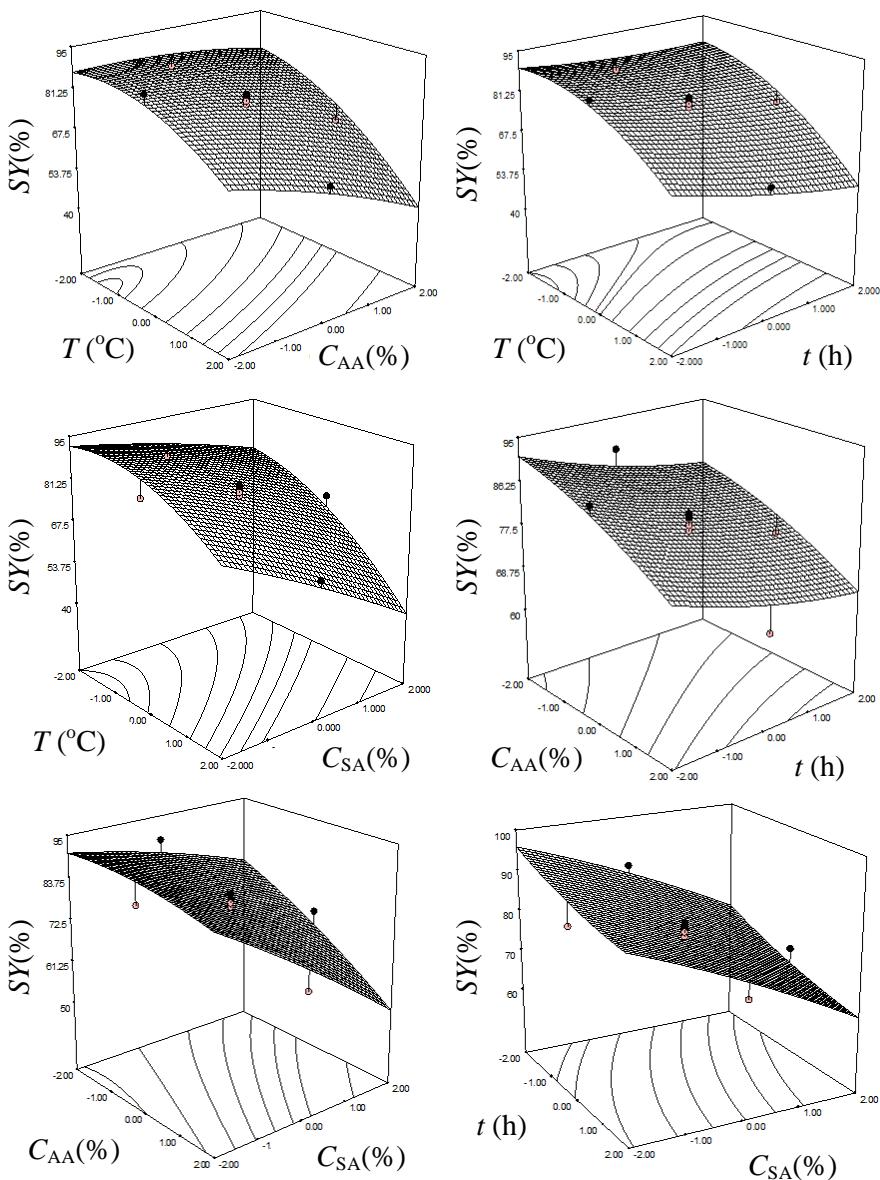
<sup>2</sup> Beijing Key Laboratory of Flavor Chemistry, Beijing Technology and Business University, Beijing 100048, China

<sup>3</sup> Key Laboratory of Industrial Biocatalysis, Ministry of Education, Tsinghua University, Beijing 100084, China

