Title
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Journal
Environmental Science and Technology, 50(23)

ISSN
0013-936X

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Publication Date
2016-12-06

DOI
10.1021/acs.est.6b04270

Peer reviewed

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Journal:	*Environmental Science & Technology*
Manuscript ID	es-2016-042708
Manuscript Type:	Policy Analysis
Date Submitted by the Author:	23-Aug-2016

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Stochastic Technology Choice Model for Consequential Life Cycle Assessment

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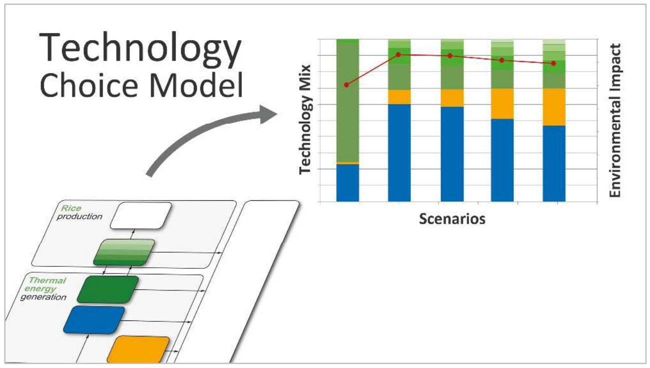
Discussions on Consequential Life Cycle Assessment (CLCA) have relied largely on partial or general equilibrium models. Such models are useful for integrating market effects into CLCA, but also have well-recognized limitations such as the poor granularity of the sectoral definition and the assumption of perfect oversight by all economic agents. Building on the Rectangular-Choice-of-Technology (RCOT) model, this study proposes a new modeling approach for CLCA, the Technology Choice Model (TCM). In this approach, the RCOT model is adapted for its use in CLCA and extended to incorporate parameter uncertainties and suboptimal decisions due to market imperfections and information asymmetry in a stochastic setting. In a case study on rice production, we demonstrate that the proposed approach allows modeling of complex production technology mixes and their expected environmental outcomes under uncertainty, at a high level of detail. Incorporating the effect of production constraints, uncertainty, and suboptimal decisions by economic agents significantly affects technology mixes and associated greenhouse gas (GHG) emissions of the system under study. The case study also shows the model's ability to

determine both the average and marginal environmental impacts of a product in response to changes in the quantity of final demand.



INTRODUCTION

Addressing global sustainability imperatives demands a substantial shift in today's production and consumption patterns. The 2 degree Celsius climate target and Sustainable Development Goals, for example, require a material change within policy, technology, market, and consumer behaviors.[1–4] Understanding the consequences of such changes for the environment, however, is challenging, in part because of our limited capacity to model the wide range of market transformations that such changes may trigger.[5] It is therefore crucial to better understand the potential effects of policies on market responses to support environmental decision-making.

An approach aiming to provide such understanding is Consequential Life Cycle Assessment (CLCA).[6–11] CLCA aspires to determine the environmental consequences of decisions such as the introduction of a new technology,[12–14] implementing a new policy,[15, 16] or an increase in product demand.[17–19] While the literature on CLCA has steadily increased in recent years, debate continues regarding its operational models for the choice of technologies, and the implications of uncertainties.[7, 20]

For modeling market effects, CLCA studies have relied largely on partial equilibrium (PE) and computational general equilibrium (CGE) models.[9, 21–25] While PE models focus on a subset of markets within an economy, CGE models consider all sectors of an economy. The advantage of both PE and CGE models lies in their ability to determine the quantity and price of products jointly based on econometrically derived underlying data. Furthermore, such models often cover multiple regions. Kløverpris et al., for example, modeled the effect of corn consumption on the use of land based on a CGE model covering 57 sectors in 87 regions.[25, 26]

Nevertheless, equilibrium models are also criticized for their underlying theoretical assumptions, which may not be observed in real markets.[27, 28] For example, equilibrium models assume that all economic agents possess perfect oversight and that independently made decisions by each agent lead to a global economic optimum. In reality, however, economic agents may make suboptimal decisions, for example due to imperfect information, and most economic decision-making by individual agents may not lead to a global optimum. Equilibrium models also assume that all markets are in equilibrium, and that prices and demands are determined based on fixed elasticities. These elasticities are, in principle, econometrically inferred, but they are often based on outdated values or proxy data.[27] In addition, in PE and CGE models, sectoral or product resolutions are generally poor. Consequently, PE and CGE models are not suitable for modeling changes introduced at a detailed process-level, or determining substitution effects among alternative technologies serving the same market. These substitution effects, however, are crucial, for example, for modeling the environmental impact of introducing a new technology producing an established product, as discussed by the authors in previous work.[29]

Moreover, CLCA is often exposed to large uncertainties.[27, 30, 31] A main source of uncertainty in CLCA arises from difficulties in modeling changes in the composition of technology mixes used to supply markets or to produce intermediate flows as a response to changes under study.[31, 32] One way to address such uncertainties is to test multiple scenarios showing the range of potential outcomes under different assumptions.[31, 32] This approach, however, may result in an extremely wide range of possible outcomes and must rely on an often subjective choice of selective scenarios. Therefore, methods to systematically address large uncertainties in CLCA have been called for.[7, 33]

While various methods for uncertainty assessment have been utilized for LCA including Analytical Error Propagation[34, 35] and Monte Carlo simulation[36–38], they are typically not applied to CLCAs. A major barrier to using such methods in CLCA lies in the choice of technologies, which is typically made independently from the mathematical formulation of the consequential model, rather than being integrated into the model. Therefore, the interdependence between technology choices and other sources of uncertainty, for example in process parameters and prices, cannot be explored by means of mathematical uncertainty assessment in existing CLCA models.

