

## A load of dioxin-like compounds in bulk of technical PCBs formulation of Chlorofen

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### Introduction

Chlorofen is a trade name for a technical polychlorinated biphenyls (PCBs) formulation manufactured in Poland in 1966-1970<sup>1,2</sup>. Actually there is a set of analytical data available on chlorobiphenyl congener composition of Chlorofen and obtained with aid of a different HRGC systems and detectors used for quantification and including HRMS<sup>3-10</sup>. Apart from a primarily chlorobiphenyl constituents of Chlorofen there are also data available on by-side dioxin-like impurities of this formulation, *e.i.* a compounds such as polychlorinated dibenzo-*p*-dioxins (PCDDs), polychlorinated dibenzofurans (PCDFs), polychlorinated naphthalenes (PCNs) and hexachlorobenzene (HCBz)<sup>4,6,11-13</sup>. Therefore, based on these of high analytical quality data available and also of volume of Chlorofen made are given amounts of important dioxin-like active substances contained in bulk of this formulation.

### Materials and Methods

Chlorofen was manufactured in 1966-1970 and in total 1000 tonnes of this formulation was made<sup>1,2</sup>. These formulation is considered as chlorobiphenyls mixture of high-chlorination type with the total chlorine content of about 60 %<sup>5,8,9</sup>. Hepta- (43 %) and octachlorobiphenyls (38 %) are considered as a major chlorobiphenyl homologue group constituents of Chlorofen, and the total number of chlorobiphenyl congeners in this formulation could be up-to 100 as reported in one study, while 40 co-eluted<sup>8</sup>.

To assess a load of a particular chlorobiphenyl, chlorodibenzo-*p*-dioxin, chlorodibenzofuran and chloronaphthalene congeners as well as of hexachlorobenzene in bulk of Chlorofen all available data regarding those compounds constituting the mixture were reviewed<sup>3-13</sup>.

To assess a load of dioxin-like constituents of Chlorofen an available data on content of non- and mono-*ortho* chlorobiphenyls, PCDDs and PCDFs as well as their dioxin-like potency – as derived by the World Health Organization (WHO) have been used. To calculate a load of by-side dioxin-like chloronaphthalenes of Chlorofen the relative potency (REPs) factors as reported for the most active members have been used<sup>14</sup>.

### Results and discussion

In Table 1 are presented absolute data as reported in the literature, calculated average concentration and relative data on a load of most important dioxin-like constituents and contaminants in Chlorofen. PCBs as primarily constituents were more frequently examined in Chlorofen when compared to PCNs, and less were PCDDs and PCDFs.

In the case of dioxin-like PCDDs 1,2,3,4,6,7,8-HpCDD and OCDD are the only compounds found, and for PCDFs are only 1,2,3,4,6,7,8-HpCDF, 1,2,3,4,7,8,9-HpCDF and OCDF (Table 1). Due to small absolute concentration values the load of dioxin-like PCDDs

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Table 1. Table 1. Reported and average absolute concentrations (ng/g or µg/g), amount produced (g or kg), TEQ or ReP values and TEQs (g), respectively, for dioxin-like PCDDs, PCDFs, PCNs and PCBs of Chlorofen