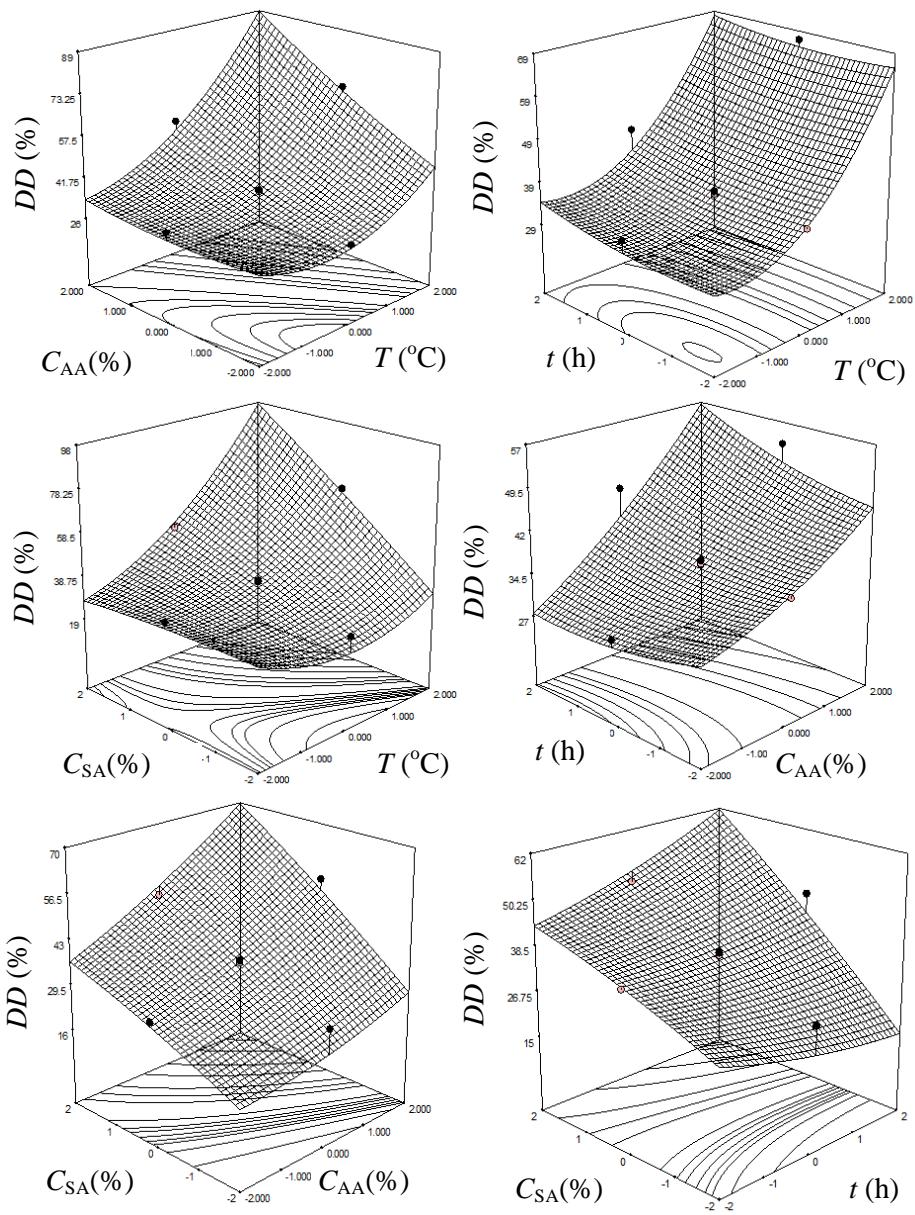
<sup>4</sup> Institute of Applied Chemistry, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

