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Market Power, Fuel Substitution and Infrastructure

A Large-Scale Equilibrium Model of Global Energy Markets

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Market power, fuel substitution and infrastructure –
A large-scale equilibrium model of global energy markets*

Daniel Huppmann† & Ruud Egging‡

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Abstract

Assessing and quantifying the impacts of technological, economic, and policy shifts in the global energy system requires large-scale numerical models. We propose a dynamic multi-fuel market equilibrium model that combines endogenous fuel substitution within demand sectors and in power generation, detailed infrastructure capacity constraints and investment, as well as strategic behaviour and market power aspects by suppliers in a unified framework. This model is the first of its kind in which market power is exerted across several fuels.

Using a dataset based on the IEA World Energy Outlook 2013 (*New Policies* scenario, time horizon 2010–2050, 30 regions, 10 fuels), we illustrate the functionality of the model in two scenarios: a reduction of shale gas availability in the US relative to current projections leads to an even stronger increase of power generation from natural gas in the European Union relative to the base case; this is due to a shift in global fossil fuel trade. In the second scenario, a tightening of the EU ETS emission cap by 80 % in 2050 combined with a stronger biofuel mandate spawns a renaissance of nuclear power after 2030 and a strong electrification of the transportation sector. We observe carbon leakage rates from the unilateral mitigation effort of 60–70 %.

Keywords: energy system model, infrastructure investment, strategic behaviour, mixed complementarity problem (MCP), generalized Nash equilibrium (GNE)

JEL Codes: Q41, C61, D43

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1 Introduction

The global energy system is constantly changing, driven by technological advances and economic shifts as well as regulatory interventions. The shale gas boom in the United States, for example, drastically shifted the economics between the different fossil fuels. Other trends are a result of governmental regulation, such as the establishment of an Emission Trading System (ETS) by the European Union, or biofuel mandates in North America and Europe. Many of these regulations are motivated by potential threats of global warming and climate change (cf. IPCC, 2014), and intend to curb greenhouse gas (GHG) emissions – most importantly carbon dioxide (CO_2) – or reduce local air pollution. Other measures are motivated by public pressure, for instance the nuclear phase-out in several OECD countries following the Fukushima incident. Another driver of energy policy interventions are concerns regarding security of supply and import dependency, which have been raised in Europe in particular by the recurring natural gas transit disputes between Russia and Ukraine (Lévêque et al., 2010).

When combined, these trends may create paradoxical effects. For example, the shale gas boom in North America led to an increase of coal exports from the US to Europe, and Germany saw an increase in the use of coal and lignite in recent years (AGEB, 2014). This occurred despite the EU ETS, as well as ambitious national policy goals to reduce CO_2 emissions and substantial renewable energy feed-in. At the same time, European policy makers express concerns about a loss of competitiveness with North America due to low energy prices overseas (IEA, 2013) – while European utilities consider mothballing natural gas power plants, because they are not able to compete with subsidized renewables and coal at current low CO_2 permit prices.

There is one further intricate aspect with regard to energy and emissions: carbon leakage. Unilateral or regional emission reduction may shift fossil fuel consumption to other regions and thus have limited benefit to the global climate. This effect can work either directly through reduced world prices for fossil fuels, increasing consumption in other regions; or it may work indirectly via the goods market channel, where production of consumer goods is shifted to regions with lower environmental standards, and the goods are then exported to the high-standards countries. Energy-intensive and trade-exposed (EITE) industries such as steel or pulp-and-paper are particularly vulnerable in this regard, further fuelling the fear of reduced competitiveness and industry relocation.

These examples illustrate the complex and integrated nature of global energy markets and climate policy. This interdependence poses various challenges to companies, governments and supra-national entities when considering long-term trends. To gauge the economic impacts of technology-related shifts as well as the effects of regulation and policy measures on the global energy system, policy makers and academics rely on large-scale numerical models of the energy sector.

There is an inherent trade-off in energy modelling: a broad research scope requires substantial aggregation, which necessarily omits many details; on the other hand, many relevant questions with regard to energy, in particular infrastructure investment, can only be tackled adequately while accounting for operational or seasonal detail. Depending on the research question posed, models therefore set different priorities and vary with respect to spatial disaggregation, the time horizon under consideration, and the level of detail with which fuels and technologies (e.g., in power generation) are modelled. They also treat different variables as endogenous (i.e., determined by the model) or exogenous (i.e., taken as a given parameter from some external source or assumption).

Energy market modelling approaches can be broadly classified into four categories, albeit the distinction is not always clear-cut and there is some overlap. *Integrated assessment models* (IAM) such as ETSAP-TIAM (Loulou and Labriet, 2008) and MIT-EPPA (Jacoby et al., 2006) typically have a global and long-term scope and explicitly capture the interaction between the economy, the energy sector, and climate. Several *computable general equilibrium* (CGE) models specifically include emissions and climate aspects, for example PHOENIX (Wing et al., 2011) or GTAP-E

(McDougall and Golub, 2007).

Energy system models (ESM) abstract from other sectors of the economy and focus only on the energy sector; this allows for an even more detailed analysis. ESM are usually based on an explicit optimization or equilibrium model.[1] Examples include the PRIMES model (EC, 2011) and the many applications based on TIMES-MARKAL.[2]

Lastly, *sector models* only cover one particular fuel (e.g., natural gas, Egging et al., 2010) or sector (e.g., power generation, Leuthold et al., 2012); this focus allows for the inclusion of a high level of detail with regard to market characteristics, infrastructure constraints (e.g., flow of electricity in a network), or variability over time. Some models in this area of research focus on market structure and strategic behaviour by certain dominant players, which we discuss in more detail below.

The model we propose in this article combines the advantages of partial-equilibrium modelling (strategic behaviour and a high level of infrastructure detail) with the broad scope of energy system modelling. In particular fuel substitution is included endogenously in the final demand sectors and in power generation. Furthermore, we make provisions for taxes and emission quota on multiple emissions and pollutants at various levels (nodal, regional, global), and we include constraints on the fuel mix in transformation and final demand to represent governmental regulation. This enables us to conduct detailed analyses of the impact of various energy and climate policies on global fossil fuel markets and the integration of renewable energy.

Compared to Egging and Huppmann (2012), this work extends the framework in the following respects: i. it is a multi-period model allowing for endogenous investments in and depreciation of all infrastructure types; ii. it includes seasonality, storage, and load variation; iii. it allows for endogenous fuel substitution in the final demand sectors; iv. the data set is more detailed in terms of geographical coverage, demand sectors, and with respect to the fuels.

The remainder of this paper is organized as follows: the next section details how different model classes tackle fuel substitution, infrastructure, and market power. Section 3 provides the mathematical formulation of the model; Section 4 gives a brief overview of the current data set and presents two scenarios to illustrate the types of analysis that can be performed with the model: a pessimistic scenario regarding the future of shale gas in North America, and a scenario where the EU unilaterally reduces its CO_2 emissions by 80 % until 2050. Section 5 concludes and proposes a number of potential avenues for further research and model development.

2 Three modelling aspects of particular interest

Numerical models for assessing potential developments of the global energy landscape have been used for decades. We refer to Hirth (2015) and Connolly et al. (2010) for a detailed classification and a comparison of models currently used for policy analyses. Instead of providing an extensive overview, we focus on three key aspects, and how they are covered in state-of-the-art models. These aspects are: fuel substitution within demand sectors as well as in power generation; infrastructure for production, transportation, storage, and transformation of different energy carriers; and finally, the explicit consideration of strategic behaviour by certain suppliers, i.e., Nash-Cournot market power exertion. This allows us to highlight how the proposed model departs from and extends the current state-of-the-art in energy modelling.

[1] Some ESM are "simulation" models, which are not based on any optimization rationale. Rather, there are certain if-then-assumptions or rules underlying the model. To simulate a scenario, the future energy demand or fuel mix is extrapolated based on these rules. Some hybrid models employ a combination of optimization and simulation approaches. For the sake of conciseness, we do not address simulation approaches in detail, but focus on optimization or partial equilibrium-based ESM.

[2] See `http://www.iea-etsap.org` for more information.

Endogenous fuel substitution

There are, in principle, two approaches for incorporating fuel substitution: a *top-down* formulation follows the computable general equilibrium methodology (CGE), using elasticities of substitution. This approach is advantageous because the energy sector can be embedded in the broader economy, thereby allowing for well-founded welfare analyses specifically including the interdependence between economic activity and energy prices. However, due to the large aggregation necessary for such models, many details are lost. In addition, a drawback of using elasticities is that, if a fuel is not used at all in the base year (or only to a small extent relative to total energy consumption), such models are rather inert and are not capable of showing large future penetration rates of these fuels even when economic considerations would warrant that. This is a significant disadvantage when modelling potentially "game-changing" technologies.

In contrast, energy system models (ESM) usually start from a *bottom-up* assessment of the energy sector such as production/generation and investments costs. They are based on optimization or partial equilibrium techniques and often follow a (linear) least-cost approach where pre-specified demand levels (often determined by another, CGE-type model) must be met at lowest total cost. Alternatively, the objective may be welfare maximization, where a decreasing willingness-to-pay for energy (or inverse demand function) is assumed. This approach may have the opposite drawbacks of CGE-type models, namely "bang-bang"-results: if a small shift in relative costs makes one fuel cheaper than the one currently used, the entire energy demand by the respective sector shifts from one fuel to the other.[3] This is obviously unrealistic, so these models need to specify (assumptions on) limits or costs of fuel substitution.

Some models only investigate fuel substitution within the electricity sector; this can be problematic due to the implicit assumption that parameters outside the scope of the analysis do not change even in drastic scenarios. For example, studying the effects of a nuclear phase-out while keeping the price of fossil fuels fixed obviously neglects the interdependence between gas and coal prices and their use in power generation to replace nuclear power (cf. Knopf et al., 2014).

Supply chain infrastructure

In typical CGE models, a long-term equilibrium perspective combined with yearly averages ensures that each sector attracts "just enough" capital to execute all activities. Hence, such models cannot account for explicit capacity constraints. This, in combination with taking yearly averages, makes such an approach unsuitable for analysing infrastructure bottlenecks in detail or addressing the many short-term operational considerations important in energy markets.

Energy system models, in comparison, can easily capture "hard" infrastructure capacity constraints, and can be extended to include seasonal or hourly variation and stochasticity. In addition, many multi-period models allow for endogenous investments, and explicitly account for the lead-time of capacity expansions, which is neglected by the "just enough" capital approach in CGE models.

The simplifications regarding the economy made in sector models allow more sector-specific peculiarities to be tackled, such as loop flows in an electricity network. This enables a correct analysis where bottlenecks occur in the transmission networks. The problem with such an approach is one of scaling; extending such a detailed model to a realistic hourly disaggregation will quickly reach the limit of computational tractability.

The model REMIND-R (Leimbach et al., 2010) and the approach proposed by Böhringer and Rutherford (2009, 2008) combine the advantages of CGE-type models to capture the economy at large and the detail allowed by sector models. In these hybrid models, the energy sector is represented with the technological detail common for partial equilibrium models, and the rest of the economy is modelled according to the top-down approach typical for CGE models. They can

[3] Mathematically speaking, the solution jumps from one corner of the feasible space to another corner (or vertex); this is a common characteristic in particular of linear optimization problems.

thereby capture the feedback loops between the market for various fuels and the economy at large, which are typically overlooked by partial equilibrium models. At the same time, their approach allows for completely inactive energy technologies to develop over time (thereby addressing the *inertia* issue discussed above) and for consideration of hard capacity limits, which standard CGE models cannot address. However, REMIND-R does not incorporate the third aspect relevant to energy markets, which we consider important – market power.

