

Optimal Multi-scale Capacity Planning for Power-Intensive Continuous Processes under Time-sensitive Electricity Prices and Demand Uncertainty, Part I: Modeling

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Abstract

With the advent of deregulation in electricity markets and an increasing share of intermittent power generation sources, time-sensitive electricity prices (as part of so-called demand-side management in the smart grid) offer potential economical incentives for large industrial customers. These incentives have to be analyzed from two perspectives. First, on an operational level, aligning the production planning with the electricity price signal might be advantageous, if the plant has enough flexibility to do so. Second, on a strategic level, investments in retrofits of existing plants, such as installing additional equipment, upgrading existing equipment, or increasing product storage capacity, facilitate cost savings on the operational level by increasing operational flexibility.

In part I of this paper, we propose an MILP formulation that integrates the operational and strategic decision-making for continuous power-intensive processes under time-sensitive electricity prices. We demonstrate the trade-off between capital and operating expenditures with an industrial case study for an air separation plant. Furthermore, we compare the insights obtained from a model that assumes deterministic demand with those obtained from a stochastic demand model. The value of the stochastic solution (VSS) is discussed, which can be significant in cases with an unclear setup, such as medium baseline product demand and growth rate, large variance or skewed demand distributions. While the resulting optimization models are very large-scale, they can mostly be solved within up to three days of computational time. A decomposition algorithm that allows solving the problems faster is described in part II of the paper.

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1 Background

1.1 Motivation

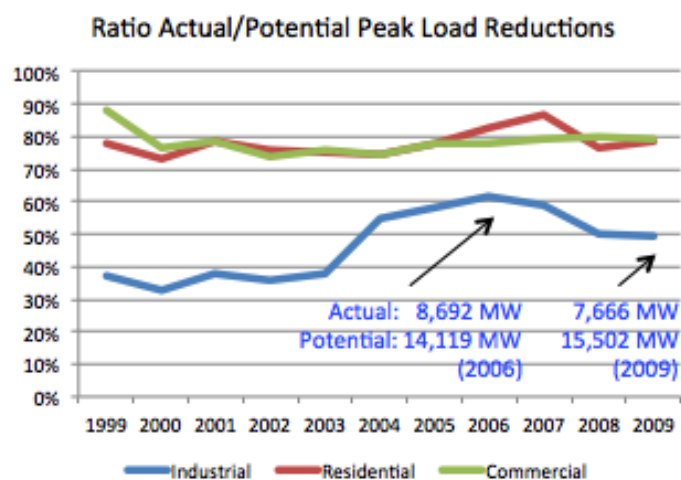
The manufacturing base in the U.S. has been eroding over the last two decades in the face of fierce international competition. However, recent developments such as the gas production from very large deposits of shale gas (Chang, 2010), as well as trends in onshoring due to rising labor cost in emerging countries (Sirkin et al., 2011), provide hope in the revitalization of U.S. manufacturing. While the economic recovery deserves further observation in the aftermath of the recession of 2008 and the current unemployment and financial market volatility, future competitiveness of industrial companies requires them to optimally design and retrofit their production facilities in anticipation of price and demand growth forecasts.

A group of chemical processes for which the design and capacity planning is very challenging is the group of power-intensive processes, such as air separation plants (compression), cement production (grinding), chlor-alkali synthesis, steel and aluminum production (electrolysis) and paper pulp production (drying). These industries in fact consume 15% of the total industrial electric power in the United States.

At the same time, the power grid is in transition to the so-called smart grid with the ambition to improve reliability, energy security, economics and greenhouse gas emissions (Samad and Kiliccote, 2012). A growing share of intermittent renewable energies, such as wind and solar, increases the challenge that grid operators face every day and every minute: balancing supply and demand of electricity on a real-time basis. A set of measures, such as co-generation, micro-grids, future storage technologies and demand-side management (DSM), is expected to play an important role in helping today's power grid, mastering the transition to the smart grid.

The societal benefit of DSM in the US is estimated to be \$59 Billion by 2019, of which 40% is attributed to large commercial and industrial consumers (McKinsey study by Davito, Tai and Uhlener, 2010). Hence, from an industrial consumer's perspective, demand-side management (DSM), consisting of Energy Efficiency (EE) and Demand Response (DR), deserves special attention. The idea of DSM is to influence the "amount and/or timing of the customers use of electricity for the collective benefit of the society, the utility and its customers" (Charles River Associates, 2005). While EE aims for permanently reducing demand for energy, DR focuses on the operational level (Voytas et al., 2007).