\* Correspondence: zhaoxb@mail.tsinghua.edu.cn

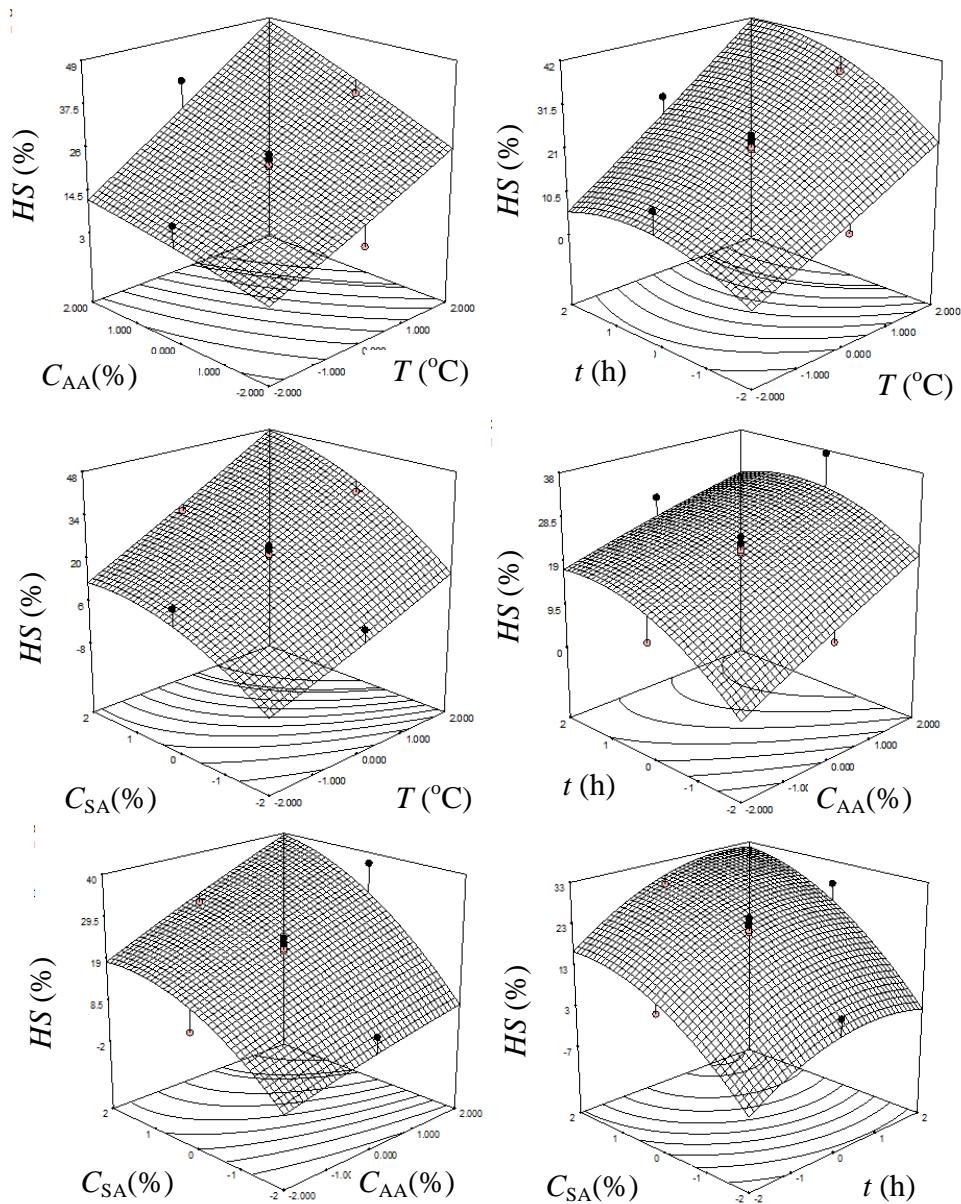
# Figures



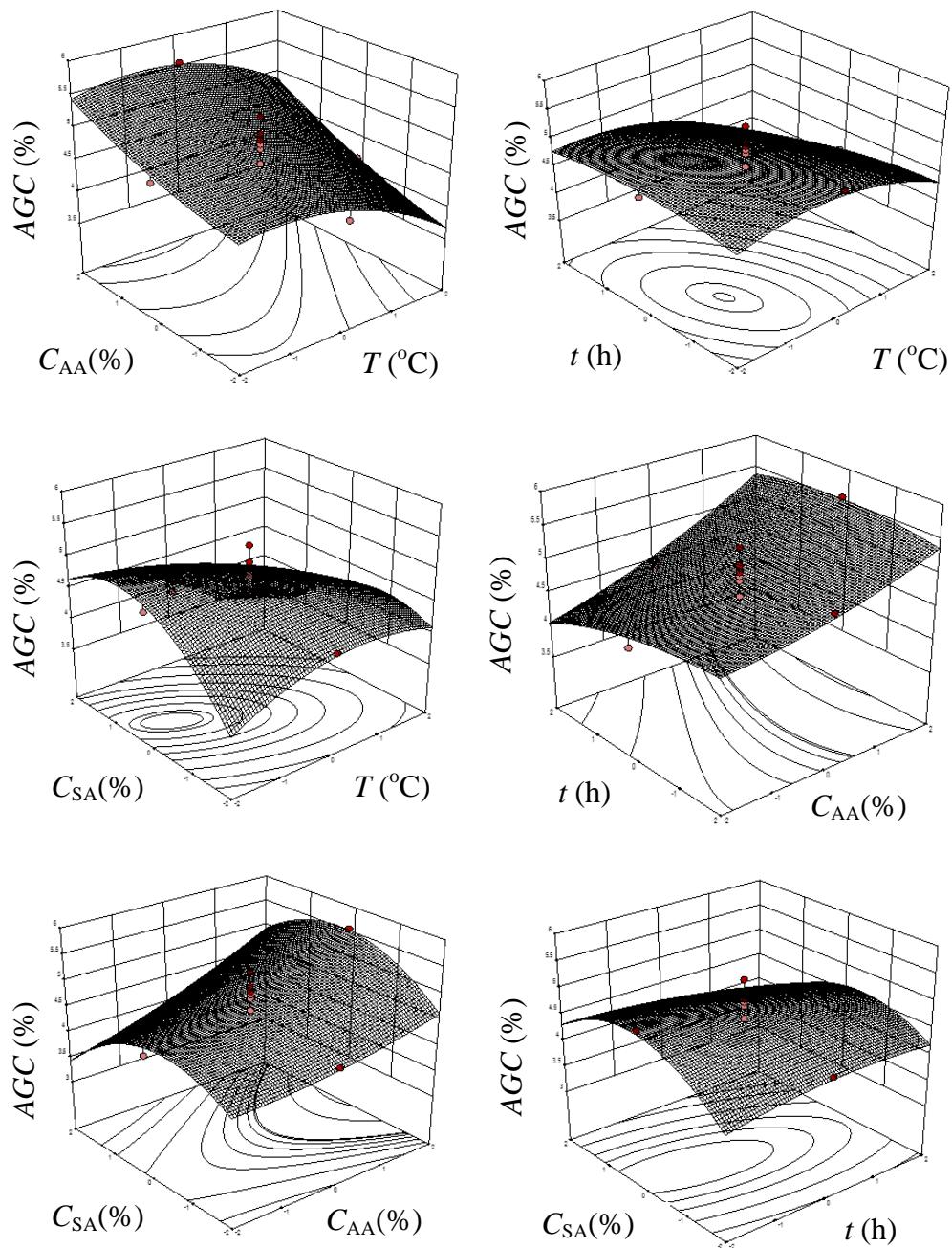
**Figure S1.** 3D surface plots of effects of temperature ( $T$ ,  $^{\circ}\text{C}$ ), AA concentration ( $C_{\text{AA}}$ , wt%), pretreatment time ( $t$ , h) and sulfuric acid concentration ( $C_{\text{SA}}$ , wt%) on solid recovery yield (SY, %).



