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A Techno-Economic Perspective on Natural Gas and Its Value Chain

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Abstract: We describe the elements and actors in the global natural gas value chains with an emphasis on characteristics relevant for large-scale energy system and market modeling. We give backgrounds on natural gas as a hydrocarbon to provide a rationale and understanding for what functional representations in mathematical programming models aim to represent. Simply taking the most advanced and detailed functional forms for all value chain characteristics and activities will typically result in numerical intractability. One should carefully determine what is needed to address a research question or analyze a business case. Recent advances in mathematical programming do allow solving large models with adequate detail for many types of analysis. We discuss which functional forms and modeling approaches can be appropriate for representing various characteristics in different types of analysis and provide a succinct and general mathematical programming formulation reflecting the optimization problems for different types of actors in the value chain. We provide an implementation for a stylized network using GAMS.

Keywords: techno-economic modeling; natural gas; value chain; network optimization

1. Introduction

Natural gas consumption and production can be found in all world regions. There are big differences between the regions regarding the maturity of the markets and the types of applications that use natural gas. For example, North America and Europe have well-developed gas pipeline systems to transport gas from suppliers to different types of consumers, possibly crossing several country borders on the way. In other parts of the world, transmission systems are much less developed, domestic distribution may only cover parts of the countries, and it can be focused on supplying some large-scale users such as electric power generation and not connect any small residential buildings or other small volume consumers.

In 2019, global gas consumption was close to 4×10^{12} m³ (trillion cubic meters), about 27% higher than global consumption in 2010 and outpacing total energy consumption growth over that same period by more than 10 percentage point (c.f., [1]). Since 2010, interregional gas trade has grown by 1/3 [1]. Whereas in 2010 interregional pipeline trade made up for 60% of total interregional trade, in 2019, liquefied natural gas (LNG) and pipeline trade had about equal shares. From 2020, the balance in the interregional pipeline trade will shift in favor of LNG.

Most natural gas is transported through high-pressure onshore pipelines, while a smaller part is transported via offshore pipelines or in ships in the form of liquefied natural gas (LNG). Until the 21st century, a global natural gas market was virtually non-existent. Several regional markets could be distinguished based on the geographical proximity of suppliers/exporters and consumers/importers. The tremendous growth in LNG trade since the turn of the century has caused regional markets to be increasingly more integrated. LNG has been traded and shipped for over sixty years; however, due to its high costs, large-scale LNG imports were limited to some rich countries with few alternative supply

options, notably Japan and South Korea. For several reasons, such as locally depleting reserves and supply security considerations, long-distance international gas trade has increased rapidly since the change of the century. Economies of scale and other drivers have increased the competitiveness of LNG as an energy carrier. Larger volumes of LNG spot trade are causing regional natural gas markets to gradually merge into a global market. This globalizing natural gas market requires an extension of the traditional modeling tools that consider regional pipeline networks mostly. Modeling tools should allow for variety in markets and infrastructure. Regionally, for instance in Europe, oligopolistic market structures still dominate, whereas in for instance North America, the market is best characterized by perfect competition. Different countries have different types of resource bases, including associated gas from crude oil production and shale gas, which have very different cost structures both in exploration and production phases.

The analysis of operational networks, including line pressure, line packing, and compressor usage, in the context of a spot market, requires a lot of engineering detail. In contrast, to analyze long-term trends in global markets, including policy impacts, and considering the role of natural gas in climate change mitigation efforts, less engineering detail is needed. Dependent on the type of analysis, modeling tools should account appropriately for different characteristics while taking into account the computational challenges and limitations connected to large-scale systems, integer decision variables, non-convex functional forms, et cetera.

Energy markets have many types of agents, and many possible interactions can occur among them. When formulating a model for an energy market, many modeling decisions must be made regarding the representation of the actors and the technical and economical detail that can be represented. In large systems and for instance climate policy or other long-term analyses, the emphasis in the model development is on the economic aspects and interactions prevalent in the natural gas market. Many technical details relevant for specific natural gas value chains and regional or national markets play less of a role in such a long-term, global analysis. Additionally, including much technical detail will hamper scalability and tractability.

There has been an increasing focus on electrification and power systems in energy markets and energy systems research. However, natural gas will have an important role in the energy system for decades to come—possibly less so in the EU but certainly globally. A succinct but thorough introduction of the natural gas sector targeting a broad audience can facilitate the appreciation of natural gas and the considerations behind established functional representations in models. This paper aims to provide such an overview and the relevant considerations and consequences of different modeling choices to represent gas sector characteristics. As such, this paper provides engineering, economic, and policy considerations and discusses a middle ground techno-economic perspective accounting for enough engineering and market detail, considering advantages and disadvantages of different functional forms and modeling approaches.

Before introducing the economic roles of natural gas market actors, we start by introducing natural gas as a fossil fuel subject to production, transport, storage, trade, and consumption.

1.1. Natural Gas

Natural gas is a hydrocarbon consisting mostly of methane (CH_4), some ethane (C_2H_6), and modest amounts of larger alkanes ($\text{C}_x\text{H}_{2x+2}$) and other components. The existence and production of natural gas are very much linked to another hydrocarbon: oil. Describing the origins of natural gas means discussing hydrocarbons more generally. Most technical detail in the following is based on unpublished chapters of my doctoral dissertation [2], with [3] as a main source.

1.1.1. Hydrocarbons

Many million years ago, dead organic material piled up on the bottom of the sea. Over time, huge layers of sediments buried the organic material. Bacteria, pressure, and heat degraded and

decayed the organic material into fluid mixtures of hydrocarbons (C_xH_y). Nowadays, these mixtures of crude oil, natural gas, and natural gas liquids (NGL) are denoted as petroleum.

Natural gas is the part of the mixture that is gaseous at ambient temperature and under atmospheric pressure. In natural circumstances, when separated from crude oil after flowing out of a reservoir, natural gas contains water vapor, hydrogen sulfide, carbon dioxide, helium, nitrogen, and dissolved NGL such as propane and butane.

Reservoirs with accumulated mixtures of hydrocarbons exist underground as subsurface porous sedimentary rocks, in and under the same sediments that buried them when the hydrocarbons were still organic material. These underground reservoirs of oil and gas are often connected to aquifers: porous rock systems containing water.