As a consequence, variability in time-sensitive electricity prices can be observed on various time scales, including hourly variations for so-called day-ahead (DA) prices that industrial consumers are exposed to in many electricity markets around the globe. However, economic benefits can be realized if the industrial consumer has the flexibility to adjust consumption



Source: EIA, Electric Power Annual 2009, April 2011, Demand Side Management, Annual Effects by Program Category

Figure 1: DSM potential for residential, commercial and industrial sectors in the US.

(Mitra et al., 2012a).

Interestingly, industrial DR still seems to be a large untapped grid resource according to data released by the Energy Information Administration (EIA, 2010). The EIA investigates the actual and potential peak load reduction (in MW) attributed to DR. While nearly 80 % of the DR potential in the residential and in the commercial sectors was realized throughout 2006-2010, only 50-60% of the DR potential was accessed in the industrial sector, as one can see in Fig. 1. We conjecture that this data can be explained by the fact that DSM is part of a complex multi-scale design, capacity planning and operations problem, which requires a sufficient set of decision-making support tools in order to facilitate optimal decisions.

With pressure on both sides, the revenue side (uncertainty in product demand) and the cost side (variability in electricity prices), new designs and plant retrofits can be viable options for power-intensive processes in the context of DSM. Retrofitting includes replacing existing equipment with more energy-efficient alternatives, improving design flexibility (with respect to DR incentives), adding further production equipment and installing additional storage tanks. All these design decisions, which could potentially lead to lower operating costs, are part of strategic capacity planning of the chemical companies. Typically, the financial analysis in terms of net present value (NPV) or return on investment (ROI) for the investment decisions is performed for a time horizon of multiple years, e.g. 10-15 years. Thus,

investigating the trade-off between the capital investment costs for new designs or retrofits, and the operating costs related to electricity prices, which can vary on an hourly basis, leads to a complex multi-scale optimization problem.

1.2 Literature review

Multi-period design and capacity planning for continuous multi-product plants has been widely studied in the literature. Sahinidis et al. (1989) propose a comprehensive deterministic MILP model for process networks. Liu and Sahinidis (1996) extend the model to account for demand uncertainty. Van den Heever and Grossmann (1999) use disjunctive programming techniques to extend the methodology to the case of multi-period design and planning of nonlinear chemical process systems. All these papers share the idea to cover a total time horizon of multiple years, which is divided into a number of time periods, typically several months or several years. Therefore, model parameters such as prices, demands are assumed to be constant over each time period.

More recent research aims at integrating multiple layers of decision-making, i.e. capacity planning with operations. For pharmaceutical product development and capacity planning, Maravelias and Grossmann (2001) propose an MILP formulation that integrate a scheduling formulation with a capacity planning model. Colvin and Maravelias (2008) model the endogenous stochastic behavior of the outcome of clinic trials with a stochastic programming framework. Sundaramoorthy et al. (2012) propose a two-stage stochastic programming formulation for the integrated capacity and operations planning that assumes exogenous stochastic clinic trials. For a chemical supply chain, Sousa, Shah and Papageorgiou (2008) propose a formulation that addresses the integrated supply chain design and operations planning. You et al. (2010) model supply chain responsiveness by integrating a simple cyclic scheduling model with the capacity planning of a supply chain. For a good overview on different modeling approaches for problems in the context of enterprise-wide optimization, such as supply chain design problems in the chemical and the pharmaceutical industry, we refer to the review papers by Grossmann (2005), Shah (2005), Varma et al. (2007) and Grossmann (2012).

Processes at the interface of power systems and the chemical industry that face similar challenges like power-intensive processes with respect to electricity prices are co-generation and poly-generation plants. Different researchers (Iyer and Grossmann (1998), Bruno et al. (1998), Aguilar et al. (2007a, 2007b)) address the integration of operations and design for co-generation plants. However, the detailed operational schedules are not modeled, since they assume that the plants are exposed to a pre-determined number of hours with on-peak and off-peak prices per year. Liu, Pistikopou-

los and Li (2010) as well as Chen et al. (2011) investigate the design of flexible poly-generation systems under uncertainty. They use a similar scenario-based approach to consider different price levels. However, for each scenario only one steady state is determined. A detailed operational modeling, which allows to account for fluctuations in electricity prices on an hourly basis in a dynamic market environment, is not performed.

Note that if prices and demands fluctuate on an hourly and seasonal basis, there is a need for a much finer discretization of time, i.e. a more detailed representation for the scheduling of the process.

Therefore, the subject of this paper is the design and capacity planning for power-intensive processes with the target of introducing flexibility in the operations to exploit changes in hourly electricity prices. The major challenge lies in the multi-scale integration of the operational level with the design and capacity planning decisions, while accounting for variability in electricity prices on an hourly basis and uncertainty in product demand. In section 2, we give a formal problem statement. The integrated model is described in section 3. An industrial case study for the retrofit of an air separation plant is presented in section 4. In section 5, we provide conclusions on our work.