| Compounds                                   | Absolute concentration<br>(ng/g) <sup>3-5,8-12</sup> | Average<br>(ng/g) | Amount<br>produced<br>(g) | TEF/ReP | TEQ<br>(mg)    |
|---|--|-------------------|---------------------------|---------|----------------|
| <b>PCDDs and PCDFs</b>                      |  |                   |                           |         |                |
| 2,3,7,8-TeCDD                               | < 0.1  | < 0.1             | 0                         | 1       | 0              |
| 1,2,3,7,8-PeCDD                             | < 0.2  | < 0.2             | 0                         | 1       | 0              |
| 1,2,3,4,7,8-HxCDD                           | < 0.1  | < 0.1             | 0                         | 0.1     | 0              |
| 1,2,3,6,7,8-HxCDD                           | < 0.07   | < 0.07            | 0                         | 0.1     | 0              |
| 1,2,3,7,8,9-HxCDD                           | < 0.1  | < 0.1             | 0                         | 0.1     | 0              |
| 1,2,3,4,6,7,8-HpCDD                         | 34   | 34                | 34                        | 0.01    | 0.34           |
| OCDD  | < 10; 99   | 50                | 50                        | 0.0001  | 0.005          |
| <b>Subtotal PCDDs</b>                       |  |                   |                           |         | <b>0.345</b>   |
| 2,3,7,8-TeCDF                               | < 0.1; < 10  | < 0.1             | 0                         | 0.1     | 0              |
| 1,2,3,7,8-PeCDF                             | < 0.2; < 10  | < 0.2             | 0                         | 0.05    | 0              |
| 2,3,4,7,8-PeCDF                             | < 0.2; < 10  | < 0.2             | 0                         | 0.5     | 0              |
| 1,2,3,4,7,8-HxCDF                           | < 10   | < 10              | 0                         | 0.1     | 0              |
| 1,2,3,6,7,8-HxCDF                           | < 0.2; < 10  | < 0.2             | 0                         | 0.1     | 0              |
| 1,2,3,7,8,9-HxCDF                           | < 0.08; < 10   | < 0.08            | 0                         | 0.1     | 0              |
| 2,3,4,6,7,8-HxCDF                           | < 0.2; < 10  | < 0.2             | 0                         | 0.1     | 0              |
| 1,2,3,4,6,7,8-HpCDF                         | 230; 800   | 520               | 520                       | 0.01    | 5.2            |
| 1,2,3,4,7,8,9-HpCDF                         | 70; 200  | 140               | 140                       | 0.01    | 1.4            |
| OCDF  | 260000; 350000                                       | 310000            | 310000                    | 0.0001  | 31             |
| <b>Subtotal PCDFs</b>                       |  |                   |                           |         | <b>37.6</b>    |
| <b>PCNs</b>                                 |  |                   |                           |         |                |
| 1,2,3,5,7-PeCN* (#52*/60)                   | 14; 70   | 42                | 42                        | 0.00001 | 0.00042        |
| 12367-PeCN (#54)                            | 6; < 10  | 6                 | 6                         | 0.00001 | 0.00006        |
| 12478-PeCN (#62)                            | 70; 230  | 150               | 150                       | 0.00001 | 0.00015        |
| 1,2,3,4,5,6-HxCN (#63)                      | 97; 100  | 100               | 100                       | 0.00001 | 0.0001         |
| 1,2,3,4,5,7-HxCN (#64)                      | < 10   | < 10              | 0                         | 0.00001 | 0              |
| 1,2,3,4,6,7- /1,2,3,5,6,7-<br>HxCN (#66/67) | < 10; 99; 140  | 80                | 80                        | 0.001   | 0.008          |
| 1,2,3,5,6,8-HxCN (#68)                      | 90; 180  | 140               | 140                       | 0.0001  | 0.014          |
| 1,2,3,5,7,8-HxCN (#69)                      | 200; 210   | 210               | 210                       | 0.00001 | 0.0021         |
| 1,2,3,4,5,6,7-HpCN (#73)                    | 5200; 5300   | 5300              | 5300                      | 0.001   | 5.3            |
| 1,2,3,4,5,6,8-HpCN (#74)                    | 2200; 3600   | 2900              | 2900                      | 0.00001 | 0.029          |
| 1,2,3,4,5,6,7,8-OcCN (#75)                  | 340000; 400000                                       | 370000            | 370000                    | 0.00001 | 3.7            |
| <b>Subtotal PCNs</b>                        |  |                   |                           |         | <b>9.05</b>    |
| <b>PCBs</b>                                 |  |                   |                           |         |                |
|   | µg/g   | µg/g              | kg                        |         | TEQ (g)        |
| 3,3',4,4'- (#77)                            | 0.065; < 1; 0.52; < 1.3; 15                          | 3.2               | 3.2                       | 0.0001  | 0.32           |
| 3,4,4',5'- (#81)                            | 0.077; < 1; < 5; < 10; < 10                          | 0.077             | 0.077                     | 0.0001  | 0.0077         |
| 2,3,3',4,4'- (#105)                         | < 1; < 2; < 5; < 10; 22; 100                         | 22                | 22                        | 0.0001  | 2.2            |
| 2,3,4,4',5'- (#114)                         | < 1; < 2; < 5; < 10; 17                              | 5                 | 5                         | 0.0005  | 2.5            |
| 2,3',4,4',5'- (#118)                        | < 1; < 2; < 5; < 10; 110; 900                        | 170               | 170                       | 0.0001  | 17             |
| 2',3,4,4',5'- (#123)                        | < 1; < 2; < 5; < 10; < 70                            | < 1               | 0                         | 0.0001  | 0              |
| 3,3',4,4',5'- (#126)                        | < 2; < 10; 0.25; 3.6; 82                             | 18                | 18                        | 0.1     | 1800           |
| 2,,3,3',4,4',5'- (#156)                     | < 1; < 2; 86; 130; 160; 400                          | 130               | 130                       | 0.0005  | 65             |
| 2,3,3',4,4',5'- (#157)                      | < 2; 8.9; 280; 2400; 4500                            | 1400              | 1400                      | 0.0005  | 700            |
| 2',3',4,4',5,5'- (#167)                     | < 1; 14; 28; 56                                      | 25                | 25                        | 0.00001 | 0.25           |
| 3,3',4,4',5,5'- (#169)                      | 0.43; < 1; < 1.8; 3.3                                | 1.2               | 1.2                       | 0.01    | 12             |
| 2,3,3',4,4',5,5'- (#189)                    | < 2; < 10; 69; 100                                   | 44                | 44                        | 0.0001  | 4.4            |
| <b>Subtotal PCBs</b>                        |  |                   |                           |         | <b>2603.68</b> |
| <b>Total TEQs (g)</b>                       |  |                   |                           |         | <b>2650.68</b> |

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and PCDFs to bulk of Chlorofen is 0.35 and 37.6 mg, respectively. Dioxin-like chloronaphthalene congeners when compared to dioxin-like active PCDD/Fs are more numerous in number in Chlorofen, while their contribution to total TEQ of bulk of this formulation is assessed for 9.0 mg (Table 1).

Dioxin-like active PCBs are highly dominant dioxin-like compounds in Chlorofen (Table 1). The load of dioxin-like non- and mono-*ortho* PCBs in bulk of Chlorofen is assessed as 2600 g TEQ, on the average. Nevertheless, both for non-*ortho* and mono-*ortho* chlorobiphenyls there is a wide range of concentrations reported in Chlorofen. If instead of the mean concentrations calculated the median values would be used in an assessment the load of dioxin-like non- and mono-*ortho* chlorobiphenyls is a much lower.

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