

An Indian-Australian research partnership

**Project Title:** **Process engineering aspects for use & synthesis of ionic liquids for extraction of aromatics from different feed**

**Project Number** IMURA0427



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## Research Academy Themes:

**Highlight which of the Academy's Theme(s) this project will address?**

*(Feel free to nominate more than one. For more information, see [www.iitbmonash.org](http://www.iitbmonash.org))*

1. **Advanced computational engineering, simulation and manufacture**
2. **Infrastructure Engineering**
3. Clean Energy
4. Water
5. Nanotechnology
6. Biotechnology and Stem Cell Research

## The research problem

*Define the problem*

The project would have 5 parts (2 Ph.D students)

- 1) Predict using an open source model such as the COSMO-SAC model the possible options for Ionic

liquids for extraction of aromatics. A selection algorithm for the ionic liquids

- 2) Verification of the prediction of the model by use of base-line experiments for checking the prediction using 2 or 3 groups of compounds : For example –
  - i) a comparison between extraction of polar and non-polar entities
  - ii) a comparison between extraction of hydrocarbon and oxygenated hydrocarbon
- 3) Experimental validation of predicted ionic liquid performance
- 4) VLE & LLE data for the feed streams
- 5) Possible synthesis of the ionic liquids

Aromatic hydrocarbons present in petrochemical streams need to be separated from the remaining aliphatic and olefinic hydrocarbons. However, this separation is difficult due to overlapping boiling points and azeotrope formation. Conventional processes for this type of separation are extraction or extractive distillation with polar, organic solvents. However, for feeds with low aromatic content (< 20%) those conventional processes are not suitable since their aromatic extraction capacity is low.

Recently it has been shown that ionic liquids can have higher capacity and selectivity in the concentration range < 20% aromatic content. Therefore, in this work ionic liquids can be used and compared to conventional solvents in order to investigate their extraction capacity for petrochemical streams with low (<20%) and high ( 50-70%) aromatics content. Hence, the aim of this work would be to evaluate the suitability of ionic liquids for the extraction of aromatic hydrocarbons from various petrochemical streams with multiple aromatics, serving as carburant fuel sources. Different petrochemical streams need to be investigated: Virgin (Straight run) Naphtha, Reformate, PyGas and FCC Gasoline. These streams have been chosen, because of their aromatic content. Hence, all streams where aromatics have to be removed. On the other hand they contain different amounts and types of aromatics which offer the possibility to study the extraction capacity of ionic liquids for several aromatic components.

## Project aims

*Define the aims of the project*

1. Selection algorithm for ionic liquid for extraction of aromatics from select petrochemical feed
2. Short list of ionic liquids
3. Experimental validation of the algorithm and the performance of the ionic liquids
4. VLE & LLE data
5. Synthesis of the ionic liquid

## Expected outcomes

*Highlight the expected outcomes of the project*

1. Literature review – ( 2 research publications)
2. COSMO- SAC model parameters and an selection algorithm

3. Short list of Ionic Liquids
4. Toxicological data from literature for EHSS
5. Experimental plan
6. Synthesis of the ionic liquids
7. VLE/ LLE data for the for the selected ionic liquids

### **How will the project address the Goals of the above Themes?**

*Describe how the project will address the goals of one or more of the 6 Themes listed above.*

The project involves the use of COSMO-SAC model to predict the possible properties of the ideal ionic liquid which can be used for experiments and hence relates to ADVANCED SIMULATION domain

Also the synthesis of the ionic liquids and the subsequent determination of the VLE and LLE data relates to the MANUFACTURE and INFRASTRUCTURE ENGINEERING domain.

### **Capabilities and Degrees Required**

*List the ideal set of capabilities that a student should have for this project. Feel free to be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can demonstrate these capabilities.*

1. Master's in Chemical Engineering or Master's in Organic Chemistry or Industrial Chemistry
2. Good report writing & communication skills
3. Hands on experience on simulation or experimentation in synthesis of chemicals/petrochemicals/fine chemicals or pharma intermediates
4. Good chemical engineering fundamentals – to be ascertained by a telephonic or personal interview