



## Shortcut applications of the Hansen Solubility Parameter for Organic Solvent Nanofiltration



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### ABSTRACT

In this paper the representation of the Hansen Solubility Parameter (HSP) in a ternary diagram is explored in order to define new applications for it in the field of Organic Solvent Nanofiltration (OSN). The use of the HSP is extended to the qualitative prediction of the behaviour of solvents or solutes in OSN as well as to estimate the HSP of ceramic membranes. This is done by representing the three components of the HSP as the axes of the ternary diagram and observing the relative positions of the HSP of solvents and solutes. In general, the closer two points are in the diagram, the larger the interactions. In membrane processes a larger solvent-membrane interaction is linked to a higher flux through the membrane; thus, plotting the flux of pure solvents through a given membrane and grouping these data by flux is postulated to give an estimation of the HSP distribution of the membrane. As a result, knowing the HSP of every component in a membrane filtration system is the first step into developing an affinity driven model for OSN with the HSP as the main parameter to describe the internal interactions not only of the solvent but also of the solute and the membrane. This is demonstrated for non-swelling ceramic membranes, for different solvents and solutes, which are scattered in the HSP diagram. It was concluded that the trend of the fluxes, ranging between 47 and 300 l h<sup>-1</sup> m<sup>-2</sup>, and rejection (−5% to −85%) match well with their position in the diagram, which opens the possibility to a more quantitative prediction of performance, and to specifically design applications based on a given membrane.

### 1. Introduction

Membrane processes are becoming more and more industrially important and their application field is growing continuously. Organic solvent nanofiltration (OSN or Solvent Resistant NanoFiltration) is an up-coming technology with a vast application potential as an alternative purification technology for molecular separation of solutes in organic solutions [1,2]. Up to 10 years ago, it was hardly possible to treat organic solutions with nanofiltration due to the lack of stable membrane materials and efficient know-how about processing of these systems. On the OSN market dynamics the study of Frost & Sullivan of 2008 [2] states the following: "According to the "Chemical Industry Vision 2020 Technology Partnership" document, separation processes account for 40–70% of both the capital and operating costs in a process industry. Those values confirm the necessity of separation technologies and simultaneously depict the tremendous market potential as well".

For a wide range of applications, OSN offers significant reductions

in energy consumption or the use of raw materials. It allows for replacement of expensive processes, like thermal distillation or evaporation [1]. However, OSN is today still applied on a trial-and-error basis, based on practical experiences with various membrane/solvent combinations; research is mostly focused on developing new polymeric membranes capable of resisting organic solvents, avoiding decay on their lifespan and selectivity while maintaining a high flux especially through new material combinations and crosslinking.

In addition to the development of new OSN membranes, understanding the fundamentals of transport of solvents and solutes through the membrane and expressing this in a practical model should attract more attention of the research community. Nowadays not even the first principles of the transport phenomena in OSN are clear and agreed on. Some research is based on viscous flow understanding of the permeation [3,4], some is based on solution-diffusion [5,6] and some is based on a mixture of both mechanisms [7–10]. Furthermore the literature on transport mechanisms in OSN shows that mutual interactions between

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the solvents and the material at the membrane top layer (*i.e.*, the separating layer) are key to determine the separation performance [10–12]. Considering that they have a large influence on the separation of solutes [5,13], however, the importance of the solute-membrane interactions has received much less attention even when it is known that equal solvent/membrane pairs show different results with different solutes [14]. The affinity between the solvent and the membrane, the solute and the membrane and between the solvent and solute determine the rejection and contrary to aqueous filtration solute affinities cannot be so easily neglected. For example, when the affinity between solute and membrane is higher than between solute and solvent, a lower rejection is expected [15]. Thus, there is a lack of “know-how” on separation of specific organic solutions due to a poor understanding of the influence of the mixtures constituents on the overall process performance, which is determined by the solvent, solute and membrane surface as well as all mutual interactions. A comprehensive transport model, which takes into account interactions and properties of the membrane, solvent and solutes, should allow for a correct prediction of the separation performance, which is necessary for general industrial applications of this separation technology.

Independently of the transport mechanism considered every model up to date is based on different parameters. Some of them introduce values for the internal interactions membrane-solvent but in general they are based on solvent and membrane parameters; following this, the behaviour of these solvents are fitted for a certain solute. The list of different parameters employed is long and includes either parameters with direct physical meaning (*e.g.*, viscosity, surface tension,...) or fitting parameters. However, there is a single one that is invariably present in every model, the solvent viscosity [16]. This is due to the fact that even dense membranes have some free volume within their structure that might act as a pore [17,18], allowing viscous flow behaviour, which is ruled by the viscosity of the solvent. However, due to the small size of these pores the role of the internal interactions increases, creating deviations from viscous flow. Consequently solvent viscosity still plays an important role in the separation but is not sufficient to provide a general explanation for solvent filtration.

