**Empirical models to predict the effect of sterilization and storage on bisphenols migration from metallic can coating into food simulants**

Sara Noureddine El Moussawia,b, Mathieu Cladièrea, Hanna Chébibb, Rosette Ouainib and Valérie Camela\*

*aUMR Ingénierie Procédés Aliments, AgroParisTech, Inra, Université Paris-Saclay, Massy, 91300, France*

*bER004 Lebanese Food Packaging, Faculty of Sciences II, Lebanese University, Fanar, 90656, Lebanon*

**Appendix A - Supplementary material**

Supplementary Material - **Table S1:** Selection ofestimated regression coefficients with their standard error and significance\* against zero for models based on Design I.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **BADGE.2H2O** | | | | |  | **BPA** | | | | |
| Term | | Scaled Estimate | Std error | p-value  scaled = 0 |  | Term | | Scaled Estimate | Std Error | p-value  scaled = 0 |
| β0 | | 30.95 | 9.74 | 0.0036 |  | β0 | | 53.16 | 10.16 | **0.0004** |
| β2*x*2 | If [S1] | -28.93 | 17.48 | 0.190 |  | β1*x*1 | If [C1] | 10.16 | 5.13 | 0.075 |
| If [S2] | -27.64 | 17.48 | 0.125 |  | If [C2] | -16.82 | 4.90 | **0.006** |
| If [S3] | -27.73 | 16.23 | 0.0985 |  | If [C3] | 6.49 | 5.08 | 0.229 |
| If [S4] | 84.30 | 16.23 | **<0.0001** |  | If [C4] | 0.16 | 4.81 | 0.974 |
| β4 | | 32.85 | 10.26 | **0.0034** |  | β2*x*2 | If [S1] | -6.22 | 5.08 | 0.248 |
|  | |  |  |  |  | If [S2] | -6.85 | 5.08 | 0.207 |
| β24*x*2 | If [S1] | -30.83 | 17.78 | 0.093 |  | If [S3] | -15.63 | 4.76 | **0.0082** |
| If [S2] | -30.15 | 17.78 | 0.101 |  | If [S4] | 28.71 | 5.03 | **0.0002** |
| If [S3] | -29.79 | 17.78 | 0.104 |  | β4 | | 8.35 | 2.84 | **0.003** |
| If [S4] | 90.7798 | 17.78 | **< 0.0001** |  | β5 | | 10.5 | 3.18 | **0.025** |
|  | |  |  |  |  | β12*x*1*x*2 | If [C1]\* [S1] | -13.14 | 8.70 | 0.161 |
|  | |  |  |  |  | If [C1]\*[S2] | -12.15 | 8.70 | 0.192 |
|  | |  |  |  |  | If [C1]\* [S3] | -24.28 | 8.68 | **0.0189** |
|  | |  |  |  |  | If [C1]\*[S4] | 49.58 | 8.68 | **0.0002** |
|  | |  |  |  |  | If [C2]\*[S1] | 13.39 | 8.56 | 0.148 |
|  | |  |  |  |  | If[C2]\*[S2] | 14.57 | 8.56 | 0.119 |
|  | |  |  |  |  | If [C2]\*[S3] | 5.90 | 7.68 | 0.459 |
|  | |  |  |  |  | If[C2]\*[S4] | -33.87 | 8.63 | **0.002** |
|  | |  |  |  |  | If [C3]\*[S1] | -7.24 | 8.66 | 0.422 |
|  | |  |  |  |  | If [C3]\*[S2] | 0.59 | 8.66 | 0.946 |
|  | |  |  |  |  | If [C3]\*[S3] | 2.93 | 8.48 | 0.735 |
|  | |  |  |  |  | If [C3]\*[S4] | 3.69 | 8.63 | 0.677 |
|  | |  |  |  |  | If [C4]\*[S1] | 6.99 | 8.51 | 0.430 |
|  | |  |  |  |  | If [C4]\*[S2] | -3.01 | 8.51 | 0.730 |
|  | |  |  |  |  | If [C4]\*[S3] | 15.43 | 7.76 | 0.074 |
|  | |  |  |  |  | If [C4]\*[S4] | -19.40 | 8.00 | **0.035** |
|  | |  |  |  |  | β15*x*1 | If [C1] | 16.65 | 5.02 | **0.007** |
|  | |  |  |  |  | If [C2] | -14.41 | 5.00 | **0.016** |
|  | |  |  |  |  | If [C3] | 0.894 | 4.95 | 0.860 |
|  | |  |  |  |  | If [C4] | -3.14 | 4.88 | 0.533 |
|  | |  |  |  |  | β25*x*2 | If [S1] | -8.72 | 4.95 | 0.108 |
|  | |  |  |  |  | If [S2] | -8.05 | 4.95 | 0.134 |
|  | |  |  |  |  | If [S3] | -8.73 | 4.96 | 0.109 |
|  | |  |  |  |  | If [S4] | 25.51 | 5.01 | **0.0005** |
|  | |  |  |  |  | β55 | | -43.20 | 11.05 | 0.0029 |