Reservoirs can contain hydrocarbons that are liquids, gases, or both. The terms gases and liquids refer to the state of the hydrocarbons under atmospheric pressure and ambient temperature. Due to high reservoir pressures, gases may have a liquid state; in contrast, liquids can have a gaseous state when temperatures are high. Dependent on the pressure and temperature in a reservoir, the mixture of hydrocarbons can be in a single-phase (either gaseous or liquid) or in the two-phase state. Thus, if the single phase is a liquid phase, there may be gases present dissolved in the oil. Alternatively, if the single phase is gaseous, any oil and NGL in the reservoir are vaporized. Typically, if the state of the reservoir is two-phase, there is a gas cap on top, and there are liquids in the lower part of the reservoir: the oil zone. Due to these various phase and substance combinations, there can exist up to four types of hydrocarbon reserves in a reservoir: free gas, dissolved gas, crude oil, and NGL [3].

The total content of a reservoir, the resource, is a fixed quantity. Generally, not all content can be recovered. How much can be depends on the production methods used, the economic circumstances, and environmental and other government regulations.

1.1.2. Reserves

Due to the physical characteristics of hydrocarbon reservoirs, it is not easy to estimate the total volume of hydrocarbon contents in them. The volume-estimating activities to gauge reserves in an area where no production is taking place yet are called “exploration”. Over time, petroleum engineers have developed an advanced toolkit, including seismographic data collection and computer simulations to gauge the total of reserves in reservoirs.

Seismology studies how seismic wave energy moves differently through various types of terrestrial surface and underground formations. Seismic waves are created artificially by machinery, and the behavior of these waves is measured using sensitive tools called geophones. Other data-gathering activities include measuring magnetic properties and the gravitational field of the Earth.

Since there is a huge variation in the reliability of the assessments and exploration activities may lead to drilling dry wells, but also to huge finds, various classifications of reserves estimates have been developed. The verbal indications proved, probable, and possible reserves are conceptually self-explanatory; however, they have varying meanings dependent on the institute that performed or reported the assessment, the assessment method used, and whether the assessment was deterministic or stochastic.

The Society of Petroleum Engineers [4,5] has made huge efforts to compare and standardize reserves likelihood methodologies. Naming conventions for reserves include: 1P for proved reserves, or Low Estimate; 2P, for proved plus probable reserves, and Best Estimate/3P, for proved plus probable plus possible reserves, or High Estimate.

When stochastic assessments are performed, in terms of proved, probable, and possible reserves, 1P is often taken equivalent to an at least 90% chance that eventually, the recovered quantity will be the estimated amount; 2P to at least 50%, and 3P to at least a 10% probability of eventual recovery. When other characteristics are taken into account, such as economic and technical recoverability, the Society of Petroleum Engineers [5] addresses that the reporting standards of many international agencies are rooted in the methodology proposed by [6]; see Figure 1.

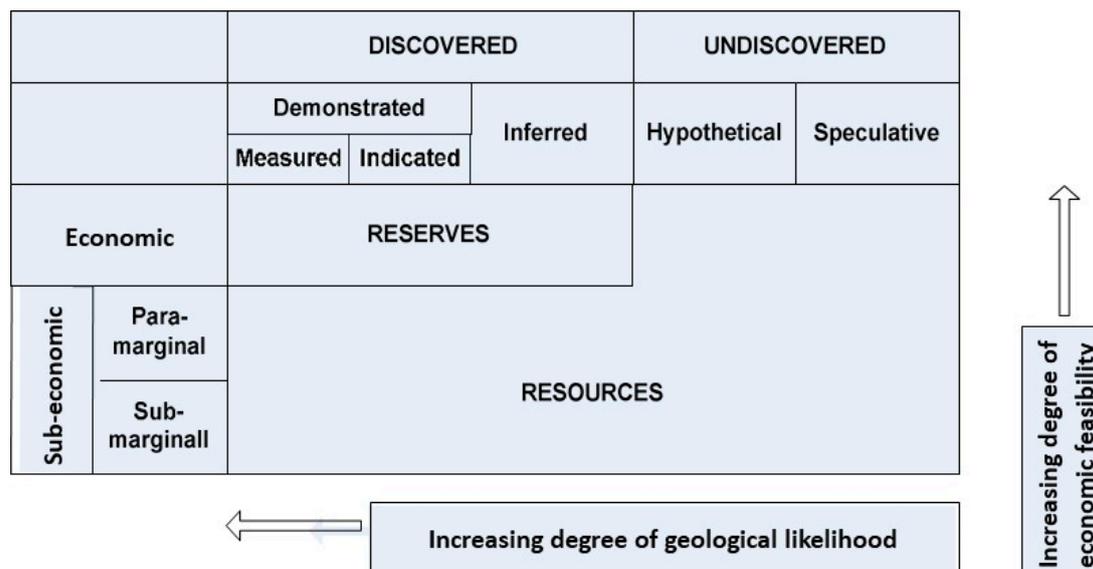


Figure 1. McKelvey Box. Recreated from [5].

As stated above, the actual volume of hydrocarbons in a reservoir is hard to assess. Whenever an exploration team decides that a site has good prospects for finding hydrocarbons, the next step will be to drill an extraction well. Permits, leases, and rights of land use need to be arranged as well as arrangements with local or federal authorities about royalty and tax regimes. If a newly drilled well hits a significant hydrocarbon deposit with development potential, it is further enhanced to become a production well.

Dependent on how big the relative share of dissolved gas in the crude oil, various types of reservoirs and wells are distinguished. Oil wells contain relatively little dissolved gas (up to a few 1000 cubic feet per barrel of crude oil). Gas-condensate reservoirs have between five thousand and one hundred thousand cubic feet of gas per barrel. In contrast, natural gas wells contain at most one barrel of hydrocarbon liquids per one hundred thousand cubic feet gas. Gas from oil wells is associated gas, which can be associated-free gas if it comes from the gas cap (in a two-phase reservoir) or associated-dissolved (or solution) gas if it was dissolved in the crude oil. Non-associated gas is from reservoirs that hardly contain any liquids. Gas from condensate reservoirs is called wet gas; that from gas reservoirs is called dry (or lean) gas [3]. Some classification aspects are situational, e.g., pressure changes during production affect the saturation level and may cause some dissolved gas to become free.

1.1.3. Production

Once a well is drilled in a reservoir, pressure differences will cause oil and gas to flow through the pores in the sedimentary rock to the well. The pressure of dissolved gas and ground water from connected aquifers pushes out oil and gas. The outflow of hydrocarbons causes the pressure and temperature to decrease over time, changing the physical properties of the hydrocarbons mixture in the reservoir. When the pressure gets lower in a two-phase reservoir, the gas saturation in the oil zone increases, eventually letting free gas start flowing to the production wells.