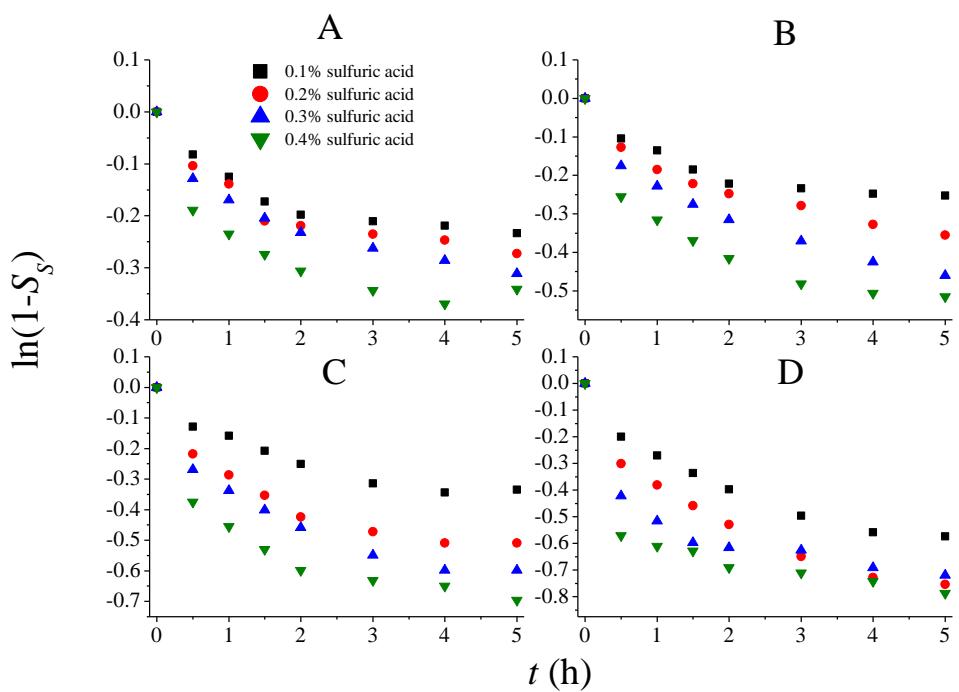
**Figure S2.** 3D surface plots of effects of temperature ( $T$ ,  $^{\circ}\text{C}$ ), AA concentration ( $C_{AA}$ , wt%), pretreatment time ( $t$ , h) and sulfuric acid concentration ( $C_{SA}$ , wt%) on degree of delignification (DD, %).



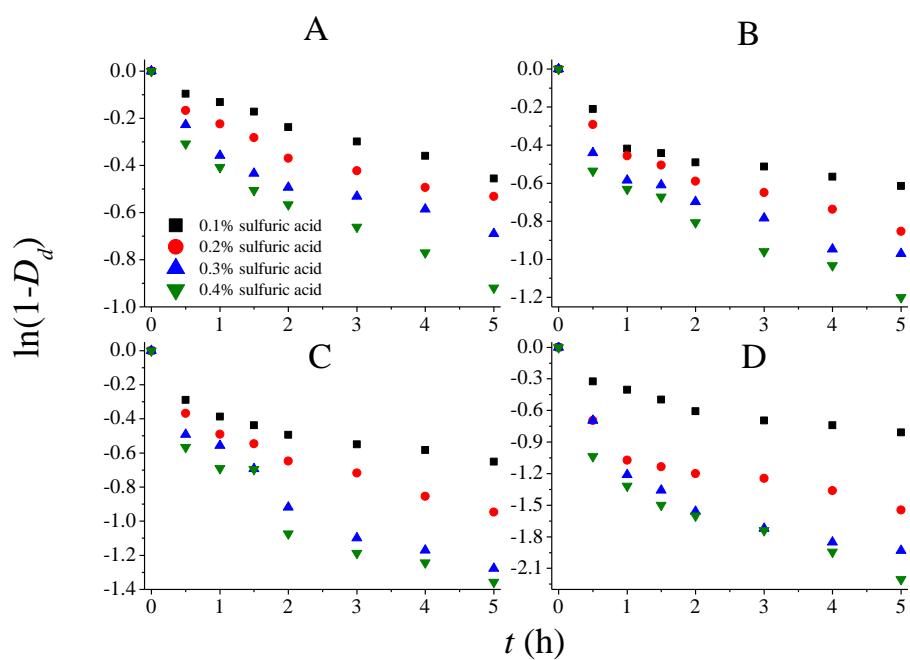
**Figure S3.** 3D surface plots of effects of temperature ( $T$ ,  $^{\circ}$ C), AA concentration ( $C_{AA}$ , wt%), pretreatment time ( $t$ , h) and sulfuric acid concentration ( $C_{SA}$ , wt %) on solubilization of holocellulose (HS, %).



