

Supplementary Information

Thiacloprid suspension formula optimization by a response surface methodology

Bei-xing Li, Wei-chang Wang, Kai Wang, Da-xia Zhang, Lei Guan and Feng Liu*

Key Laboratory of Pesticide Toxicology & Application Technique, Shandong Agricultural University, Tai'an, P. R. China. Fax/Tel: 86 0538 8242611; E-mail: fliu@sdau.edu.cn

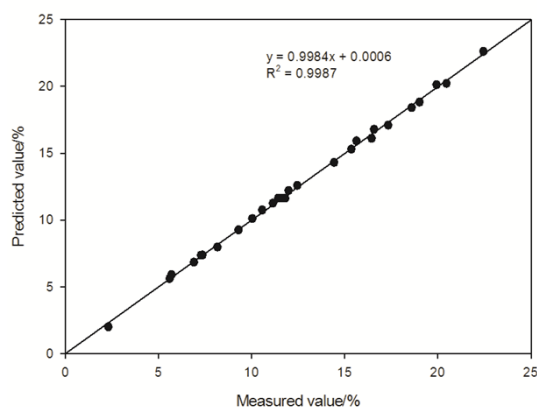


Figure S1. Measured values vs. predicted values for modeled centrifugal sedimentation ratio.

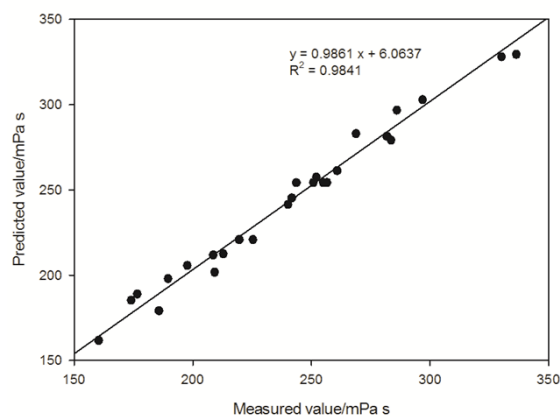


Figure S2. Measured values vs. predicted values for modeled viscosity.

Table S1. Proposed experiments by RSM and their corresponding output parameters.

