White paper by *Akshay Patel*, adpatel@sustanalyze.com, +31644232526

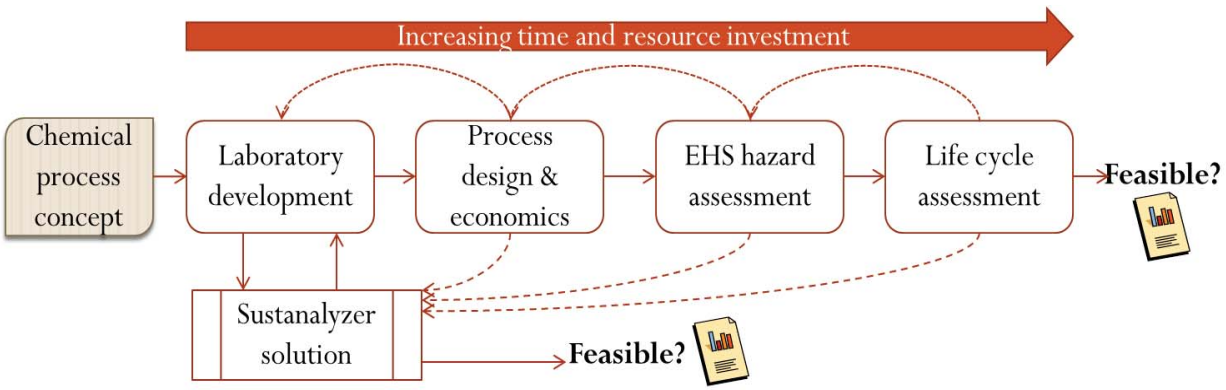
Effective and holistic chemical R&D with Sustanalyze

Salient points

- Speed up chemical innovation while adopting a holistic approach
- Simplify integration of sustainability in day-to-day decision making
- Prioritize chemical processes and resource allocation
- Scientific assessment methodology
- High quality integrated database and data support
- Chemical data: Properties, Prices, Hazards, Life cycle impacts…
- Process data: Mass balance, technical information…
- Advanced output reports
- Process/Product intelligence

How can we speed up chemical innovation and decision making

The sustanalyze tool brings in key pieces of information from various different domains (departments) to provide a rapid feedback at an early stage in the development cycle. Enables chemists to iterate faster and provides R&D managers key actionable information and overview about the potential of various process routes.

