**SUPPLEMENTARY MATERIAL TO**

**Validation and uncertainity estimation of analitycal method for determination of phenolic compounds in concrete**

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The needed information for uncertainty calculations for both methods (GUM and Monte Carlo) for the other 8 phenolic compounds (2-chloro phenol, 2,4-dimethyl phenol, 2,4-dichlorophenol, 2,6-dichlorophenol, 4-chloro-3-methyl phenol, 2,4,6-trichlorophenol, 2,3,4,6-tetrahlorophenol, pentachlorophenol) are summarized in Tables I, III, V, VII, IX, XI, XIII, XV.

The results obtained by processing the set of available information by GUM uncertainty approach and corresponding statistical parameters obtained by Monte Carlo simulation for the other 8 phenolic compounds (2-chloro phenol, 2,4-dimethyl phenol, 2,4-dichlorophenol, 2,6-dichlorophenol, 4-chloro-3-methyl phenol, 2,4,6-trichlorophenol, 2,3,4,6-tetrahlorophenol, pentachlorophenol) are presented in Tables II, IV, VI, VIII, X, XII, XIV, XVI.

**2-chloro phenol**

TABLE I. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2-chloro phenol compound

|  |  |  |
| --- | --- | --- |
| Uncertainty source | Distribution | Parameters of a distribution |
| Volume (*V*) | Normal | Mean: *75 ml*; SD: *2.55 ml* |
| Mass (*m*) | Normal | Mean: *10 g*; SD: *0.22g* |
| Recovery (*R*) | Student’s t Location-Scale | Mean: *87.02 %*; SD: *5.67 %*; DF: *3* |
| The area of peak (*y*) | Student’s t Location-Scale | Mean: *177131*; SD: *9000*; DF: *3* |
| Slope (*a*) | Student’s t Location-Scale | Mean: *-9888*; SD: *4938*; DF: *3* |
| Intercept (*b*) | Student’s t Location-Scale | Mean: *416101 l/mg*; SD: *9593 l/mg*; DF: *3* |
| Purity of standard | Uniform | Min: *-0.0201 mg/kg*; Max: *0.0201mg/kg* |

\*SD – Standard Deviation; DF – Degrees of Freedom

TABLE II. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2-chloro phenol compound

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter (GUM) | Value | Parameter (MC) | Value |
| Mean | *3.87 mg/kg* | Median | *3.87 mg/kg* |
| Combined standard uncertainty | *0.38 mg/kg* | Low endpoint for 95% | *2.79 mg/kg* |
| Expanded uncertainty for 95% | *0.83 mg/kg* | High endpoint for 95% | *5.13 mg/kg* |

**2,4-dimephyl phenol**

TABLE III. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,4-dimephyl phenol compound

|  |  |  |
| --- | --- | --- |
| Uncertainty source | Distribution | Parameters of a distribution |
| Volume (*V*) | Normal | Mean: *75 ml*; SD: *2.55 ml* |
| Mass (*m*) | Normal | Mean: *10 g*; SD: *0.22g* |
| Recovery (*R*) | Student’s t Location-Scale | Mean: *33.71%*; SD: *3.47 %*; DF: *3* |
| The area of peak (*y*) | Student’s t Location-Scale | Mean: *73259*; SD: *4000*; DF: *3* |
| Slope (*a*) | Student’s t Location-Scale | Mean: *-10495*; SD: *7726*; DF: *3* |
| Intercept (*b*) | Student’s t Location-Scale | Mean: *500447 l/mg*; SD: *15007l/mg*; DF: *3* |
| Purity of standard | Uniform | Min: *-0.0193 mg/kg*; Max: *0.0193 mg/kg* |

\*SD – Standard Deviation; DF – Degrees of Freedom

TABLE IV. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,4-dimephyl phenol compound

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter (GUM) | Value | Parameter (MC) | Value |
| Mean | *3.72 mg/kg* | Median | *3.72 mg/kg* |
| Combined standard uncertainty | *0.58 mg/kg* | Low endpoint for 95% | *1.99 mg/kg* |
| Expanded uncertainty for 95% | *1.30 mg/kg* | High endpoint for 95% | *5.83 mg/kg* |