Strategic behaviour and market power

Energy system models usually apply a least-cost or welfare maximization approach, and therefore, they cannot incorporate strategic behaviour. Rather, market structure analysis is frequently conducted using a sector-specific modelling approach: for example, Trüby (2013) and Haftendorn and Holz (2010) test several market power assumptions for the global coal market in a partial-equilibrium framework; Huppmann and Holz (2012) conduct a similar analysis for crude oil, with a specific emphasis on the role of OPEC members. For natural gas, a large number of models have been developed over the last years; several of these compute market equilibria for the next decades taking into account Nash-Cournot behaviour by certain suppliers (e.g., Abada et al., 2013; Egging et al., 2010; Lise and Hobbs, 2008). The generalization of Nash-Cournot market power are conjectural variations (CV): each supplier has an expectation (or conjecture) regarding how its rivals will react to a variation in its own output. This allows to model "intermediate" cases of market power exertion. As recently discussed by Huppmann (2013b), the assumption of Nash-Cournot behaviour (or any fixed CV parameter) to represent strategic interaction is in itself a strong simplification, but it may still be a useful approximation.

CGE-type models can – in principle – incorporate imperfect competition; however, to our knowledge, most large-scale applications used in the policy evaluation arena assume perfectly competitive behaviour by all players. Böhringer et al. (2014) are the exception; in their article, they compare several assumptions concerning OPEC market power in a CGE framework and discuss the implications on carbon leakage. However, they only treat oil as a homogeneously traded fuel, and thus (to some extent) omit carbon leakage via other fossil fuels.[4]

Another application of a CGE-type model with market power is presented by Golombek et al. (2013): they use the market power version of the LIBEMOD model (Aune et al., 2008) to investigate how different energy market liberalization trajectories affect prices and social welfare in Western Europe.[5] They model market power through incorporating price mark-ups, representing various market imperfections, to the supply cost curves. The values of these mark-ups are based on data observations and determined in the model calibration phase. As such, the origins and magnitudes of the various market imperfections are neither assessed nor quantified. Merely the aggregate effect in each agent's behaviour is accounted for. The market liberalization in a specific market can then be represented by removing the mark-ups for the agents involved in that market.

The approach used by Golombek et al. follows the reasoning of Smeers (2008); he argues that just adding a mark-up in addition to marginal costs is an easier way to include non-competitive behaviour than conjectural variations. We disagree; in spite of some theoretical shortcomings, using a CV allows to incorporate a relation between the level of market power exertion and the market share of the respective supplier in various markets. As a consequence, a supplier exerting market power will seek to diversify its sales. Standard optimization energy models, in contrast, implicitly minimize transportation costs. For this reason, one will not observe trade flows of the same fuels in opposite directions in such models – but such trade flows do occur in the real world. Assuming Cournot behaviour or a CV by (some) suppliers result in trade flows that are more

[4]Böhringer et al. (2014) assume that there exists a global integrated market only for crude oil; they use Armington elasticities for other fossil fuels, which implicitly assumes that coal or gas from different regions are not perfect substitutes.

[5]Strictly speaking, the LIBEMOD model is a hybrid between a CGE model and a bottom-up energy system model. It is a partial equilibrium model for the energy sectors using mathematical expressions that are commonly used in CGE models, in particular nested constant elasticity of substitution (CES) functions.

diverse, and thus allow for a better matching of actually sales and trade patterns; just increasing marginal costs cannot capture such an effect. Using CV assumptions therefore offers a significant practical advantage when calibrating a model to replicate real-world observations.

We discuss the solution approach and some mathematical and game-theoretic considerations in more detail in Section 3.8, after presenting the structure and the mathematical formulation of the model.

Combining fuel substitution, infrastructure, and market power

The model presented in this article follows the bottom-up approach and allows for linear substitution between fuels in the final demand sectors. Nevertheless, to avoid the problem of bang-bang-results, we introduce fuel-specific end use costs increasing in the amount of each specific fuel used in a sector. This represents stickiness of fuel usage due to existing capital stock, the fact that fuels are used for various purposes within a sector, as well as the costs associated with installing additional equipment.

Regarding infrastructure, we allow for the level of technological detail common in bottom-up energy system models. In particular, we consider endogenous investment in production capacity and transport, transformation, and storage infrastructure. The model covers multiple periods (i.e., years) and includes seasonality within each year. It is therefore able to address both short-term operational concerns as well as long-term trends.

Because the model is formulated as a partial equilibrium model derived from individual players' profit maximization problems (mathematically, a mixed complementarity problem, MCP), it allows for the inclusion of Nash-Cournot market power of several suppliers using a conjectural variations (CV) approach. To our knowledge, this is the first large-scale model that is spatially disaggregated and explicitly models "cross-fuel" market power – a supplier is able to consider how its sales of one fuel affect not only the price of that fuel, but also the price of other fuels it is selling in the same market.

3 A multi-fuel market equilibrium model

The model represents the entire supply chain of multiple fossil fuels and renewable energy sources in a spatially disaggregated framework. It captures game-theoretic considerations (i.e., supplier market power), infrastructure capacity constraints, endogenous fuel substitution by consumers in various end use sectors, multiple governmental regulatory constraints, and greenhouse gas or other pollutants' emission caps in an integrated mathematical framework.

There are three levels of the supply chain: first, fuels are produced (upstream activities); then, they are transformed, stored and/or transported to other nodes by the service providers (midstream); and finally, they are sold to the demand sectors (downstream). We solve for a Nash equilibrium of profit-maximizing players using a deterministic open-loop approach (i.e., assuming perfect foresight and full information). The players are suppliers and infrastructure operators, each aiming to maximize profits. Final demand sectors seek to optimize their welfare from consuming energy. When formulating the model, we took great care to develop a flexible and generic framework; the following examples should be understood as motivation for the model formulation and functionality.

The *suppliers* produce various energy carriers and use infrastructure services purchased from *service providers* to transport fuels, to transform them into other types of energy, and to store fuels across seasons. They ultimately sell the fuels to *final demand sectors* which endogenously substitute between different fuels depending on relative costs, efficiencies, as well as regulatory and technical constraints. The suppliers may be modelled as Nash-Cournot players, exerting market power vis-à-vis consumers, or as price-takers (i.e., perfectly competitive). Suppliers may control production capacity at several nodes and of several fuels.

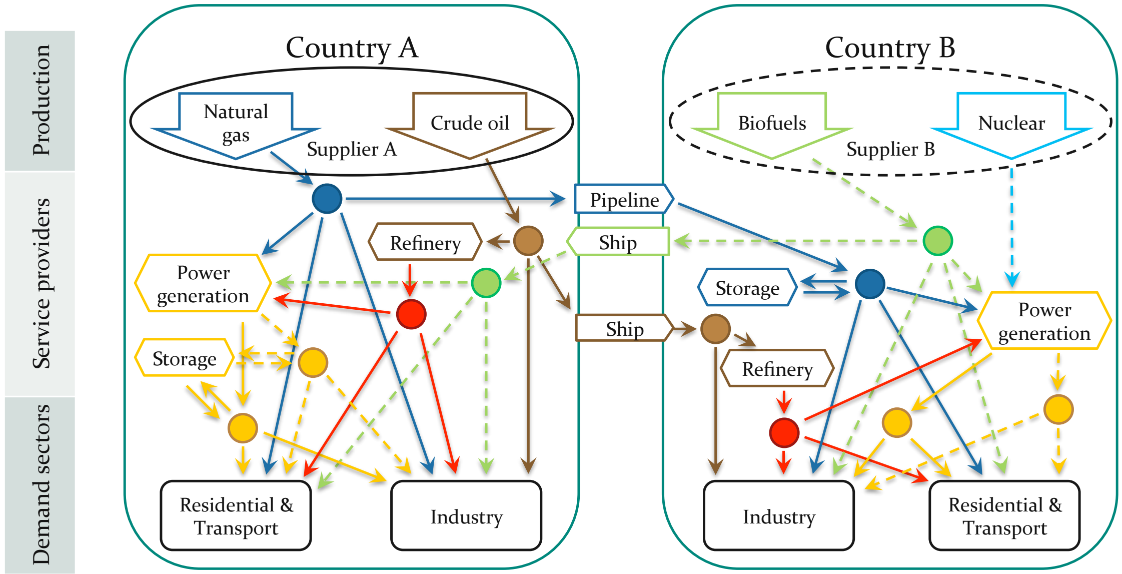

Figure 1: Illustration of the supply chain in a two-node, six-fuel setup; ◯ represents the nodal mass balance of each supplier regarding a fuel at the node.

The *transformation technology operators* can be parametrized with multiple input fuels and several output fuels; hence, this can represent crude oil refineries, power generation, and combined power-and-heat plants. This setup also provides flexibility to model different technologies for the same input-output combination, for example single vs. combined cycle gas turbines to generate electricity from natural gas.

The *arc operators* can represent pipelines, tanker ships, the LNG supply chain components, and power transmission lines (albeit no consideration is given to alternate-current power flow characteristics). The *storage operators* allow the supplier to shift fuels between different seasons within a year; one may think of natural gas storage (summer-winter) or pump-hydro electricity storage (night-day). All service providers are assumed to act perfectly competitive; whenever capacity is scarce, an implicit auction between the suppliers using the infrastructure allocates capacity according to the highest willingness-to-pay.

The *emission permit auctioneer* allocates permits and collects taxes on emissions of greenhouse gases or other pollutants. Both the taxes and the emission quota can be set on a nodal, regional and global level, and are additive. The model is thereby able to replicate a situation where, for example, Norway is part of the EU ETS, but levies an additional methane emissions tax within its borders. The constraints can also be set such that only one sector is faced with a tax or a quota, so that the model is able to replicate sector-specific carbon prices (IEA, 2013).

The suppliers and the service providers face infrastructure constraints, i.e., limited production, transportation or transformation capacity, or maximum injection (extraction) rates into (from) storage. The players invest endogenously in additional capacity if this is economically viable.

Figure 1 illustrates how the supply chain is modelled in a simplified two-node, four-fuel setup: In *Country A*, *Supplier A* produces both natural gas and crude oil, which it can either sell domestically or export via ship (oil) or pipeline (natural gas). There are two demand sectors, *Industry* and *Residential & Transport*. Only the industry sector can use crude oil directly; natural gas, oil products (crude oil processed by a refinery), biofuels, and electricity can be used by both sectors. Nuclear power, “produced” by *supplier B* in *country B*, is modelled as an input to the power sector. For illustrative purposes, the power sector is very stylized here: it converts any input fuel except crude oil into electricity. There exists a natural gas storage facility in country

B and an electricity storage plant in country A; the latter can be used by both suppliers, since both can convert some of their fuels into electric power.

In this example, there is one supplier per node to keep the illustration simple, but one could easily include a supplier active at several nodes, or multiple suppliers producing identical fuels at the same node, each supplier with an individual capacity and cost function. We assume that each supplier remains the owner of the fuel it produces, even after transformation and storage. This is necessary to properly account for market power exertion. We discuss this in more detail below.

3.1 General notation

First, we introduce some general notation before presenting the optimization problem of each player in detail. Table 1 lists the most important sets and mappings used in the model. The remaining notation is introduced in the explanation of each player's problem. A complete list of sets, parameters and variables is provided in Appendix A. In general, $q^{\circledast}$ are decision variables of the supplier, where $^{\circledast}$ is to be replaced by a letter representing the activity in the supply chain. Accordingly, $f^{\circledast}$ are decision variables of the service providers, and $z^{\circledast}$ are the respective infrastructure investment variables.

The relative duration of season h is given by dur_h; the sum of all season durations (over a year) must equal to 1. The discount factor of future revenues and costs is df_y. We use $y' < y$ as shorthand for "all years y' prior to year y", and $y' > y$ for the inverse statement.