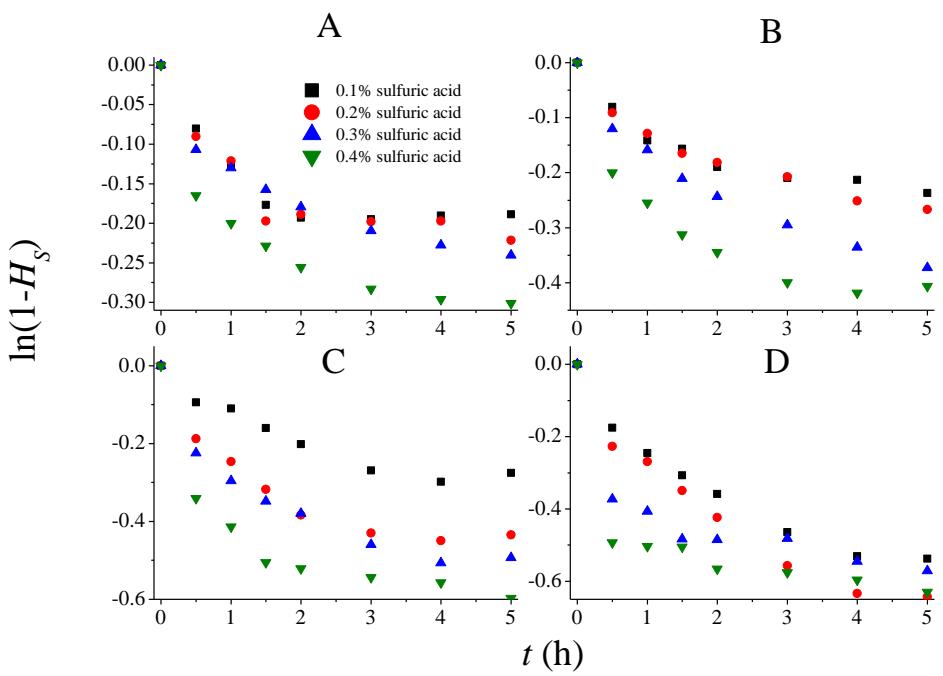
**Figure S4.** 3D surface plots of effects of temperature ( $T$ ,  $^{\circ}\text{C}$ ), AA concentration ( $C_{\text{AA}}$ , wt%), pretreatment time ( $t$ , h) and sulfuric acid concentration ( $C_{\text{SA}}$ , wt%) on acetyl group content (AGC, %) of pretreated substrates.



**Figure S5.** Plots of  $\ln(1-S_s)$  with  $t$  at different temperatures. A: 80 °C; B: 90 °C; C: 100 °C; D: 110 °C.



**Figure S6.** Plots of  $\ln(1-D_d)$  with  $t$  at different temperatures. A: 80 °C; B: 90 °C; C: 100 °C; D: 110 °C.



**Figure S7.** Plots of  $\ln(1-H_s)$  with  $t$  at different temperatures. A: 80 °C; B: 90 °C; C: 100 °C; D: 110 °C.

## Tables

**Table S1.** ANOVA for Response Surface Quadratic model for SY.

Source	Sum of Squares	df	Mean squares	F value	P-Value <i>P &gt; F</i>
Model	2653.27	14	189.52	11.89	< 0.0001
$X_1$	1100.80	1	1100.80	69.05	< 0.0001
$X_2$	341.26	1	341.26	21.41	0.0003
$X_3$	147.71	1	147.71	9.26	0.0082
$X_4$	879.67	1	879.67	55.18	< 0.0001
$X_1X_2$	25.00	1	25.00	1.57	0.2297
$X_1X_3$	9.39	1	9.39	0.59	0.4546
$X_1X_4$	26.27	1	26.27	1.65	0.2188
$X_2X_3$	2.500E-003	1	2.500E-003	1.568E-004	0.9902
$X_2X_4$	29.81	1	29.81	1.87	0.1916
$X_3X_4$	0.39	1	0.39	0.025	0.8777
$X_1^2$	80.48	1	80.48	5.05	0.0401
$X_2^2$	6.36	1	6.36	0.40	0.5370
$X_3^2$	3.16	1	3.16	0.20	0.6624
$X_4^2$	2.27	1	2.27	0.14	0.7110
Residual	239.14	15	15.94		
Lack of Fit	231.37	10	23.14	14.89	0.0041
Pure Error	7.77	5	1.55		
Cor Total	2892.41	29			

