Software for the selection of chemical protective materials.
Description of ProtecPo and recent developments

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Introduction

The selection of chemical protective materials is a major problem due to the number of chemicals used in workplaces. REACH estimates that there are more than 100 000 chemical substances on the market. It is well known that no protective polymer material exists that protects against all classes of chemicals. The predictive software ProtecPo based on the Hansen solubility parameters approach HSP allows select the best protective materials for single and mixture of chemicals.

The Hansen Solubility Parameters approach

Hansen stated that the solubility parameter δ_t results of the contribution of three types of interactions: polar interactions, hydrogen bonds, and dispersion forces;

$$\delta_t = \sqrt{\delta_d^2 + \delta_p^2 + \delta_h^2}$$

More similar the solubility parameters of two substances , higher the solubility between them (*Like dissolves like*). The solubility of a chemical into a polymer can be estimated as follows:

$$A = \sqrt{4*\left(\delta_d^P - \delta_d^S\right)^2 + \left(\delta_p^P - \delta_p^S\right)^2 + \left(\delta_h^P - \delta_h^S\right)^2}$$

A is the **dissimilarity factor,** and the superscripts **P** the polymer and S the chemical. For a **binary mixture** of chemicals, A becomes …

$$A = \sqrt{4*\left(\delta_d^P - \delta_d^M\right)^2 + \left(\delta_p^P - \delta_p^M\right)^2 + \left(\delta_h^P - \delta_h^M\right)^2}$$

δ_t can be represented by a point with its three-dimensional coordinates in a figure with δ_d, δ_p and δ_h axes.

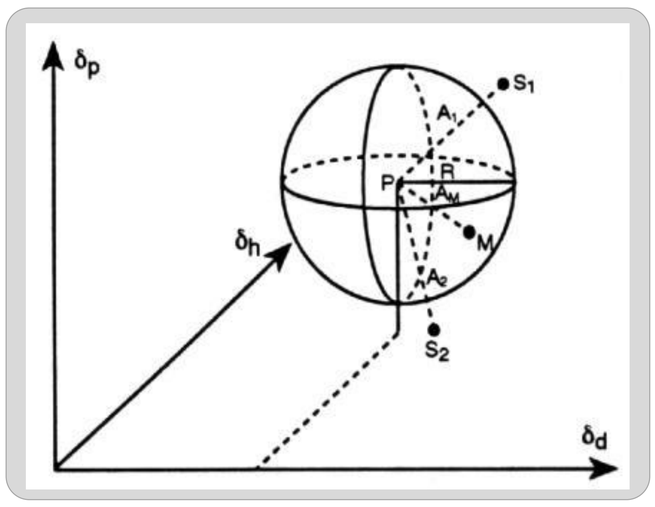

Figure 1 represents the Hansen solubility concept. The center of the sphere corresponds to δ_d, δ_p and δ_h of a polymer with **radius R** (the solubility limit).

S_1 and S_2 are the coordinates of chemicals with values A_1 and A_2 values higher that the radius R. The chemicals are not soluble into the polymer.

The A value for a mixture of S_1 + S_2 (M) fall inside the sphere (A<R). The chemical mixture is soluble into the polymer

Hansen defined the **Relative Energy Difference** (**RED**) as follows ;

$$RED = \frac{A}{R}$$

Relative Energy Difference

For **RED > 1**
the chemical is **non soluble into the polymer**.

For **RED < 1**
the chemical is soluble into the polymer.

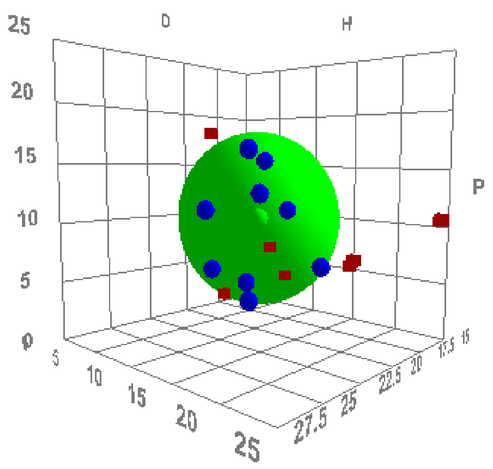

Figure 3 is the calculated solubility sphere for a polymer material. In red are the chemicals that are not soluble into the polymer and in blue, the chemicals that are soluble.

The development of the ProtecPo software

Given that Chemical protective clothing and gloves are made in polymer materials, the Hansen approach was used to develop ProtecPo.

The Algorithm

Figure 3 show the sequence followed in the development of ProtecPo. Each polymer material was submitted to swelling tests with 40 selected solvents. The R and HSP for protective materials (Nitrile, Neoprene, Butyl, Latex and Viton) were calculated using the SPHERE software. More than 3000 swelling tests were performed.

The algorithm assumes that the radius of the sphere, is not a frozen value but can be represented by a zone of uncertainty (in **yellow** on Figure 4). The polymer is resistant for the chemicals that are located in the **green zone** and is not resistant for those in the **red zone**.

The limits, RED_{min} and RED_{max} values, are specific for each material.

The developed algorithm was validated by comparing ProtecPo's predictions to experimental results found in the scientific literature and glove manufacturers, as well as by comparing these predictions with standardized permeation tests.