$y \in Y$	... years
$h \in H$	... hours/days/seasons
$v \in V$	... loading (injection/extraction) cycles of storage
$s \in S$	... suppliers
$n, k \in N$	... nodes
$d \in D$	... demand sectors
$a \in A$	... arcs
$c \in C$	... transformation technology (e.g., oil refineries, power plants)
$o \in O$	... storage operators/technology
$e, f \in E$	... energy carriers/fuels
$r \in R$	... regions
$g \in G$	... emission types (greenhouse gases)
$n, k \in N_r$	... node-to-region mapping
$r \in R_n$	... region-to-node mapping (any node can be part of several regions)
$a \in A^+_{ne}$	... subset of arcs ending at node n transporting fuel e
$a \in A^-_{ne}$	... subset of arcs starting at node n transporting fuel e
$e \in E^A_a$	... fuel(s) transported via arc a (singleton)
$n^{A+}(a)$	... end node of arc a (singleton)
$n^{A-}(a)$	... start node of arc a (singleton)
$f \in E^{C+}_c$	... subset of output fuel(s) f obtained from transformation technology c
$e \in E^{C-}_c$	... subset of input fuel(s) e for transformation technology c
$(e, f) \in E^C_c$	... input/output fuel mapping of transformation technology c
$o \in O^E_e$	... subset of technologies storing fuel e
$h \in H^V_{vo}$	... mapping between loading cycle and hour/day/season

Table 1: Selected sets and mappings

3.2 The supplier

The supplier maximizes its profits earned by producing and selling fuels while considering costs for production, transport, transformation and storage. Losses during each step of the supply chain are considered by the supplier in the nodal mass balance constraint. Final demand emission costs as well as fuel-specific end use costs are paid by the consumers, which are introduced later. The supplier's profit optimization problem is given by the following; variables in parentheses denote the duals of the constraints.

$$
\begin{aligned}
\max_{\substack{q^P,q^A,q^C\\ q^{O-},q^{O+},q^D\\ z^P}} \sum_{\substack{y\in Y,h\in H\\ n\in N,e\in E}} df_y dur_h \Bigg(& \sum_{d\in D}\left[cour^S_{ysnd}\Pi^D_{yhnde}(\cdot) + (1-cour^S_{ysnd})p^D_{yhnde}\right] q^D_{yhsnde} \\
& - cost^P_{yhsne}(\cdot) - \sum_{a\in A^+_{ne}} p^A_{yha} q^A_{yhsa} - \sum_{c\in C} p^C_{yhnce} q^C_{yhsnce} \\
& - \sum_{o\in O^E_e}\left(p^{O-}_{yhno} q^{O-}_{yhsno} + p^{O+}_{yhno} q^{O+}_{yhsno}\right) \\
& - \sum_{g\in G} p^G_{yng} ems^P_{ysneg} q^P_{yhsne} - inv^P_{ysne} z^P_{ysne} \Bigg)
\end{aligned}
\tag{1a}
$$

$$
\text{s.t.} \qquad q^P_{yhsne} \le avl^P_{yhsne}\left(cap^P_{ysne} + \sum_{y'<y} dep^P_{y'ysne} z^P_{y'sne}\right) \quad (\alpha^P_{yhsne}) \tag{1b}
$$

$$
\sum_{h\in H^V_{vo}} dur_h q^{O+}_{yhsno} = \sum_{h\in H^V_{vo}} dur_h (1-loss^{O-}_o) q^{O-}_{yhsno} \quad (\alpha^O_{yvsno}) \tag{1c}
$$

$$
\begin{aligned}
& (1-loss^P_{sne}) q^P_{yhsne} - \sum_{d\in D} q^D_{yhsnde} \\
& + \sum_{c\in C, f\in E^{C-}_c} transf^C_{yncfe} q^C_{yhsncf} - \sum_{c\in C} q^C_{yhsnce} \\
& + \sum_{a\in A^+_{ne}} (1-loss^A_a) q^A_{yhsa} - \sum_{a\in A^-_{ne}} q^A_{yhsa} \\
& + \sum_{o\in O^E_e}\left(q^{O+}_{yhsno} - q^{O-}_{yhsno}\right) = 0 \quad (\phi_{yhsne})
\end{aligned}
\tag{1d}
$$

$$
z^P_{ysne} \le exp^P_{ysne} \quad (\zeta^P_{ysne}) \tag{1e}
$$

$$
\sum_{y\in Y,h\in H} dur_h q^P_{yhsne} \le hor^P_{sne} \quad (\gamma^P_{sne}) \tag{1f}
$$

The linear combination of price and inverse demand function is multiplied by the quantity sold to final demand q^D to yield the revenue in the supplier's objective function (Equation 1a). As discussed in Section 2, the supplier may either act competitively (i.e., price-taking behaviour) or as a Cournot player. In the competitive case, the parameter $cour^S$ is set to 0, and the supplier takes the final demand price p^D as given in its optimization. In contrast, if the supplier acts as a pure Cournot player ($cour^S = 1$), it is aware of the inverse demand function $\Pi^D(\cdot)$, and hence the impact of its own sales on the market price.[6] A similar approach is applied by several models

[6] The term $cour^S$ may lie in the range $[0, 1]$. The standard conjectural variations literature uses a slightly

using a CV representation if market power, as discussed in the previous section. In order to properly account for market power, all fuels remain the property (and hence under the control) of the supplier throughout the entire supply chain; therefore, the supplier is aware not only of the impact of its sales of one fuel on the price for that specific fuel ("direct" market power), but also of its impact on the price of other fuels ("cross-fuel" market power).

The supplier faces production costs $cost^P(\cdot)$, specified below. It also has to pay the market-determined price p^A for each unit transported via arcs, q^A; price p^C for each unit of fuel put into a transformation unit, q^C; and the prices p^{O-} and p^{O+} for each unit of fuel injected into storage q^{O-} and extracted from storage q^{O+}, respectively. The prices charged by the service operators are derived from a market-clearing constraint; they include operating costs, emission charges incurred by the service providers, and congestion rent. Only the price for emissions p^G during production q^P have to be paid by the supplier directly, where ems^P gives the emission intensity. The investment costs in additional production capacity are given by inv^P, and z^P denotes the capacity expansion (i.e., investment) variable of the supplier.

The supplier must satisfy a production capacity constraint (Equation 1b) at each node where he is active, where avl^P is the availability factor of capacity, cap^P is the existing capacity (with depreciation included for future periods) and dep^P is the depreciation factor of newly-built capacity.

Equation (1c) is a mass-balance constraint regarding storage; the amount extracted from storage must equal the amount injected, after losses ($loss^{O-}$), over each loading cycle. The nodal mass balance constraint (1d) states that production, sales to final demand, transformation into other fuels (where $transf^C$ is the transformation rate), imports and exports, and injection into and extraction from storage must be balanced at each node, for each fuel, and in each time period.

The parameter exp^P sets the maximum production capacity expansion level (Equation 1e); the reserve horizon hor^P gives the maximum cumulative production over the model horizon by the supplier (Equation 1f) of a specific fuel at a node.

Last, let us specify the production cost function and its partial derivatives (Equations 2a–2c): it follows the functional form proposed by Golombek et al. (1995). The logarithmic part allows to add two interesting effects to be included, compared to a simpler linear or quadratic cost function. First, marginal costs increase sharply when producing close to capacity; this is realistic for natural gas or crude oil production. Second, since costs depend on total capacity, an investment reduces production costs for all future periods, ceteris paribus (cf. Huppmann, 2013a). For conciseness, $\widehat{cap}^P_{yhsne}$ defines the available capacity including prior expansions as defined in Equation 1b. The parameters lin^P, qud^P, and gol^P specify the shape of the cost function.

$$\begin{aligned}
cost^P_{yhsne}(\cdot) &= (lin^P_{ysne} + gol^P_{ysne})q^P_{yhsne} + qud^P_{ysne}(q^P_{yhsne})^2 \\
&\qquad + gol^P_{ysne}\left(\widehat{cap}^P_{yhsne} - q^P_{yhsne}\right)\ln\left(1 - \frac{q^P_{yhsne}}{\widehat{cap}^P_{yhsne}}\right) && \text{(2a)} \\
\frac{\partial\, cost^P_{yhsne}(\cdot)}{\partial\, q^P_{yhsne}} &= lin^P_{ysne} + 2qud^P_{ysne}q^P_{yhsne} - gol^P_{ysne}\ln\left(1 - \frac{q^P_{yhsne}}{\widehat{cap}^P_{yhsne}}\right) && \text{(2b)} \\
\frac{\partial\, cost^P_{yhsne}(\cdot)}{\partial\, z^P_{\hat{y}sne}} &= gol^P_{ysne}avl^P_{yhsne}dep^P_{\hat{y}ysne}\left(\ln\left(1 - \frac{q^P_{yhsne}}{\widehat{cap}^P_{yhsne}}\right) + \frac{q^P_{yhsne}}{\widehat{cap}^P_{yhsne}}\right) \qquad \text{if } \hat{y} < y && \text{(2c)} \\
&\text{where } \widehat{cap}^P_{yhsne} = avl^P_{yhsne}\left(cap^P_{ysne} + \sum_{y'<y} dep^P_{y'ysne}z^P_{y'sne}\right)
\end{aligned}$$

different notation, so the CV values applied there are in the range $[-1, 0]$. The interpretation, however, is identical: a value at the lower end of the range indicates competitive behaviour, while a high value represents standard Nash-Cournot behaviour.

3.3 The arc operator

The arc operator maximizes its profits from transporting fuel f^A considering operation costs trf^A and emission costs.[7] Each arc is fuel-specific; losses are accounted for in the supplier's mass balance constraint (Constraint 1d). The operator allocates congested capacity to suppliers, such that the market clearing constraint (Equation 4) is satisfied. The dual variable to this constraint is the price p^A for using the arc. Capacity investment z^A is undertaken if the shadow price of future congestion (τ^A) is greater than investment costs inv^A.

$$\max_{f^A, z^A} \sum_{y \in Y, h \in H} df_y dur_h \left((p^A_{yha} - trf^A_{ya}) f^A_{yha} - \sum_{g \in G} p^G_{yng} ems^A_{yag} f^A_{yha} - inv^A_{ya} z^A_{ya} \right) \tag{3a}$$

$$\text{s.t.} \qquad f^A_{yha} \leq cap^A_{ya} + \sum_{y' < y} dep^A_{y'ya} z^A_{y'a} \quad (\tau^A_{yha}) \tag{3b}$$

$$z^A_{ya} \leq exp^A_{ya} \quad (\zeta^A_{ya}) \tag{3c}$$

Market clearing

$$\sum_{s \in S} q^A_{yhsa} = f^A_{yha} \quad (p^A_{yha}) \tag{4}$$

3.4 The transformation technology operator

The transformation technology operator transforms fuels into other energy carriers. The input into the unit is denoted by f^C; the share of output fuels produced $transf^C$ is fixed, but depends on the input fuel. There is one unit per technology at each node, which represents total (aggregate) capacity; the capacity constraint (Equation 5b) is stated in terms of output quantities. In order to capture technical or regulatory constraints, Equation (5c) allows us to impose that a certain minimum share shr^C of total output must be produced from a certain input fuel.

$$\max_{f^C, z^C} \sum_{\substack{y \in Y, h \in H \\ e \in E^{C-}_c}} df_y dur_h \left((p^C_{yhnce} - trf^C_{ync}) f^C_{yhnce} - \sum_{g \in G} p^G_{yng} ems^C_{yceg} f^C_{yhnce} - inv^C_{ync} z^C_{ync} \right) \tag{5a}$$

$$\text{s.t.} \qquad \sum_{(e,f) \in E^C_c} transf^C_{yncef} f^C_{yhnce} \leq cap^C_{ync} + \sum_{y' < y} dep^C_{y'ync} z^C_{y'nc} \quad (\tau^C_{yhnc}) \tag{5b}$$

$$shr^C_{ynce} \sum_{(e',f) \in E^C_c} transf^C_{ynce'f} f^C_{yhnce'} \leq \sum_{f \in E^{C+}_c} transf^C_{yncef} f^C_{yhnce} \quad (\beta^C_{yhnce}) \tag{5c}$$

$$z^C_{ync} \leq exp^C_{ync} \quad (\zeta^C_{ync}) \tag{5d}$$

Market clearing

$$\sum_{s \in S} q^C_{yhsnce} = f^C_{yhnce} \quad (p^C_{yhnce}) \tag{6}$$

[7]All emissions are accounted for at the starting node of the arc.