Dependent on the physical properties of the hydrocarbons mixture, various production methods can be used. Primary production methods are based on different types of pressure in the reservoir. This includes pressure due to dissolved gas, water inflow from connected aquifers, capillary expulsion (water creeping up pores in rocks pushing out oil) and gravity drainage (oil moving to wells in lower parts of a reservoir). Secondary recovery methods aim at repressurizing the reservoir. These methods include the injection of water (water flooding), carbon dioxide, or natural gas (gas cycling), or using pumps. Injected natural gas can usually be recovered at the end of the oil production phase.

Tertiary recovery methods (improved or enhanced recovery) aim at lowering oil viscosity (stickiness) by the injection of chemicals or increasing oil temperature by injecting steam.

In addition to hydrocarbon wells, there are other sources adding to the total gas supply. Examples of such supplemental supplies include blast furnace gas, refinery gas, propane–air mixtures, and synthetic natural gas (SNG) manufactured from biomass, hydrocarbons, or coal. Although locally these supplies can be significant, at present, they do not have significant shares in the global gas supply. In the future, biogas (e.g., captured from organic waste at wastewater treatment facilities or from manure at dairy farms) and the gasification of coal in combination with carbon capture and storage could play significant roles in the supply of natural gas.

Biogas arises from the degeneration of organic material in the absence of oxygen. Due to the generally large carbon dioxide share in biogas, it often needs to be upgraded to allow injection into the natural gas grid, but it can often be used as is in local gas-fired power generation. The huge potential for biogas and its status as a renewable energy source may affect the reserve base of natural gas, but this depends very much on subsidies and other incentives.

Many not-so-deep reservoirs, the low-hanging fruit among the oil and gas wells, have been exploited. New hydrocarbon wells in the 2000s have become increasingly deeper and offshore. Deeper reservoirs contain more gas and condensates due to higher pressures. Naturally, drilling deeper is more costly, which has incentivized the exploration of other sources, such as shale oil and gas. Shale gas has gained market share rapidly, especially in the US but also in some other regions. It is produced from shale rock using hydraulic fracturing (fracking): injecting a mixture of water, sand, and chemicals under high pressure via drilled holes to break the rock and create and keep open pores to release the gas inside.

1.1.4. Processing

Produced natural gas is referred to as raw natural gas. It may or may not be wet and contain large amounts of condensate, which affect the calorific value. In addition, it may or may not be sour, containing sulfur dioxide and/or carbon dioxide, which may cause the corrosion of pipelines. Therefore, most gas needs processing before it can be transported to final consumers.

Raw natural gas may contain all kinds of substances such as water vapor, hydrogen sulfide, carbon dioxide, helium, nitrogen, dissolved oil and gas condensates, sand, and other large particles. Processing removes these to get dry natural gas: mostly methane and a modest fraction of ethane. Some technically uncomplicated processing steps, such as removing sand and water, are done close to the wellhead, whereas more advanced steps including sulfur and carbon dioxide are done in large-scale facilities.

1.1.5. Producers

Companies involved in natural gas production include Exxon-Mobil, BP, Shell, Equinor, Gazprom, Sonatrach, and CNOOC. A main difference between the first three and the other is that they are publicly listed and operate globally, and the other are not and operate (mostly) regionally.

In many countries, the production of gas is nationalized, especially in the countries that would potentially participate in a global gas cartel (c.f., [7,8]).

Much of the company data for oil and gas producing firms—for instance, on production costs—is not publicly available, or only at a very aggregate level. In fact, natural gas production rates and costs vary by reservoir and over time, as do costs for, and the success rates of, drilling new wells. However, data for costs and reserves of individual reservoirs are not publicly available. One may buy data from consulting firms, e.g., Rystad or Wood Mackenzie, or rely on own source reviews and assumptions (e.g., [9]) and increasingly more on open data repositories.

Many academic gas market models consider countries rather than companies. This can be warranted when the analysis focuses on climate policy, long-term developments, supply security, or global cartelization issues. In such analyses, it can be viable to limit the representation of the

production side of the gas market to the economically most relevant aspects. Then, the technical characteristics from production and processing can be summarized into supply cost curves, production capacities, and economically recoverable reserves.

Summarizing all (marginal) supply costs into one curve is a simplification very common in the literature, and it is representative enough for many types of analysis. Golombek et al. [10] introduced a rather general functional form for production costs that accounts for aspects such as different marginal costs for differently sized fields and increasingly higher costs when production is close to capacity limits. The marginal costs for production level q , for non-negative parameter values $a, b, c, d, CAP \geq 0$ is expressed as:

$$C'(q) = a + bq - c \ln\left(\frac{CAP - q}{CAP}\right). \quad (1)$$

Variants and extensions of Function (1) consider the reserves base and accumulative production Q via a term:

$$- d \ln\left(\frac{RES - Q}{RES}\right). \quad (2)$$

Although the functional form proposed by Golombek et al. is quite elegant, the logarithmic term(s) challenge numerical tractability. In addition, considering that input data is often based on assumptions, and typically the resulting parameter values have an error margin of several 10%, a piecewise quadratic cost approximation (hence piecewise linear marginal costs) will be close enough in function value and with much better numerical tractability.

1.1.6. Wholesale Trade

Most companies that physically trade natural gas also perform other activities. Often, gas companies are active in oil, too, and they tend to be vertically or horizontally integrated. Such integrated companies may be active in all aspects of the natural gas market, from production and trade, to liquefaction, regasification, LNG transport, pipeline operation, and storage. All seven companies listed above as producers have major trading activities. Examples of pure traders are (before 2006) Gazexport, the trading arm for Gazprom, and (until 2024) GasTerra, a Dutch trader without its own production (but owned by two gas majors and the Dutch government). Retail trade by local gas utilities who deliver to final consumers is typically not of interest in global-scale analyses. We elaborate on some aspects relevant for gas trade.

1.1.7. Market Power

Market power is the ability to change prices from the level that would prevail under competition. In the European market, both intended and unintended supply shocks in the past have proven the existence of market power (if not always the conscious exertion of it). At several points in time, the disruption of Russian supplies to Ukraine has caused price hikes in Ukraine and other European countries. In contrast, Norway's testing of a new major pipeline to the UK some years ago caused negative prices. The objectives of the Gas Exporting Countries Forum (GECF, <https://www.gecf.org/about/mission-objectives.aspx>) are some indication that members are or would be willing to exercise market power.