In this work, we propose the Technology Choice Model (TCM) as a new operational framework for CLCA. The model simultaneously determines technology choices in multiple markets, while systematically considering parameter uncertainties, suboptimal decisions, and factor constraints. As a result, TCM enables the modeling of both market effects and environmental impacts at a high level of detail.

In the following section, we introduce the basic structure of TCM. The basic structure integrates technology choices and lays the foundation for a comprehensive uncertainty assessment. The model inherits its basic structure from the Rectangular Choice-of-Technology (RCOT) model,[39] which is an economic input-output model that allows for more than one technology for producing one product. Practical applications of the RCOT model have been presented for the analysis of the choice between irrigation technologies for agricultural production,[40] and the choice between bio- and petroleum-based fuels.[41]

In the subsequent section, we expand the basic structure of TCM to account for uncertainty and variability in process parameters, prices, factor constraints, and final demand. In addition, we allow for suboptimal decisions by economic agents. The application of TCM is demonstrated in a hypothetical case study on rice production.

BASIC STRUCTURE OF THE TECHNOLOGY CHOICE MODEL (TCM)

In RCOT, technology choices directly result from the model: given all existing technology options, a cost minimization objective determines which technologies are used to which extent, taking into account constraints in factor availability. In this section, the RCOT model of the economic input-output literature is adapted into a CLCA formulation. For this purpose, we follow the notations of the generalized calculus for LCA by Heijungs and Suh,[42 43] which are shortly summarized in the following.

Generalized calculus for LCA

In Heijungs and Suh,[42] the life cycle inventory model is described as a product system consisting of unit processes that exchange intermediate flows (functional flows) and elementary flows (to and from the environment). The exchange of intermediate flows between unit processes is described in the technology matrix A. In this matrix, rows represent intermediate flows, while columns represent processes. A coefficient a_{ij} of the technology matrix A describes the intermediate flow i, which is produced (for $a_{ij} > 0$) or absorbed (for $a_{ij} < 0$) by process j. The net intermediate flows leaving the product system are specified in the functional unit vector f representing the unit quantity that the LCA study is based upon. For an invertible technology matrix A and a given functional unit vector f, a scaling vector s can be calculated from

$$s = A^{-1}f. \tag{1}$$

The elementary flow matrix B describes the elementary flows of the unit processes. In the ISO standards on LCA (ISO 14040[44] and 14044[45]), elementary flows are defined as "material or energy entering the system being studied that has been drawn from the environment without previous human transformation, or material or energy leaving the system being studied that is released into the environment without subsequent human transformation". In the elementary flow matrix, elementary flows are represented by rows, while the columns represent the same processes as in the technology matrix A. The matrix is defined such that a coefficient b_{ej} shows the elementary flow e of unit process j entering (for $b_{ej} < 0$) or leaving (for $b_{ej} > 0$) the system. Multiplying the elementary flow matrix B with the scaling vector s yields the Life Cycle Inventory (LCI) vector g representing the total elementary flows associated with the functional unit f:

$$g = Bs = BA^{-1}f. \tag{2}$$

The characterization matrix Q contains characterization factors transforming the elementary flows into environmental impact flows. The characterization factor of elementary flow e for impact category z is represented by the coefficient q_{ze} of the characterization matrix Q. The total environmental impacts expressed in impact vector h are calculated such that

$$h = Qg = QBA^{-1}f. \quad (3)$$

Basic formulation of the Technology Choice Model

The generalized calculus for LCA by Heijungs and Suh[42] presented in the previous section requires a square technology matrix A, i.e., the same number of processes and intermediate flows. Which technology is utilized to produce which intermediate flow is thus pre-determined for the application of Equations 1-3. In contrast, the RCOT model provides a platform under which technology choices are determined by the model within market conditions and constraints.

Following RCOT, suppose that intermediate flows (functional flows such as products) can be produced by more than one process, in which case the number m of processes in the product system exceeds the number n of intermediate flows.[39] The resulting $n \times m$ technology matrix is rectangular since there are more columns than rows. For a given functional unit f and a rectangular technology matrix A, multiple feasible solutions for the scaling vector s may exist, because intermediate flows can be produced by more than one process. In other words, the system is *underdetermined*. To determine a unique solution, one or more additional criteria are needed to choose between feasible solutions, which in fact serve as criteria for technology choices.