3.5 The storage operator

The storage operator allows suppliers to transfer fuels between different hours/days/seasons. We assume one or several loading (f^{O-})/unloading (f^{O+}) cycles for each technology, and all costs, losses and emissions are accounted for during injection. The capacity constraint (i.e., maximum quantity stored, Equation 7b) is the summation over all energy injected during one loading cycle. In addition, there is a capacity constraint on injection (Equation 7c) and extraction (Equation 7d), and the respective investment variables may also be constrained (Equations 7e–7g).

$$\max_{\substack{f^{O-},f^{O+}\\ z^{O},z^{O-},z^{O+}}} \sum_{y\in Y,h\in H} df_y dur_h \Bigg((p^{O-}_{yhno} - trf^{O-}_{yno}) f^{O-}_{yhno} + p^{O+}_{yhno} f^{O+}_{yhno}$$

$$- \sum_{g\in G} p^{G}_{yng} ems^{O-}_{yog} f^{O-}_{yhno} - inv^{O}_{yno} z^{O}_{yno} - inv^{O-}_{yno} z^{O-}_{yno} - inv^{O+}_{yno} z^{O+}_{yno} \Bigg) \quad (7a)$$

$$\text{s.t.} \quad \sum_{h\in H^V_{vo}} dur_h f^{O-}_{yhno} \leq cap^{O}_{yno} + \sum_{y'<y} dep^{O}_{y'yno} z^{O}_{y'no} \quad (\tau^{O}_{yvno}) \quad (7b)$$

$$f^{O-}_{yhno} \leq cap^{O-}_{yno} + \sum_{y'<y} dep^{O-}_{y'yno} z^{O-}_{y'no} \quad (\kappa^{O-}_{yhno}) \quad (7c)$$

$$f^{O+}_{yhno} \leq cap^{O+}_{yno} + \sum_{y'<y} dep^{O+}_{y'yno} z^{O+}_{y'no} \quad (\kappa^{O+}_{yhno}) \quad (7d)$$

$$z^{O}_{yno} \leq exp^{O}_{yno} \quad (\zeta^{O}_{yno}) \quad (7e)$$

$$z^{O-}_{yno} \leq exp^{O-}_{yno} \quad (\zeta^{O-}_{yno}) \quad (7f)$$

$$z^{O+}_{yno} \leq exp^{O+}_{yno} \quad (\zeta^{O+}_{yno}) \quad (7g)$$

Market clearing

$$\sum_{s\in S} q^{O-}_{yhsno} = f^{O-}_{yhno} \quad (p^{O-}_{yhno}) \quad (8a)$$

$$\sum_{s\in S} q^{O+}_{yhsno} = f^{O+}_{yhno} \quad (p^{O+}_{yhno}) \quad (8b)$$

Quantities must be extracted within the same loading cycle in which they were injected, but we do not model the storage level explicitly. This and the consideration that only amounts injected (after losses) can be extracted is included in the supplier's optimization problem (Equation 1c).

3.6 The emission permit auctioneer

The emission permit auctioneer allocates constrained emission quota. This mechanism represents an implicit auction of permits. It is possible to have multiple constraints on global ($quota^{glob}$), regional ($quota^{reg}$) or nodal ($quota^{nod}$) levels. In addition, a tax can be introduced for any emission type, again on a global, regional and/or nodal level (tax^{glob}, tax^{reg}, tax^{nod}); the equilibrium price at any node cannot be lower than the respective tax(es), so this can be interpreted as a floor price. [8] If a node belongs to more than one region, the taxes and shadow prices (dual variables to Equations 9b–9d) from both regions apply.

[8] Mathematically speaking, the dual to a constraint and a tax (i.e., mark-up) are equivalent, since each supplier and service provider takes the emission price as given. However, one may want to investigate scenarios with specific carbon prices, in which setting a parameter is a more straightforward approach; hence, we include both options to provide more flexibility when defining scenarios.

The optimization problem of the emission permit auctioneer reads as follows:

$$\max_{f^G} \sum_{\substack{y\in Y,n\in N\\ g\in G}} df_y \left(p^G_{yng} - tax^{glob}_{yg} - \sum_{r\in R_n} tax^{reg}_{yrg} - tax^{nod}_{yng} \right) f^G_{yng} \tag{9a}$$

$$\text{s.t.} \qquad \sum_{n\in N} f^G_{yng} \le quota^{glob}_{yg} \quad (\mu^{glob}_{yg}) \tag{9b}$$

$$\sum_{n\in N_r} f^G_{yng} \le quota^{reg}_{yrg} \quad (\mu^{reg}_{yrg}) \tag{9c}$$

$$f^G_{yng} \le quota^{nod}_{yng} \quad (\mu^{nod}_{yng}) \tag{9d}$$

Market clearing

$$\begin{aligned}\sum_{h\in H,e\in E} dur_h \Bigg(\sum_{s\in S} ems^P_{ysneg} q^P_{yhsne} + \sum_{s\in S,d\in D} ems^D_{ydeg} q^D_{yhsnde} + \sum_{a\in A^+_{ne}} ems^A_{yag} f^A_{yha} \\ + \sum_{c\in C} ems^C_{yceg} f^C_{yhnce} + \sum_{o\in O} ems^{O-}_{yog} f^{O-}_{yhno} \Bigg) = f^G_{yng} \quad (p^G_{yng})\end{aligned} \tag{10}$$

3.7 Final demand

The final demand sector aims to maximize its utility from using energy services, where each fuel provides a certain level of service (eff^D). When taking the derivative of the utility maximization problem with respect to the amount of a particular fuel, one obtains the inverse demand curve for this fuel (Equation 11); this is the inverse demand function Π^D included in the supplier's objective function (1a):

$$\begin{aligned}p^D_{yhnde} = \mathit{eff}^D_{ynde} \left[int^D_{yhnd} - slp^D_{yhnd} \left(\sum_{s\in S,f\in E} \mathit{eff}^D_{yndf} q^D_{yhsndf} \right) \right] \\ - eucc^D_{yhnde} - eucl^D_{yhnde} \left(\sum_{s\in S} q^D_{yhsnde} \right) - \sum_{g\in G} p^G_{yng} ems^D_{ydeg}\end{aligned} \tag{11}$$

Final demand price of a fuel p^D equals the following: the first part of the equation is a composite sector price index in terms of energy services, weighted by the efficiency of the particular fuel in supplying the service. Parameters int^D and slp^D give the form of the sector's energy service demand function.

The second part concerns the fuel-specific end use costs. We use a linear function with parameters $eucc^D$ and $eucl^D$ to capture stickiness of usage of a fuel. The third part of the inverse demand curve represents the emission costs for consuming the fuel.

In addition to emission constraints and end use costs, consumers may face restrictions in their energy consumption due to governmental regulation, technical constraints or a limited capital stock. The first constraint type (denoted L) concerns the fuel mix of demand for a certain sector: a minimum share shr^L of total consumption of demand sector(s) $d \in D^L$ satisfied from fuels $e \in \widehat{E}^L$ must be supplied using fuel(s) $e \in E^L$.

$$shr^L_{ynl} \sum_{\substack{s\in S,d\in D^L_l\\ e\in \widehat{E}^L_l}} \mathit{eff}^D_{ynde} q^D_{yhsnde} \le \sum_{\substack{s\in S,d\in D^L_l\\ e\in E^L_l}} \mathit{eff}^D_{ynde} q^D_{yhsnde} \quad (\beta^L_{yhnl}) \tag{12}$$

The second constraint type (denoted M) concerns the "origin" or transformation of fuels. A minimum share shr^M of consumption of fuel(s) $e \in E^M$ must be supplied from transformation technology(s) $c \in C^M$ at that node n.

$$shr^M_{ynm} \sum_{\substack{s\in S, d\in D\\ f\in E^M_m}} q^D_{yhsndf} \leq \sum_{\substack{s\in S,(e,f)\in E^C_c\\ c\in C^M_m}} transf^C_{yncef} q^C_{yhsnce} \quad (\beta^M_{yhnm}) \tag{13}$$

3.8 Solution approach

We formulate the problem as a Mixed Complementarity Problem (MCP, cf. Facchinei and Pang, 2003) by deriving the first-order (Karush-Kuhn-Tucker, or KKT) conditions of each player's optimization problem and solving them simultaneously. This can be interpreted as a Nash equilibrium solution of the market, in which some players act as price-takers (i.e., perfectly competitive), while others may exert Cournot market power vis-à-vis final demand. We use an exogenous conjectural variations parameter ($cour^S$) to incorporate this behaviour and allow intermediate cases. Each player's optimization problem is convex and all constraints are linear, so the KKT conditions are necessary and sufficient for optimality. Nevertheless, since not all optimization problems are strictly convex, we cannot guarantee uniqueness of the equilibrium. This is an inherent problem common to all large-scale energy models that are (partly) linear.

The KKT conditions are stated in Appendix B. The equilibrium price p^D is replaced by the inverse demand curve to reduce the number of variables and equations. Hence, there is no equivalent to Equation 11 in the KKT conditions.

Since the demand sectors do not have specific decision variables, the constraints (12) and (13) are included in the profit maximization problem of the suppliers. We therefore have a Generalized Nash Equilibrium (GNE), because the suppliers face so-called "shared constraints": the constraints are identical, but in principle, each supplier may value the constraint differently. Mathematically, this is equivalent to assigning a different Lagrange multiplier to it. Hence, the MCP would no longer be a square system. We follow the approach by Harker (1991) and assume that each supplier values a shared constraint identically. Several recent models of generalized Nash games in energy markets use a similar approach (e.g., Abada et al., 2013; Oggioni et al., 2012).

A challenging task of building a large-scale bottom-up equilibrium model is the calibration to match observed values in the base year and projections from a reference source reasonably well. While data on production and transformation costs as well as other technology aspects (e.g., transformation efficiency, losses) are available, making defensible assumptions concerning the demand side is more difficult (e.g., willingness-to-pay for energy services, possibility for fuel substitution). Furthermore, one has to avoid the aforementioned problem of "bang-bang"-results. To this end, we introduce the concept of fuel-specific end use costs in the final demand curve. We also implement an iterative semi-automated calibration algorithm; the end use costs and this algorithm are discussed in more detail in Appendix C.

For the reference data set (explained further in the next section), the resulting model contains approximately 150,000 variables and equations. It is solved in GAMS using the PATH solver (Ferris and Munson, 2000). Due to the logarithmic function used in the model, the solver does not necessarily converge without initializing from a well-chosen starting point. We implemented several subroutines to facilitate obtaining a valid starting point.

4 Some illustrative results

In the following section, we illustrate that this model can be used to solve large-scale applications of the global energy system. We provide a brief overview of the underlying data set and two scenarios to demonstrate the advantages of our approach compared to both energy system models and fuel-specific equilibrium models.

4.1 The base case

The base year of the data set is 2010; the model proceeds in 10-year steps until 2050. Data on quantities produced, transformed and consumed in the base year are compiled from the Extended World Energy Balances of the International Energy Agency (IEA).[9] Reference demand values for future years are derived from the IEA's World Energy Outlook (WEO IEA, 2013), *New Policies* scenario; however, since our assumptions on demand sector and fuel disaggregation partly differ from the WEO, one must be careful when comparing our results with the IEA's publications. For EU members countries, we compared the IEA projections to the Energy Roadmap 2050 (EC, 2011) and the European Commission's Reference Scenario (EC, 2013) to obtain projections on a more disaggregated level.