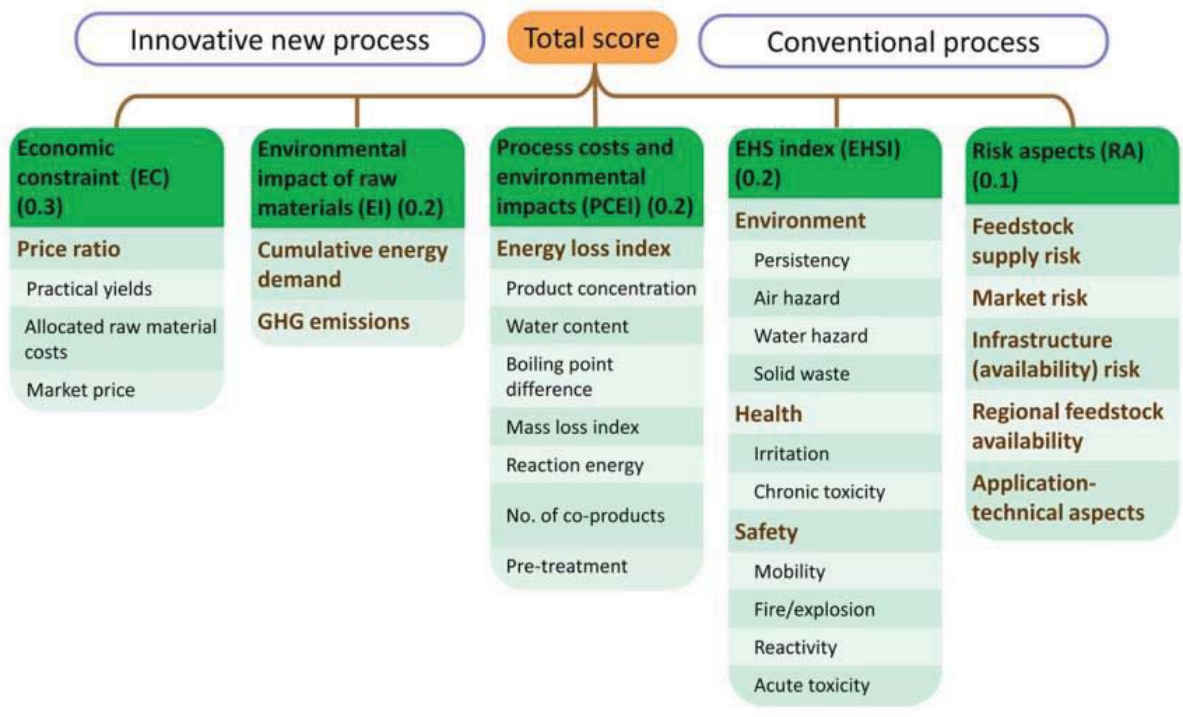


Advantages over conventional approach

	Conventional	Sustanalyze
Development approach	Staged	Real time simulation
Iterative loops	Longer or absent	Instantaneous
Optimization scope (e.g. sustainability integration)	In Silos	Holistic
Decision making timeframe and information	Longer and unstructured	Quick and structured
Innovation and route discovery	Limited scope	Faster and diverse
Basic problem discovery	6 -12 months	0.5 – 3 months

Assessment Methodology

Assessment is based on a 5 pillar methodology. Reaction mass balance information for the process being developed in the laboratory is entered by the user. This process is benchmarked against conventional processes. The assessment takes into account economics, environmental impacts, EHS hazards and general commercial risks.



Patel et al., Sustainability Assessment of Novel Chemical Processes at Early-stage: Application to Biobased Processes, Energy Environ. Sci., 2012, 5 (9), 8430 – 8444

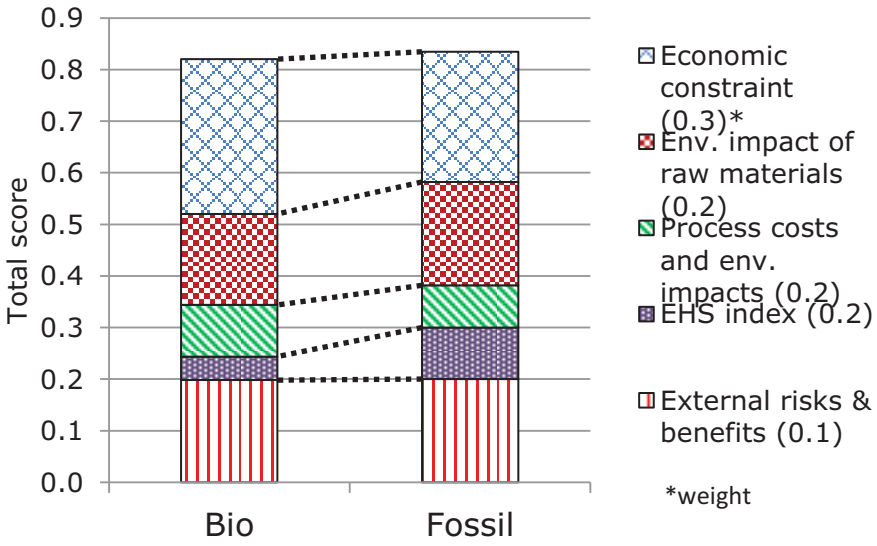
Applications

Process analysis and optimization

Analyze the performance of a process based on different parameters. The outcome can be used to explore other alternatives with rapid feedback. The case study depicted below compares butadiene production via a novel ethanol based process with the naphtha based process.