No.	^a Independent variable				Aqueous separation ratio/%	Centrifugal sedimentation ratio/%	Viscosity/mPa·s	Dispersibility	Suspensibility/%	
	Tersperse 2700	AE1601	Xanthan gum	Veegum					Before storage	After hot storage
1	-1	-1	-1	-1	16.83 ± 0.12 a	22.45 ± 0.37 a	176.60 ± 1.16 t	Excellent	94.78 ± 0.53 abcdef	93.79 ± 0.58 cdefg
2	1	-1	-1	-1	15.11 ± 0.14 b	19.93 ± 0.25 b	160.34 ± 0.10 u	Excellent	96.05 ± 0.23 abc	94.71 ± 0.42 abcde
3	-1	1	-1	-1	10.47 ± 0.12 d	16.58 ± 0.09 e	189.62 ± 0.08 r	Excellent	95.70 ± 0.89 abcd	93.09 ± 0.52 defghi
4	1	1	-1	-1	8.82 ± 0.14 e	14.43 ± 0.39 g	209.22 ± 0.20 p	Excellent	96.34 ± 0.53 ab	96.16 ± 0.33 a
5	-1	-1	1	-1	7.67 ± 0.07 f	16.45 ± 0.11 e	241.76 ± 0.39 kl	Fine	95.45 ± 0.19 abcde	94.06 ± 0.23 bcdef
6	1	-1	1	-1	4.70 ± 0.07 h	11.14 ± 0.33 jk	240.16 ± 0.19 l	Excellent	95.97 ± 0.42 abc	91.40 ± 0.49 i
7	-1	1	1	-1	6.35 ± 0.11 g	11.99 ± 0.09 hi	243.64 ± 0.81 k	Fine	93.68 ± 0.42 cdef	93.90 ± 0.33 bcdefg
8	1	1	1	-1	4.67 ± 0.10 h	7.28 ± 0.19 o	281.92 ± 0.11 f	Fine	95.17 ± 0.45 abcdef	95.27 ± 0.26 abc
9	-1	-1	-1	1	9.98 ± 0.05 d	18.60 ± 0.07 c	212.90 ± 0.13 o	Fine	93.30 ± 0.48 def	91.33 ± 0.30 i
10	1	-1	-1	1	6.60 ± 0.08 g	15.64 ± 0.32 f	174.02 ± 0.60 t	Excellent	95.22 ± 0.85 abcdef	94.11 ± 0.62 bcdef
11	-1	1	-1	1	4.55 ± 0.12 h	12.46 ± 0.31 h	252.16 ± 0.14 j	Fine	96.06 ± 0.25 abc	95.12 ± 0.26 abcd
12	1	1	-1	1	1.50 ± 0.11 no	10.04 ± 0.51 l	260.92 ± 0.59 h	Excellent	95.49 ± 0.61 abcde	94.37 ± 0.58 abcde
13	-1	-1	1	1	4.48 ± 0.12 hi	10.57 ± 0.24 kl	268.86 ± 0.28 g	Fine	93.19 ± 0.27 def	93.31 ± 0.28
14	1	-1	1	1	1.81 ± 0.10 n	5.70 ± 0.28 p	283.66 ± 0.83 ef	Fine	94.10 ± 0.37 bcdef	93.94 ± 0.23 bcdef
15	-1	1	1	1	3.92 ± 0.10 ij	6.91 ± 0.19 o	330.22 ± 0.87 c	Fine	95.43 ± 0.46 abcde	94.42 ± 0.25 abcde
16	1	1	1	1	1.22 ± 0.03 o	2.31 ± 0.15 q	345.78 ± 0.08 a	Fine	94.80 ± 0.32 abcdef	94.25 ± 0.22 abcde
17	-2	0	0	0	6.90 ± 0.10 g	15.36 ± 0.21 f	219.58 ± 0.62 n	Fine	93.29 ± 0.53 def	92.12 ± 0.50 fghi
18	2	0	0	0	2.74 ± 0.07 m	8.17 ± 0.24 n	225.38 ± 0.08 m	Excellent	96.05 ± 0.40 abc	95.88 ± 0.36 ab
19	0	-2	0	0	8.91 ± 0.06 e	17.34 ± 0.35 d	208.64 ± 0.14 p	Excellent	93.12 ± 0.75 ef	91.89 ± 0.30 ghi
20	0	2	0	0	3.04 ± 0.13 lm	7.36 ± 0.14 o	286.08 ± 0.11 e	Excellent	94.94 ± 0.25 abcdef	94.61 ± 0.36 abcde
21	0	0	-2	0	11.42 ± 0.17 c	20.47 ± 0.25 b	185.76 ± 0.10 s	Excellent	94.77 ± 0.35 abcdef	93.65 ± 0.01 cdefg
22	0	0	2	0	1.77 ± 0.08 no	5.60 ± 0.26 p	336.46 ± 1.01 b	Fine	93.55 ± 0.42 cdef	92.92 ± 0.36 efghi
23	0	0	0	-2	14.83 ± 0.13 b	19.02 ± 0.19 c	197.68 ± 0.08 q	Excellent	92.84 ± 0.16 f	91.54 ± 0.16 hi
24	0	0	0	2	3.64 ± 0.08 jk	9.30 ± 0.29 m	296.94 ± 0.48 d	Fine	97.02 ± 0.21 a	94.25 ± 0.26 abcde
25	0	0	0	0	3.50 ± 0.08 jkl	11.64 ± 0.16 ij	255.10 ± 0.49 i	Fine	94.21 ± 0.41 bcdef	93.47 ± 0.36 cdefgh
26	0	0	0	0	3.40 ± 0.08 jkl	11.80 ± 0.17 hij	256.66 ± 0.48 i	Fine	94.96 ± 0.20 abcdef	93.93 ± 0.38 bcdefg
27	0	0	0	0	3.14 ± 0.09 klm	11.43 ± 0.11 ij	250.88 ± 0.08 j	Fine	94.52 ± 0.34 abcdef	93.77 ± 0.35 cdefg

^aThe levels of adjuvants were coded value. Each data of dependent variable is the mean ± SE. Data of the same index with different lowercase letters are significantly different at $p < 0.05$ level by Tukey test.