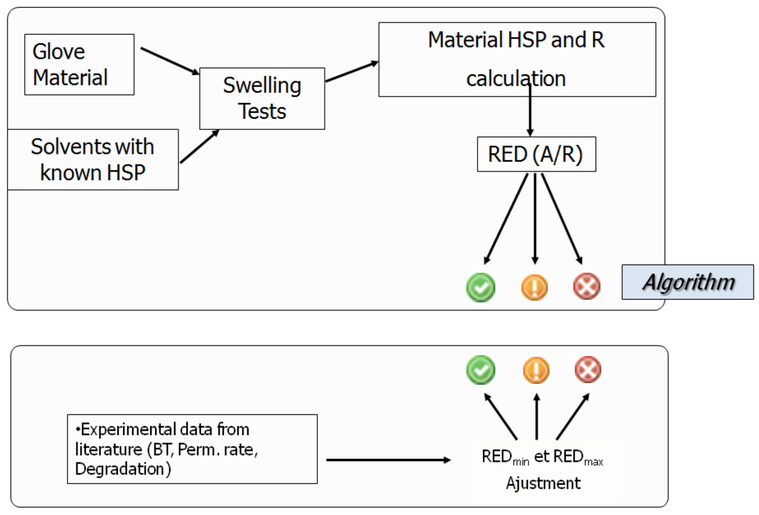

Figure 4

The ProtecPo Software

https://protecpo.inrs.fr/

The predictive software contains information on the five more frequently used protective materials and 1200 chemicals substances. The search can be made by substance name or CAS number to create chemical mixture compositions (**Figure 5**). The search can also be made by chemical family (**Figure 6**) or by protective material.

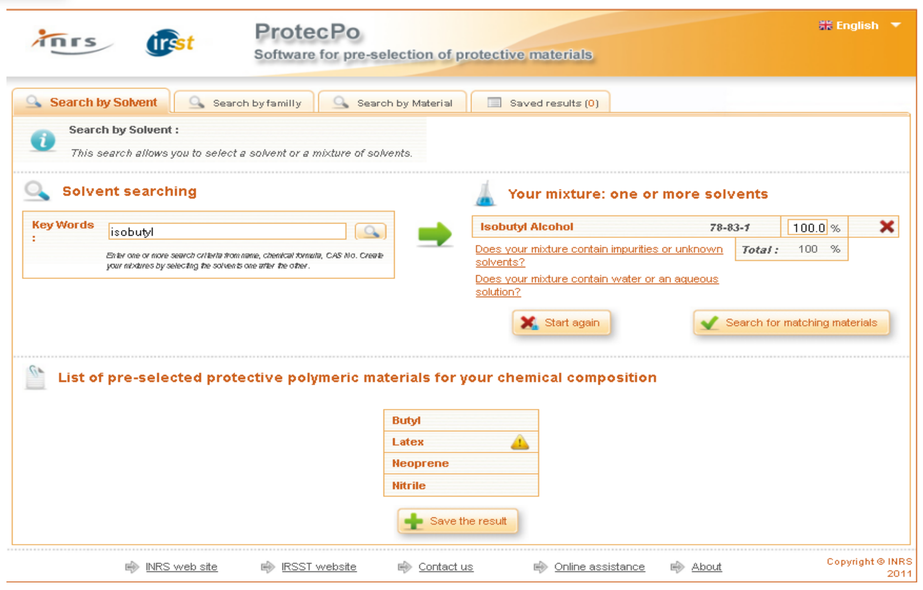

Figure 5: Screenshot of a Search made by chemical substance

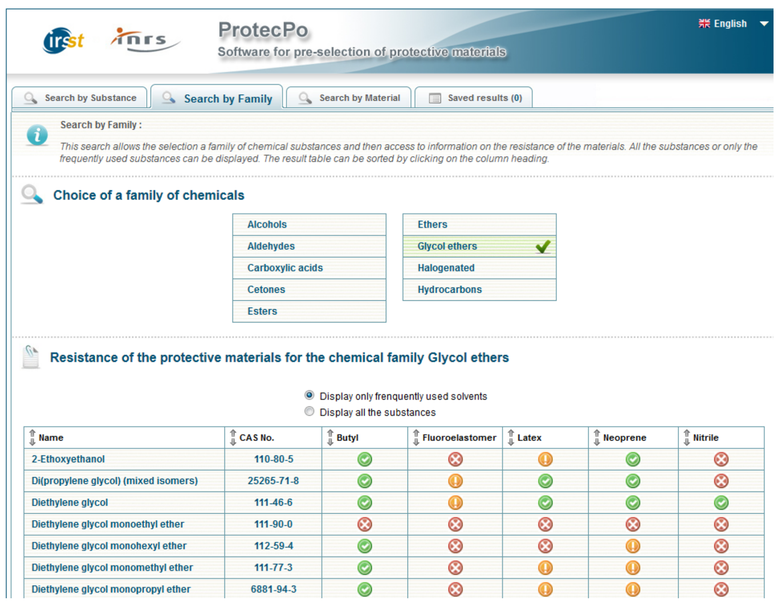

Figure 6: Screenshot of a Search made by chemical family

New Developments

In a collaborative international effort, a project to develop a new database containing 10000 chemicals is in progress. Swelling and permeation test on randomly selected chemical-materials pairs will be performed. If necessary, adjustments on the calculated HSP and RED_{max} and RED_{min} will be done.