Further suppose that products will be produced in the most economical way, i.e. using technologies that belong to the least expensive production pathway. The term “production pathway” is thereby defined as the entire chain of processes used to produce a product, from the extraction of raw materials to the production of the final product. In addition, factor constraints determine the maximum potential production volume of technologies. The production of agricultural products, for example, is constrained by the amount of cropland available. To implement criteria for technology choices and factor constraints in CLCA, we introduce the linear programming formulation of the RCOT model[39] to the generalized calculus for LCA.[42]

We define a $o \times m$ factor requirement matrix F containing the factor inputs of the unit processes measured in physical units. Typical factors are labor, taxes, and natural resources. The factor requirement matrix F is constructed such that a coefficient f_{kj} describes the amount of factor k needed by process j. We further define a $o \times 1$ unit price vector κ. An element κ_k of κ represents the unit price of factor k. In addition, we define a vector c of factor constraints (the term noted as 'factor endowment' in Duchin and Levine[39]). An element c_k of c quantifies the maximum available amount of factor k. The coefficients for unconstrained factors are set to ∞. Finally, we define a final demand vector y containing the final demand y_i for each commodity i. In contrast to the functional unit vector f in the previous section, the final demand vector y in this model contains the total final demand for products from the production system. The formulation of basic TCM follows:

$$Min\, Z = \kappa' \; Fs \tag{4}$$

$$s.t. \quad As = y$$

$$s_j \geq 0$$

$$Fs \leq c.$$

The objective function Z of the model represents the factor costs associated with the final demand y. The constraint $As = y$ ensures that the final demand y is produced. The constraint $s_j \geq 0$ specifies that the output of each process is positive. The last constraint ensures that the total factor use calculated by Fs does not exceed the factor availability expressed by the constraints vector c.

Finally, once the scaling vector s is calculated, the total elementary flows g as well as the environmental impacts h associated with the final demand y can be calculated from

$$g = Bs \tag{5}$$

and

$$h = Qg = QBs. \tag{6}$$

Basic TCM has the following properties:

(1) All processes are chosen in a way that minimizes the factor costs associated with the final demand y.

(2) If an intermediate flow can be produced only by processes with identical outputs along the production chain (either single outputs or the same combination of multiple outputs), it is supplied by exactly one process.

(3) If an intermediate flow can be produced by processes with different multiple outputs along the production chain (co-products), it will be supplied by either one process or by a combination of processes.

(4) If there are binding factor constraints for any process on the least expensive production pathway, this production pathway will be used until the constraint applies and then complemented by one or several other production pathways representing the next-lowest-cost option for the supply of the final demand.

TCM, as a generalized framework, is independent of the resolution in the underlying data. Therefore, it can utilize detailed, engineering-level data suitable for process LCAs, as well as input-output tables that RCOT utilizes. This feature also enables connecting detailed foreground systems with an input-output background system via hybrid approaches.[43, 46]

In addition to economic factor constraints, product systems may also be constrained in the availability of environmental factors of production, e.g. emissions of pollutants, generation of waste, use of natural resources and ecosystem services. The implementation of environmental factor constraints in basic TCM is discussed in section 1 of the supporting information.

STOCHASTIC TECHNOLOGY CHOICE MODEL

The basic TCM presented in the previous section estimates the environmental impacts h associated with the final demand y in a deterministic way based on the specified input parameters. This deterministic approach disregards the uncertainty inherent in these input parameters and may therefore yield misleading results.[47] For example, the results of a comparative LCA of two products may be misleading if the differences are not significant. Addressing uncertainties in LCA is therefore crucial for reliable decision support.[47]

Uncertainties in LCA are manifold and have been categorized in various ways.[48] Huijbregts[49] distinguishes between (1) parameter uncertainty, (2) model uncertainty, (3) uncertainty due to choices, (4) spatial variability, (5) temporal variability, and (6) variability between objects/sources. While all of these uncertainties are applicable to basic TCM, in this work, we focus on (1), and (3) to (6). The term “uncertainty” is understood as discrepancy between a quantity used in the study and the true value of that quantity,[10] whereas the term “variability” refers to inherent variations in the real world, e.g. seasonal and spatial variation of precipitation.[50, 47] In addition to uncertainties in the data typically used in LCA, TCM is subject to uncertainties in factor constraints and in the final demand. For example, the amount of natural resources classed as a factor constraint, and future final demands are generally estimated. Various methods have been used to quantify uncertainties in LCA, e.g. analytical error propagation,[34] calculations with fuzzy logic,[51] and stochastic methods such as Monte Carlo simulation.[36–38] While the application of these methods is becoming increasingly common in attributional LCA, examples and methods for a comprehensive quantitative uncertainty assessment in CLCA are still missing.

In this section, we expand basic TCM (Equations 4-6) to account for uncertainties and variability. We therefore first identify parameters subject to uncertainty and variability in TCM, and discuss their impact on technology choices and environmental impacts. Subsequently, we stochastically propagate these uncertainties into the CLCA results using Monte Carlo simulation. The combination of basic TCM and Monte Carlo simulation is denoted 'stochastic Technology Choice Model (stochastic TCM)'.

