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A model for cost- and greenhouse gas optimal material and energy allocation of biomass and hydrogen

Markus Millinger [a,b,*], Philip Tafarte [c,d], Matthias Jordan [a], Frazer Musonda [a], Katrina Chan [a], Kathleen Meisel [e], Danial Esmaeili Aliabadi [a]

[a] Department of Bioenergy, Helmholtz Centre for Environmental Research - UFZ, Permoserstraße 15, 04318 Leipzig, Germany
[b] Department of Space Earth and Environment, Chalmers University of Technology, 412 96, Göteborg, Sweden
[c] Department of Economics, Helmholtz Centre for Environmental Research - UFZ, Permoserstraße 15, 04318 Leipzig, Germany
[d] Research Group MultiplEE, Faculty of Economics and Management Science, Institute for Infrastructure and Resources Management, University of Leipzig, Ritterstraße 12, 04109 Leipzig, Germany
[e] Department of Bioenergy Systems, Deutsches Biomasseforschungszentrum Gemeinnützige GmbH—DBFZ, Torgauer Straße 116, 04347 Leipzig, Germany

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ABSTRACT

BENOPT, an optimal material and energy allocation model is presented, which is used to assess cost-optimal and/or greenhouse gas abatement optimal allocation of renewable energy carriers across power, heat and transport sectors. A high level of detail on the processes from source to end service enables detailed life-cycle greenhouse gas and cost assessments. Pareto analyses can be performed, as well as thorough sensitivity analyses. The model is designed to analyse optimal biomass and hydrogen usage, as a complement to integrated assessment and power system models.

Code metadata

Current code version	v2.1
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX_2020_97
Legal Code License	GNU-GPL 3.0
Code versioning system used	git
Software code languages, tools, and services used	Matlab, GAMS, Cplex solver
Support email for questions	markus.millinger@chalmers.se

1. Motivation and significance

Biomass and hydrogen play important roles in a transition to renewable energy and materials. Their use as storable and dispatchable renewable energy carriers make them well suited to complement wind and solar photovoltaic power. Through sector coupling, heat, transport and industry are expected to be increasingly electrified, where this is possible, with biomass and hydrogen derivatives as a complement.

However, in many studies and integrated assessment models (IAMs) these options are often handled in a highly aggregated form [1], whereby information on the diverse characteristics of different pathways is lost, such as regarding GHG emissions and temporal resolution [2]. Also, they mostly lack gaseous fuels and heat production, as well as often depicting energy demands rather than service demands [3], which are significant for being able to depict an efficient resource usage [4–6]. Within future energy scenarios and dedicated energy system models, biomass usage is often crudely depicted, with low detail on biomass types, conversion options, land use, costs, greenhouse gas emissions and connected resource use and environmental effects [7]. Also, these models as well as IAMs are often computationally intensive, which hinders thorough sensitivity analyses [2,8,9], despite the

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[*] Corresponding author at: Department of Space Earth and Environment, Chalmers University of Technology, 412 96, Göteborg, Sweden.
E-mail address: markus.millinger@chalmers.se (Markus Millinger).

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importance thereof, considering the substantial data uncertainties regarding e.g. biomass usage [3] and hydrogen [10].

The BioENergy OPTimisation model (BENOPT) operates within this research and modelling gap, in order to provide more detailed information on the role of biomass and hydrogen derivatives within a sustainable transition. The model is developed for:

- System modelling across energy and bioeconomy sectors with a high detail on biomass crops and conversion pathways, as well as on power-to-X/electrofuels.
- Analysis throughout the entire biomass and renewable energy carrier supply chain, using a systems perspective

The model was developed to integrate the most important aspects of the complex biomass usage and PtX within a systems perspective. A systems perspective does not merely consider each usage option or pathway independently, but their development in a system and is in the framework of industrial ecology manifested through the following areas [11,12]: (i) a life-cycle perspective, (ii) material and energy flow analyses, (iii) systems modelling and ideally (iv) interdisciplinary analyses. A further important aspect, (v) technological change, should also be mentioned in this context [11,13]. Aspects i–iii and v are included directly in the model [14], which enables a more holistic analysis than for instance LCAs of singular pathways. The results can be embedded within broader, interdisciplinary analyses.

The research questions assessed with the help of the model generally fall under the question: *What role could biomass and other renewable energy options play within the energy and bioeconomy system transformation process in order to achieve climate targets in the most cost- and GHG-optimal way?*

Detailed input–output and cost information on the processes along the whole pathway from the source to the end use enables a detailed analysis of greenhouse gas emissions and cost developments. An analysis across power, heat and transport sectors with sub-sectors enables a systems perspective and thus a solid decision support framework.