Table S2. The ANOVA for the aqueous separation ratio

Source	Coefficient	F-value	Sequential <i>p</i> -value
Model	-	248.39	< 0.0001
Lack of Fit	-	4.51	0.1951
Intercept	3.35	-	-
X ₁	-1.17	231.62	< 0.0001*
X ₂	-1.56	409.53	< 0.0001*
X ₃	-2.43	995.17	< 0.0001*
X ₄	-2.62	1158.72	< 0.0001*
X ₁ X ₂	0.10	1.20	0.2941
X ₁ X ₃	-0.01	0.02	0.9037
X ₁ X ₄	-0.24	6.21	0.0284*
X ₂ X ₃	1.29	187.43	< 0.0001*
X ₂ X ₄	0.14	2.36	0.1503
X ₃ X ₄	1.04	121.54	< 0.0001*
X ₁ ²	0.39	22.89	0.0004*
X ₂ ²	0.68	69.05	< 0.0001*
X ₃ ²	0.83	104.28	< 0.0001*
X ₄ ²	1.49	334.59	< 0.0001*

Note: * indicates significant impact.

Table S3. Fitness of centrifugal sedimentation ratio to different models.

Model	Sequential <i>p</i> -value	Lack of fit <i>p</i> -value	Adjusted R ²	Predicted R ²
Linear	< 0.0001	0.0320	0.9645	0.9546
2FI	0.0429	0.0462	0.9765	0.9770
Quadratic polynomial	< 0.0001	0.4323	0.9980	0.9951
Cubic polynomial	0.6310	0.2804	0.9977	0.9638

Table S4. The ANOVA for the centrifugal sedimentation ratio

Source	Coefficient	F-value	Sequential <i>p</i> -value
Model	-	940.72	< 0.0001
Lack of Fit	-	1.67	0.4323
Intercept	11.62	-	-
X ₁	-1.83	1511.99	< 0.0001*
X ₂	-2.43	2677.50	< 0.0001*
X ₃	-3.65	6005.32	< 0.0001*
X ₄	-2.39	2590.99	< 0.0001*
X ₁ X ₂	0.11	3.76	0.0763
X ₁ X ₃	-0.59	104.50	< 0.0001*
X ₁ X ₄	-0.01	0.04	0.8540
X ₂ X ₃	0.48	70.14	< 0.0001*
X ₂ X ₄	0.06	0.94	0.3526
X ₃ X ₄	-0.29	26.02	0.0003*
X ₁ ²	0.01	0.01	0.9066
X ₂ ²	0.15	9.34	0.0100*
X ₃ ²	0.32	42.11	< 0.0001*
X ₄ ²	0.60	146.85	< 0.0001*

Note: * indicates significant impact.

Table S5. Fitness of the viscosity to different models.

Model	Sequential <i>p</i> -value	Lack of fit <i>p</i> -value	Adjusted R ²	Predicted R ²
Linear	< 0.0001	0.0319	0.8988	0.8675
2FI	0.0208	0.0513	0.9399	0.9144
Quadratic polynomial	0.0004	0.1696	0.9836	0.9572
Cubic polynomial	0.7274	0.0831	0.9783	0.5590

Table S6. The ANOVA for the viscosity

Source	Coefficient	F-value	Sequential p-value
Model	-	112.04	< 0.0001
Lack of Fit	-	5.28	0.1696
Intercept	254.21	-	-
X ₁	2.16	2.74	0.1235
X ₂	21.25	265.43	< 0.0001*
X ₃	37.57	829.37	< 0.0001*
X ₄	24.32	347.70	< 0.0001*
X ₁ X ₂	7.76	23.58	0.0004*
X ₁ X ₃	5.86	13.47	0.0032*
X ₁ X ₄	-2.49	2.42	0.1456
X ₂ X ₃	-1.31	0.67	0.4287
X ₂ X ₄	9.01	31.78	0.0001*
X ₃ X ₄	3.55	4.94	0.0462*
X ₁ ²	-8.36	36.53	< 0.0001*
X ₂ ²	-2.14	2.40	0.1474
X ₃ ²	1.29	0.88	0.3680
X ₄ ²	-2.16	2.43	0.1452

Note: * indicates significant impact.

Table S7. Constraints for the multiple-response optimization.

Name	Goal	Lower limit	Upper limit	Lower weight	Upper weight	Importance
X ₁ : Tersperse2700	Range	-2.00	2.00	1	1	3
X ₂ : AE1601	Range	-2.00	2.00	1	1	3
X ₃ : Xanthan gum	Range	-2.00	2.00	1	1	3
X ₄ : Veegum	Range	-2.00	2.00	1	1	3
Aqueous separation ratio/%	Minimize	1.22	5.00	1	1	3
Centrifugal sedimentation ratio/%	Minimize	2.31	5.00	1	1	3
Viscosity/ mPa·s	Minimize	160.34	345.78	1	1	1