Market power is often ignored in modeling energy markets. One reason is that for a long time, it was believed that a typical Cournot oligopoly cannot be represented as a linear or quadratic program (e.g., [11]), which hindered the numerical tractability of large-scale problems. However, Egging-Bratseth et al. [12] show that a simple adjustment to the standard welfare maximizing problems allows representing market power characteristics such as Cournot behavior with convex optimization programs, surpassing the need for mixed complementarity problems in many cases.

In—perceived—lieu of scalable modeling alternatives, some authors have favored adding mark-ups to the competitive, marginal-cost based prices, or conjectured supply variation approaches. One main drawback of such approaches is that they fail to capture endogenously the incentive for market power exerting actors to geographically diversify their supplies. (c.f., [13]). As a result, gas is

being shipped over longer distances in an oligopolistic market compared to perfectly competitive markets, and typically counterflows will occur; flows in both directions between two countries is not welfare-efficient due to costs and losses and would not happen in any social welfare maximizing or system cost minimization approach.

The author's own experience with large-scale energy market models indicates that a full-fledged Cournot oligopoly in the (upstream) natural gas market is an unreasonable assumption. More moderate market power assumptions are warranted with different levels of market power for different suppliers. Conjectural variation is an approach with theoretical limitations but in practice, it is simple to implement and calibrate. For a discussion see, e.g., [14].

1.1.8. Contracts

A major determinant of global gas trade flows is contracts, especially long-term contracts. Although decreasing in relative volume, long-term contracts are still a very important factor in natural gas markets. Contracts in place can often easily be accommodated with appropriate lower bounds on volumes. To reflect the contracting process, one needs a multi-stage model, with contracting and spot-market stages (c.f., [15,16]). For the portfolio optimization of an energy company, reflecting this multi-stage decision process may be warranted. For global analyses focusing on climate change mitigation or other policy impacts over a multi-decade horizon, contracts are of much less interest, and new contracts endogenously decided by a model would accommodate the long-term equilibrium.

For LNG trade, GIIGNL [17] lists all contracts in place. To the best of the author's knowledge, for pipeline contracts, no such complete information exist in the public domain.

1.1.9. Traders

Legal requirements forcing an unbundling of production and trade operations pushed by the U.S. Federal Energy Regulatory Commission (FERC, www.ferc.gov/order-no-636-restructuring-pipeline-services) and the European Commission [18] may favor modeling traders as actors separate from producers in some regions. This would make not so much sense when considering state-controlled companies such as Gazprom and Qatargas. However, the approach in [12] caters to both vertically integrated and unbundled production and trade, and profits may be calculated ex-post in accordance with the represented company and market structure relevant in each region.

1.2. Liquefied Natural Gas

When natural gas is cooled to below its boiling point of about -160 Celsius (-260 Fahrenheit), it liquefies and becomes over 600 times denser. Capital investment costs for a liquefaction facility are significant, and a loss of 10–12% of the natural gas used to power the liquefaction process is a major operational cost. However, distance-related losses for transport over long distances are only about 1/10 of the losses in pipelines. Therefore, to overcome long distances, or when pipelines just cannot be built, LNG is a viable and competitive option to transport natural gas. GIIGNL [17] provides an overview of liquefaction and regasification terminals, ships, and contracts.

1.2.1. Liquefaction

Some of the major actors in LNG are Qatargas, Shell, Engie, and BP. Where Qatargas operates LNG export activities sourced from a single country, the other three are present in several LNG exporting countries. Figure 2 characterizes the main elements of the LNG supply chain.



Figure 2. Liquefied natural gas (LNG) supply chain.

On the upstream (supply) side, there is gas production and liquefaction; then, the liquefied gas is shipped overseas. In the consuming region, an importing facility re-gasifies the gas and pumps it into the local pipeline system.

In 2019, there were 21 LNG exporting countries, with about 50 terminals in total (many with multiple plants and *trains*) for a total capacity of about $570 \times 10^9 \text{ m}^3$ (billion m^3 per annum, bcma).

The liquefaction of natural gas is a capital-intensive and technologically-advanced process. A large part of the operational liquefaction costs is due to the gas usage in the compressors. Differences in the gas constituents in various production fields and the requirements in the importing markets need to be overcome. Local circumstances can drastically impact the construction of facilities as well as operational characteristics. For instance, arctic conditions in the Norwegian northern North Sea, the Russian Barents Sea, and Sakhalin Island may impede the development of LNG infrastructure and the accessibility of the facilities by ships. On the upside, the much colder sea water in the arctic regions as compared to Middle Eastern countries such as Qatar allows for significantly lower losses in the operational liquefaction.

Impurities and non-combustible components (such as carbon dioxide) do not add any value to the end users and are removed from the gas to transport more energy content in the available shipping capacity. The same processing steps on the raw gas as described above apply, however with stricter requirements on purity, therefore resulting in a gas (still in gaseous form) with significantly higher calorific value than pipeline gas. Additional to these processing steps, there are the liquefaction steps: compression and heat exchange (cooling and pressurizing the natural gas), expansion (bringing the liquefied gas to atmospheric pressure), storage (between the liquefaction and the loading of the ship), and loading (bringing the LNG onto the ship). For more details on the design of liquefaction plants, see for example [19,20].

Since liquefaction terminals are expensive, often several billion dollars, there is significant financial risk involved. This is mitigated by joint ownership structures and long-term contracts securing high utilization rates and a return on investment. In many countries, LNG terminals are owned and operated by joint ventures between local producers and international oil majors. Notably, Qatar has significant uncontracted liquefaction capacity, allowing it to seek the most profitable destinations in the spot markets and a pivotal arbitrage role between the Atlantic and the Pacific basins.

Many aspects of the liquefaction process potentially cause non-linearities and non-convexities when representing them in a mathematical model, which hampers tractability. The same is true for capacity expansions, which are integer-valued, and economies of scale, which induces the concavity of minimization objectives. From a global, multi-decade, perspective, it often suffices to account for capacity limits, loss rates, capital, and operational costs.

1.2.2. LNG Shipment

The bulk of LNG is transported in dedicated large-scale LNG shipping vessels. Such ships have large tanks to hold the liquid LNG. A major concern is that due to ship movement (sloshing), some LNG evaporates: the so-called boil-off. This causes pressure increases in the tanks. Some new ships use the boil-off to fuel the ship's engines. According to [21], there are about 600 LNG vessels. The largest of LNG vessels carry up to 270,000 cubic meters of LNG, the equivalent of about $0.16 \times 10^9 \text{ m}^3$ (bcm) in gaseous form.