The model is suited for policy support on optimal deployment of biomass and hydrogen based energy carriers across transport, heat and energy sectors. With the help of the model, analyses for the case of Germany on renewable fuel policy analysis for the Federal Ministry of Food and Agriculture (BMEL) [15,16] have been performed, as well as an analysis on biomass use across all energy sectors within long-term scenarios for the Federal Ministry for Economic Affairs and Energy (BMWi) [17,18].

The model is programmed in Matlab and GAMS and has been tested with the use of the CPLEX solver, with process data and dependencies read from Excel and csv files. Data setting is done in an Excel file as well as within the model code.

2. Software description

2.1. Software architecture

BENOPT is a deterministic, recursive, bottom-up, perfect foresight, linear optimization model for modelling cost-optimal and/or GHG abatement optimal allocation of renewable energy carriers across power, heat and transport sectors. The sectors are further divided into sub-sectors. The model has an up to 15-min resolution, which can be aggregated depending on the task. The model has been developed in Matlab and GAMS, which are both required for running the software.

The model includes modules for crop price developments (based on the premise that farmers want to achieve the same profit regardless of the crop grown), automatic GHG emission and cost calculations based on input–output, opex and capex data, and it has been hard coupled with a Variable Renewable Electricity (VRE) module. Some 30+ technologies with 20+ biomass residues and crop types, which can be used across 10+ subsectors enable a myriad of biomass pathway options, which can be easily extended. Sector coupling based on the power mix or excess electricity is included with numerous usage pathways, such as hydrogen, electric vehicles (EV) or heat pumps. The whole pathway from source to end use service is captured across all sectors, allowing a systems perspective. Thanks to short run-times, extensive sensitivity analyses can be performed.

BENOPT contains sectors for transport (road passenger, road goods, shipping and aviation), power and heat (industry, household and commercial). The model functions on a yearly resolution (with the exception of the power sector, which can be broken down to a 15-min resolution or less depending on available data) and is not spatially explicit. Detailed input–output, capex and opex data are integrated for feedstocks, conversion and supply, which allows detailed cost analyses and combined with relevant emission factors also GHG analyses.

The model process is as follows (Fig. 2). Data setting is mainly performed in the Excel-sheet, for the conversion technologies and feedstocks. These as well as the VRE data for the base years are imported and converted to mat-files. The data are attributed to the specific variables, as well as additional data set. With these data, GHG emissions are calculated for the feedstocks and processes. Scenarios are set by setting chosen scenario specific variables. The future VRE development is calculated and based on this the excess renewable electricity (ERE) data are aggregated. Biomass crop and residue prices are calculated, as well as opex and capex costs of the processes. The data ensemble required for GAMS is set in the correct format and sent to GAMS, where developments are optimized. The results can then be plotted in the chosen format. The process chain can also be parallelized in a Monte-Carlo sensitivity analysis, where the complete process is repeated a set number of times with variations in chosen variables.

2.2. Software functionalities

The key model functions are presented here, with a mathematical formulation of the model presented in the supplementary material.

Country specific data. The country code as well as a weather year is specified, and country specific data are read from the power system data as well as from the excel file. These include solar and wind power generation time-series, demands, technology and vehicle fleet capacities.

Process data, opex and capex costs. The process data includes CAPEX data, infrastructure, operation and maintenance cost, personnel cost and inputs and outputs, including by-products and secondary feedstocks. The input and output data enables a detailed calculation of the costs and is elaborated in Millinger et al. [19]. Within the Excel-file, process and feedstock data can be adapted, and allowable feedstock-technology and technology-market combinations set (through which also technologies can be excluded from the modelling).

VRE and excess electricity modules. Variable renewable electricity generation and power load in the baseline year is scaled according to the scenario specific future wind and solar PV capacity expansion and electricity demand development, resulting in VRE share and excess electricity developments. Electricity storage is included and other (fossil or renewable) must-run generation can be added [20]. The temporally high resolution data can be subsequently aggregated depending on the task, by sorting the data to residual load duration curves (RLDC) and dividing the data into a set number of slices (50 in the standard version), which reduces the computational burden substantially [4].

