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Article

Dataset for a Monte Carlo Based Techno-Economic Assessment of the Synthetic Methanol-to-Jet Fuel Production Pathway

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Abstract

This article presents a dataset generated for a techno-economic assessment (TEA) of the methanol-to-jet (MtJ) fuel production pathway. The dataset was produced using a large-scale Monte Carlo (MC) sampling approach applied to a steady-state process model implemented in Aspen Plus V14. The techno-economic evaluation was conducted using an external cost model, with subsequent data processing performed in Python. In total, three million individual data points were generated by varying key technical and economic input parameters within predefined ranges and are under public access. For each MC sample, the net production cost on a mass basis (NPC_m, EUR kg_{jet-fuel}⁻¹) of synthetic jet fuel was calculated as the primary economic performance indicator. The dataset comprises both the sampled input parameters and the corresponding techno-economic output variables and is intended to support transparency, reproducibility, and further uncertainty analysis of MtJ fuel production pathways.

Keywords: Monte Carlo; techno-economic assessment; synthetic aviation fuel (SAF); methanol-to-jet

1. Summary

This data article provides an open-access dataset for a Monte Carlo-based techno-economic assessment of the synthetic methanol-to-jet (MtJ) fuel production pathway. The dataset comprises three million individual simulations generated by coupling a steady-state Aspen Plus V14 process model with an external techno-economic cost framework and Python-based data processing. Key economic, technical, and operational parameters were systematically varied within literature-based uncertainty ranges to quantify their combined impact on the mass-specific net production cost of synthetic jet fuel. By jointly reporting all sampled inputs and corresponding outputs, the dataset enables probabilistic cost analysis, uncertainty and sensitivity studies, and the development of surrogate or machine-learning models for Power-to-Liquid systems. It supports transparency, reproducibility, and comparability of techno-economic evaluations of MtJ-based sustainable aviation fuel pathways.

2. Data Description

TEAs are commonly used to evaluate the economic performance of Power-to-Liquid (PtL) fuel production pathways. In the existing literature, such assessments are typically conducted using scenario analyses or sensitivity studies, in which individual parameters are varied while others remain fixed (univariate) [1–7]. Although these approaches are computationally efficient, they do not capture the combined variability and interaction of multiple economic, technical, and operational parameters.

MC methods provide a methodology to represent uncertainty by simultaneously varying multiple input parameters according to predefined ranges. However, the application of MC-based TEAs to complex PtL systems remains limited as stated by Wu et al. [8]. Existing literature remains scarce and, where available, predominantly focuses on Fischer-Tropsch (FT) based pathways [4,9]. The dataset presented here was compiled to enable a large-scale MC-based techno-economic evaluation of the methanol-to-jet (MtJ) fuel production pathway. The data were to include both the randomly sampled input parameters and the resulting net production costs. This work enables reuse for uncertainty analysis and surrogate model development.

The dataset is hosted in a public data repository (Mendeley data) [10] and is organized into structured files to ensure transparency and reproducibility. The main dataset is provided as a comma-separated values (CSV) file:

“mc_results_3mio.csv” with 264 MB

It contains all MC simulation results. Each row corresponds to a single MC sample. Columns include input parameters (economic, technical, and operational variables) and the corresponding techno-economic output variable (net production cost, NPC_m). To ensure that data handling is possible with lower quality computers, there are also minor data files with 1 million, 100 thousand, and 10 thousand points:

“mc_results_1mio_V3.csv” with 88.8 MB

“mc_results_100k.csv” with 21.5 MB

“mc_results_10k.csv” with 1.59 MB

An additional metadata file is provided to describe the dataset structure:

“variable_description.csv”

Lists all variables contained in the main dataset, including variable name, and physical unit and description.