Case study: Ethanol to Butadiene

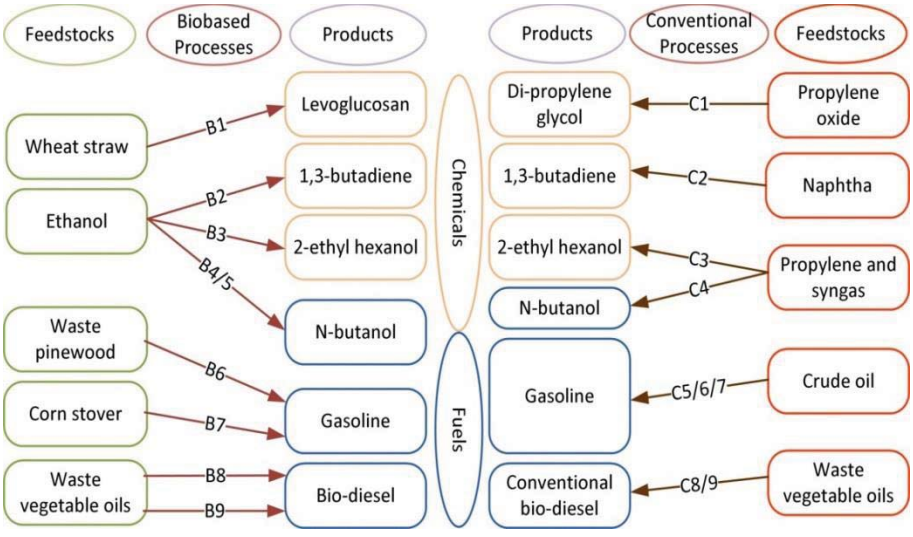
Sustainability index ratio: 0.98 (Bio/Fossil)



Evaluation and comparison of multiple process routes

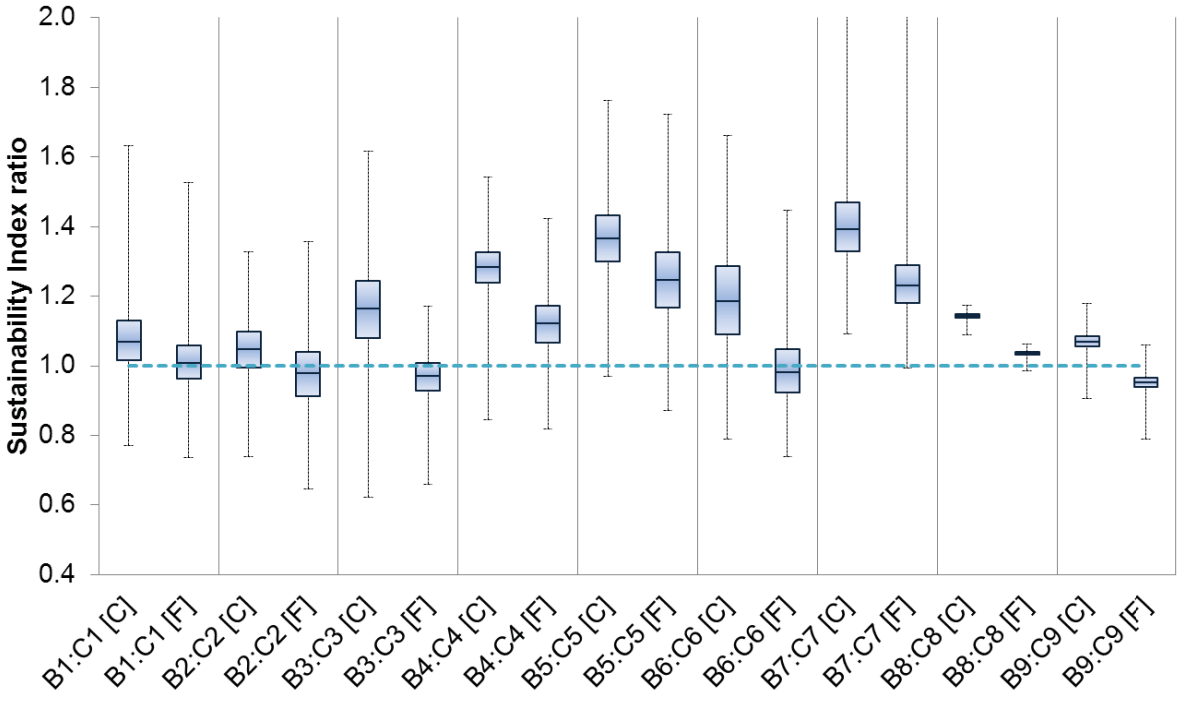
Simultaneously compare the performance of different process routes. The use of sustainability index ratio ensures that you compare apples with apples. Each process is benchmarked against a conventional process leading to the same product with similar functionality.