Production capacities and costs, both for the base year of 2010 as well as the development over the next decades, are taken from our research group's sector models (Egging, 2013; Schröder et al., 2013; Huppmann and Holz, 2012; Leuthold et al., 2012; Haftendorn and Holz, 2010). Cost estimates and the potential of different renewable energy sources are taken from the respective IEA publications; for Europe, we use data based on the Re-shaping project.[10] During calibration, we compiled reference values for future production and the fuel mix in power generation from the WEO 2013, various publications by the US Energy Information Administration (EIA), and BP (2014); however, since we derive and use our own cost estimates for production and transformation, model results may deviate with respect to production and fuel mix in power generation.[11]

The fuels included are: crude oil, (refined) oil products, natural gas, coal, lignite, electricity, biofuels, renewables, and (as input for power generation only) nuclear and hydro. We intend to use this data set mainly for studies with a European focus, so Europe is represented by 15 nodes, of which eleven are EU member states (or aggregates thereof). The rest of the world is aggregated into thirteen nodes by continent or major regions. Noting that capacity constraints in global liquefied natural gas (LNG) trade are due to the liquefaction and regasification infrastructure (rather than along the shipping routes), we add 34 nodes to represent LNG terminals. There are two seasons per year, summer and winter, with natural gas storage facilities to shift this fuel from the low demand to high demand months.

The Russian production of crude oil and natural gas is assumed to be controlled by one strategic supplier. In the Middle East, the production of crude oil and natural gas is divided between two suppliers: a strategic supplier representing the OPEC members in the region (93 % of crude oil and 87 % of natural gas production in the Middle East region in 2010), and a competitive supplier controlling the remaining capacity. The reserves in the Middle East are separated by OPEC membership as well. We assume a CV value of 0.5 for the strategic suppliers (cf. Huppmann, 2013b), except for their respective domestic markets where they act competitively.

[9] IEA (2013), "Extended world energy balances", *IEA World Energy Statistics and Balances* (database). doi: 10.1787/data-00513-en

[10] See `http://www.reshaping-res-policy.eu` for a list of publications.

[11] The numerical results presented below are based on the data set as of March 17, 2014. We intend to continue improving the underlying data and assumptions, in particular with respect to renewable energy sources, and to incorporate updated projections from IEA, EIA, BP, and other publications.

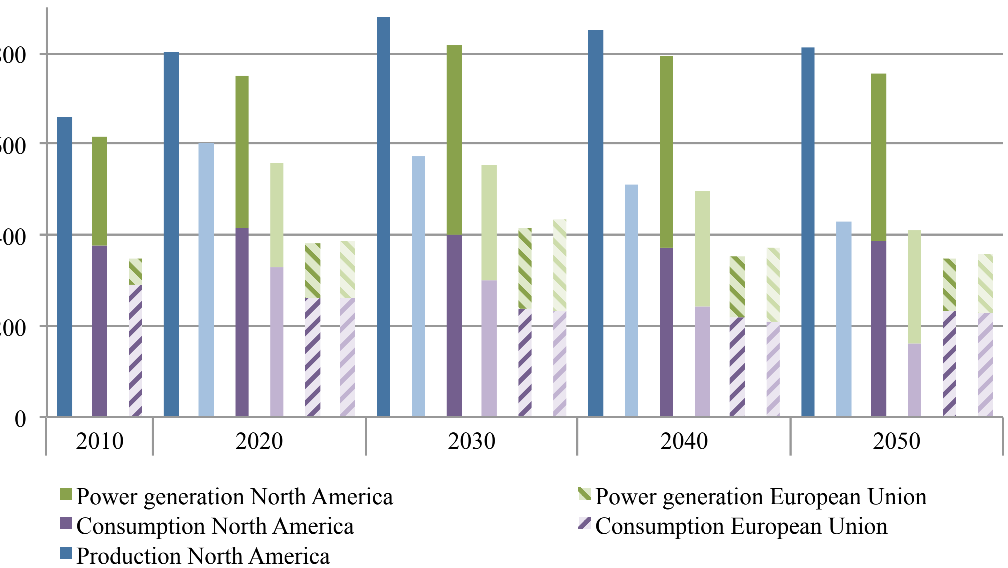

Figure 2: Scenario *A shale disappointment*: Natural gas production and consumption in North America and the European Union, in mtoe/y (base case: dark; scenario results: light colours)

4.2 *Shale disappointment* – A reduction of the US natural gas supply

The strongly increasing production of shale gas in the US over the past years has dramatically changed expectations regarding the future energy landscape. Only a few years ago, substantial investment went into regasification terminals in North America to import liquefied natural gas (LNG). Now, the IEA and the Energy Information Administration (EIA) project that North America will be a net exporter of natural gas in the near future (EIA, 2014).

Richter (2013) discusses how current projections of US shale gas production may be substantially over-optimistic. He uses a single-fuel partial-equilibrium model to analyse shifts in trade flows as well as production and consumption patterns if the shale gas potential does not meet current expectations. We replicate his work, but our model allows to analyse endogenous fuel substitution due to reduced availability of shale gas compared to our base case derived from the WEO and other sources.

Production and consumption of natural gas in North America and the European Union is presented in Figure 2: instead of increasing natural gas production in North America, as projected by the EIA and others, output decreases steadily until 2050 in this scenario. Direct consumption and use in power generation in North America decline accordingly.

The interesting effect from this scenario can be seen in the use of natural gas in European power generation: it increases more than in the base case. This can be explained by a shift in global fossil fuel trade: North America makes up for reduced availability of domestic natural gas by increasing their imports of crude oil and coal; it even starts to import natural gas by 2030 from South America, as predicted by the EIA as recent as a decade ago (cf. Richter, 2013). The EU in turn compensates for higher world prices of coal and oil by importing more natural gas by pipeline from Russia and the Caspian region.

4.3 *Ambitious EU* – Strengthening the EU ETS and biofuel standards

The European Commission recently announced its intention to reduce greenhouse gas emissions by 40 % until 2030 relative to 1990 levels, amongst other objectives (EC, 2014); a reduction by

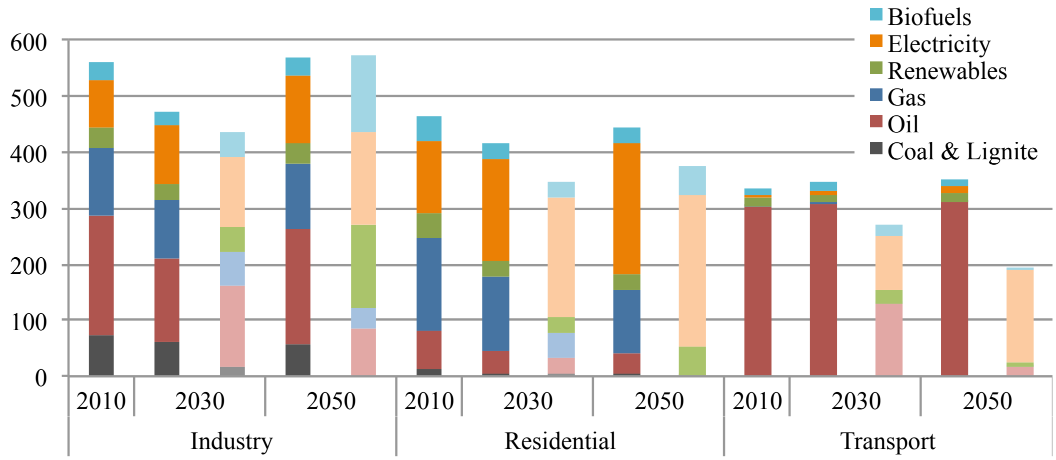

Figure 3: Scenario *Ambitious EU*: Energy consumption by sector in the European Union, in mtoe/y (base case: dark; scenario results: light colours)

80 % until 2050 is regularly discussed (EC, 2011), even though no legally binding decisions have been made. We simulate a scenario where all emissions from the energy sector are reduced by 40 % until 2030 and 80 % until 2050.[12] We assume that all energy consumed is covered by this mandate, in contrast to the current setup of the ETS. In addition, we introduce an increasing biofuel mandate, reaching 25 % of all oil products consumed in the transportation sector by 2050.

The energy mix in the demand sectors is depicted in Figure 3: the sector most affected is transportation, where the combination of a biofuel mandate and the emissions quota induces a strong shift to electrification. Coal is phased out almost completely by 2050, both in direct use and in power generation, as shown in Figure 4.

The underlying cost assumptions which we use for nuclear power are substantially higher than those assumed by the IEA and EC (2011, 2013). Hence, we do not observe substantial nuclear power plant construction in the base case. However, in the *Ambitious EU* scenario, there is investment in nuclear power in Europe after 2030, supplying approximately a third of European power consumption. In both the base case and the scenario, we do not see any construction of carbon capture and sequestration (CCS) power plants.

In the scenario, the CO_2 emission permit price in the EU ETS increases to 54 USD/t CO_2 in 2030 and 155 USD in 2050, compared to the base case emission costs of 40 USD in 2030 (according to the WEO) and 60 USD in 2050 (own assumption).

Last, let us turn to emission reductions and carbon leakage, which is illustrated in Figure 5: Emissions from coal and oil are reduced most drastically, while natural gas serves as a transition fuel until nuclear capacity becomes operational in 2040. Leakage rates are in the range of 60–70 %. At first, most of the leakage occurs in the European periphery (the Balkans and Ukraine): power generators use their comparative cost advantage of not being covered by the EU ETS and export electricity to Eastern EU member states, in spite of relatively high losses of power transmission. After 2030, the major part of the leakage shifts to Asia, where China and other countries increase their consumption of fossil fuels due to reduced prices on the world market.

[12] Since we do not include non-energy sector emissions (e.g., industrial process emissions), we abstract from those. The difference between the WEO reference emission values presented in Figure 5 and model results is mostly due to this omission, as well as the aggregation to keep our data set sufficiently small to be numerically tractable. To avoid distortion due to the model aggregation and calibration, we set the reduction relative to model results of emissions in 2010.

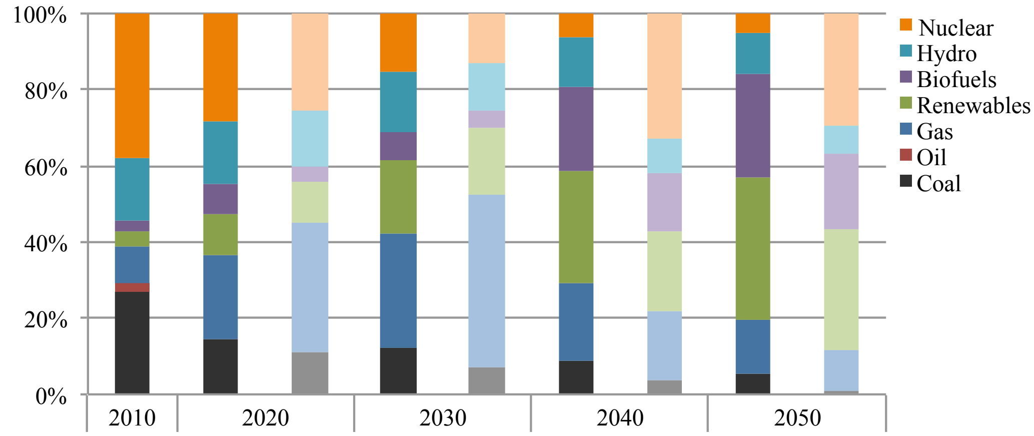

Figure 4: Scenario *Ambitious EU*: Aggregate relative fuel mix in power generation in the European Union (base case: dark; scenario results: light colours)

5 Conclusions and outlook

Understanding the global energy system and quantifying the impacts of technological and economic changes as well as the effects of policy measures requires large-scale numerical models. A multitude of such models exist and are widely used for policy evaluation and scenario simulations. They either follow a *top-down* methodology, which allows embedding the energy sector in the economy at large, or a *bottom-up* approach, which allows for a detailed analysis of the energy system and infrastructure constraints. Market structure analysis is usually done in a sector- or fuel-specific modelling framework.

We present a first-of-its-kind large-scale model that combines endogenous fuel substitution, detailed infrastructure constraints, and strategic behaviour by suppliers in a unified framework. Most importantly, in the model proposed here, suppliers can exert market power across several fuels; strategic firms are aware how their sales of one fuel impact not only the price of that fuel ("direct" market power), but also the revenue they earn from selling other fuels in the same market. We believe that this is the first large-scale market equilibrium model that captures such an effect.

