



Process to Manufacture Branched Caprolactone

IP Status: Pending US Patent; **Application #:** 16/562,971

Two-stage process manufactures methyl- ϵ -caprolactone (MCL)

A cost effective, new two-stage chemical process manufactures methyl- ϵ -caprolactone (MCL) from cresol, a fossil or bio-renewable feedstock. Details for designing a process optimized for net present value (including unit operation design of two reactors, distillation and integrated heat transfer) were determined via process simulation. The two-reaction process first hydrogenates cresol to methyl-cyclohexanone, which is then followed by Baeyer-Villiger oxidation to MCL. Improvements in overall selectivity via catalytic performance of the Baeyer-Villiger oxidation catalyst boost the overall economics of the process, rendering it a low-cost process broadly applicable to multiple classes of alkyl-phenol feedstocks. The novel process can manufacture MCL for use in polymer/plastics.

Technology ID

2019-011

Category

Engineering & Physical Sciences/Chemicals
Engineering & Physical Sciences/Materials
Engineering & Physical Sciences/Sustainable Technology

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Combines all reaction, separation and purification operations

Polymers related to poly- ϵ -caprolactone (PCL), which have many biomedical and industrial field applications, could be derived from biobased starting materials, but the challenge has been finding a cost effective route to the starting monomer. This new process uses already-existing chemistry in a brand new way, putting all reaction, separation and purification operations together in a cost-competitive manner. The result is a high yield and inexpensive method of producing 4-methyl- ϵ -caprolactone (and other alkyl caprolactones) from lignin or petroleum-based starting materials.

Phase of Development

- Proof of concept. Simulation models with technical description of chemical process conditions and unit connectivity with economic analysis.

Benefits

- Low-cost process; potential for extremely lucrative chemical product
- High process yield potential
- Broadly applicable to multiple classes of alkyl-phenol feedstocks
- Aspen model based technoeconomic analysis available

Features

- Manufactures methyl- ϵ -caprolactone (MCL) (and other alkyl caprolactones) from biobased cresol, lignin or petroleum based starting materials
- Two-stage chemical process
- Baeyer-Villiger oxidation catalyst improves overall selectivity
- Combines all reaction, separation and purification operations together

Applications

- Chemicals/polymers
- Caprolactone
- Monomers
- Methyl- ϵ -caprolactone (MCL) manufacture

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Publications

[*Techno-Economic Analysis of a Chemical Process to Manufacture Methyl- \$\epsilon\$ -Caprolactone from Cresols*](#)

ACS Sustainable Chem. Eng., Publication Date (Web): September 28, 2018

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