HyChem

PHD RESEARCH PROPOSAL

Doutoramento em Engenharia da Refinação, Petroquímica e Química (EngIQ)

LIQUID ORGANIC HYDROGEN CARRIERS OPTIMIZATION

Summary / Framework

Liquid Organic Hydrogen Carriers (LOHC) are very promising materials that will allow the industry to overcome two of most serious challenges to the New Hydrogen Economy: hydrogen's low storage energy density (MWh/m^3) and safety issues, with the consequent problems concerning logistics of both storage and supply, mainly due to high pressures or low temperatures. These compounds are capable of store and transport hydrogen at atmospheric pressure and room temperature, without the conventional problems. Another important factor for these reactions is the catalyst used. It must be a catalyst with hydrogenation capacity (and dehydrogenation) capacity. The catalysts that are usually used are noble metals (for example platinum (Pt), palladium (Pd), ruthenium (Ru) and rhenium (Re)) deposited on inert supports (for example alumina (Al_2O_3), activated carbon and silica (SiO_2).

LOHC materials have in common the possibility of a reversable hydrogenation reaction, allowing their reuse. The system is composed by a hydrogen-lean molecule, that is hydrogenated and becomes a hydrogen-rich molecule. This hydrogen-rich molecule is then dehydrogenated, releasing the stored hydrogen and returning to its hydrogen-lean state, thus achieving a full cycle. The hydrogenation reaction is carried out between 50 and 250 ºC and between 20 and 50 bar and is exothermic. On the other hand, the dehydrogenation reaction is carried out at high temperatures, between 200 and 420 ºC, low pressures, between atmospheric and 5 bar and is endothermic, which means that it is necessary to supply it with the necessary energy.

There are numerous potential LOHC compounds, being the most attractive the ones that present the following characteristics, among others:

- Liquid state in a large range of temperature and low vapor pressure. This will allow an easier separation between LOHC and H_2;
- Storage capacity of hydrogen must be reasonable, between 5.7 and 7.3 % weight of hydrogen;
- Low Toxic Potential Indicator (TPI) (the lower, the less toxic);
- Stable at the reaction conditions (hydrogenation and dehydrogenation) to allow a cyclic process;
- Low production cost;
- Available;
- Non-flammable.

There is yet a lot to be developed in this very promising area, both in the hydrogenation and de-hydrogenation stages, which still require optimization of the process conditions and the choice/development of the adequate LOHC and catalysts.

The aim of this PhD proposal is to optimize the process conditions, identifying adequate catalysts for both hydrogenation and dehydrogenation and achieve an effective LOHC solution at industrial scale.