The model covers multiple time periods and allows for endogenous investment in production and mid-stream infrastructure capacity. We include seasonality and storage, and are thus able to incorporate short-term operational concerns, which are highly relevant for energy market analysis.

We illustrate the model functionality using a data set compiled from the IEA's "Extended World Energy Balances" and other sources. The first scenario analyses the impacts of strongly reduced shale gas availability in North America, in contrast to current optimistic projections of LNG exports from the US in the next years. The decreasing output of North American natural gas is compensated in the scenario with increased imports of crude oil and coal. This induces a shift in global trade patterns, and Europe increases its use of natural gas in power generation due to higher world market prices of coal and oil.

In the second scenario, we assume a tightening of the EU ETS emission cap by 80 % in 2050 combined with a stronger biofuel mandate. This induces a renaissance of nuclear power after 2030 and a strong electrification of the transportation sector. We observe significant carbon leakage ratios from the unilateral mitigation effort in the order of 60–70 %. In the first decades, the leakage mostly takes place in the European periphery (the Balkans and Ukraine), which benefits from being adjacent to the ETS jurisdiction and exports electricity to Eastern European countries. As more renewable and nuclear generation capacity comes online after 2030, the leakage shifts

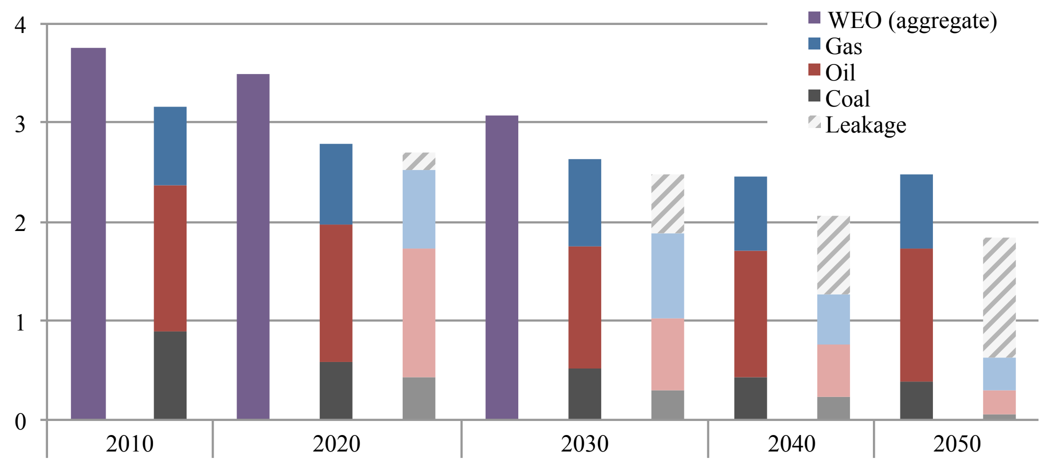

Figure 5: Scenario *Ambitious EU*: CO_2 emissions, model results by fossil fuel, and WEO projections, in Gt/y (base case: dark; scenario results: light colours)

to the Asian region, where China and other countries soak up the global fossil fuel supplies not exported to Europe.

Both scenarios illustrate fuel substitution effects which can hardly be captured using single-fuel sector models. At the same time, the market power aspects ignored by ESM, IAM (and most CGE models) affect supply, trade and infrastructure developments and fuel prices.

We plan to extend this modelling framework in two directions: on the one hand, we will use the model for detailed policy analysis, going beyond the two illustrative scenarios presented here. This will require regular updates of the underlying data set and continuous improvement regarding implicit assumptions, in particular with respect to renewable energy sources. Furthermore, we have not yet discussed the impact of market power, which is included in the calibration of our base case and the scenarios. Egging et al. (2009) analyse the impact of a counterfactual cartel of "GasPEC" member countries in the natural gas market; the model presented here allows us to replicate their analysis for market power exertion by a joint OPEC-GasPEC cartel in both crude oil and natural gas.

On the other hand, we will extend the model mathematically: one avenue is to include stochasticity, which was recently implemented in other large-scale sector models (e.g., Egging, 2013). Short-term stochasticity could be interpreted as operational or seasonal uncertainty. Long-term stochasticity may represent the ambiguity of resource availability or the "threat" of a global climate change mitigation agreement. Uncertain prospects over an extended time horizon are especially relevant when one considers long-lived infrastructure investment.

Another interesting question to be tackled in the context of energy markets, strategic behaviour, and emissions is the issue of carbon leakage: mitigation efforts in one region may just displace GHG emissions to other regions. This may happen either directly via the channel of fossil fuel prices, as exemplified in the second illustrative scenario. But it may also occur indirectly via the goods channel, including relocation of firms to regions with less stringent climate policies. To properly capture both channels simultaneously requires combining a detailed bottom-up energy system model with a CGE-type module to reflect the impact of energy prices on the economy (Böhringer and Rutherford, 2008). This would allow to more accurately quantify the extent of carbon leakage due to unilateral or regional climate policies with particular regard to strategic behaviour by fossil fuel suppliers.

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A Nomenclature

Sets and mappings

Sets

$y \in Y$	... years (#1)
$h \in H$	... hours/days/seasons
$v \in V$	... loading (injection/extraction) cycles of storage
$s \in S$	... suppliers
$n, k \in N$	... nodes
$d \in D$	... demand sectors
$l \in L$	... sector fuel mix constraints
$m \in M$	... transformation mix constraints
$a \in A$	... arcs (#2)
$c \in C$	... transformation technology (e.g., oil refineries, power plants)
$o \in O$	... storage operators/technology (#2)
$e, f \in E$	... energy carriers/fuels
$r \in R$	... regions
$g \in G$	... emission types (greenhouse gases)

Mappings

$n, k \in N_r$	... node-to-region mapping
$r \in R_n$	... region-to-node mapping (any node can be part of several regions)
$a \in A^+_{ne}$	... subset of arcs ending at node n transporting fuel e
$a \in A^-_{ne}$	... subset of arcs starting at node n transporting fuel e
$e \in E^A_a$	... fuel(s) transported via arc a (singleton)
$n^{A+}(a)$	... end node of arc a (singleton)
$n^{A-}(a)$	... start node of arc a (singleton)
$f \in E^{C+}_c$	... subset of output fuel(s) f obtained from transformation technology c
$e \in E^{C-}_c$	... subset of input fuel(s) e for transformation technology c
$(e, f) \in E^C_c$	... input/output fuel mapping of transformation technology c
$e^O(o)$	... fuel stored by technology o (singleton)
$o \in O^E_e$	... subset of technologies storing fuel e
$h \in H^V_{vo}$	... mapping between loading cycle and hour/day/season
$v^H(h, o)$	... loading cycle of hour/day/season (singleton)
$e \in E^L_l$	... fuel(s) that satisfies fuel mix constraint l
$e \in \widehat{E}^L_l$	... fuel(s) that are included in fuel mix constraint l
$e \in E^M_m$	... fuel(s) that satisfies transformation mix constraint m
$d \in D^L_l$	... demand sector(s) to which fuel mix constraint l applies
$c \in C^M_m$	... transformation technologies that satisfy transformation mix constraint m

Parameters and functions

General Parameters

df_y	... discount factor
dur_h	... relative duration of hour/day/season h (with $\sum_h dur_h = 1$; #3)

Supplier

$cour^S_{ysnd}$	... Cournot market power parameter of supplier s at node n regarding sector d
$cost^P_{yhsne}(\cdot)$	... production cost function faced by supplier s at node n for fuel e
lin^P_{ysne}	... linear term of the production cost function ($lin^P \geq 0$)
qud^P_{ysne}	... quadratic term of the production cost function ($qud^P \geq 0$)
gol^P_{ysne}	... logarithmic (Golombek) term of the production cost function ($gol^P \geq 0$)
cap^P_{ysne}	... gross production capacity (#4)
avl^P_{yhsne}	... availability factor of production capacity
exp^P_{ysne}	... production capacity expansion limit
inv^P_{ysne}	... production capacity expansion (per-unit) costs
$dep^P_{yy'sne}$	... production capacity expansion depreciation factor (#6)
hor^P_{sne}	... production horizon (reserves)
$loss^P_{sne}$	... loss rate during production of fuel e at node n
ems^P_{ysneg}	... emission of type g during production of fuel e at node n by supplier s

Arc operator

trf^A_{ya}	... tariff for using arc a
cap^A_{ya}	... gross capacity of arc a (#4)
exp^A_{ya}	... arc capacity expansion limit
inv^A_{ya}	... arc capacity expansion (per-unit) costs
$dep^A_{yy'a}$	... arc capacity expansion depreciation (#6)
$loss^A_{a}$	... loss rate during transportation through arc a
ems^A_{yag}	... emission of type g during transportation through arc a

Transformation technology operator

trf^C_{ync}	... tariff for using transformation technology c for input fuel e
cap^C_{ync}	... capacity of transformation technology c (as measured in output fuel, #4)
exp^C_{ync}	... transformation technology capacity expansion limit
inv^C_{ync}	... transformation technology expansion (per-unit) costs
$dep^C_{yy'nc}$	... transformation capacity expansion depreciation (#6)
$transf^C_{yncef}$	... transformation rate by technology c at node n from input e to output f
shr^C_{ynce}	... minimum share of (input) fuel e by transformation technology c
ems^C_{yceg}	... emission of type g during transformation of (input) fuel e

Storage technology operator

trf^{O-}_{yno}	... tariff for injecting into storage technology o
cap^{O}_{yno}	... capacity for total fuel stored in storage technology o over one loading cycle (#4)
exp^{O}_{yno}	... yearly storage capacity expansion limit
inv^{O}_{yno}	... yearly storage capacity expansion (per-unit) costs
$dep^{O}_{yy'no}$	... yearly storage capacity expansion depreciation (#6)
cap^{O-}_{yno}	... capacity for fuel injection into storage
exp^{O-}_{yno}	... storage injection capacity expansion limit
inv^{O-}_{yno}	... storage injection capacity expansion (per-unit) costs
$dep^{O-}_{yy'no}$	... storage injection capacity expansion depreciation (#6)
cap^{O+}_{yno}	... capacity for fuel extraction rate from storage technology o (#4)
exp^{O+}_{yno}	... storage extraction capacity expansion limit
inv^{O+}_{yno}	... storage extraction capacity expansion (per-unit) costs
$dep^{O+}_{yy'no}$	... storage extraction capacity expansion depreciation (#6)
$loss^{O-}_{o}$	... loss rate of storage technology o (accounted at injection)
ems^{O-}_{yog}	... emission of type g of storage technology o (accounted at injection)

Emissions auctioneer

$quota^{glob}_{yg}$	... quota for global emissions
$quota^{reg}_{yrg}$	... quota for regional emissions
$quota^{nod}_{yng}$	... quota for nodal emissions
tax^{glob}_{yg}	... tax for emission g (global)
tax^{reg}_{yrg}	... tax for emission g in region r
tax^{nod}_{yng}	... tax for emission g at node n

Demand

$\Pi^{D}_{yhnde}(\cdot)$	... inverse demand curve of sector d for fuel e
int^{D}_{yhnd}	... intercept of inverse demand curve at node n
slp^{D}_{yhnd}	... slope of inverse demand curve at node n
eff^{D}_{ynde}	... efficiency of demand satisfaction of sector d by fuel e at node n
$eucc^{D}_{yhnde}$	... constant end use cost parameter
$eucl^{D}_{yhnde}$	... linear end use cost parameter
ems^{D}_{ydeg}	... emission of type g during consumption of fuel e at node n
shr^{L}_{ynl}	... minimum share of sector fuel mix constraint l (in energy services)
shr^{M}_{ynm}	... minimum share of generation mix constraint m (in gross energy)

