

A Theoretical Multivariate Algorithm to Optimize Catalytic Conditions

One-factor-at-a-time (OFAT) method used for screening each catalytic variable

OFAT

- Time consuming
- Laborious
- Low turnover number (TON)

Carbon Dioxide (CO₂)
↓
Dimethoxymethane (C₃H₈O₂)

Catalytic variables

Y, S, C, T, L, I, A

CO₂

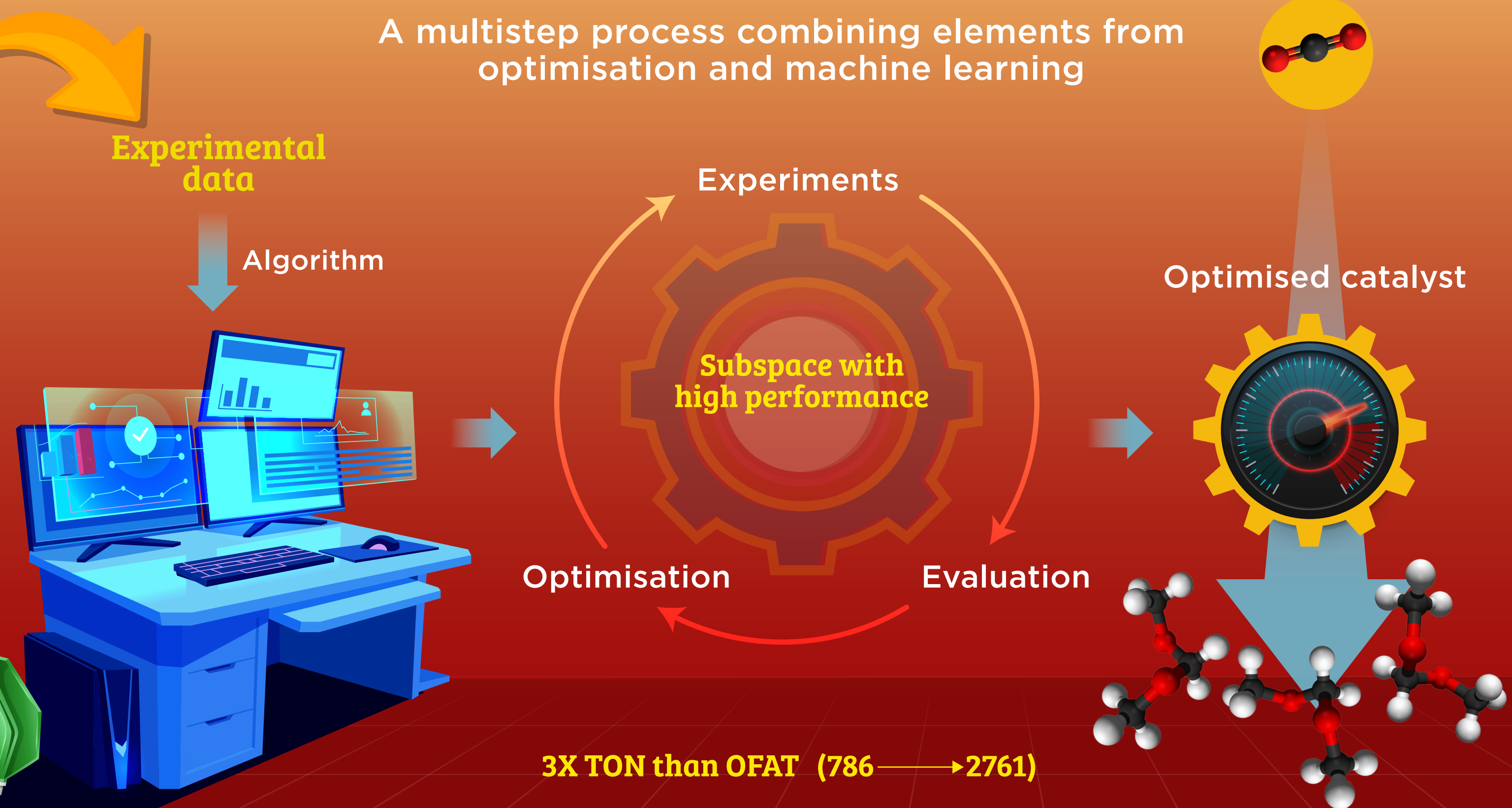
C₃H₈O₂

A scientist in a white lab coat stands in a laboratory setting with various glassware and a microscope. A green fuel nozzle is also visible.

A theoretical multivariate approach is proposed for screening high efficiency catalysts



A multistep process combining elements from optimisation and machine learning



Using the optimised conditions obtained from the algorithm, the highest TON for the investigated catalysis can be obtained with minimum time, cost, and energy