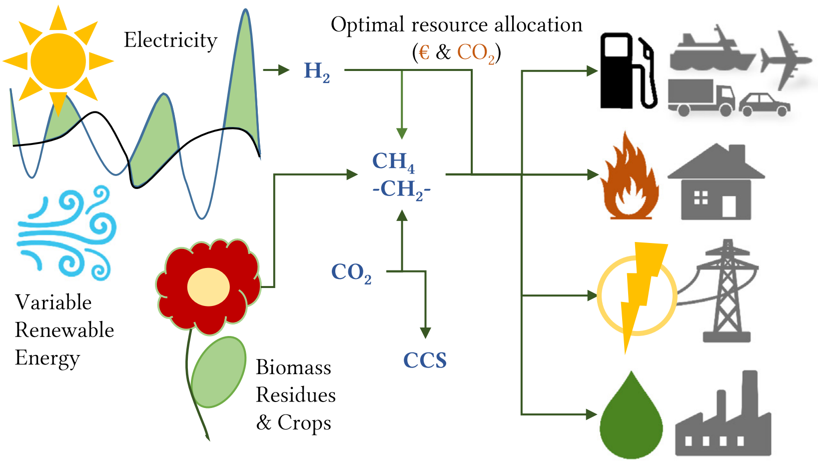

Fig. 1. Simplified model scope overview.

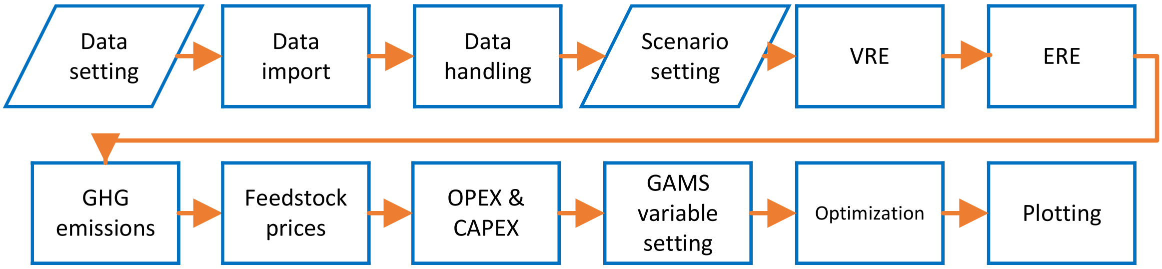

Fig. 2. Process flow in the model. Sensitivity analyses can be performed involving the whole chain or for submodules.

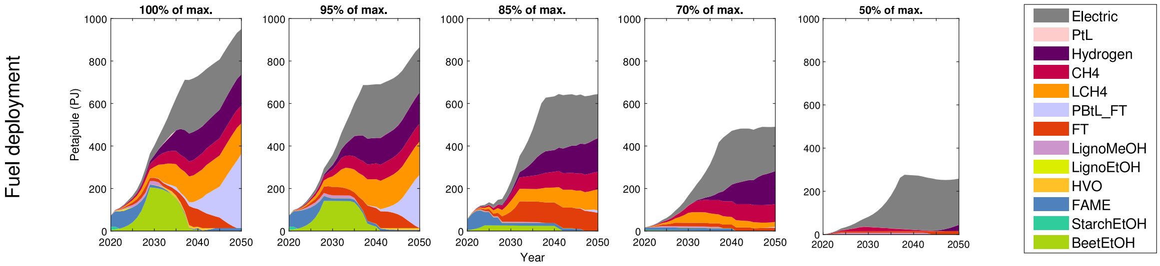

Fig. 3. Cost-optimal transport energy carrier deployment at different GHG-abatement budget targets. Electric = electric vehicles, PtL = Power-to-Liquid, CH4 = methane (from different conversion pathways), LCH4 = liquefied methane, PBtL_FT = Power-to-Biomass-to-Liquid (Fischer–Tropsch), FT = Fischer–Tropsch-diesel, LignoMeOH = lignocellulose based methanol, LignoEtOH = lignocellulose based ethanol, HVO = Hydrogenated vegetable oils, FAME = Fatty-acid methyl esters, StarchEtOH = starch crop based ethanol, BeetEtOH = sugar beet based ethanol.

GHG emissions. The agricultural and conversion process input and output data combined with emission factors enable the calculation of detailed pathway GHG emissions including the allocation of emissions to the by-products [21].

Feedstock price module. Crop price developments are calculated by adding the per hectare profit of a benchmark crop (wheat) to the per hectare production cost of each energy crop [22]. The future price developments are calculated based on a set yearly development of the wheat price. The price of biomass residues is likewise tied to the set development, while the electricity prices (mix and ERE) are set according to assumptions based on e.g. literature.

Optimization module. Input data for the optimization are formatted to suit the GAMS data format and transferred to the optimization module in GAMS. The data are transferred back to Matlab for data handling and plotting. The crops grown on the arable land, investment and deployment is optimized, with the fuel demand in the transport sector endogenously determined through vehicle fleet adaptations. In the standard set-up, the GHG-abatement over the whole time-span is first maximized without cost restrictions. Then, the GHG-abatement is set as a target that has to be achieved while minimizing costs. Any level below this target can be set, also in a step-wise approach for a pareto analysis. The target sets a GHG abatement budget which needs to be met in sum over the whole analysed time span, but no targets for individual years are set.

