**Homework 4 - Solvent Substitution: CHEM21 Solvent Selection Guide**

*Readings and Resources:*

Using the open access article (required reading): <https://pubs.rsc.org/en/content/articlelanding/gc/2016/c5gc01008j#!divAbstract>

CHEM21 selection guide of classical- and less classical solvents, Green Chem., 2016, 18, 288-296.

Also use the CHEM21 open-access resources available here: <http://learning.chem21.eu/methods-of-facilitating-change/tools-and-guides/solvent-selection-guides/>

*Solvents in Printer Ink Formulations:*

Most of us are familiar with inkjet printers in the home or office. Within each printer is a cartridge of ink and a printhead which squirts out ink onto paper through a printhead consisting of a multitude of fine nozzles. The ink in these printers is composed of primarily water (~80%) and a colorant, but also contains a multitude of other components for which sustainability choices can be made.

Typical components and function of water-based inkjet ink formulations are:

* Water – the main component 60~90%
* Colorant – Soluble dye or pigment 2~10%
* Humectant co-solvent – Retains water in the ink to prevent drying of ink in the nozzles 5~20%
* Penetrant co-solvent – Wets paper fibers to allow ink to wick into the paper 1~10%
* Surfactant - Reduces the ink surface tension to allow for ink to ‘jet’ well in addition to controlling the ink spread on paper 0.2~5%
* Antimicrobial agents – prevents the growth of fungi and microbes 0.1~0.5%
* Others: polymers for viscosity control, pH buffers and sequestering agents 0~1%

For this homework, we will be focusing on the *co-solvents* that are used within water-based inkjet ink formulations. Two formulations are given below. Follow the steps to identify which formulation has more sustainable solvents. Identify opportunities in each for substituting solvents based on their properties using the CHEM21 selection guide. What alternatives would you suggest substituting in these formulations?

**Inkjet Ink Formulation 1:**

|  |  |  |
| --- | --- | --- |
| **Chemical** | **CAS#** | **Amount (grams)** |
| Water |  | 743 |
| *Ethylene Glycol* | 107-21-1 | 51.5 |
| *Diethylene glycol monomethyl ether* | 109-86-4 | 48.3 |
| *Dimethyl formamide* | 68-12-2 | 23.6 |
| Potassium heptadecafluoro-1-octanesulfate (Potassium perfluorooctanesulfonate) | 2795-39-3 | 2.0 |
| Pigment yellow 83 (diarylide) (2,2'-[(3,3'-Dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]) | 5567-15-7 | 30 |

**Inkjet Ink Formulation 2:**

|  |  |  |
| --- | --- | --- |
| **Chemical** | **CAS#** | **Amount (grams)** |
| Water |  | 743 |
| *Propylene Glycol* | 57-55-6 | 104 |
| *Isopropanol* | 67-63-0 | 39.3 |
| *Propylene glycol ether acetate* | 108-65-6 | 48.5 |
| *Glycerol* | 56-81-5 | 31.3 |
| Acetylinic diol Surfonyl 104 (2,4,7,9-Tetramethyldec-5-yne-4,7-diol | 126-86-3 | 2 |
| Pigment yellow 74 (2-[(2-Methoxy-4-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide) | 6358-31-2 | 30 |

The solvents are italicized in each of the formulations. Look up the solvents on the CHEM21 solvent selection guide table: <http://learning.chem21.eu/methods-of-facilitating-change/tools-and-guides/solvent-selection-guides/guide-tables/> and gather the data in the following tables.