Effect of uncertainty in TCM

Uncertainty and variability in input parameters

In TCM, the input parameters in A, B, Q, F, κ, c and y may be subject to both uncertainty and variability. Uncertainties in A, F, and κ affect the factor costs of the product system, which determine the choice of technologies. To illustrate the effect of uncertainties in A, F, and κ on the choice of technologies, we assume a product system in which the final demand can be produced via 3 different production pathways. The factor costs of the 3 production pathways are illustrated in Figure 1, and represent the sum of factor costs along the entire production pathway that are associated with the production of one unit of output. The bars show single value estimates of the factor costs, while the error bars specify the uncertainties. Without uncertainties, the choice of technologies is obvious: all technologies on production pathway P_1 are chosen, because P_1 is the lowest-cost option. Considering uncertainty, however, we find that there is a certain probability for each production pathway to be the lowest-cost option. Pathway P_3, for example, may be cheaper than the other pathways if its factor cost is overestimated while the costs of the other pathways are underestimated. Thus, the expected environmental impact associated with the final demand is not equal to the environmental impact of a single production pathway. It is given by the sum of the environmental impacts of all 3 production pathways weighted by their respective probability of being the lowest-cost option.

Uncertainties in y directly affect the total amount of products produced, while uncertainties in both y and c may affect technology mixes if factor constraints are binding. The effect of changes in y is further discussed in the case study section.

Uncertainties in B and Q affect the elementary flows and environmental impact flows associated with a given scaling vector s. Uncertainties in B and Q may also affect the choice of technology in the model with environmental factor constraints (see Equation S1).

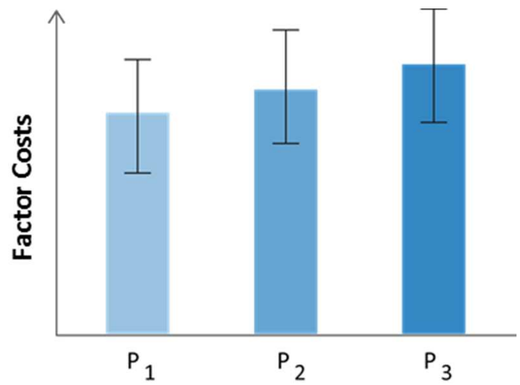


Figure 1: Factor costs of three hypothetical production pathways P_1, P_2, P_3 for a product. The columns show the expected values, while the error bars refer to the inherent uncertainty.

Uncertainty due to suboptimal decisions

In basic TCM, technologies are chosen based on minimization of factor costs. This approach reflects the assumption that economic agents make optimal decisions to minimize their factor costs. In reality, however, decisions in the market may not be optimal for several reasons. One is imperfect information or information asymmetry in the market.[52] Due to imperfect information, decision-makers may not know all decision alternatives (e.g. suppliers for a certain raw material) and the potential outcome of the decision alternatives (e.g. present and future prices). Another reason lies in non-market influences such as personal relationships and patriotism. A business owner, for example, may choose a supplier with whom he/she has a friendly relationship or family ties. More fundamentally, human decisions are not always rational.[53, 54]

In TCM, the effect of suboptimal decisions can be simulated as random noise in the choice of technologies. This random noise causes a diversification of raw material supplies and technologies used. The integration of uncertainties and suboptimal decisions is discussed in the following section.

Modeling of uncertainties in stochastic TCM

Stochastic TCM addresses uncertainties in basic TCM using Monte Carlo simulation. Monte Carlo simulation is a widely accepted method to quantify uncertainties in LCA.[10] The idea of Monte Carlo simulation is to stochastically propagate uncertainties in input parameters into the model's results. To perform a Monte Carlo simulation of TCM, we first need to quantify the uncertainties inherent in the model.

Uncertainties and variability in input parameters can be quantified as probability distributions. Data on probability distributions of process parameters can be obtained from LCA databases. Ecoinvent,[55] for example, specifies probability distributions for almost all data items. Probability distribution for prices can be determined based on historic data under the assumption that the volatility of future prices equals the volatility of a certain timeframe in the past.

The quantification of uncertainties due to suboptimal decisions is more difficult, because no literature values on these uncertainties exist. In the context of TCM, suboptimal decisions are understood as random noise in decision-making, and hence technology choices. The choice of technologies is based on the costs of individual processes determined by factor requirements and prices. Introducing a random error to the determination of the factor cost therefore results in a random error in the choice of technologies. In this way, uncertainty due to suboptimal decisions can be translated into additional parameter uncertainty.

To simulate the effect of suboptimal decisions, we add an additional row to the factor requirement matrix F. This row specifies the requirement of an additional factor representing suboptimal decisions, which is normally distributed and has an expected value of zero. The standard deviation of the amount of this additional factor required by each process is defined as percentage i of the expected cost of running the respective process. Consequently, the standard deviations for the additional row in F are calculated by

$$\sigma_{C,add} = i\kappa' F. \quad (7)$$

In this equation, κ contains the expected factor prices and F the expected factor requirements before adding the additional row. Subsequently, we add an additional entry to the factor price vector κ, which corresponds to the newly added row in F. This additional entry has an expected value of 1 and a standard deviation of 0. Due to the modifications in F and κ, we introduce an error in the factor cost calculations for each process representing suboptimal decisions.

Once the probability distributions of all input parameters are defined, we can perform the Monte Carlo simulation. The Monte Carlo simulation is a stepwise procedure: in each step v, the parameters of TCM are varied according to their respective probability distribution, and the scalars s_v, g_v, and h_v are calculated. After n steps, we determine the arithmetic mean of the n results from the Monte Carlo simulation for all elements in s, g, and h. The mean values represent the expected values of these elements, and hence the CLCA results.

