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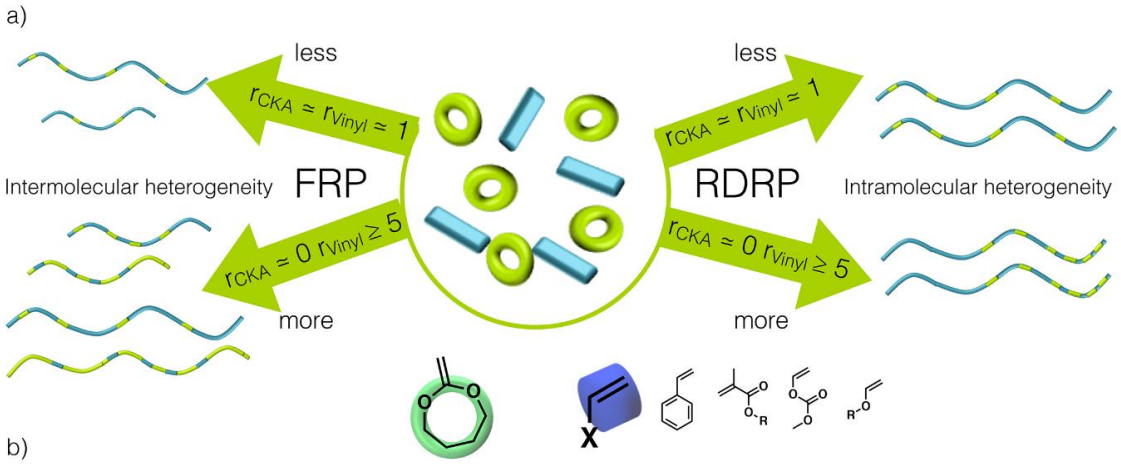
# Modelling of sustainable vinyl polymer production

## Aim

Finding reactor operator conditions to tune the molecular structure of renewable vinyl polymers.

## Justification

Traditional vinyl polymers are not biodegradable but display excellent material properties. In contrast, biodegradable polymers such as polyesters can be easily (bio)degraded via hydrolysis but lack high mechanical strength. The best of both worlds can be achieved by incorporating ester moieties along the vinyl backbone, providing susceptibility to hydrolysis and achieving (bio)degradation, which is an ambitious task as monomers for polycondensation and radical polymerization processes can't react in one single process. One promising route is the radical polymerization (FRP) of traditional vinyl monomers and novel cyclic ketene acetals (CKA) monomers, the ring opening of which provides the critical (bio)degradable ester moiety during FRP (see green monomer in the Figure below).




Many chemists are investigating batch processes in which the reactivity of the CKA type is tuned based on the reactivity of the vinyl monomer (styrene, (meth)acrylates, vinyl ether, *etc.*). This chemical approach reduces composition drifting to some degree, incorporating the CKA at regular distances along the vinyl backbone, providing efficient biodegradation. However, composition drifting can be nearly completely avoided by using semi-batch feeding of reactors, in which the more reactive "CKA" monomer is slowly fed over time to a reactor containing all the "'slower" vinyl monomer, thereby greatly uniformizing the vinyl segment length and achieving optimal (bio)degradability. Such reactor operation provides opportunities for advances in polymer reaction engineering to complement advances in polymer chemistry recently achieved by research labs in Marseille and Singapore, paving the way to sustainable polymers production without compromising material properties of vinyl polymers.

## Program

1. Surveying the literature and constructing a database of reactivity ratios of vinyl-CKA pairs.
2. Adapting an existing polymerization model (for batch vinyl homopolymerization) toward semi-batch copolymerization.
3. Based on the model outcome, construction of the correlations between operating conditions (batch time, feeding regime, *etc.*) and the molecular structure of polymers (vinyl segment length, composition drifting, *etc.*).
4. Revealing the best operating conditions for optimal molecular structure of sustainable polymers.