Sensitivity analysis module. Monte Carlo sensitivity analysis [21, 22] can be performed with parallel computing, enabling faster runs. Any parameter can be added for variation and plotting related to individual parameters can be performed. The analysis can be done for both singular functions as well as for the whole model process chain (Fig. 5).

Plotting. Extensive plotting can be performed and more added, with examples shown in Figs. 1–3 and more can be found in the cited body of literature.

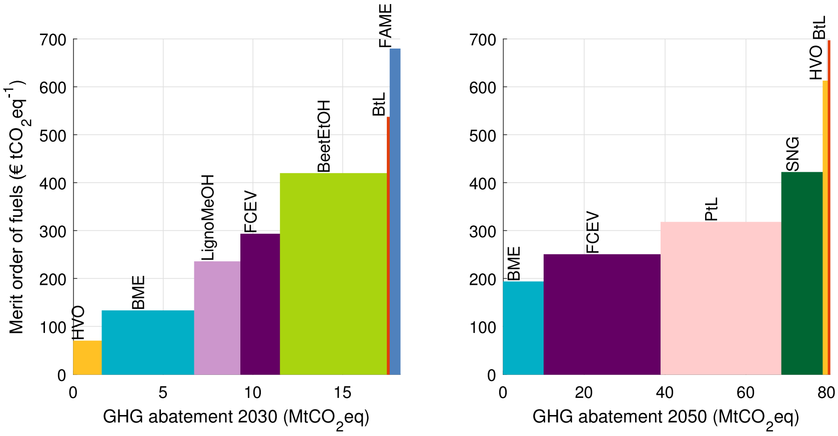

Fig. 4. Merit order of fuel options in two years. HVO = Hydrogenated vegetable oils, BME = biomethane, LignoMeOH = lignocellulose based methanol, FCEV = fuel cell electric vehicles, BeetEtOH = sugar beet based ethanol, BtL = Biomass-to-Liquid, FAME = Fatty-acid methyl esters, PtL = Power-to-Liquid, SNG = Substitute natural gas.