Charter rates for a common-sized LNG ship (160,000 cum) in recent normal years have been between 50,000 and 100,000 USD/day. A 1000 sea mile (1800 km) journey takes about 2.5–3 days, plus time loading and unloading brings it to 4–5 days in total.

In increasingly more countries, including the United States, France, and Belgium, LNG is transported by trucks to supply not-grid-connected power plants, industry facilities, and LNG refueling stations. Some LNG import terminals, for instance Singapore and Rotterdam, have "break-bulk" facilities. Such facilities reload LNG onto smaller tankers that deliver to smaller destinations on coasts and river banks. Environmental policy, e.g., concerning small particles and sulfur dioxide emissions,

incentivizes LNG replacing diesel in freight road transport and fuel in short sea shipping, similar to gas replacing coal in power generation. Still, these applications account for a small fraction of total LNG supply only. At present, such applications are niche markets, and the bulk of LNG still follows the value chain depicted in Figure 2.

LNG vessel routing and scheduling optimization has a much different perspective than long-term market development analysis. It would take the outcomes of the latter as one of the starting points for planning from a single company perspective with a portfolio of LNG infrastructure and contracts. The large-scale integer programs to model this often need dedicated advanced solution algorithms, (c.f., [22–24]). Aspects such as minimizing the number of ships, schedule regularity, fuel usage minimization, inventory level management, stabilizing the number of charter ships hired, etc. are important cost drivers. In a long-term global market perspective, the importance of LNG is that it connects otherwise disconnected regional markets into a global market, albeit with significant transaction costs (including losses), which allows significant price differences between regions, but also providing the means to physically arbitrage away very large price differences.

1.2.3. Regasification

When an LNG shipment arrives at its destination, the vessel must be unloaded and the gas brought back into a gaseous state to inject it into the gas grid. Some actors that are active in regasification are Engie, British Gas, Cheniere, and Fluxys. In 2019, there were over a hundred terminals in 42 countries with total regasification capacity of about $1250 \times 10^9 \text{ m}^3$ per annum (bcma).

Regasification is a much simpler process than liquefaction. Therefore, the infrastructure for the regasification of gas tends to be less capital-intensive than for liquefaction. Naturally, when LNG is exposed to ambient temperature and atmospheric pressure, it will return to a gaseous state. Regasification happens automatically when the temperature of the fluid LNG reaches its boiling point of -160 Celsius, which can be accelerated by using sea water in heat exchangers. Sometimes, the sea water is heated by boilers, using a small portion of the gas that is regasified.

The main steps in the regasification process are the following: unloading (of LNG shipping vessels), vaporization (of the liquefied gas to bring it back to a gaseous state), storing the gas (to allow quick unloading of the vessel while not immediately bringing the gas into the pipeline system), processing (sometimes, some components must be added to meet local requirements), and finally, injection into the pipeline system (the high-pressure network to transport the gas to local distribution systems and end users).

In the wake of the rapidly growing shale gas production, many terminals in the USA that were planned originally for LNG imports have been repurposed for LNG export. A consideration is that regasification and consequent reliquefaction is very costly and should be avoided. Rather, liquefied gas that has been unloaded and stored but not yet vaporized can be loaded back onto ships and shipped to other destinations. Some LNG receiving terminals have installed such (re)loading facilities, while others have break-bulk facilities to split large LNG loads into smaller cargos. Such kinds of loading equipment allow market actors to benefit from short-term arbitrage opportunities and may provide swing supply in some markets.

Since regasification terminals are technically less challenging than liquefaction terminals, investment costs per unit of capacity are typically a half order of magnitude lower; operational cost, especially losses, are even more modest.

1.2.4. Storage

Natural gas storage is used for various reasons, including daily balancing, speculation, seasonal balancing, and as a strategic backup supply to overcome temporary supply disruptions or to meet peak demand on extremely cold winter days. There are several types of gas storage: depleted reservoirs in oil and gas fields, aquifers, salt caverns, and integrated in LNG liquefaction and regasification terminals. Each has different characteristics relative to the amount of gas that can be stored and the

speed with which the gas can be injected or extracted (deliverability). Storage is typically located close to demand centers so that bottlenecks in the transportation system do not harm the deliverability of gas to consumers. Alternatively, it may be located at critical nodes in the gas network with ample transmission capacity toward different demand centers. Some volume of gas in the storage, the cushion gas, should maintain a high enough pressure level and is never extracted. This cushion gas may take 50–80% of the available space in the storage. The amount of gas available for operation is the working gas.

Typically, gas installations have minimum and maximum injection and extraction rates. Deliverability depends on the pressure in the facility, which is higher when the total stored amount is larger. To be able to inject gas into storage, compressors are used to increase pressure. These compressors use some of the gas as their energy source; therefore, there is a loss rate typically of about 1%.

Storage infrastructure in many countries is subject to third party access (TPA), which means that they facilitate others to use injection, storage, and extraction services. In such cases, the storage operators provide services but do not own the gas stored in their facilities. Many storage facilities are not owned by specific storage operating companies but rather by other actors in the gas market, such as producers, traders, or grid network owners. Examples of companies involved in gas storage are Gazprom, TAQA, Royal Dutch Shell, and E.ON.

1.3. Gas Transmission System

Ownership, management, and operation of the gas transmission system, a pipeline network with compressors and valves, is done differently in different countries. In the past, it was very common that pipeline owners also traded the gas. However, regulatory authorities have recognized that the ownership of a pipeline provides the owner with a monopoly position in the transportation of the gas and thereby too much leverage in negotiations. Regulatory bodies such as FERC in the USA and the EC in Europe have taken measures to enhance the access to transport infrastructure for third parties. Notably, the US and Europe are the regions with the most mature gas markets and best developed large-scale pipeline network systems.

In Northwest Europe, there is a second high-pressure pipeline system to accommodate gas exports from the large onshore Groningen field, whose gas has significantly lower calorific value than much other gas due to a nitrogen content of about 20%. In a global setting, this is of limited relevance, and with rapidly declining production from the Groningen field, this will also be the case in the European setting in the near future.