The resulting mean-scaling vector s_{mean} allows us to determine the expected production volumes of each process, as well as technology mixes for the production of each flow. Production volumes are determined by the scaling vector entry of a technology in s_{mean} multiplied by the expected value of the output of this technology specified in A. The share of a technology in a technology mix is determined by the ratio of the production volume of this technology and the sum of the production volumes of all technologies producing the same product. The elements in g_{mean} and h_{mean} represent the expected elementary flows and environmental impacts of the production system, respectively.

CASE STUDY

In this section, we apply stochastic TCM to a case study investigating the environmental impacts of producing processed rice. The results from stochastic TCM are compared with those from basic TCM to show the effect of uncertainties and suboptimal decisions. In the case study, the final demand for processed rice is 1 Mt, while the functional unit is defined as "production of 1 kg processed rice". The case study is designed to demonstrate the application of the model and does not aim to provide implications for real-life rice production. It is therefore based on hypothetical data. The rice production system, however, is inspired by an existing production site in the Punjab Province in Pakistan. The data base for this case study, as well as the Matlab[56]-file used to determine the case study results are available in the supporting information.

Rice production system

The rice production system is illustrated in Figure 2. Producing processed rice in the rice factory requires raw rice, electricity, and thermal energy. The raw rice is produced in small-scale farms surrounding the factory. Electricity is provided by a coal-fired power plant. Thermal energy can be generated by three different types of boilers fueled by natural gas, wood pellets, and rice husk, respectively. Natural gas is supplied by the national gas grid. Wood pellets are produced in the vicinity of the rice factory. Rice husk is co-produced with raw rice at the farms. The use of rice husk for thermal energy generation, however, requires the collection of rice husk at farms, involving an additional transportation demand. For simplicity, we assume that the farms are located in five different zones with average transportation distances of 100 km (zone 1), 200 km (zone 2), 300 km (zone 3), 400 km (zone 4), and 500 km (zone 5). The amount of rice husk available in each zone is assumed to be sufficient to satisfy about 20% of the thermal energy demand of the rice factory. Rice husk not used at the factory is burned at the fields.

Consequently, there are technology choices for the supply of rice husk and for thermal energy. Rice husk can be provided by farms in 5 different zones, while thermal energy can be produced from rice husk but also from natural gas and wood pellets. These technology choices ultimately lead to 7 potential fuel choices for thermal energy generation: rice husk from 5 zones, natural gas, and wood pellets.

For the 7 fuel types, we assume the following order of factor costs associated with thermal energy production beginning with the lowest: (1) rice husk from zone 1, (2) rice husk from zone 2, (3) natural gas, (4) rice husk from zone 3, (5) wood pellets, (6) rice husk from zone 4, and (7) rice husk from zone 5. The expected values of these factor costs and their standard deviations are illustrated in Figure S1 of the supporting information.

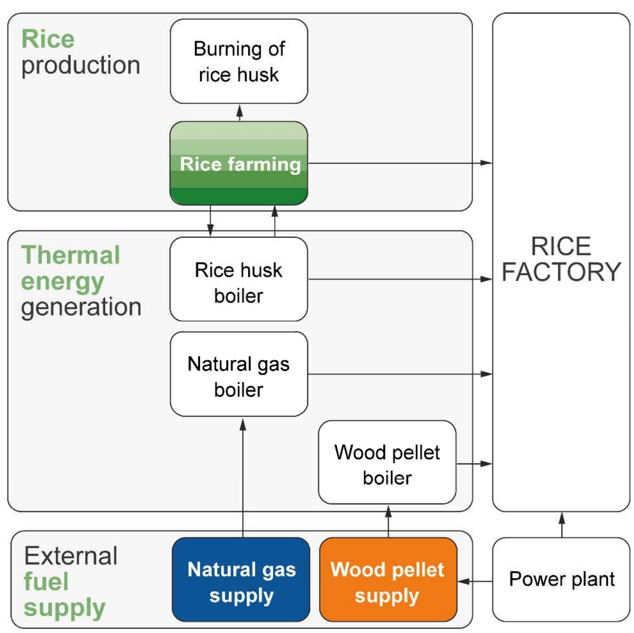


Figure 2: Process flow sheet of the rice production system

Mathematical formulation of TCM for the case study

The product system is comprised of the following 15 processes: rice factory, rice farming, rice husk boiler, natural gas boiler, wood pellet boiler, 5 processes for rice husk collection, natural gas supply, wood pellet supply, burning of rice husk, power plant, and transportation by truck. The unit processes are represented by the columns of the matrices A, B, and F. The product flows include processed rice, unprocessed rice, thermal energy, rice husk at factory, rice husk at farm, natural gas, wood pellets, electricity, and transportation. These flows are specified by the rows of the technology matrix A and the coefficients of the final demand vector y. Furthermore, 11 production factors are defined: operation of rice factory, cultivation of land, 5 factors representing purchases of rice husk in the 5 zones, extraction of natural gas, operation of power plant, extraction of coal (used in power plant), and operation of truck. The cost factors are collected in the cost factor matrix F, while the respective prices are expressed by the price vector κ. For simplicity, we only consider 2 elementary flows, namely CO_2 and CH_4, which are expressed by the rows of the intervention matrix B. The respective characterization factors are specified in the characterization matrix Q. Finally, factor constraints are defined in the constraints vector c for the quantity of rice husk available in each zone.