Case study: Biobased routes within CatchBio[2]



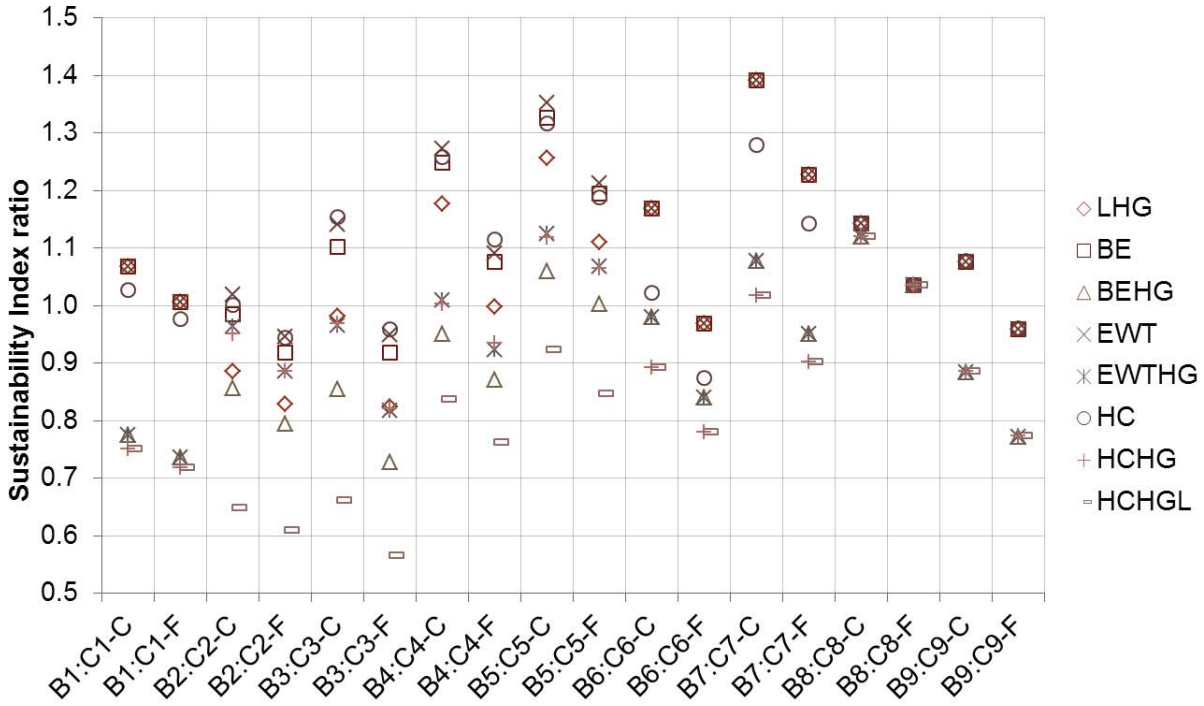
Base case and uncertainty analysis

A lower median sustainability index ratio indicates a more favorable process. The uncertainty analysis gives an indication of the possible outcomes with variation in underlying data and assumptions. Subscript [C] and [F] in figure below refer to the current state of development and a future one.