In Europe between countries, and in the USA between states, there are often multiple pipeline connections. Actual high pressure pipelines within countries and states may not accommodate (large) transits to (all) neighboring countries (c.f., Switzerland). Although sometimes regionally critical, in a global context, it often suffices to aggregate pipelines to a single connection from one country to another in either relevant direction. In contrast to the LNG vessel fleet, which imposes a restriction on the aggregate shipped volume but can essentially accommodate flexible shipments, pipeline capacities do restrict supplied volumes on specific links from producers to end users, and they need to be considered in a techno-economic natural gas market model. A big issue is that pipeline capacities depend on flows and pressure differences in neighboring pipelines and that these dependencies are nonlinear. The optimal operation of pipeline systems requires decisions on the flow direction in bi-directional pipelines, the use of specific valves, and compressors (c.f., [25,26]). If integer variables would hamper the tractability, linearization techniques can be used to convexify feasible regions, often very adequately and rooted in steady-state analysis, to represent the non-linear relations [27–29]. Midthun et al. [30] discussed that ignoring the physical characteristics gas flows in a pipeline network will often lead to wrong conclusions regarding the maximum flows that can be transported through the network, specifically when compressors are absent as is the case on the Norwegian continental shelf. For analyses not considering periods shorter than days, these operational considerations become much less relevant.

Typically, pipelines are designed with a safety margin and can bear significantly higher pressure than the nominally listed one. Combined with the operational flexibility provided by *linepack*, temporarily increasing the amount of gas and hence the pressure in part of the network, actual capacities are often higher than the listed, publicized nominal capacities.

The number of gas transmission companies varies by country. In some countries, there is one organization responsible for the entire gas network; for instance, in the Netherlands, this is Gas Transport Services. In other countries, such as Denmark and the United Kingdom, there is one organization responsible for both the electricity and the natural gas grid. In other countries, there are several companies responsible for different parts of the gas transport network. For example, in Germany, there are sixteen companies, and regional networks, and in the United States, there are about two hundred (by 2010).

1.4. Capacity Expansions

In a multi-period setting with a long enough model horizon, capacity changes become relevant. Both investing and divesting may be considered, and they may involve increments and decrements in existing and new infrastructure. Typically, there are yes/no decisions, economies of scale, and lead times to allow for permitting procedures and construction periods. For example, consider an LNG export facility and the number of trains and plants. One decision concerns the number and size of gas turbines powering the compressors. LNG processing equipment does not come in an unlimited variety of sizes. More or larger turbines will result in a significant cost increase but a more than linear increase in capacity. In a global setting, with already about 50 LNG export facilities in place, such integer characteristics are less relevant, and the impact of integer variables on numerical tractability may be detrimental. In practice, researchers often fix the level of investments exogenously, thereby circumventing the issue completely, or allow continuous decision variables, which offer a viable approximation in a global, long-term setting. A middle road is provided by so-called semi-continuous variables (e.g., [31]), which allow for economies of scale with a capacity choice within some bandwidth, but at the expense of higher solution times. A depreciation of existing infrastructure can be accounted for implicitly via operation and maintenance costs, or explicitly (e.g., [32]).

1.5. Marketing, Distribution, and Consumption Sectors

The last step in the natural gas supply chain is the distribution to final consumers. In Europe, retailers (marketing and distribution companies) include RWE and Engie, which are both active in several countries. In the United States, examples include San Diego Gas & Electric and the Southern California Gas Co, which are active in some of the Southern U.S. states, and Baltimore Gas and Electric Company and Washington Gas, who market their gas in Maryland and Washington DC. Often, there is some vertical integration with producers, and horizontal integration, e.g., when utilities also sell electricity.

Final demand levels may be exogenously given, or there may be a need for representing different types of (price-responsive) demand. There are various sectors using natural gas. Mostly, natural gas is used as a source of energy; however, there are also non-energy uses, such as fertilizer production. The International Energy Agency provides information for the natural gas use for sectors, types of usage, prices, and taxes.

In the EU, the wholesale price of gas is less than half of the retail price paid by consumers. The myriad of pricing structures, taxes, and subsidies in countries poses an impossible task to those who would like in-depth insight globally. Additionally, there is a lack of information on the critical characteristic as how demand responds to price changes (both short-term and long-term price-demand elasticities). For high-level, global, and long-term analyses of world gas markets, it is neither relevant nor feasible to include all different sectors and marketers in each country. To account for different uses and the substitution and lock-in effects (e.g., compare the sectors' electric power generation, transport, and residential heating), distinguishing some different aggregate sectors may be warranted.

Then, these sectors will each have their own demand curve. To allow large-scale models, often linear (inverse) demand curves are used. Considering an intercept and (negative) slope $a, b > 0$, a price depends on quantity as follows:

$$p(q) = a - bq. \quad (3)$$

Intercept and slope must be estimated or calibrated based on reference values and demand elasticities. Non-linear expressions for demand can be more realistic, but if demand levels only vary modestly around reference levels, and given the unavailability and low quality of elasticity estimates, linear expressions can capture most of the desired response in the model.

2. Mathematical Programming for Long-Term Gas Market Analysis

Developing mathematical programming models to represent the optimization problems of actors in the natural gas market or the market as a whole requires making tradeoffs in aggregation levels for actors, sectors, and infrastructure, spatiotemporal scope and detail, information structures and the sequencing of decisions, market, and economic and technical characteristics (c.f., [33]). What are good tradeoffs is motivated by the analysis goals, data availability and quality, the desired solution time in relation to accessible resources, and the available time for model development. Naturally, a simpler type of model should be used if possible to facilitate finding solutions more quickly. Often, quite some detail can be recovered by ex-post calculations. If that is the case, it is preferable to opt for a more aggregate model (and dataset).

Here, we present a general mathematical programming formulation reflecting aspects relevant in a global natural gas market perspective. The optimization problem captures all the steps in the value chains discussed above, and it accommodates different choices in the tradeoffs discussed, including market structures and market power exertion by different actors. We present possible extensions and give references for details.

2.1. Assumptions

All actors have perfect information. Suppliers and service providers maximize profits, while consumers maximize their surplus. (Consumer surplus is an economic term reflecting the utility or benefit of consumption considering the difference between consumers' willingness to pay and the prevailing market price.) If output requirements, i.e., demand levels, are exogenously given, absent market power, this boils down to a minimization of discounted costs.

The only actor type that may exert market power is the supplier. The exertion of market power to the consumer sectors is done by strategically withholding part of the supply according to a pre-specified market power parameter value (c.f., conjectural variation). The consequences of this are captured by including a market power adjustment term in the objective function (Equation (7)).

