**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/>. The following information is needed to generate a score from the interactive tool:

* Boiling point, flash point, auto-ignition temperature, resistivity;
  + This data can generally be found on reliable Safety Data Sheets, or other reliable data websites (SigmaAldrich.com will have reliable SDS’s)
* Whether or not it is an ether that forms explosive peroxides;
* GHS statements and symbols;
  + This data can generally be found on reliable Safety Data Sheets, or other reliable data websites (SigmaAldrich.com will have reliable SDS’s)
* Whether or not it is hazardous to the ozone layer;
* Whether or not it is fully registered for REACH.
  + To inquire whether the chemical is fully registered for REACH: <https://echa.europa.eu/information-on-chemicals/registered-substances>

**Student Data Sheet**

**Inkjet Ink Formulation 1:**

***Solvent Physical Properties***

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Chemical** | **CAS#** | **BP (°C)** | **FP (°C)** | **Hazard Statements** |
| *Ethylene Glycol* | 107-21-1 |  |  |  |
| *Diethylene glycol monomethyl ether (Methoxy ethanol)* | 109-86-4 |  |  |  |
| *Dimethyl formamide* | 68-12-2 |  |  |  |

***Chemical Ranking Information***

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Chemical** | **Safety Score** | **Health Score** | **Env. Score** | **Ranking by default** | **Ranking after discussion** |
| *Ethylene Glycol* |  |  |  |  |  |
| *Diethylene glycol monomethyl ether (Methoxy ethanol)* |  |  |  |  |  |
| *Dimethyl formamide* |  |  |  |  |  |

**Inkjet Ink Formulation 2:**

***Solvent Physical Properties***

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Chemical** | **CAS#** | **BP (°C)** | **FP (°C)** | **Hazard Statements** |
| *Propylene Glycol* | 57-55-6 |  |  |  |
| *Isopropanol* | 67-63-0 |  |  |  |
| *Propylene glycol ether acetate* | 108-65-6 |  |  |  |
| *Glycerol* | 56-81-5 |  |  |  |

***Chemical Ranking Information***

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Chemical** | **Safety Score** | **Health Score** | **Env. Score** | **Ranking by default** | **Ranking after discussion** |
| *Propylene Glycol* |  |  |  |  |  |
| *Isopropanol* |  |  |  |  |  |
| *Propylene glycol ether acetate* |  |  |  |  |  |
| *Glycerol* |  |  |  |  |  |

***Additional Questions:*** Please justify your answers with your reasoning.

1. Please list the sources where you gathered the above data. If the solvent was found in the CHEM21 solvent selection guide table, please note that.

|  |  |
| --- | --- |
| **Chemical** | **Data Source(s) for BP, FP, Hazard Statements, and Safety, Health, Env. Scores and Ranking data** |
| *Ethylene Glycol* |  |
| *Diethylene glycol monomethyl ether (Methoxy ethanol)* |  |
| *Dimethyl formamide* |  |

|  |  |
| --- | --- |
| **Chemical** | **Data Source(s) for BP, FP, Hazard Statements, and Safety, Health, Env. Scores and Ranking data** |
| *Propylene Glycol* |  |
| *Isopropanol* |  |
| *Propylene glycol ether acetate* |  |
| *Glycerol* |  |

1. Which formulation would you recommend based on the rankings from the CHEM21 Solvent Selection Tool?
2. Which solvents do you still have concerns about?
3. What solvents would you recommend to formulators as alternatives that could be considered in attempts to create a formulation with greener solvents?