2 Generic Problem Statement

Given is a set of products $g \in G$ that can be produced in a continuously operated plant. While some products can be stored on-site, others must be delivered directly to customers. It is possible to make the following long-term investments at the plant over a time horizon of several years: a) Add new equipment $n \in N$; b) Perform upgrades (replacements) $u \in U$ of existing equipment; c) Install additional storage facilities $st \in ST$. The time horizon is divided into time periods $t \in T$ and investments are allowed during the periods $T_{invest} \subset T$. All investments have fixed standard sizes and the associated costs are known and discounted appropriately. The plant has to satisfy product demands, specified on a weekly, daily or hourly basis. We assume that the operating costs due to electricity prices within period t , vary for every hour $h \in H$ and undergo seasonal changes. With this setup, we can consider day-ahead (DA) prices, which vary on an hourly basis, as well as time-of-use (TOU) pricing, for which blocks of hours either follow off-peak, mid-peak or on-peak prices. We assume that a seasonal electricity price forecast for a typical week is specified on an hourly basis. Hence, the design or retrofit of a plant involves strategic, long-term design decisions, and operational, short-term decisions for determining what equipment to turn on or shut down and when. At the strategic level, the problem is to determine what design investments to make and when they should take place. Operationally, production levels, modes of operation, inventory levels

and sales must be determined on an hourly basis, so that the given demand is met. The objective is to minimize the total cost, consisting of investment and operating costs.

3 Model Formulation

3.1 Modeling strategy and multi-scale representation

A major modeling challenge is the integration of the different time scales that are involved in the problem. On the one hand, electricity prices fluctuate on an hourly basis in most electricity markets, e.g. if day-ahead (DA) prices are considered. On the other hand, strategic capacity planning decisions have to be justified for a time horizon of multiple years. However, based on an analysis of multiple years (2004-2010) of PJM data (PJM, 2011), we identified typical profiles that reflect seasonal behavior in electricity prices. It is known that these typical patterns are also present in other electricity markets (Conejo, 2010).

Therefore, we propose four major periods of operation for each year, corresponding to the seasonal behavior of electricity prices: spring, summer, fall and winter. Furthermore, in each season we consider a representative week that is repeated cyclically and in which electricity prices are specified on an hourly basis (see Fig. 2). In this way, the model for one year consists of 672 hrs (4 seasons each with a week of 168 hrs) in which electricity prices change. In contrast to the 8,760 hours in a year, this represents one order of magnitude reduction.

Another complication is the timing of investment decisions, which are typically reviewed on a yearly basis. Investment decisions are driven by the amount of demand that needs to be met. The demand forecast, which consists of an estimate of the average weekly demand for each product, and a weekly demand profile, contains a large amount of economic uncertainty.

As one can see in Fig. 2, the investment planning problem is a multi-stage problem, where investments are annually reviewed (each year corresponds to one stage), and operational decisions are made as the actual demand is realized. However, the resulting multi-stage stochastic programming problem is extremely large and hard to solve computationally. Therefore, we approximate the multi-stage programming problem with a two-stage stochastic program (Birge and Louveaux, 2011) as shown in Fig. 3, where all investment decisions are first-stage variables (here-and-now) and all operational decisions such as production and inventory levels, modes of operation and sales are second-stage decisions (wait-and-see) according to the demand realization of scenario s in time period t . Note that the second-stage variables contain integer decisions related to the modes of operation and associated transitions, which make the resulting two-stage stochastic programming problem hard to solve.

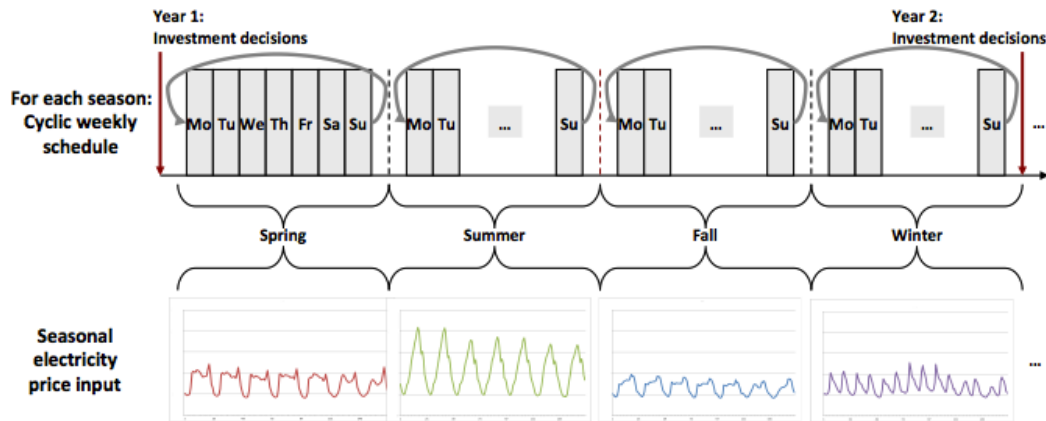


Figure 2: Multi-scale representation of the multi-period capacity planning problem with hourly varying electricity prices.