Variables

q^P_{yhsne}	... quantity produced
q^A_{yhsa}	... quantity transported through arc a
q^C_{yhsnce}	... quantity put into transformation technology c
q^{O-}_{yhsno}	... quantity injected into storage o
q^{O+}_{yhsno}	... quantity extracted from storage o
q^D_{yhsnde}	... quantity sold to final demand sector d
z^P_{ysne}	... expansion of production capacity (#5)
α^P_{yhsne}	... dual for production capacity constraint
α^O_{yvsno}	... dual for injection/extraction constraint
γ^P_{sne}	... dual for production horizon constraint
ζ^P_{ysne}	... dual for production capacity expansion limit
ϕ_{yhsne}	... dual for mass-balance constraint
f^A_{yha}	... quantity transported by the arc operator
z^A_{ya}	... expansion of arc capacity (#5)
τ^A_{yha}	... dual for arc capacity constraint
ζ^A_{ya}	... dual to arc capacity expansion limit
p^A_{yha}	... market-clearing price of arc capacity
f^C_{yhnce}	... quantity of fuel e put into transformation technology c
z^C_{ync}	... expansion of transformation technology capacity (#5)
τ^C_{yhnc}	... dual for capacity constraint of transformation technology c
β^C_{yhnce}	... dual for minimum input share of fuel e to transformation technology c
ζ^C_{ync}	... dual to transformation technology capacity expansion limit
p^C_{yhnce}	... market-clearing price of transformation technology capacity
f^{O-}_{yhno}	... quantity injected into storage
f^{O+}_{yhno}	... quantity extracted from storage
z^O_{yno}	... expansion of yearly storage capacity (#5)
z^{O-}_{yno}	... expansion of injection capacity (#5)
z^{O+}_{yno}	... expansion of extraction capacity (#5)
ζ^O_{yno}	... dual to yearly storage capacity expansion limit
ζ^{O-}_{yno}	... dual to injection capacity expansion limit
ζ^{O+}_{yno}	... dual to extraction capacity expansion limit
p^{O-}_{yhno}	... market-clearing price for injection into storage
p^{O+}_{yhno}	... market-clearing price for extraction from storage
τ^O_{yvno}	... dual for capacity constraint of storage technology in loading cycle v
κ^{O-}_{yhno}	... dual for injection capacity constraint of storage technology
κ^{O+}_{yhno}	... dual for extraction capacity constraint of storage technology

f^G_{yng} ... quantity of emissions of type g at node n
μ^{glob}_{yg} ... dual for emission constraints of type g (global)
μ^{reg}_{yrg} ... dual for emission constraints of type g in region r
μ^{nod}_{yng} ... dual for emission constraints of type g at node n
p^G_{yng} ... market-clearing price for emission of type g
p^D_{yhnde} ... final demand price by fuel
β^L_{yhnl} ... dual for fuel mix constraint l
β^M_{yhnm} ... dual for generation mix constraint m

Comments

#1 The notation $y' < y$ indicates "all years y' prior to year y", and $y' > y$ the reverse.

#2 Arcs and storage technologies can be used for exactly one fuel. This saves indices, but may be a problem later (e.g., capacity constraints of oil products pipelines).

#3 We want to maintain flexibility of the model, and there is no general "natural" time unit for a multi-fuel model (such as mcm/d for natural gas or kWh for power). All variables have to be interpreted as "full-year equivalent (i.e., the quantities produced, transported, transformed, or consumed if that time slice lasted one year).

#4 Initial capacity in the base year net of depreciation or planned shut-down; capacities are given in gross terms (before losses).

#5 Investment in additional capacity is available from the following period at the earliest.

#6 The first subscript (y) refers to the time period at which the expansion was undertaken; the second subscript refers to the "current" period. The parameter specifies how much of an expansion is still available in the current period. (Note that $dep^{\circledast}_{yy'\ldots} = 0$ if $y \geq y'$, since any expansion can only be available after the investment period.)

B The Karush-Kuhn-Tucker conditions

We write $f(x) \geq 0 \perp x \geq 0$ to indicate the complementarity constraint $f(x) \cdot x = 0$. This allows to have the KKT conditions below to be written exactly as they are coded in GAMS.

$$df_y dur_h \left[\frac{\partial \, cost^P_{yhsne}(\cdot)}{\partial \, q^P_{yhsne}} + \sum_{g \in G} p^G_{yng} ems^P_{ysneg} \right] + \alpha^P_{yhsne} - (1 - loss^P_{sne})\phi_{yhsne} + \gamma^P_{sne} \geq 0 \quad \perp \quad q^P_{yhsne} \geq 0 \tag{14}$$

$$df_y dur_h p^A_{yha} + \phi_{yhsn^{A-}(a)e} - (1 - loss^A_a)\phi_{yhsn^{A+}(a)e} \geq 0 \quad \perp \quad q^A_{yhsa} \geq 0 \tag{15}$$

$$df_y dur_h p^C_{yhnce} + \phi_{yhsne} - \sum_{f \in E^{C+}_c} transf^C_{yncef} \phi_{yhsnf} - \sum_{\substack{m \in M, f \in E^{C+}_c \\ \text{if } c \in C^M_m}} transf^C_{yncef} \beta^M_{yhnm} \geq 0 \quad \perp \quad q^C_{yhsnec} \geq 0 \tag{16}$$

$$df_y dur_h p^{O-}_{yhno} - dur_h (1 - loss^{O-}_o) \alpha^O_{yvH(ho)sno} + \phi_{yhsne} \geq 0 \quad \perp \quad q^{O-}_{yhsno} \geq 0 \tag{17}$$

$$df_y dur_h p^{O+}_{yhno} + dur_h \alpha^O_{yvH(ho)sno} - \phi_{yhsne} \geq 0 \quad \perp \quad q^{O+}_{yhsno} \geq 0 \tag{18}$$

$$\begin{aligned} df_y dur_h \Bigg[& \left(-int^D_{yhnd} + slp^D_{yhnd} \left(\sum_{s' \in S, f \in E} eff^D_{yndf} q^D_{yhs'ndf} \right) \right) eff^D_{ynde} \\ & + eucc^D_{yhnde} + eucl^D_{yhnde} \sum_{s' \in S} q^D_{yhs'nde} + \sum_{g \in G} p^G_{yng} ems^D_{ydeg} \\ & + cour^S_{ysnd} \left(eff^D_{ynde} slp^D_{yhnd} \sum_{f \in E} eff^D_{yndf} q^D_{yhsndf} + eucl^D_{yhnde} q^D_{yhsnde} \right) \Bigg] \\ & + \phi_{yhsne} + \sum_{\substack{l \in L \\ \text{if } d \in D^L_l}} \left\{ \begin{array}{ll} (shr^L_{ynl} - 1) eff^D_{ynde} \beta^L_{yhnl} & \text{if } e \in E^L_l \\ shr^L_{ynl} eff^D_{ynde} \beta^L_{yhnl} & \text{if } e \in \widehat{E}^L_l, e \notin E^L_l \end{array} \right\} \\ & + \sum_{\substack{m \in M \\ \text{if } e \in E^M_m}} shr^M_{ynm} \beta^M_{yhnm} \geq 0 \quad \perp \quad q^D_{yhsnde} \geq 0 \end{aligned} \tag{19}$$

$$df_y inv^P_{ysne} + \sum_{y' > y, h \in H} \left[df_{y'} dur_h \frac{\partial \, cost^P_{y'hsne}(\cdot)}{\partial \, z^P_{ysne}} - avl^P_{y'hsne} dep^P_{yy'sne} \alpha^P_{y'hsne} \right] + \zeta^P_{ysne} \geq 0 \quad \perp \quad z^P_{ysne} \geq 0 \tag{20}$$

$$avl^P_{yhsne} \left(cap^P_{ysne} + \sum_{y' < y} dep^P_{y'ysne} z^P_{y'sne} \right) - q^P_{yhsne} \geq 0 \quad \perp \quad \alpha^P_{yhsne} \geq 0 \tag{21}$$

$$\sum_{h \in H^V_{vo}} dur_h \left((1 - loss^{O-}_o) q^{O-}_{yhsno} - q^{O+}_{yhsno} \right) = 0 \quad \perp \quad \alpha^O_{yvsno} \text{ (free)} \tag{22}$$

$$
\begin{aligned}
(1-loss^P_{sne})q^P_{yhsne} - \sum_{d\in D} q^D_{yhsnde} + \sum_{c\in C, f\in E^{C-}_c} transf^C_{yncfe} q^C_{yhsncf}& \\
- \sum_{c\in C} q^C_{yhsnce} + \sum_{a\in A^+_{ne}} (1-loss^A_a) q^A_{yhsa} - \sum_{a\in A^-_{ne}} q^A_{yhsa}& \\
+ \sum_{o\in O^E_e} \left(q^{O+}_{yhsno} - q^{O-}_{yhsno}\right) = 0 &\quad , \quad \phi_{yhsne} \text{ (free)} \qquad (23)
\end{aligned}
$$

$$exp^P_{ysne} - z^P_{ysne} \geq 0 \quad \perp \quad \zeta^P_{ysne} \geq 0 \qquad (24)$$

$$hor^P_{sne} - \sum_{y\in Y, h\in H} dur_h q^P_{yhsne} \geq 0 \quad \perp \quad \gamma^P_{sne} \geq 0 \qquad (25)$$

$$-shr^L_{ynl} \sum_{\substack{s\in S, d\in D^L_l \\ e\in \widehat{E}^L_l}} eff^D_{ynde} q^D_{yhsnde} + \sum_{\substack{s\in S, d\in D^L_l \\ e\in E^L_l}} eff^D_{ynde} q^D_{yhsnde} \geq 0 \quad \perp \quad \beta^L_{yhnl} \geq 0 \qquad (26)$$

$$-shr^M_{ynm} \sum_{\substack{s\in S, d\in D \\ f\in E^M_m}} q^D_{yhsndf} + \sum_{\substack{s\in S, (e,f)\in E^C_c \\ c\in C^M_m}} transf^C_{yncef} q^C_{yhsnce} \geq 0 \quad \perp \quad \beta^M_{yhnm} \geq 0 \qquad (27)$$

$$df_y dur_h \left(-p^A_{yha} + trf^A_{ya} + \sum_{g\in G} p^G_{ynA^-(a)g} ems^A_{yag}\right) + \tau^A_{yha} \geq 0 \quad \perp \quad f^A_{yha} \geq 0 \qquad (28)$$

$$df_y inv^A_{ya} - \sum_{y'>y, h\in H} dep^A_{yy'a} \tau^A_{y'ha} + \zeta^A_{ya} \geq 0 \quad \perp \quad z^A_{ya} \geq 0 \qquad (29)$$

$$cap^A_{ya} + \sum_{y'<y} dep^A_{y'ya} z^A_{y'a} - f^A_{yha} \geq 0 \quad \perp \quad \tau^A_{yha} \geq 0 \qquad (30)$$

$$exp^A_{ya} - z^A_{ya} \geq 0 \quad \perp \quad \zeta^A_{ya} \geq 0 \qquad (31)$$

$$
\begin{aligned}
df_y dur_h \left(-p^C_{yhnce} + trf^C_{ync} + \sum_{g\in G} p^G_{yng} ems^C_{yceg}\right) + \sum_{f\in E^{C+}_c} transf^C_{yncef} \tau^C_{yhnc}& \\
+ \sum_{(e',f)\in E^C_c} shr^C_{ynce'} transf^C_{yncef} \beta^C_{yhnce'} - \sum_{f\in E^{C+}_c} transf^C_{yncef} \beta^C_{yhnce} \geq 0 &\quad \perp \quad f^C_{yhnce} \geq 0 \qquad (32)
\end{aligned}
$$

$$df_y inv^C_{ync} - \sum_{y'>y, h\in H} dep^C_{yy'nc} \tau^C_{y'hnc} + \zeta^C_{ync} \geq 0 \quad \perp \quad z^C_{ync} \geq 0 \qquad (33)$$