We assume that parameters in A, B, F, κ, and c, except for the main process outputs in A, follow a normal distribution with a standard deviation of 10%. The main outputs of processes in A have a standard deviation of 0, because the uncertainty of other parameters is defined in relation to the main outputs. Furthermore, all uncertainties are assumed to be independent from each other.

All matrices and vectors used in the case study are provided in the Excel-file ‘TCM Case Study Data.xlsx’ in the supporting information.

Case study results

Results of basic TCM

The case study results of basic TCM are shown in columns (1) and (2) in Figure 3. Without considering factor constraints (column (1)), all thermal energy is produced from rice husk from zone 1 in the basic model. Rice husk from zone 1 is chosen, because it has the lowest expected factor costs, and is assumed to be available without any limits. In the model with factor constraints (column (2)), in contrast, thermal energy is produced from rice husk from zones 1 and 2, as well as from natural gas. Multiple production pathways are chosen, because the amount of rice husk available in each zone is constrained. Rice husk from zone 1 represents the lowest cost option, but can only satisfy about 20% of the total thermal energy demand due to factor constraints. It is therefore complemented by rice husk from zone 2, which is the second lowest-cost option and can provide another 20% of the total energy demand. After all rice husk from zones 1 and 2 is utilized, additional thermal energy needed is generated from natural gas. This production pathway represents the next-lowest cost option and is available without limits in the model.

In a decision-making context, it is important to note that the global warming impact in the model result is substantially higher when considering factor constraints (about 0.9 kg CO2e/kg v.s. 1.3 kg CO2e/kg), because rice husk must be fetched from afar. Fetching rice husk from afar increases the transportation needs, and hence, also the cost of rice husk to the extent that natural gas becomes economically favorable. Without considering such constraints, costs, and associated market responses, the environmental benefit of a new technology can be overestimated.

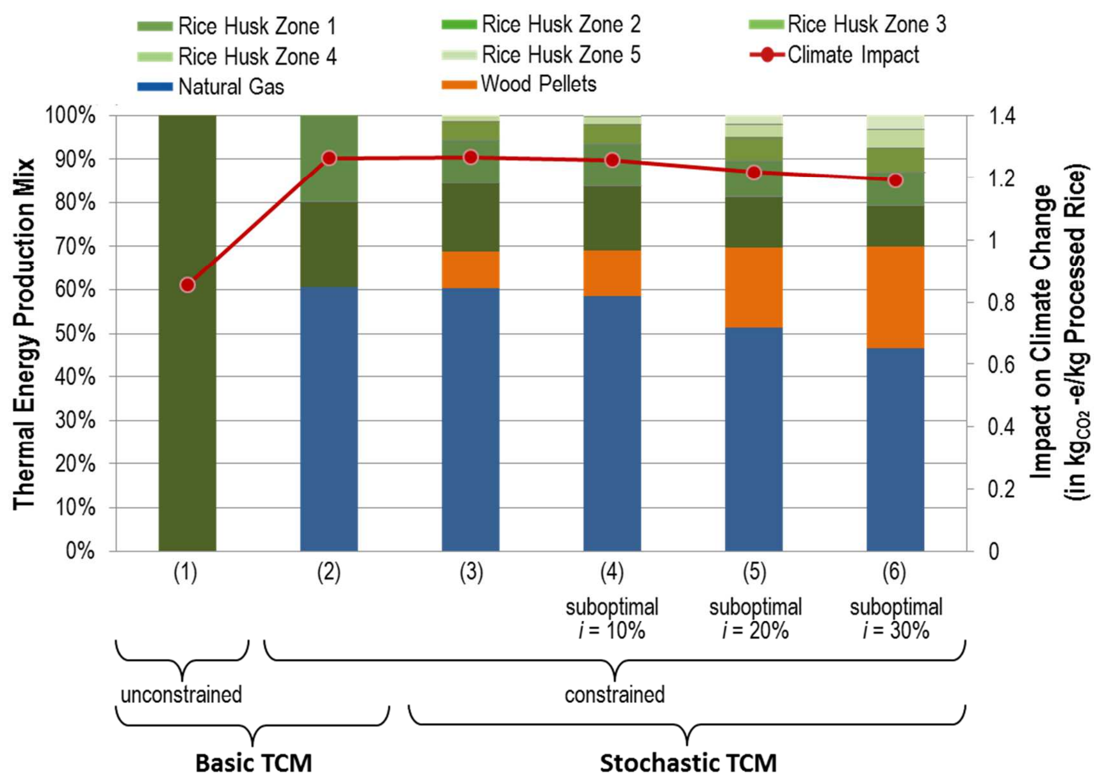


Figure 3: Thermal energy production mixes (columns, left axis) and resulting climate change impacts (markers on solid line, right axis) based on basic TCM and stochastic TCM with and without binding factor constraints and suboptimal decisions.