Actual models lack a general predictive ability. They are able to predict the behaviour of series of solvents (solvents of the same type, *e.g.* alcohols, ethers, *etc.*) for a determined membrane but cannot make a general prediction, failing to explain the performance of some other solvents tested. This is usually related to the necessity of calculating a fitting parameter for each membrane-solvent pair [16]. However, a new parameter has been recently introduced in OSN in order to explain the interactions present in the system; the Hansen Solubility Parameter (HSP). The work of Buekenhoudt et al. on ceramic nanofiltration membranes [19] proved that the HSP has a great potential to explain the membrane-solvent interactions as the HSP of the solvent correlates very well to a wide range of solvent fluxes. The previous exploration of other solvent variables such as the dielectric constant or the polarity are covered and complemented by the HSP, as this parameter takes into account all the intermolecular forces that drive molecular affinity (dispersion, polarity and hydrogen bonding). More recent work of the same group [24] shows that the HSP of the solvent is also relevant in considering retentions of grafted ceramic membranes in OSN. The introduction of the HSP parameter provides the necessary importance to the interactions between components (solvents, solutes and membranes) and thus opens the option of understanding OSN as an affinity driven process.

The work of Buekenhoudt et al. [19] provides a starting point for the use of the HSP by employing the HSP of the solvent; however, the explanation should be extended to include solute and membrane solubility parameters, which can be relatively easily calculated by a group contribution method if they are both organic compounds/materials [20,21]. In the case studied by Buekenhoudt et al. [19] a new problem appears due to the use of TiO<sub>2</sub> ceramic membranes that – contrary to polymeric membranes – do not allow the use of a group contribution

method to estimate the HSP. That is because titanium and its bonds are not present in the existing group contribution data bases [20,21].

This paper deals with different new practical applications of the HSP in OSN beyond the point of calculating to which extent two solvents are miscible. These applications can be split in two groups; (1) estimating the HSP of ceramic membranes and (2) using the HSP in order to estimate performance of different solvents or solutes beforehand. All applications will be based on a graphical representation of the HSP in a ternary diagram, a concept that was first introduced by Teas et al. in the late 1960s [22] and has attracted much interest in the literature for its usefulness in selecting solvents for making polymer solutions, even nowadays [23].

In this work we focus on ceramic membranes, as the flux and retention data for these membranes is not influenced by swelling, an effect further complicating interpretation, prediction and modelling of OSN performance. Remark that for these non-swelling ceramic membranes, solvents and solutes will not solve in the bulk of the membrane as for polymeric membranes; they can merely adsorb on the membrane pore surface. This paper will show that these adsorption/interaction phenomena important for OSN can be well assessed using the HSPs of all components.

## 2. Methods

### 2.1. Use of the ternary HSP diagram

In a Teas plot or ternary HSP diagram [22], the three components of the HSP are used as reference axes in a diagram. The axes form a triangular diagram with the three axes representing the values of dispersion, polarity and hydrogen bonding components of the HSP of a compound in percentages, so that the sum of the three coordinates is always 100%. Eq. (1) is an example for the coordinates on the dispersion axis.

$$\%_{d\text{Teas}} = \frac{\delta_d}{\delta_d + \delta_p + \delta_h} \cdot 100 \quad (1)$$

Fig. 1 shows an example of such a Teas plot, representing the HSP of common solvents taking the values from the work of Hansen [21]. Setting the diagram as a ternary distribution of HSP values makes it easy to see in 2D the relationships between the dispersion, polarity and

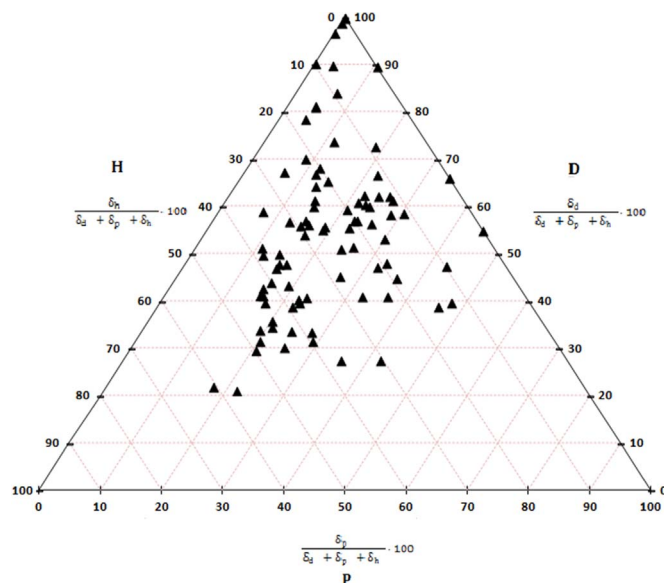


Fig. 1. Example of the triangular representation of the HSP where D is for dispersion forces, P for polar forces and H for hydrogen bonding forces. The points represent common solvents.

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