$$cap^C_{ync} + \sum_{y'<y} dep^C_{y'ync} z^C_{y'nc} - \sum_{(e,f)\in E^C_c} transf^C_{yncef} f^C_{yhnce} \geq 0 \quad \perp \quad \tau^C_{yhnc} \geq 0 \qquad (34)$$

$$-shr^C_{ynce} \sum_{(e',f)\in E^C_c} transf^C_{ynce'f} f^C_{yhnce'} + \sum_{f\in E^{C+}_c} transf^C_{yncef} f^C_{yhnce} \geq 0 \quad \perp \quad \beta^C_{yhnce} \geq 0 \qquad (35)$$

$$exp^C_{ync} - z^C_{ync} \geq 0 \quad \perp \quad \zeta^C_{ync} \geq 0 \qquad (36)$$

$$df_y dur_h \left(-p^{O-}_{yhno} + trf^{O-}_{yno} + \sum_{g\in G} p^G_{yng} ems^{O-}_{yog}\right) + dur_h \tau^O_{yv^H(h,o)no} + \kappa^{O-}_{yhno} \geq 0 \quad \perp \quad f^{O-}_{h,n,o} \geq 0 \qquad (37)$$

$$-df_y dur_h p^{O+}_{yhno} + \kappa^{O+}_{yhno} \geq 0 \quad \perp \quad f^{O+}_{yhno} \geq 0 \qquad (38)$$

$$df_y inv^O_{yno} - \sum_{y'>y, v\in V} dep^O_{yy'no}\tau^O_{y'vno} + \zeta^O_{yno} \geq 0 \quad \perp \quad z^O_{yno} \geq 0 \tag{39}$$

$$df_y inv^{O-}_{yno} - \sum_{y'>y, h\in H} dep^{O-}_{yy'no}\kappa^{O-}_{y'hno} + \zeta^{O-}_{yno} \geq 0 \quad \perp \quad z^{O-}_{yno} \geq 0 \tag{40}$$

$$df_y inv^{O+}_{yno} - \sum_{y'>y, h\in H} dep^{O+}_{yy'no}\kappa^{O+}_{y'hno} + \zeta^{O+}_{yno} \geq 0 \quad \perp \quad z^{O+}_{yno} \geq 0 \tag{41}$$

$$cap^O_{yno} + \sum_{y'<y} dep^O_{y'yno} z^O_{y'no} - \sum_{h\in H^V_{v,o}} dur_h f^{O-}_{yhno} \geq 0 \quad \perp \quad \tau^O_{yvno} \geq 0 \tag{42}$$

$$cap^{O-}_{yno} + \sum_{y'<y} dep^{O-}_{y'yno} z^{O-}_{y'no} - f^{O-}_{yhno} \geq 0 \quad \perp \quad \kappa^{O-}_{yhno} \geq 0 \tag{43}$$

$$cap^{O+}_{yno} + \sum_{y'<y} dep^{O+}_{y'yno} z^{O+}_{y'no} - f^{O+}_{yhno} \geq 0 \quad \perp \quad \kappa^{O+}_{yhno} \geq 0 \tag{44}$$

$$exp^O_{yno} - z^O_{yno} \geq 0 \quad \perp \quad \zeta^O_{yno} \geq 0 \tag{45}$$

$$exp^{O-}_{yno} - z^{O-}_{yno} \geq 0 \quad \perp \quad \zeta^{O-}_{yno} \geq 0 \tag{46}$$

$$exp^{O+}_{yno} - z^{O+}_{yno} \geq 0 \quad \perp \quad \zeta^{O+}_{yno} \geq 0 \tag{47}$$

$$df_y \left(-p^G_{yng} + tax^{glob}_{yg} + \sum_{r\in R_n} tax^{reg}_{yrg} + tax^{nod}_{yng} \right) + \mu^{glob}_{yg} + \sum_{r\in R_n} \mu^{reg}_{yrg} + \mu^{nod}_{yng} \geq 0 \quad \perp \quad f^G_{yng} \geq 0 \tag{48}$$

$$quota^{glob}_{yg} - \sum_{n\in N} f^G_{yng} \geq 0 \quad \perp \quad \mu^{glob}_{yg} \geq 0 \tag{49}$$

$$quota^{reg}_{yrg} - \sum_{n\in N_r} f^G_{yng} \geq 0 \quad \perp \quad \mu^{reg}_{yrg} \geq 0 \tag{50}$$

$$quota^{nod}_{yng} - f^G_{yng} \geq 0 \quad \perp \quad \mu^{nod}_{yng} \geq 0 \tag{51}$$

$$f^A_{yha} - \sum_{s\in S} q^A_{yhsa} = 0 \quad , \quad p^A_{yha} \text{ (free)} \tag{52}$$

$$f^C_{yhnce} - \sum_{s\in S} q^C_{yhsnce} = 0 \quad , \quad p^C_{yhnce} \text{ (free)} \tag{53}$$

$$f^{O-}_{yhno} - \sum_{s\in S} q^{O-}_{yhsno} = 0 \quad , \quad p^{O-}_{yhno} \text{ (free)} \tag{54}$$

$$f^{O+}_{yhno} - \sum_{s\in S} q^{O+}_{yhsno} = 0 \quad , \quad p^{O+}_{yhno} \text{ (free)} \tag{55}$$

$$\begin{aligned} f^G_{yng} - \sum_{h\in H, e\in E} dur_h \Bigg(& \sum_{s\in S} ems^P_{ysneg} q^P_{yhsne} + \sum_{s\in S, d\in D} ems^D_{ydeg} q^D_{yhsnde} \\ & + \sum_{a\in A^+_{ne}} ems^A_{yag} f^A_{yha} + \sum_{c\in C} ems^C_{yceg} f^C_{yhnce} + \sum_{o\in O} ems^{O-}_{yog} f^{O-}_{yhno} \Bigg) = 0 \quad , \quad p^G_{yng} \text{ (free)} \end{aligned} \tag{56}$$

C End use costs and model calibration

As discussed in Section 2, linear fuel substitution may yield "bang-bang"-results. Given that a fuel is usually used for many different purposes even within a sector, a certain measure of "stickiness" of fuel usage is plausible. Furthermore, fuel-switching often requires a change of equipment, which entails investment costs. One may also consider start-up costs as a rationale for sticky fuel-switching in a seasonal model. Overall, we expect substitution to occur gradually, purpose-by-purpose. However, this is difficult to capture while keeping the model linear, which is an important consideration for the sake of efficient numerical computation.

We therefore introduce the concept of fuel-specific end use costs to mimic this gradual substitution; they are represented by an affine function. Parameters are chosen such that, in equilibrium, each demand sector chooses exactly the reference demand quantity of each fuel in its consumption mix.

An illustration of end use costs

The end use costs are depicted, in a stylized example, in Figure 6. There are two fuels (1 and 2) used in the sector; reference consumption values are given by q^{D1} and q^{D2}. For simplicity, we assume that both fuels have the same *efficiency*, i.e., the same level of *energy service* provided per unit of fuel.

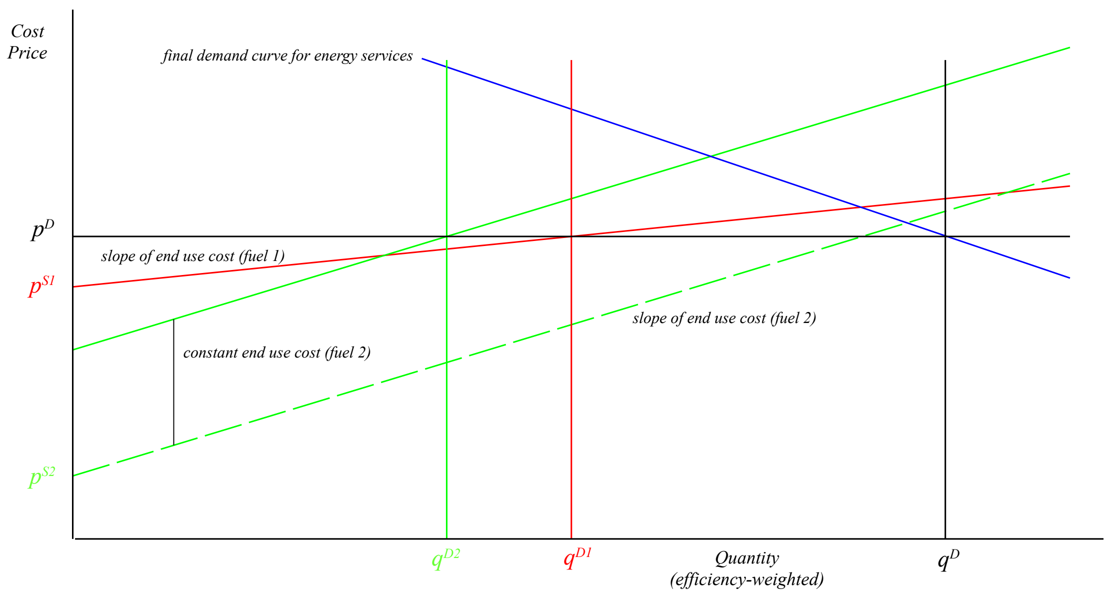

Figure 6: Illustration of end use costs in a sector which can consume two fuels

The prices on the y-axis (p^{S1} and p^{S2}) can be interpreted as supply price, i.e., how much does it cost to deliver (supply) the reference quantity of the respective fuel to that node. The consumer has to pay the supply costs plus the end use costs, depicted by the intercept and slope of the end use cost function. The slope of the end use cost curve of fuel 1 is flatter, which means that consumption of this fuel is more elastic. The slope is determined from assumptions on the relative elasticity of substitution between the fuels in the sector.

When comparing the intersection of the demand cost curves (supply cost plus linear end use costs) with the reference demand quantity for both fuels, one notices that the "price" to be paid by the consumer for fuel 2 is much lower than the price for fuel 1; hence, this would not be a plausible equilibrium for the consumer to choose less of fuel 2 than of fuel 1. We therefore shift the demand cost curve upwards by adding a constant end use cost term; this could be, for example, interpreted as distribution costs to deliver the fuel.

Now, the intersection of the demand cost curve and the reference demand quantity for both fuels are equal; hence, it is indeed optimal for the consumer to use exactly the reference quantities, paying the final demand price p^D for a unit of either.

Summing up the reference demand quantities, we obtain the total quantity (energy service) consumed (q^D). Now, we can use the standard approach in partial equilibrium energy sector models, fitting a linear inverse demand curve through the reference point (q^D, p^D). The slope of the inverse demand curve at that point is derived from the elasticity of the entire sector.

An iterative calibration algorithm

As we stated in the main article, calibrating a large-scale model is a challenge. We use the concept of the end use costs and supply prices to implement a semi-automatic calibration algorithm.

0 *Initialize:* Assume a supply price for each node/fuel/sector combination

1 Derive the end use cost parameters and the inverse demand function based on the supply prices

2 Solve the model

3 Compare model results (quantities consumed) with demand reference values; if model results are too high, decrease the supply price of this fuel; otherwise, increase the supply price

4 Repeat from step 1; end after n iterations

At first glance, it may seem counter-intuitive to decrease the fuel supply price when this fuel is used too much relative to the reference quantity, so let us elaborate on the rationale: if this fuel is not the most expensive one (including end use costs), a change in this fuel's supply price will not influence the final demand price p^D, set by the most expensive fuel. Instead, the constant end use cost term will be increased, making the fuel relatively more expensive in the next model run. In contrast, if a fuel is already the most expensive, reducing its supply price will also reduce the final demand price. This will also reduce all other fuels' constant end use cost parameter, making all other fuels relatively cheaper. Either way, the share of this fuel in the sector's total consumption will decrease in the next model run, which should get model results closer to reference values.

Obviously, this algorithm only seeks to match the demand reference quantities. Therefore, after a sufficient number of iterations, we compare production, transformation, and trade flow results to the reference values, and adapt relative costs and other parameters accordingly (and manually). Then, we repeat steps 1–4. In practical application, this algorithm works quite well.