**2,4-dichlorophenol**

TABLE V. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,4-dichlorophenol compound

|  |  |  |
| --- | --- | --- |
| Uncertainty source | Distribution | Parameters of a distribution |
| Volume (*V*) | Normal | Mean: *75 ml*; SD: *2.55 ml* |
| Mass (*m*) | Normal | Mean: *10 g*; SD: *0.22g* |
| Recovery (*R*) | Student’s t Location-Scale | Mean: *86.61%*; SD: *7.84%*; DF: *3* |
| The area of peak (*y*) | Student’s t Location-Scale | Mean: *165832*; SD: *8000*; DF: *3* |
| Slope (*a*) | Student’s t Location-Scale | Mean: *-10262*; SD: *5325*; DF: *3* |
| Intercept (*b*) | Student’s t Location-Scale | Mean: *394626 l/mg*; SD: *10345 l/mg*; DF: *3* |
| Purity of standard | Uniform | Min: *-0.0201mg/kg*; Max: *0.0201 mg/kg* |

\*SD – Standard Deviation; DF – Degrees of Freedom

TABLE VI. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,4-dichlorophenol compound

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter (GUM) | Value | Parameter (MC) | Value |
| Mean | *3.86 mg/kg* | Median | *3.87 mg/kg* |
| Combined standard uncertainty | *0.45 mg/kg* | Low endpoint for 95% | *2.59 mg/kg* |
| Expanded uncertainty for 95% | *1.06 mg/kg* | High endpoint for 95% | *5.46 mg/kg* |

**2,6-dichlorophenol**

TABLE VII. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,6-dichlorophenol compound

|  |  |  |
| --- | --- | --- |
| Uncertainty source | Distribution | Parameters of a distribution |
| Volume (*V*) | Normal | Mean: *75 ml*; SD: *2.55 ml* |
| Mass (*m*) | Normal | Mean: *10 g*; SD: *0.22g* |
| Recovery (*R*) | Student’s t Location-Scale | Mean: *91.03 %*; SD: *7.21%*; DF: *3* |
| The area of peak (*y*) | Student’s t Location-Scale | Mean: *154874*; SD: *8000*; DF: *3* |
| Slope (*a*) | Student’s t Location-Scale | Mean: *-6017*; SD: *3182*; DF: *3* |
| Intercept (*b*) | Student’s t Location-Scale | Mean: *343841 l/mg*; SD: *6181 l/mg*; DF: *3* |
| Purity of standard | Uniform | Min: *-0.0200 mg/kg*; Max: *0.0200 mg/kg* |

\*SD – Standard Deviation; DF – Degrees of Freedom

TABLE VIII. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,4-dichlorophenol compound

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter (GUM) | Value | Parameter (MC) | Value |
| Mean | *3.86 mg/kg* | Median | *3.86 mg/kg* |
| Combined standard uncertainty | *0.41 mg/kg* | Low endpoint for 95% | *2.63 mg/kg* |
| Expanded uncertainty for 95% | *0.94 mg/kg* | High endpoint for 95% | *5.19mg/kg* |

**4-chloro-3-methyl phenol**

TABLE IX. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 4-chloro-3-methyl phenolcompound

|  |  |  |
| --- | --- | --- |
| Uncertainty source | Distribution | Parameters of a distribution |
| Volume (*V*) | Normal | Mean: *75 ml*; SD: *2.55 ml* |
| Mass (*m*) | Normal | Mean: *10 g*; SD: *0.22g* |
| Recovery (*R*) | Student’s t Location-Scale | Mean: *83.88%*; SD: *7.79%*; DF: *3* |
| The area of peak (*y*) | Student’s t Location-Scale | Mean: *80524*; SD: *4000*; DF: *3* |
| Slope (*a*) | Student’s t Location-Scale | Mean: *-4857*; SD: *2310*; DF: *3* |
| Intercept (*b*) | Student’s t Location-Scale | Mean: *201366 l/mg*; SD: *4487 l/mg*; DF: *3* |
| Purity of standard | Uniform | Min: *-0.0394 mg/kg*; Max: *0.0394 mg/kg* |

\*SD – Standard Deviation; DF – Degrees of Freedom

TABLE X. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 4-chloro-3-methyl phenolcompound

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter (GUM) | Value | Parameter (MC) | Value |
| Mean | *3.79 mg/kg* | Median | *3.79 mg/kg* |
| Combined standard uncertainty | *0.44 mg/kg* | Low endpoint for 95% | *2.53 mg/kg* |
| Expanded uncertainty for 95% | *1.05 mg/kg* | High endpoint for 95% | *5.37 mg/kg* |