Value of the data:

- The dataset provides a large-scale, techno-economic parameter space for the methanol-to-jet fuel production pathway, enabling probabilistic analysis of economic performance.
- The data can be reused for uncertainty and sensitivity analyses, allowing to investigate how variations in economic and technical parameters influence net production costs in Power-to-Liquid systems.
- The dataset is suitable for machine learning applications, such as training surrogate models for techno-economic modeling.
- The data supports reproducibility and comparability across various techno-economic studies, as all input ranges, assumptions, and outputs are documented and provided in open-access format.

Limitations:

- The dataset is based on a steady-state techno-economic model and therefore does not capture dynamic operation, transient effects, or start-up and shutdown behaviour of the MtJ process.
- Input parameters were sampled assuming uniform distributions, which may not reflect real-world probability distributions in all cases.
- Cost estimation relies on literature values and market assumptions which introduce uncertainty. Regional effects, policy instruments, and future market developments are not explicitly represented beyond the selected parameter ranges.
- The dataset represents a specific process configuration and therefore a set of “hard” assumptions (e.g. operating conditions, conversion, selectivities) inherent in the MtJ pathway. Consequently, results may not be directly transferable to alternative process designs without modification.

3. Method

The dataset was generated using a steady-state techno-economic assessment model of the methanol-to-jet fuel production pathway. The simulation process was performed using Aspen Plus

V14. The Mtj process includes three-stage methanol synthesis, dehydration to olefine and subsequent upgrading to jet fuel as explained in detail in [11].

The applied framework for the TEA in this study was developed and described in detail by the authors in previous publications [11,12] and is in large parts based on the frameworks presented by Peters et al. [13]. For a more detailed description, the reader is referred to the original work of Peters et al. [13] or different studies adopting the methodology [3,5,6]. The economic performance is evaluated using the mass specific net production costs (NPC_m in EUR kg_{SAF}^{-1}) which is calculated by dividing the total annualized costs by the annual fuel output, as in Equation **Error! Reference source not found..**

$$NPC_m = (ACC + ARC + OPEX) / \dot{m}_{SAF} \quad (1)$$

The annualized capital costs (ACC in EUR a^{-1}) are derived from the fixed capital investment (FCI in EUR) and working capital (WC in EUR) using the capital charge factor (CCF) as given in Equation **Error! Reference source not found..**

$$ACC = (FCI + WC) * CCF - (WC/PL) \quad (2)$$

The CCF [6] is defined according to Equation **Error! Reference source not found.:**

$$CCF = (IR * (1 + IR)^{PL}) / ((1 + IR)^{PL} - 1) \quad (3)$$

IR denotes the interest rate and PL the lifetime of the plant. The FCI is calculated from equipment costs (derived from Aspen Plus) using the established factorial method described by Peters et al. [13]. The WC is assumed to be 10% of the total capital investment (sum of FCI and WC). The annual replacement costs (ARC in EUR a^{-1}) account for the periodic replacement of the electrolysis stacks. Operating expenditures (OPEX) are composed of fixed and variable contributions. Fixed OPEX comprises labor, maintenance and overheads, whereas variable OPEX are made up of electricity demand, feedstock supply, utilities and consumables.

Input variables and uncertainty

The dataset includes a predefined set of input variables selected to represent the dominant sources of techno-economic uncertainty for Mtj production pathway. All input variables, their units, classification, baseline values, uncertainty bounds and data sources are summarized in Table . Economic variables include plant lifetime (PL), fixed interest rate (IR), hourly wage (HW), electricity price (EP), specific investment costs (SIC) of the alkaline electrolysis unit, purified water price (WP), CO₂ price, oxygen price (OP), and the fixed capital investment (FCI). Technical uncertainty is represented by the electrolysis stack lifetime (SL), which is linked to cell degradation mechanisms that are subject to current research. SIC are likewise treated as a semi technical parameter, as they are also strongly influenced by technological learning, meaning that design improvements and production scale-up could offer future cost reduction. The baseline values correspond to a representative reference case for a large scale Mtj plant, while the specified ranges define the uncertainty space in the MC analysis. The authors recognize that alternative probability density functions (e.g. beta or gamma distributions) could be used to model asymmetric uncertainty or greater confidence around nominal values for specific variables as shown in [8]. However, in the absence of statistical evidence for most of the defined variables in this study, all input variables are sampled using uniform distributions withing their respective bounds.