Scenario analysis

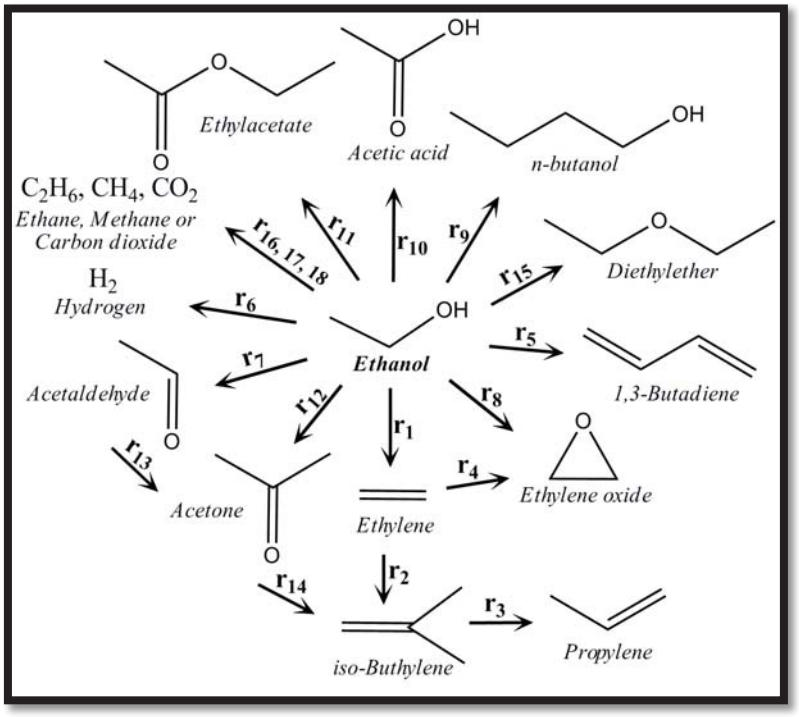
Enables to evaluate the change in outcome with different scenarios (e.g. high crude oil prices)



Case study: Promising routes from Bioethanol[3]

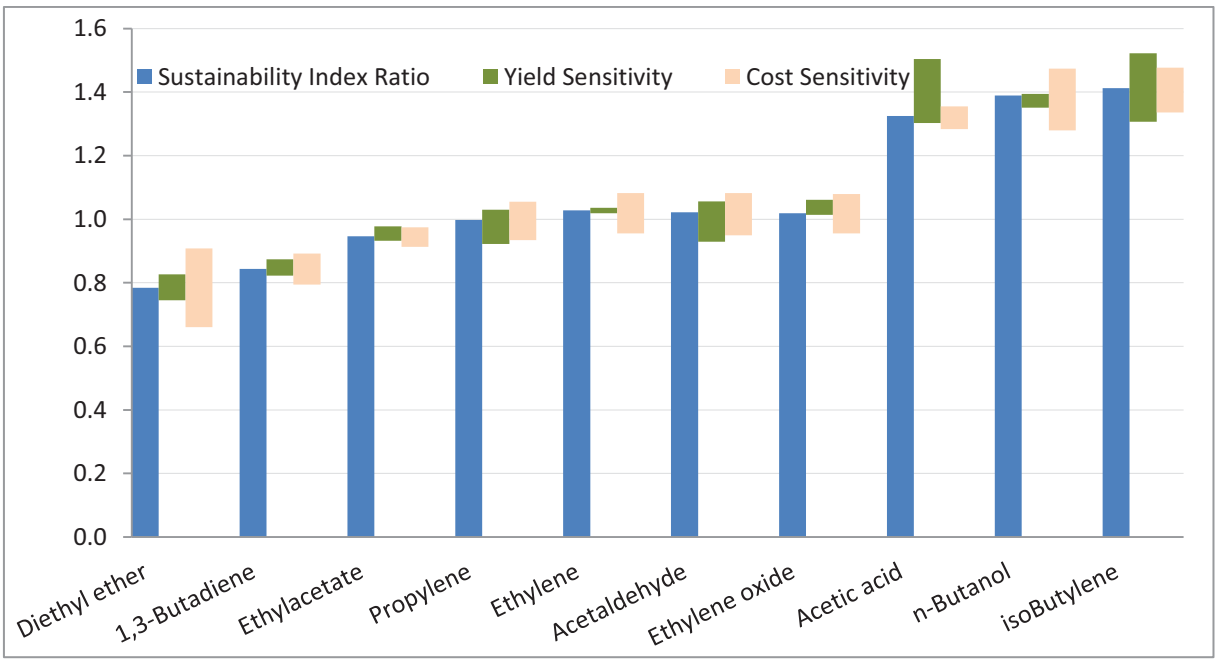
What could be the potentially interesting routes for use of bioethanol?

