Fossil vs. Renewable Sources for Chemicals Production: A New Process for the Production of Acetonitrile from Bioethanol Compared with the Sohio Process

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Abstract

Acetonitrile is mainly used as a solvent for pharmaceutical and laboratory applications (nearly 70%), but is also used in the extractive separation of butadiene from C_4 alkanes and in other similar processes. It is a byproduct of the acrylonitrile synthesis (6 Mton in 2010) and its yield depends on how the main process is operated. This intrinsic dependence is the underlying reason for the recognized mismatch between its demand and availability worldwide.
Routes to acetonitrile as the main reaction product have been sought and an efficient atom-economy could be achieved by using C_2 substrates, such as ethanol, ethane and ethylene. Ethanol as a reactant is a promising alternative being a renewable resource, readily available from established fermentation processes and usable for this process without particular purification requirements.
A new fully integrated ethanol-to-acetonitrile production plant has been designed here from the grass roots on a pilot scale (10 kg/h) from ethanol, ammonia and air. Besides the reaction section, the full separation train for pure acetonitrile recovery (> 99%) has been optimized and integrated with the recovery of all the byproducts (CO_2, HCN) and unreacted NH_3. The recovery and valorisation of the marketable byproducts (cyanide salts and NH_4HCO_3) is also discussed. Finally, the process consumes more CO_2 than what constitutes the reactor byproduct, allowing the further sequestration of this greenhouse gas.
In order to evaluate the potential benefits of the bio-based synthesis of acetonitrile a Life Cycle Assessment (LCA) approach was applied by comparing the environmental scores of the renewable route with those achieved by the traditional fossil-based pathway. A cradle to gate perspective, from raw material extraction up to the acetonitrile production, has confirmed the lower impacts in terms of resources depletion and environmental burdens for the innovative and renewable synthetic process.