Suppliers do not own any infrastructure but rent infrastructure services needed for the transportation and storage of natural gas from service providers. Service providers are an economic mechanism to efficiently allocate scarce capacity. They do not withhold capacity from the market in order to create artificial scarcity (and thereby manipulating congestion and scarcity rents). Capacity reservation markets are ignored. Infrastructure services are considered to be third-party-access based with negotiable tariffs, and suppliers and service providers are all price-takers in markets for infrastructure services. However, different access or regulatory regimes can be implemented by defining (limiting) the access of specific suppliers and an ex-post assignment of congestion charges. Congestion charges can be derived from dual values of capacity bounds (Equation (8)). The service providers are responsible for capacity management, operation, and investment (Equations (8), (12) and (13)). Suppliers can only source gas from a subset of production locations (specified as part of set Z_{snt}^+ , see below). Suppliers sell gas to markets in countries that are accessible via arcs they have access to (pipelines or LNG supply chain steps, cf., set Z_{snt}^-).

Pipeline transport, liquefaction, LNG shipping, regasification, storage injection, and the extraction of gas are modeled with costs (Equation (7)), capacity bounds, and loss rates (Equation (8)). Deliverability, for instance storage extraction, does not depend on stored volumes. Storage inventory is restricted by a capacity (Equation (12)). Minimum operating limits are not represented.

Bi-directional natural gas pipelines are included as separate capacities in both directions. There is no *netting* of flows. This provides market-power exerting suppliers with the possibility to congest pipelines in both directions. This will not happen in perfect competition, since in a minimal cost solution (assuming positive costs or losses), at most, one pipeline of the pair representing the bidirectional pipeline will be used (see, e.g., [13]).

To preserve convexity, all capacity expansion variables are continuous.

2.2. Notation and Units of Measurement

For reference, volumes can be considered to be m^3 and capacities are in m^3/y . Operational costs and prices are in $\$/m^3$ and investment costs are in $\$/m^3/y$.

In the model, we consider the supplier as the central actor. Suppliers $s, s' \in S$ source gas from production locations and sell gas to end users. The use of any infrastructure other than own production is organized via renting capacity from dedicated infrastructure service providers.

Consider a network with nodes $n, m \in N$, some of which are connected by links $a \in A$. Nodes and links respectively contain and represent value chain activities. Activities involving infrastructure are denoted by $z \in Z$, with subsets and superscripts allowing customized referencing, grouping, and selection. For example, Z_{spt}^P is the set of production facilities that are accessible to supplier s in period t . Other superscripts used are A for transmission arcs (including LNG value chain steps), W for storage working gas (*inventory*), and I and X for storage injection and extraction, respectively. Injection and extraction are connected to working gas via parameters z_{zW}^I and z_{zW}^X . Activities in Z_n^+ source gas into node n (production, arc inflows, storage extractions), while activities in Z_n^- source them away (arc outflows, storage injections, sales). To select flow-based activities (excluding the volume-based activity storage inventory), we use $Z^F = P \cup A \cup I \cup X$. To reflect liquefaction, LNG vessels, and regasification, auxiliary nodes can be defined.

In the dataset, activities may be disaggregated to allow a quadratic cost representation or aggregated to represent activities similar enough from the perspective of the desired analysis; e.g., a production reservoir field with different wells with their own characteristics can be reflected by multiple production activities $z \in Z^P$ on a node. However, wells in different reservoirs, storages, or LNG trains with similar characteristics may be aggregated.

The shortest relevant periods with equal period lengths, e.g., days or weeks, are denoted by $t, t' \in T$. Activity levels are flows: $q_{szt'}^Z$; volumes can be calculated by aggregating flows over multiple periods. Preinstalled capacity is given by CAP_{zt}^Z with t being the first period that it is available.

Capacity expansion is given by Δ_{zt}^Z . All operational costs (Equation (4)) are quadratic, and all investment costs Equation (5) are linear.

$$c_{zt}^Z \left(\sum_{s \in Z_{zt}^Z} f_{szt}^Z \right) \quad (4)$$

$$c_{zt}^\Delta (\Delta_{zt}^Z) \quad (5)$$

The depreciation rate for capacity is $g_{zt} t$. The lead time for capacity to become available after the investment decision is t_z^{lead} . Parameter l_{zt}^Z accounts for the loss rate of the specific activity z . With a minor abuse of notation, let f_{snt}^D be the quantity sold at node n in a period by a specific supplier. Denote demand intercept and slope as a_{zt} and b_{zt} respectively; prices depend on sold quantities via

$$p_{zt} = a_{zt} - b_{zt} \sum_s f_{szt}^D \quad (6)$$

The discount rate is r_t . Market power levels are specified via $cv_{snt} \in [0, 1]$; the higher the value, the higher the market power exertion.

2.3. Model Formulation

The objective function sums up sales revenues and consumer surpluses, minus the market power adjustment terms (c.f., [12]) and total costs for production, infrastructure usage, and investments.

Objective function:

$$\max \sum_t r_t \left[\begin{array}{l} \sum_{s', z \in Z^D} \left(a_{zt} - b_{zt} \sum_s q_{szt}^D \right) q_{s'zt}^D + \frac{1}{2} \sum_{z \in Z^D} b_{zt} \left(\sum_s q_{szt}^D \right)^2 \\ - \frac{1}{2} \sum_{z \in Z^D} b_{zt} \sum_s cv_{szt} \left(q_{szt}^D \right)^2 - \sum_z c_{szt}^Z \left(\sum_s q_{szt}^Z \right) - \sum_z c_{zt}^\Delta \Delta_{zt}^Z \end{array} \right]. \quad (7)$$

The feasible region is defined by the actor-specific restrictions given below. For infrastructure restrictions and mass balances, it is crucial to consider them at the relevant actor level.