**2,4,6-trichlorophenol**

TABLE XI. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,4,6-trichlorophenol compound

|  |  |  |
| --- | --- | --- |
| Uncertainty source | Distribution | Parameters of a distribution |
| Volume (*V*) | Normal | Mean: *75 ml*; SD: *2.55 ml* |
| Mass (*m*) | Normal | Mean: *10 g*; SD: *0.22g* |
| Recovery (*R*) | Student’s t Location-Scale | Mean: *88.41%*; SD: *8.80%*; DF: *3* |
| The area of peak (*y*) | Student’s t Location-Scale | Mean: *106234*; SD: *5000*; DF: *3* |
| Slope (*a*) | Student’s t Location-Scale | Mean: *-6070*; SD: *3479*; DF: *3* |
| Intercept (*b*) | Student’s t Location-Scale | Mean: *246943 l/mg*; SD: *6759 l/mg*; DF: *3* |
| Purity of standard | Uniform | Min: *-0.0401 mg/kg*; Max: *0.0401 mg/kg* |

\*SD – Standard Deviation; DF – Degrees of Freedom

TABLE XII. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,4,6-trichlorophenol compound

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter (GUM) | Value | Parameter (MC) | Value |
| Mean | *3.86 mg/kg* | Median | *3.86 mg/kg* |
| Combined standard uncertainty | *0.48 mg/kg* | Low endpoint for 95% | *2.48 mg/kg* |
| Expanded uncertainty for 95% | *1.17 mg/kg* | High endpoint for 95% | *5.56 mg/kg* |

**2,3,4,6-tetrahlorophenol**

TABLE XIII. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,3,4,6-tetrahlorophenol compound

|  |  |  |
| --- | --- | --- |
| Uncertainty source | Distribution | Parameters of a distribution |
| Volume (*V*) | Normal | Mean: *75 ml*; SD: *2.55 ml* |
| Mass (*m*) | Normal | Mean: *10 g*; SD: *0.22g* |
| Recovery (*R*) | Student’s t Location-Scale | Mean: *89.03%*; SD: *11.86%*; DF: *3* |
| The area of peak (*y*) | Student’s t Location-Scale | Mean: *43749*; SD: *2000*; DF: *3* |
| Slope (*a*) | Student’s t Location-Scale | Mean: *-4218*; SD: *2948*; DF: *3* |
| Intercept (*b*) | Student’s t Location-Scale | Mean: *109197 l/mg*; SD: *5727 l/mg*; DF: *3* |
| Purity of standard | Uniform | Min: *-0.0385 mg/kg*; Max: *0.0385 mg/kg* |
| \*SD – Standard Deviation; DF – Degrees of FreedomTABLE XIV. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,3,4,6-tetrahlorophenol compound

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter (GUM) | Value | Parameter (MC) | Value |
| Mean | *3.70 mg/kg* | Median | *3.71 mg/kg* |
| Combined standard uncertainty | *0.62 mg/kg* | Low endpoint for 95% | *1.92 mg/kg* |
| Expanded uncertainty for 95% | *1.51 mg/kg* | High endpoint for 95% | *6.14 mg/kg* |

 |
|  |

**Pentachlorophenol**

TABLE XV. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the pentachlorophenol compound

|  |  |  |
| --- | --- | --- |
| Uncertainty source | Distribution | Parameters of a distribution |
| Volume (*V*) | Normal | Mean: *75 ml*; SD: *2.55 ml* |
| Mass (*m*) | Normal | Mean: *10 g*; SD: *0.22g* |
| Recovery (*R*) | Student’s t Location-Scale | Mean: *85.13 %*; SD: *14.16%*; DF: *3* |
| The area of peak (*y*) | Student’s t Location-Scale | Mean: *28669*; SD: *1400*; DF: *3* |
| Slope (*a*) | Student’s t Location-Scale | Mean: *-5042*; SD: *3019*; DF: *3* |
| Intercept (*b*) | Student’s t Location-Scale | Mean: *82373 l/mg*; SD: *5864 l/mg*; DF: *3* |
| Purity of standard | Uniform | Min: *-0.0375 mg/kg*; Max: *0.0375 mg/kg* |

\*SD – Standard Deviation; DF – Degrees of Freedom

TABLE XVI. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the pentachlorophenol compound

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter (GUM) | Value | Parameter (MC) | Value |
| Mean | *3.61 mg/kg* | Median | *3.61 mg/kg* |
| Combined standard uncertainty | *0.76 mg/kg* | Low endpoint for 95% | *1.42 mg/kg* |
| Expanded uncertainty for 95% | *1.86 mg/kg* | High endpoint for 95% | *6.95 mg/kg* |