

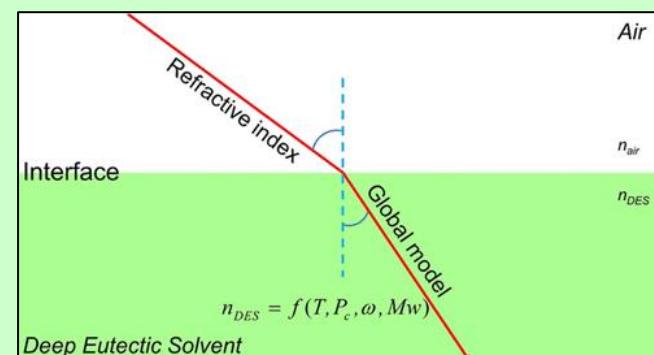


## Ongoing work – DES Thermodynamic Modelling

Des.solve Research Group, in collaboration with Shiraz University, has proposed two models applicable to DES: one to estimate the refractive indices of various types of DES and other for viscosities.

### Generalized Model to Estimate the Refractive Indices of Deep Eutectic Solvents

The goal was to develop an accurate, global, simple, and easy-to-use model for estimating the refractive indices of large numbers of DES having different natures. For this purpose, a large up-to-date data bank for DES was collected, consisting of 1203 data points from 153 different DES. The proposed model requires critical pressure, molecular weight, and acentric factor as the input parameters and these parameters are calculated by suggested procedures. Therefore, in essence, to be used, the refractive index model does not need any experimental data. The overall absolute average relative deviation, AARD%, of the proposed model for all of the investigated DES was 1.03%, which indicates high accuracy, as well as generality, for the estimation of the refractive indices of DES.



Mehrdad Taherzadeh, Reza Haghbakhsh, Ana Rita C. Duarte, Sona Raeissi, "Generalized Model to Estimate the Refractive Indices of Deep Eutectic Solvents". *J. Chem. Eng. Data*, 2020, 65(8), 3965–3976

### A Simple Model for the Viscosities of Deep Eutectic Solvents

Based on a databank covering 156 DES of different natures, a straightforward, simple, accurate, and global correlation was proposed. This model, which covers wide ranges of temperatures, requires the critical pressure, critical temperature, and one reference viscosity data as its input parameters. Since the model has one set of global constants, it can be used for any DES. Apart from this correlation, a second approach was also taken in this study, which was to obtain the constants of the Vogel-Fulcher-Tamman (VFT) model for all of the investigated DES. With this approach, the constants are individually fit to each DES, therefore, no physical properties are required as input. The results indicate that the proposed correlation, in addition to its acceptable accuracy and simplicity, is a general model for the estimation of the viscosities of different-natured DES.

Ali Bakhtyari, Reza Haghbakhsh, Ana Rita C. Duarte, Sona Raeissi, "A simple model for the viscosities of deep eutectic solvents". *Fluid Phase Equilibria*, 2020, 521(112662)

## Deep Eutectic Systems on the spotlight to fight COVID-19

Dexamethasone, a widely known steroid drug, has demonstrated, in a clinical study performed by Oxford University researchers, to reduce the risk of death for Covid-19 patients on a ventilator by 35%, and for those on oxygen by 20%. Although it does not treat the disease, it can help its management in more severe patients. Once the drug can dramatically improve Covid-19 survival for these patients in hospital, much more lives can be saved. The drug should now become "standard of care" in Covid-19 patients requiring ventilation or oxygen, according to researchers.

THEDES based on Choline Chloride and Ascorbic Acid significantly enhance the bioavailability of **dexamethasone** in physiological media

**65-fold increase in solubility**  
**Almost doubled permeability**  
**Non cytotoxic up to 1.5 mg/mL**

In this context, THEDES (Therapeutic Deep Eutectic Systems) may play an important role. THEDES are composed of two or more compounds in which one of them is an active pharmaceutical ingredient (API), whose bioavailability can be increased by the system. In a study, carried out by Des.Solve and 3B's Research Group, it was found that THEDES based on Choline Chloride and Ascorbic Acid significantly enhance the bioavailability of dexamethasone in physiological media. This means that the therapeutic effect of dexamethasone is more efficient when the drug is administered in specific THEDES, once it is more easily absorbed by the body. In this sense, allying dexamethasone to a specific THEDES could be of great value, not only to the fight of Covid-19, but also of other pathological conditions requiring this drug.

Silva, et al., *ACS Sustainable Chem. Eng.* 2018,6, 10355-10363

## Publications

- "Optimal Design of THEDES Based on Perillyl Alcohol and Ibuprofen" – *Pharmaceutics*
- "Organic Salts Based on Isoniazid Drug: Synthesis, Bioavailability and Cytotoxicity Studies" – *Pharmaceutics*

Despite some confinement periods at home in this atypic year, due to COVID-19 pandemic, Des.Solve team tried to ally professional obligations with well-being and healthy habits.



Des.Solve team gathered for a teambuilding activity in nature. It involved one day walking and simultaneous mentoring, with the aim to slow down, reconnect, focus and gain perspective to take action. During the activity, the team discussed some professional challenges and proposed future solutions.