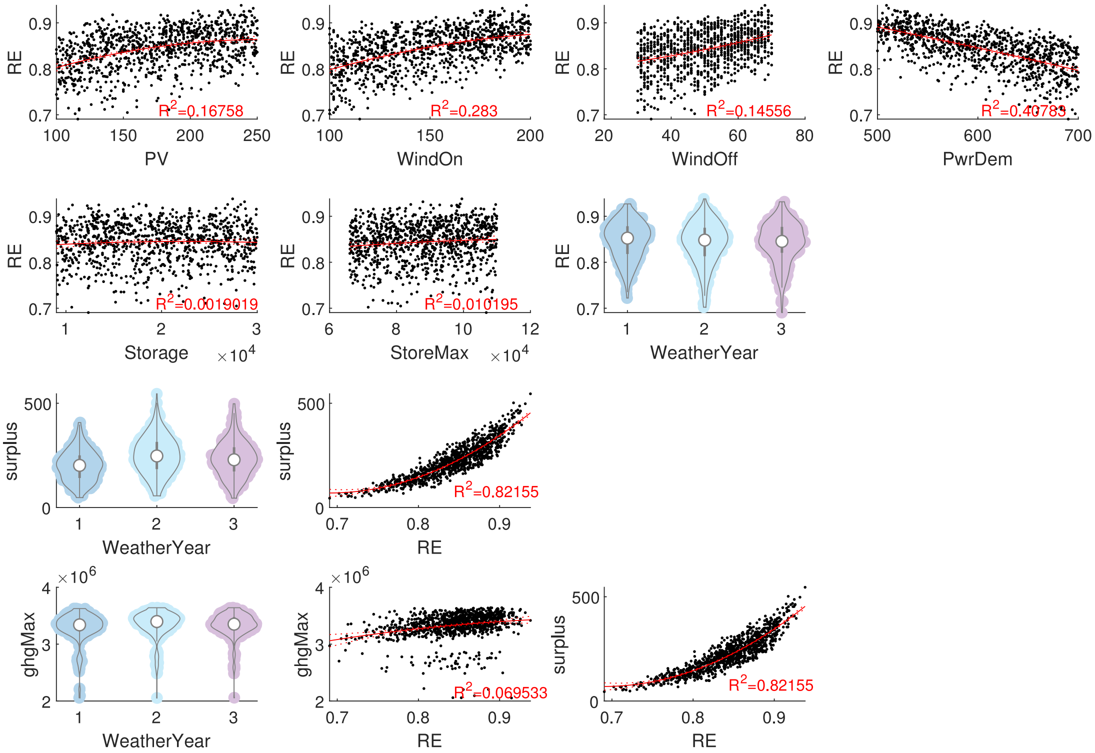

Fig. 5. Example Monte Carlo sensitivity analysis of a sample of variables. RE = renewable energy share of the power supply, surplus = excess electricity, PV = photovoltaics, WindOn = onshore wind power, WindOff = offshore wind power, WeatherYear = weather year on which the PV and wind power generation and power demand patterns are based, ghgMax = maximum achievable greenhouse gas abatement.

3. Illustrative examples

We show the main functions of the model through an application for the transport sector in Germany. An assessment of cost-optimal fuel deployment at different GHG-budget targets is performed (Fig. 3). As can be seen in the example for the transport sector, the model chooses at what time-point changes between runs at different targets occur. For instance, at the maximal GHG-target, some capacities of BeetEtOH (sugar beet-based bioethanol) are only used for a few years. At a slightly lower target, these over-capacities do not emerge. Also, PBtL (Power-to-Biomass-to-Liquid) is less deployed, in order to fully disappear at lower targets. With decreasing targets, the diversity of options decreases. Electric vehicles appear across all targets and can thus be seen as the most robust option in the example.

A merit order plot shows the resulting GHG abatement costs and potentials of different options given feedstock and demand restrictions under competition (Fig. 4). Depending on which resources are used at different time-points and whether there are over-capacities compared to the produced amounts, the costs of technology options may differ over time, as can be seen for instance HVO in the figure. The usage of electrofuels expands the possible GHG abatement in 2050 compared to 2030, while biofuels remain largely with the same GHG abatement but with different end products.

A global Monte Carlo sensitivity analysis can be performed, which provides a solid basis for analysing the effect of different parameter values on the results, and thus on the robustness of results. Plots of a 1000 Monte Carlo runs on the VRE and excess electricity modules are shown in Fig. 5. Through such analyses one can visualize the spread of results across different parameters, which helps in determining the importance of the parameters. For instance, in this case the capacities of PV and on- and offshore wind power taken individually are not that decisive for the achieved renewable shares, and the excess electricity is sensitive to the weather year assessed, whereas the renewable electricity share is not, as seen in the violin plots. Both biomass usage and PtX are coupled with large uncertainties across the pathways, which are important to assess in order to get a thorough understanding of the analysed systems.

4. Impact

Compared to IAMs, an increased level of detail regarding VRE, sector coupling and across the more diverse supply chain options from source to end service is given. Compared to power system models, biomass and other sectors are depicted in more detail. The model is also well suited to investigate the sensitivity of developments, on which a large number of parameters have an influence, especially in the complex area of biomass use. Thus, a modelling gap can to an extent be bridged with BENOPT.

The model has been used for numerous analyses for Germany. Assessments of biofuels regarding costs [19,22] and greenhouse gas emissions [21], as well as optimal biofuel deployment [5] and renewable fuel policy analysis for the BMEL [15,16] have been published. An analysis on biomass use across transport, heat and power sectors within long-term scenarios for the BMWi has been performed [17]. Coupling with a general equilibrium agricultural model and a land use model [23,24] have been performed, as well as an analysis of electrofuels/power-to-X [4].

Future Work. Stand-alone versions focusing on chemical products [25,26] as well as on the heat sector [6,27–30] have been developed, with details being planned for integration into the main model. Aspects concerning sustainable agriculture, nutrition [31] and industry are underway. Sector coupling and (renewable) power based options as well as carbon capture are increasingly included in the modelling, which enables a holistic analysis of renewable futures in the sectors considered. The model allows for analyses for any country or region, based on available data.

5. Conclusions

An optimal material and energy allocation model has been outlined. The model includes transport, heat and power sectors, with additions possible. The whole supply chains from source to end service are analysed under resource competition, enabling a systems perspective. Biomass and electricity-based options (PtX, EVs) are included and are deployed by either maximizing the GHG abatement or by achieving a GHG target cost-optimally. Pareto analyses at different GHG targets can be performed, as well as thorough sensitivity analyses. The model is designed to analyse sector coupling and biomass usage, as a more detailed complement to IAMs and power system models, and has been used for policy advice on the context of Germany.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.softx.2022.101264. This includes detailed descriptions of model equations, sets, parameters, variables and nomenclature.

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