Simulation and Optimization of Volatile Fatty Acid Upgrading Strategies for Sustainable Transportation Fuel Production

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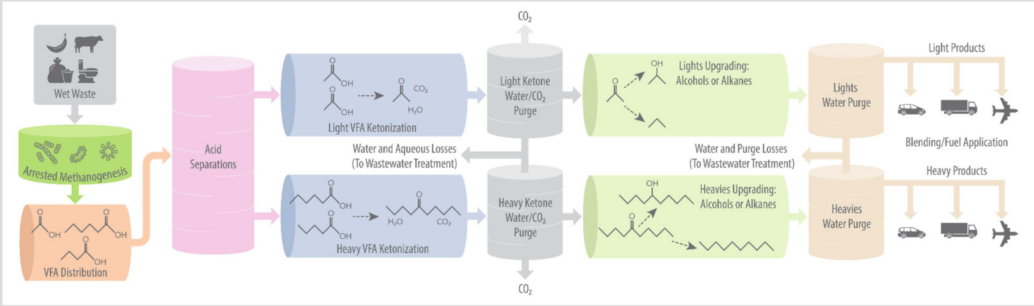
Introduction

- Volatile fatty acids (VFAs) derived from arrested methanogenesis of wet waste are a promising liquid transportation fuel feedstock.
- Optimal upgrading strategies for mixtures of VFAs not obvious (Make one fuel or two fuels? Make alcohols or alkanes? Make gasoline, jet, or diesel fuel?).
- **V**FA **U**pgrading to **L**iquid **T**ransportation f**U**els **R**efinery **E**stimation (VULTURE), developed in this work, predicts upgrading configurations maximizing bio-derived fuel content based on predicted fuel properties and blending limits in petrofuels.
- VULTURE rapidly identifies 2-3 promising scenarios from hundreds of possible upgrading strategies, facilitating more detailed modeling and fuel property estimation of promising scenarios.



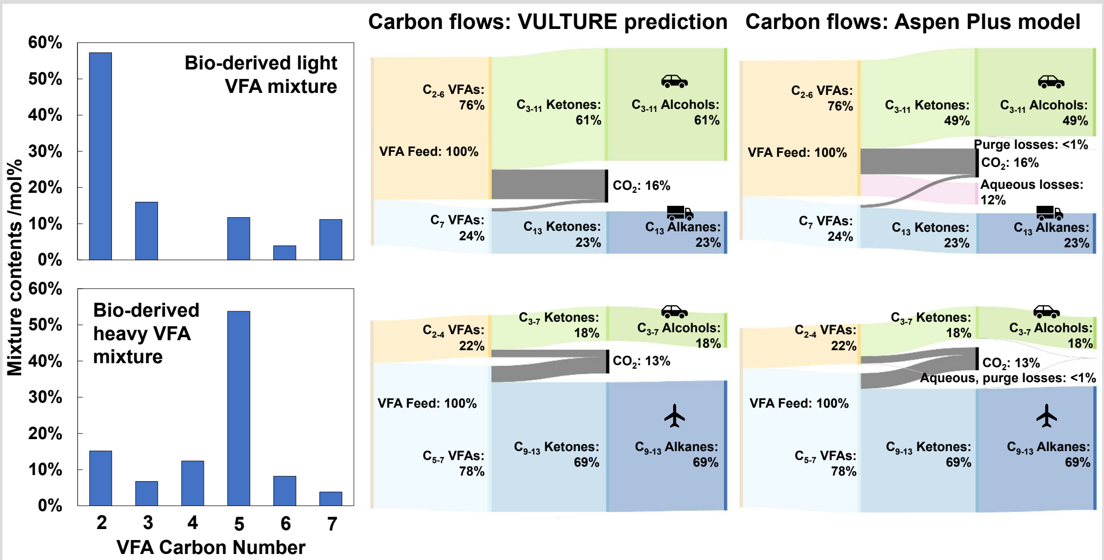
Proposed VFA upgrading pathway(s) to liquid transportation fuels. Another alteration involves ketonizing the entire acid stream without separations, then separating upgraded products for end fuel uses.

VFA Upgrading Process, Models

- VFA upgrading process includes catalytic ketonization, catalytic hydrotreatment (to n-alkanes or alcohols), and associated separation of streams into light and heavy fractions.
- VULTURE makes simple process assumptions (100% conversion/selectivity, based off lab-scale demonstrations) and simulates all possible combinations of upgrading, separations, and fuel end applications.
- Maximum blending levels of upgraded feedstock in petrofuels predicted via modeling of key fuel properties: boiling point, flash point, energy density, viscosity, melting point, water solubility, and cetane/octane number.
- Surrogate measurements match most predicted fuel properties accurately.

Optimal VFA Upgrading Strategies

- Upgrading strategies with maximal utilization of bio-carbon depend on carbon distribution of VFA feedstock.
- Generally, light (C_{2-3}) VFAs best upgraded to alcohol gasoline, heavy (C_{4-7}) VFAs best upgraded to alkane jet blendstock.
- Heaviest alkanes (C_{7-13}) are not well suited for diesel compared to jet applications (too light), while C_{7-13} alcohols blend in diesel at lower levels than alkanes in jet (high viscosity, melting point).
- Aspen Plus models show light (C_{3-4}) ketones highly soluble in water (ketonization co-product), causing substantial VFA upgrading carbon losses unanticipated by VULTURE.



VFA profiles from arrested methanogenesis of slaughterhouse wastes (left column), carbon flows of optimal upgrading processes identified by VULTURE (middle column), and carbon flows in same processes estimated by detailed modeling in Aspen Plus (right column).

Techno-economic and Life-cycle Analyses

- Assuming fixed transportation fuel prices based on 7-year US averages, maximum VFA purchase prices range from \$-0.01 to 0.13/kg for 250 (wet) ton food waste/day plant in promising scenarios selected by VULTURE for five VFA profiles.
- Economic viability (higher VFA purchase price) and carbon yield both increase as average influent VFA carbon number increases due to (i) lower fraction of CO_2 losses from ketonization and (ii) lower post-ketonization aqueous-phase losses.
- Carbon intensities (CI) of promising scenarios range from 22-36 g CO_2eq/MJ; 57%-74% emissions reduction compared to fossil fuel analogs.
- Largest CI decrease associated with scenario directing VFAs to jet blendstocks due to high process carbon yield.

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