Although the annual operating hours are included as an operational parameter, they are kept fixed in this study assuming continuous operation of the plant. An effective operating time of 7,884 hours per year is applied, which is calculated by multiplying 8,760 possible operating hours per year by an availability factor of 0.9 to account for maintenance and planned shutdowns [5]. Process-internal parameters, such as reaction conversions, operating temperatures and pressures, residence times, separation efficiencies and yields, etc. are not varied and are treated as fixed design parameters. This follows the approach from Bube et al. [3,14] who classified these parameter as “hard” process parameters, since changing them would require changes to the process design iteratively rather than representing uncertainty within a defined fixed configuration. The influence of such process-internal

parameters of the performance of the MtJ process in a similar configuration is analysed in [14], to which the reader is referred.

Table 1. Input variables for the MC experiment on the MtJ process pathway.

Variable	Abbreviation	Unit	Type	Baseline	Range	Source
Plant lifetime	PL	a	Economic	20	15-30	[4,6]
Fixed interest rate	IR	%/100	Economic	0.1	0.05-0.15	[4]
Operating hours	-	h a ⁻¹	Operational	7,884	Fixed	[5]
Hourly wage	HW	€ h ⁻¹	Economic	40	15-50	[15]
Electricity price	EP	€ MWh ⁻¹	Economic	100	10-200	[1,3,15]
Specific investment costs	SIC	€ kW ⁻¹	Economic/ Technical	800	300-1000	[16]
Stack lifetime	SL	h	Technical	60,000	40,000-100,000	[16]
Purified water price	WP	€ m ⁻³	Economic	10	5-15	[17]
CO ₂ price	-	€ kg ⁻¹	Economic	0.11	0.04-0.20	[11]
Oxygen price ¹	-	€ kg ⁻¹	Economic	0	0.00-0.15	[1,15]
Fixed capital investment	FCI	€	Economic	3.4×10 ⁷	(2.36-4.42)×10 ⁷	Aspen cost estimation (APEA)

¹... For oxygen, two approaches can be found in the literature, with some studies considering oxygen as a valuable co-product [1,2,5,15], while others neglect or conservatively set potential revenues [6,9,11]. A baseline value of zero is assumed in this study, while possible future valorisation is accounted for by the uncertainty bounds.

Monte Carlo sampling

MC sampling was implemented in Python (version ≥ 3.11) using the NumPy and Pandas libraries. All simulations were executed on a workstation equipped with an Intel® Core™ Ultra 9 285K processor. For each MC run, a set of input parameters was randomly sampled within literature-based or assumption-driven bounds, while fixed parameters were held constant across all simulations. Each sampled parameter set was automatically transferred to the techno-economic model, and the NPC_m was calculated as the primary output variable, with a consuming time of approximately 22 sets per second. The resulting input and output pairs were stored directly in CSV format without further filtering or post-processing. Time consumption for the 3 million sets was timed at approximately 37 hours, 52 minutes and 12 seconds.

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Abbreviations

The following abbreviations are used in this manuscript:

MDPI	Multidisciplinary Digital Publishing Institute
MtJ	Methanol-to-Jet
SAF	Sustainable Aviation Fuel
PtL	Power-to-Liquid
TEA	Techno-Economic Assessment
MC	Monte Carlo
NPC _m	Mass-specific Net Production Cost
ACC	Annualized Capital Costs
ARC	Annual Replacement Costs
OPEX	Operating Expenditures
FCI	Fixed Capital Investment
WC	Working Capital
CCF	Capital Charge Factor
IR	Interest Rate
PL	Plant Lifetime
HW	Hourly Wage
EP	Electricity Price
SIC	Specific Investment Costs
SL	Stack Lifetime
WP	Purified Water Price
CSV	Comma-Separated Values
APEA	Aspen Process Economic Analyzer
DOAJ	Directory of Open Access Journals

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