*\* based on p-value from a t‑test assessing if the estimated values are statistically different from zero*

Supplementary Material - **Table S2:** Estimated regression coefficients of the models built to fit data from Design II.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **BADGE.2H2O** | | |  | **BPA** | | |  |
| Term | | Scaled estimate |  | Term | | Scaled estimate |  |
| β0 | | 494.10 |  | β0 | | 97.38 |  |
| β1*x*1 | If [C1] | -8.33 |  | β1*x*1 | If [C1] | 53.93 |  |
| If [C2] | -123.24 |  | If [C2] | -37.09 |  |
| If [C3] | 249.25 |  | If [C3] | 7.73 |  |
| If [C4] | -117.68 |  | If [C4] | -24.57 |  |
| β2*x*2 | If [S1] | -38.84 |  | β3 | | 45.98 |  |
| If [S2] | 38.84 |  | β4 | | 2.64 |  |
| β3 | | 300.79 |  | β5 | | -19.75 |  |
| β4 | | 9.25 |  | β13*x*1 | If [C1] | 23.23 |  |
| β12*x*1*x*2 | If [C1]\*[S1] | -10.86 |  | If [C2] | -22.48 |  |
| If [C1]\*[S2] | 10.86 |  | If [C3] | 16.93 |  |
| If [C2]\*[S1] | 32.84 |  | If [C4] | -17.67 |  |
| If [C2]\*[S2] | -32.84 |  | β15*x*1 | If [C1] | -42.80 |  |
| If [C3]\*[S1] | -40.53 |  | If [C2] | 18.24 |  |
| If [C3]\*[S2] | 40.53 |  | If [C3] | 5.04 |  |
| If [C4]\*[S1] | 18.56 |  | If [C4] | 19.51 |  |
| If [C4]\*[S2] | -18.56 |  | β33 | | -117.62 |  |
| β13*x*1 | If [C1] | -27.25 |  | β44 | | 82.02 |  |
| If [C2] | -117.37 |  |  | |  |  |
| If [C3] | 249.60 |  |  | |  |  |
| If [C4] | -104.98 |  |  | |  |  |
| β23*x*2 | If [S1] | -32.73 |  |  | |  |  |
| If [S2] | 32.73 |  |  | |  |  |
| β24*x*2 | If [S1] | -19.76 |  |  | |  |  |
| If [S2] | 19.76 |  |  | |  |  |
| β33 | | -187.99 |  |  | |  |  |
|  | |  |  |  | |  |  |

Supplementary Material - **Table S3**: Adequacy and significance tests of regression models.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Model Fit** | | | | | | | | | | | | | | | | |
| **Design I** | | | | | | | | | |  | **Design II** | | | | | | |
|  | | BADGE.2H2O | | | | BPA | | | |  | BADGE.2H2O | | | | BPA | | |
| R2 a | | 0.693 | | | | 0.999 | | | |  | 0.989 | | | | 0.912 | | |
| R2adjustedb  R2predicted | | 0.617  0.948 | | | | 0.994  0.956 | | | |  | 0.981  0.977 | | | | 0.854  0.937 | | |
|  | | **Analysis of variance** | | | | | | | | | | | | | | | |
|  | | **Design I** | | | | | | | |  | **Design II** | | | | | | |
|  | | BADGE.2H2O | | |  | | BPA | | |  | BADGE.2H2O | | |  | BPA | | |
|  | | Model | Error | Total |  | | Model | Error | Total |  | Model | Error | Total |  | Model | Error | Total |
| Degree of freedom (d*f*)c | | 7 | 28 | 35 |  | | 32 | 3 | 35 |  | 15 | 20 | 35 |  | 14 | 21 | 35 |
| Sum of Squares (SS)d | | 213651 | 94384 | 308035 |  | | 6924 | 34.9 | 69280 |  | 4492456 | 49790 | 4542246 |  | 212182 | 20444 | 232626 |
| Mean Square (MS)e | | 30522 | 3371 |  |  | | 2164 | 11.6 |  |  | 299497 | 2489 |  |  | 15156 | 973 |  |
| F-ratiof | | 9.05 |  |  |  | | 186 |  |  |  | 120.3 |  |  |  | 15.57 |  |  |
| P-valueg | | <0.0001\* |  |  |  | | 0.0006\* |  |  |  | <0.0001\* |  |  |  | <0.0001\* |  |  |

*\* Significant effect if p<0.05*

*a: coefficient of determination defined as R2 = 1 – SS (error)/ SS (Total) (0 ≤ R2 ≤ 1)*

*b: adjusted coefficient of determination defined as R2adjusted= 1 – (SS (error) / n-p)/ (SS (Total)/n-1), where (n) is the number of observations and (p) is the number of regression coefficients*

*c: number of free units of information*

*d: calculated by summing the squared factor effect for each run*

*e: MS = SS/df*

*f: F-ratio = MS (model)/ MS (error)*

*g: looked up in the F table*