**Table S2.** ANOVA for Response Surface Quadratic model for *DD*.

Source	Sum of Squares	df	Mean squares	F value	P-Value <i>P &gt; F</i>
Model	4773.11	14	340.94	19.68	< 0.0001
$X_1$	1805.44	1	1805.44	104.24	< 0.0001
$X_2$	736.16	1	736.16	42.50	< 0.0001
$X_3$	16.80	1	16.80	0.97	0.3403
$X_4$	1476.74	1	1476.74	85.26	< 0.0001
$X_1X_2$	108.06	1	108.06	6.24	0.0246
$X_1X_3$	0.30	1	0.30	0.017	0.8966
$X_1X_4$	304.68	1	304.68	17.59	0.0008
$X_2X_3$	12.22	1	12.22	0.71	0.4142
$X_2X_4$	29.81	1	29.81	1.72	0.2093
$X_3X_4$	51.77	1	51.77	2.99	0.1044
$X_1^2$	215.33	1	215.33	12.43	0.0031
$X_2^2$	7.36	1	7.36	0.43	0.5243
$X_3^2$	4.43	1	4.43	0.26	0.6204
$X_4^2$	2.78	1	2.78	0.16	0.6946
Residual	259.80	15	17.32		
Lack of Fit	259.30	10	25.93	255.67	< 0.0001
Pure Error	0.51	5	0.10		
Cor Total	5032.91	29			

**Table S3.** ANOVA for Response Surface Quadratic model for HS.

Source	Sum of Squares	df	Mean squares	F value	P-Value <i>P &gt; F</i>
Model	3021.88	14	215.85	11.42	< 0.0001
$X_1$	1277.50	1	1277.50	67.59	< 0.0001
$X_2$	348.69	1	348.69	18.45	0.0006
$X_3$	219.86	1	219.86	11.63	0.0039
$X_4$	1024.95	1	1024.95	54.23	< 0.0001
$X_1X_2$	11.59	1	11.59	0.61	0.4457
$X_1X_3$	11.22	1	11.22	0.59	0.4529
$X_1X_4$	9.21	1	9.21	0.49	0.4958
$X_2X_3$	5.11	1	5.11	0.27	0.6108
$X_2X_4$	8.56	1	8.56	0.45	0.5113
$X_3X_4$	2.40	1	2.40	0.13	0.7264
$X_1^2$	0.57	1	0.57	0.030	0.8650
$X_2^2$	0.25	1	0.25	0.013	0.9102
$X_3^2$	47.18	1	47.18	2.50	0.1350
$X_4^2$	60.91	1	60.91	3.22	0.0928
Residual	283.51	15	18.90		
Lack of Fit	279.28	10	27.93	33.02	0.0006
Pure Error	4.23	5	0.85		
Cor Total	3305.40	29			

**Table S4.** ANOVA for Response Surface Quadratic model for AGC.

Source	Sum of Squares	df	Mean squares	F value	P-Value <i>P &gt; F</i>
Model	4.27	14	0.31	6.66	0.0004
$X_1$	0.79	1	0.79	17.28	0.0008
$X_2$	1.56	1	1.56	34.05	< 0.0001
$X_3$	0.13	1	0.13	2.88	0.1103
$X_4$	0.045	1	0.045	0.98	0.3371
$X_1X_2$	9.025E-003	1	9.025E-003	0.20	0.6635
$X_1X_3$	0.032	1	0.032	0.71	0.4136
$X_1X_4$	0.34	1	0.34	7.47	0.0154
$X_2X_3$	0.026	1	0.026	0.56	0.4664
$X_2X_4$	0.060	1	0.060	1.31	0.2704
$X_3X_4$	0.062	1	0.062	1.36	0.2611
$X_1^2$	0.24	1	0.24	5.14	0.0385
$X_2^2$	0.024	1	0.024	0.53	0.4773
$X_3^2$	0.039	1	0.039	0.85	0.3709
$X_4^2$	0.97	1	0.97	21.09	0.0004
Residual	0.69	15	0.046		
Lack of Fit	0.40	10	0.040	0.69	0.7105
Pure Error	0.29	5	0.058		
Cor Total	4.96	29			