Optimization of the reaction mixture and validation of the microreactor platform for the stereoselective hydrogenation in presence of ionic liquids

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Stereoselective hydrogenation can be performed using Ruthenium BINAP complex (2,2'-bis(diphenyl-phosphino)-1,1'-binaphtyl) [1]. A pseudo-immobilisation of this complex into an ionic liquid allows for an easy separation of this stereoselective catalyst [2]. In combination with a microreactor platform, which is capable of enhancing the mass and heat transfer, a very flexible reactor for such purposes can be built up.
An optimization of a colloidal reaction mixture, containing the Ruthenium BINAP complex in an ionic liquid, methanol, water, source of hydrogen and reactant, consists of various parts:

(i) A suitable ionic liquids should be selected. A series of tetraalkylaamonium bistriflamides (N[R,222][Tf2N]) with N = 4, 6, 8, 10 and 12 were tested.

(ii) An optimum amount of water to keep the reaction mixture homogeneous has to be found, because bistriflamide ionic liquids and water show limited miscibility. The three-phase diagram of a mixture IL (N = 8), methanol and water was predicted using the COSMO-RS methodology.

(iii) A suitable source of hydrogen has to be chosen – either a donor or gaseous hydrogen.

A validation of the microreactor platform for the stereoselective hydrogenation has also been realized:

(i) A calibration of a micro-pump for the volume flow rate was carried out.

(ii) Inputs of all reactants including the possibility of gaseous hydrogen were prepared.

(iii) A correction for the pressure drop on entrance effects was approached by performing comparable measurements using a bypassing of the microreactor.

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