Potential routes



Base case and sensitivity analysis

In the figure below lower scores for sustainability index ratio mean more promising process routes.



Scenario analysis

Explore the effect of various geographical and process scenarios on the outcome for potential interesting routes from ethanol.

Type of BR	Country/ Region	Diethyl ether	1,3-butadiene	Ethyl acetate	Propylene	Ethylene	Acetaldehyde	Ethylene oxide	Acetic acid	*n*-Butanol	Isobutyl-ene	Hydrogen	Acetone
Non-integrated biorefinery	EU	G-I	G-I	G-II	G-II	G-II	G-II	G-II	G-III	G-III	G-III	G-III	G-III
	USA	G-I	G-I	G-I	G-I	G-I	G-II	G-II	G-III	G-III	G-III	G-III	G-III
	Brazil	G-I	G-I	G-I	G-I	G-I	G-I	G-I	G-III	G-III	G-III	G-III	G-III
	China	G-I	G-I	G-I	G-I	G-I	G-II	G-II	G-III	G-III	G-III	G-III	G-III
Integrated biorefinery	EU	G-I	G-I	G-I	G-I	G-I	G-I	G-I	G-III	G-III	G-III	G-III	G-III
	USA	G-I	G-I	G-I	G-I	G-I	G-I	G-I	G-III	G-III	G-III	G-III	G-III
	Brazil	G-I	G-I	G-I	G-I	G-I	G-I	G-I	G-II	G-II	G-II	G-II	G-III
	China	G-I	G-I	G-I	G-I	G-I	G-I	G-I	G-III	G-III	G-III	G-III	G-III
	2020 (low)	G-I	G-I	G-I	G-I	G-I	G-I	G-I	G-II	G-II	G-II	G-II	G-II
	2020 (high)	G-I	G-I	G-I	G-I	G-I	G-I	G-I	G-II	G-II	G-II	G-II	G-III

GI: Group I, most favorable compounds to be produced from bioethanol.
GII: Group II, promising candidates.
GIII: Group III, unfavorable derivatives from bioethanol.

Conclusions

Use of Sustanalyzer can help significantly increase the effectiveness of R&D resources. It can help identify opportunities and bottlenecks early on in the process development phase. While doing so it also provides an opportunity to optimize the process from a holistic perspective by integrating information from different domains.

Key publications

1. Patel et al., Sustainability Assessment of Novel Chemical Processes at Early-stage: Application to Biobased Processes, Energy Environ. Sci., 2012, 5 (9), 8430 – 8444
2. Patel et al., Early-stage comparative sustainability assessment of novel biobased processes, ChemSusChem, 2013, 6 (9), 1724-1736
3. Posada et al., Potential of bioethanol as a chemical building block for biorefineries: Preliminary sustainability assessment of 12 bioethanol-based products, Bioresource Technology, 2013, 135, 490-499

Contact information

Akshay Patel
Heidelberglaan 2, 3584CS, Utrecht, The Netherlands
Phone: +31644232526
Email: adpatel@sustanalyze.com; patelakshayd@gmail.com
Website: www.sustanalyze.com