Results of stochastic TCM

Columns (3) to (6) in Figure 3 show the results of stochastic TCM reflecting uncertainties in A, B, F, κ , and c. The consideration of these uncertainties leads to a diversification of the thermal energy production mix, where wood pellets and rice husk from zone 5 enter the market, absorbing part of the nearby rice husk supplies and natural gas. Parametric uncertainties considered in these results can arise from various origins including price fluctuations, measurement errors, and seasonality in supplies. Additionally, the effect of suboptimal decisions is illustrated in columns (4) to (6) in Figure 3. The percentage i specified in the column labels states the factor i used to model suboptimal decisions in the respective scenario (cf. Equation 7). The higher this factor i is, the more equally distributed the shares of individual technologies in technology mixes are. Hence, suboptimal decisions lead to an increase in market share of less competitive technologies in TCM. In our particular example, the consideration of uncertainties and suboptimal decisions in stochastic TCM reduces the expected global warming impact of rice production (solid line in Figure 3). Modeling the potential outcome of suboptimal decisions, e.g. due to market imperfections and behavioral aspects, is important, because it helps understand the potential discrepancy between the designed and real outcomes of a policy.

Figure 4 shows the effect of varying the final demand from 0 to 1 Mt, using TCM with factor constraints and suboptimal decisions ($i = 10\%$). Varying the final demand allows us to show what would happen if consumers made different consumption decisions, e.g. due to changes in prices and incomes, legislation, or desire to contribute to sustainability. The shaded areas illustrate the shares of energy carriers in the technology mix (left vertical axis). The dashed line represents the marginal climate impact per functional unit, while the solid line shows the average climate impact per functional unit. For a final demand below 0.2 Mt of processed rice, no factor constraints apply. In this range, the amount of rice husk available in each zone is sufficient to satisfy the total thermal energy demand. Consequently, mostly rice husk from zone one is used, because it has the lowest factor costs. As long as no factor constraints apply, the technology mix is constant and the marginal climate impact equals the average climate impact per functional unit. For a final demand above 0.2 Mt, one or more factor constraints become binding: the thermal energy demand of the rice factory exceeds the amount of thermal energy that can be generated from rice husk from zone 1. This constraint results in an increased use of rice husk from other zones, natural gas, and wood pellets. Since these changes in the technology mix are

436 induced by changes in final demand, the resulting climate impact also depends on the final demand. Consequently, in presence of factor constraints, the marginal climate impact per functional unit differs from the average climate impact per functional unit. The non-linear relationship between climate impact and final demand can be determined using TCM.

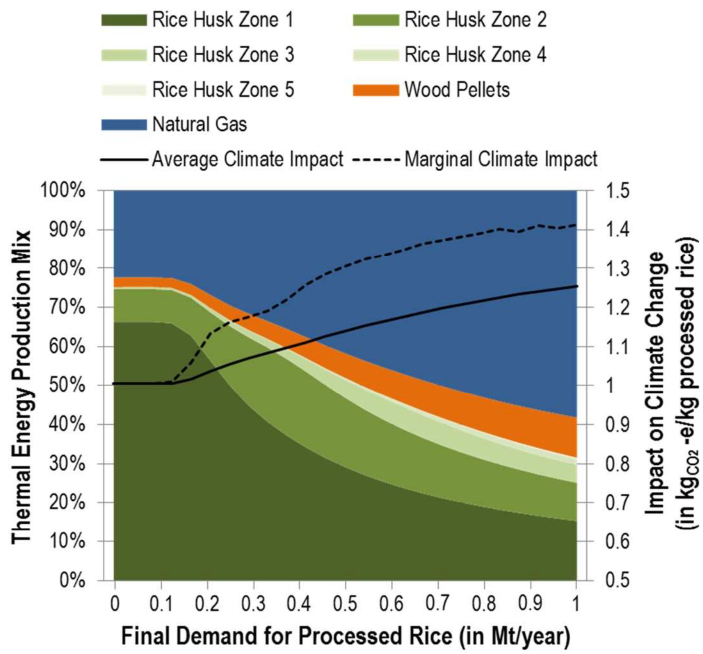


Figure 4: Effect of varying the final demand in TCM with factor constraints and suboptimal decisions ($i = 10\%$; cf. Equation 7) on thermal energy production mix (shaded areas, left vertical axis), marginal climate impact per functional unit (dashed black line, right vertical axis), and average climate impact per functional unit (solid black line, right vertical axis)

This result casts light on another important variable for decision-making that traditional LCAs often ignore: the scale of production and consumption.[57–60] In the presence of constraints, the market may favor different technologies under different scales of production and consumption, which in turn affect the policy outcome. Figure 4 shows that the system may generate larger-than-expected GHG emissions when the demand for processed rice rises beyond 0.2 Mt/year.

DISCUSSION

There is no doubt that understanding the environmental consequences of an action, which consequential LCA aims at measuring, is of great importance for policy-makers. An operational framework enabling the modeling of technology choices at an engineering-level detail, however, has been lacking in CLCA literature. In this paper, we presented an operational approach to model discrete technology choices at process-level detail, while systematically considering parameter uncertainty, suboptimal decisions, and factor constraints. In TCM, products are produced by technology mixes rather than single technologies, where the shares of individual technologies within these technology mixes are determined by the cost of production, factor constraints, uncertainties, and suboptimal decisions. By this means, TCM models market effects and environmental impacts of a product system and its changes at a high level of detail. The case study shows that considering uncertainty is not only essential for understanding the quality of CLCA results but may also lead to substantially different results.