If the solvent cannot be found on the solvent selection guide table, use the CHEM21 interactive tool to generate a score: <http://learning.chem21.eu/methods-of-facilitating-change/tools-and-guides/solvent-selection-guides/interactive-tool-chem21-guide/>

**Inkjet Ink Formulation 1:**

**Answer Key:**

***Solvent Physical Properties***

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Chemical** | **CAS#** | **BP (° C)** | **FP (° C)** | **Hazard Statements** |
| *Ethylene Glycol (from solvent guide table)* | 107-21-1 | 198 | 116 | H302 |
| *Diethylene glycol monomethyl ether (Methoxy ethanol) (from solvent guide table)* | 109-86-4 | 125 | 45 | H360 |
| *Dimethyl formamide (from solvent guide table)* | 68-12-2 | 153 | 58 | H360 |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Chemical** | **Safety Score** | **Health Score** | **Env. Score** | **Ranking by default** | **Ranking after discussion** |
| *Ethylene Glycol (from solvent guide table)* | 1 | 2 | 5 | Recommended | Recommended |
| *Diethylene glycol monomethyl ether (Methoxy ethanol) (from solvent guide table)* | 3 | 9 | 3 | Hazardous | Hazardous |
| *Dimethyl formamide (from solvent guide table)* | 3 | 9 | 5 | Hazardous | Hazardous |

**Inkjet Ink Formulation 2:**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Chemical** | **CAS#** | **BP (° C)** | **FP (° C)** | **Hazard Statements** |
| *Propylene Glycol (from data sources)* | 57-55-6 | 187 | 103 | none |
| *Isopropanol (from solvent guide table)* | 67-63-0 | 82 | 12 | H319 |
| *Propylene glycol ether acetate (from data sources)* | 108-65-6 | 145 | 45.5 | H226, H360 |
| *Glycerol (from solvent guide table)* | 56-81-5 | 290 | 177 | none |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Chemical** | **Safety Score** | **Health Score** | **Env. Score** | **Ranking by default** | **Ranking after discussion** |
| *Propylene Glycol (from the interactive tool)* | 1 | 1 | 5 | Recommended | Recommended |
| *Isopropanol (from solvent guide table)* | 4 | 3 | 3 | Recommended | Recommended |
| *Propylene glycol ether acetate (from interactive tool)* | 3 | 9 | 5 | Hazardous | Hazardous |
| *Glycerol (from solvent guide table)* | 1 | 1 | 7 | Problematic | Problematic |

*Propylene Glycol, CAS# 57-55-6:*

* Boiling point, flash point, auto-ignition temperature, resistivity; 187 C (BP), 103 C (FP), auto-ignition temp – 420C; resistivity – 0.34
* Whether or not it is an ether that forms explosive peroxides; No
* GHS statements and symbols; none
* Whether or not it is hazardous to the ozone layer; No
* Whether or not it is fully registered for REACH. Full registration

*Propylene glycol ether acetate, CAS#*108-65-6

* Boiling point, flash point, auto-ignition temperature, resistivity; 145-146 C (BP), 45.5 C (FP), auto-ignition temp 333 C; resistivity -
* Whether or not it is an ether that forms explosive peroxides;
* GHS statements and symbols; has 3 pictograms – GHS statements: H226, H360 GHS02: Flammable GHS07: Health hazard
* Whether or not it is hazardous to the ozone layer; and
* Whether or not it is fully registered for REACH. – Full registration

Data sources: Propylene Glycol, <http://www.inchem.org/documents/icsc/icsc/eics0321.htm>

SigmaAldrich SDS, Propylene Glycol, CAS# 57-55-6 (will have physical data, GHS statements and symbols information): <https://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=US&language=en&productNumber=P4347&brand=SIAL&PageToGoToURL=https%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fsearch%3Fterm%3D57-55-6%26interface%3DCAS%2520No.%26N%3D0%26mode%3Dmatch%2520partialmax%26lang%3Den%26region%3DUS%26focus%3Dproduct>

SigmaAldrich SDS, *Propylene glycol ether acetate*, 108-65-6 (will have physical data, GHS statements and symbols information): <https://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=US&language=en&productNumber=484431&brand=SIAL&PageToGoToURL=https%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fsearch%3Fterm%3D108-65-6%26interface%3DCAS%2520No.%26N%3D0%26mode%3Dmatch%2520partialmax%26lang%3Den%26region%3DUS%26focus%3Dproduct>

To inquire whether the chemical is fully registered for REACH: <https://echa.europa.eu/information-on-chemicals/registered-substances>