Flow capacity:

$$\forall z \in Z^F, t : \sum_s q_{szt}^Z \leq (1 - g_{z1t}) CAP_{zt}^Z + \sum_{0 < t' \leq t - t_z^{lead}} (1 - g_{zt't}) \Delta_{zt'}^Z \quad (8)$$

Nodal mass-flow balance:

$$\forall s, n, t : \sum_{z \in Z_{snt}^+} (1 - l_z^Z) q_{szt}^Z = \sum_{z \in Z_{snt}^-} q_{szt}^Z \quad (9)$$

Reserves:

$$\forall z \in Z^P : \sum_{s \in Z_{szt}^P} q_{szt}^P \leq RES_z^P \quad (10)$$

Storage extractions cannot exceed net injections:

$$\forall s, z \in Z^W : \sum_{z_z^X, t' \leq t} q_{szt}^X \leq (1 - l_z^I) \sum_{z_z^I, t' < t} q_{szt}^I \quad (11)$$

Storage inventory limitation:

$$\forall z \in Z^W, t : \sum_s \left[(1 - l_z^I) \sum_{z_z^I, t' \leq t} q_{szt}^I - \sum_{z_z^X, t' < t} q_{szt}^X \right] \leq (1 - g_{z1t}) CAP_{zt}^W + \sum_{0 < t' \leq t - t_z^{lead}} (1 - g_{zt't}) \Delta_{zt'}^W \quad (12)$$

Limit to infrastructure expansion:

$$\forall z \notin Z^D, t : \Delta_{zt}^Z \leq \overline{\Delta_{zt}^Z} \quad (13)$$

3. Extensions

To allow for taxes and distribution fees, the inverse demand curves in Equation (7) can simply be adjusted. If sector discrimination is needed, multiple demand curves can be specified for a single node, or a geographic region can be split into multiple nodes.

Production costs can be extended to variants discussed above by [10] but with negative impact on scalability and solution times. As discussed, quadratic approximations can be fit very well.

Flow capacity (Equation (8)) for pipelines can be made dependent on pressure via the techniques discussed in [27–29]. Similarly, storage deliverability can be made dependent on the inventory level in Equation (8). This can be done using linearization. Limits to global LNG vessel capacity can be included as a variant of Equation (8). To account for different ship sizes and shipping routes is computationally very expensive and will harm scalability.

Capacity expansion variables can be made using the integer valued in Equation (7). However, this cannot be combined with non-zero values for cv_{snt} , as the uniqueness of solutions would not be guaranteed otherwise. Limits to infrastructure expansions can be included for multiple periods. This requires a variant of Equation (13). Reserve additions can be implemented by including the reserve expansions in Equation (10) and the exploration costs in the objective (Equation (7)). The left-hand-side summation in Equation (10) must be adjusted to reflect the production periods up until the reserve additions become available. The inclusion of other gas sources such as biomethane or SNG does not require formulation adjustments. It can be done by dataset adjustments for production nodes, capacities, and costs. Multiple energy carriers including energy carrier transformation requires very significant changes (c.f., [34]).

Considering uncertainty requires the representation of multiple futures, for instance via scenarios (c.f., [35]). For considering information structures other than *open loop*, consider, e.g., [36,37].

The (real-time) operational optimization of hybrid multi-energy carrier systems may require completely different approaches, such as simulation (e.g., [38]).

To illustrate that the compact formulation presented above can reflect the main aspects of a market, we have implemented the model using GAMS [39]. The example and solution are available in the Appendix A, and the GAMS code is available online (Supplementary Materials).

Supplementary Materials: The following are available online at <http://www.mdpi.com/2673-5628/1/1/1/s1>, GAMS implementation for stylized natural gas market problem.

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Appendix A. Implementation Example

Consider a four-node network: one production node with two production facilities each accessible by a different supplier, one liquefaction node with a liquefaction facility, one regasification node with a regasification facility, and one consumption node with two demand sectors and a storage facility. Supplier 1 exerts monopoly power to the first demand sector only, supplier 2 is a price taker. A pipeline arc from the production node to the consumption node is accessible to supplier 1. The LNG value chain from the production node to the consumption node via the liquefaction and regasification node is only accessible to supplier 2. Initially, the liquefaction capacity is 0. There are two periods. Investment in liquefaction capacity in the first period can be used in the second period. The discount rate is 10%. Ignore capacity depreciation.

Table A1. Data for implementation example.

N	Facility	Type	Access	Capacity	Oper Costs	Loss	Inv costs	
PN	P1	Prod	S1	10	Linear, $1q$	0%		
PN	P2	Prod	S2	6	Quadr $0.2q^2$	0%		
PN	PC	Pipe	Arc to CN	S1	10	Linear, $1.8q$	3%	
PN	PL	Liquef	Arc to LN	S2	0	0	10%	1
LN	LR	Vessel	Arc to RN	S2	99	Linear, $1q$	1%	
RN	RC	Regas	Arc to CN	S2	10	Linear, $1q$	2%	
CN	I1	Inject	Into W1	S1	3	Linear, $1q$	2%	
CN	X1	Extract	From W1	S1	4	Linear, $1q$	0%	
CN	W1	storage	Inventory	S1	5	0	0%	
CN	D1,D2	Demand	S1,S2		$p_{z,1} = 10 - \sum_s q_{s,z,t}^D$; $p_{z,2} = 20 - \sum_s q_{s,z,t}^D$			

Figure A1 depicts the solution. Values on arcs are gross quantities, not yet corrected for losses. The GAMS code generates a file with name *report.gdx* showing mass balance and other results.

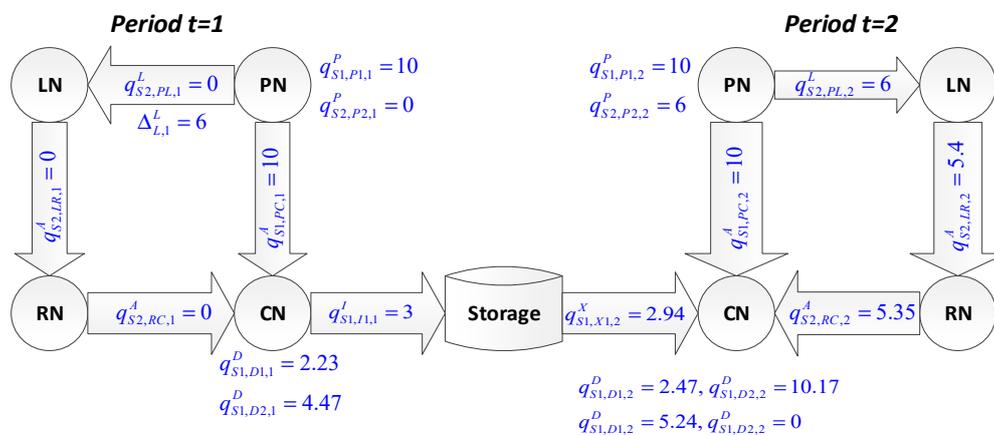


Figure A1. Results of implementation example.

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