Equilibrium models v.s. Technology Choice Model

Here we briefly discuss the advantages and limitations of TCM as compared to other modeling approaches widely used for CLCAs. In the literature, Partial Equilibrium (PE) models and General Equilibrium Models (GEMs)—and CGE models as their operational form—are frequently used as a modeling framework for CLCA. Unlike PE and CGE models, TCM can be formulated as a purely process-based model based on engineering estimates and measurement data. PE and CGE models, in contrast, are based on elasticities derived from econometric analyses. These elasticities are determined on an aggregated sector basis which typically distinguishes less than 60 sectors per country. Therefore, the level of detail of PE and CGE models is substantially lower compared to TCM. A high level of detail as provided by TCM is crucial, for example, for modeling substitution effects among technologies producing the same product, or to explore the effect of a policy on technological change.[29]

PE and CGE models are criticized for assuming perfect cost-minimization for all economic agents. This assumption has been relaxed in stochastic TCM by allowing for suboptimal decisions. In the case study, considering suboptimal decisions has been shown to significantly affect technology choices as well as expected climate impacts. In this work, suboptimal decisions are understood as technology choices that do not result in the minimization of factor costs.

In contrast to TCM, on the other hand, PE and CGE models determine demand changes due to price changes in all considered markets. In TCM, these changes are captured for intermediate products, but not for final product markets, i.e. markets of products with non-zero entries in y. Nevertheless, if reliable data on the price elasticity of demand is available, TCM can be expanded to account for changes in final product demand due to price change. For this purpose, the demand at time t + 1 can be determined in response to the price in time t using the price elasticity of demand.[29] Also, the data requirement for TCM can be higher than for PE or CGE, and unlike CGE models, TCM captures only a part of the entire economic system. However, TCM can be extended to cover broader economic systems by employing hybrid approaches, where the foreground system is modeled in process-level detail, while the rest of the economy is modeled using input-output data.[43, 46]

Limitations and future research

In TCM, suboptimal decisions are treated as random phenomena. In reality, however, suboptimal decisions may be systematic: a potential reason for suboptimal decisions is that decision-makers may have objectives other than cost minimization. A company, for example, may decide to use renewable feedstocks along the entire supply chain to demonstrate commitment to environmental protection, even if these feedstocks may be more expensive. In this case, technology choices are suboptimal regarding the cost minimization objective, but optimal with regard to the decision-makers' objective. Furthermore, in this case, decisions on feedstock choices are correlated. Correlations between suboptimal decisions, as well as conflicting objectives are currently not captured in TCM and remain a topic for future research. In addition, the degree to which economic agents make suboptimal decisions still needs to be investigated in the context of TCM. Thus, our modeling approach for suboptimal decisions represents only an initial step towards acknowledging the effect of suboptimal decisions in the model, and needs further refinement to capture the full complexity of the topic.

TCM allows the consideration of factor constraints in LCA, which have rarely been addressed quantitatively in the literature. These constraints may largely affect technology mixes, as shown in the case study. While our case study demonstrated the use of constraints for factor availability only, in reality, production systems may be subject to additional constraints. Chemical industries, for example, may be constrained in the use of certain chemicals imposing material health risks.[61] Operation of energy technologies is affected by regulation, transmission and storage capacity, among other things.[62, 63] Additional constraints may be further incorporated into the general TCM framework.

It is also important to note that all parameter uncertainties in our case study were assumed to be independent from each other. In reality, uncertainties may be correlated, in which case, this correlation can be incorporated into the Monte Carlo simulation, if the correlation between input parameters can be estimated.[49]

TCM presented in this paper aims at operationalizing CLCA focusing on the question of technology choice based on a transparent and reproducible modeling framework. While taking into account economic principles, uncertainty, and suboptimal decisions in technology choices, there are many more aspects to be further explored, including technology lock-in and path dependency, rebound effect, delay mechanisms, and inertia in market behavior, to name a few. Follow-up research on such topics as well as additional case studies using TCM would be desirable.

Operationalizing TCM at a large scale requires additional information to existing and established process life cycle inventory (LCI) databases. In particular, reliable price data is crucial in applying TCM to existing process LCI databases. In addition, understanding factor constraints and capacity limitations would be essential in transforming existing process LCI databases for TCM. In order to materialize the benefits of TCM, efforts must be made to develop related meta-data protocols and collect additional data required.

ASSOCIATED CONTENT

Supporting information. TCM with environmental factor constraints, factor costs of thermal energy generation, implementation of TCM in MATLAB, MATLAB-code and data (Excel-file) used to calculate the case study results. This material is available free of charge via the internet at http://pubs.acs.org

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ACKNOWLEDGEMENT

This work has been carried out in part within the project “enCO_2re - enabling CO_2 re-use”, which is funded by the Climate Knowledge and Innovation Community (Climate-KIC) by the European Institute of Innovation and Technology (EIT). André Bardow and Arne Kätelhön gratefully acknowledge support by the German Academic Exchange Service (DAAD) through its thematic network „ACalNet“ funded by the German Federal Ministry of Education and Research (BMBF). Sangwon Suh was supported by the US National Science Foundation (NSF) (grant #: 1360445), and by the US Environmental Protection Agency (EPA) (grant #: 8-442650-22870-2 RFEP70).

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