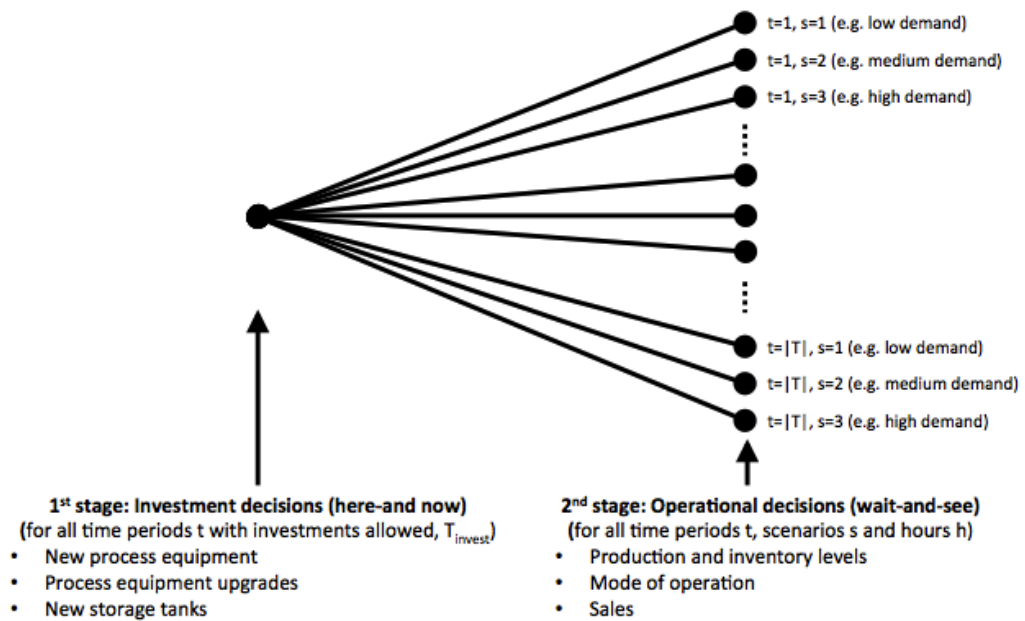


Figure 3: Two-stage representation of investment and operational decisions.

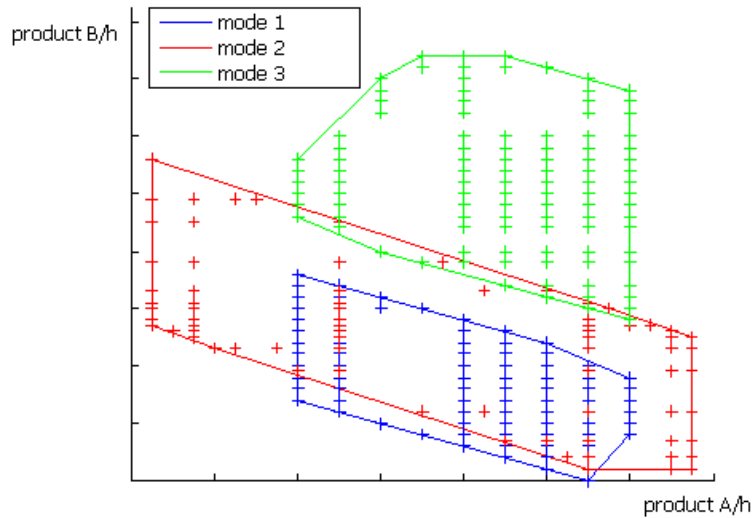


Figure 4: **Example of a feasible region (feasible production rates according to time discretization) with distinct operating modes (from Mitra et al., 2012a).**

3.2 Operational representation

Since a full-scale model that includes detailed non-linear process models can become prohibitively hard to solve for longer time horizons, we use a surrogate model to represent the operational behavior of the plant for each time period t and scenario s . The surrogate operational model (Mitra et al., 2012a, 2012b) is based on two concepts, which will be explained later in this paper. First, the feasible region of operation is represented in the product space according to the chosen time discretization (here $\Delta h = 1$ hour, index h) as shown in Fig. 4. Second, there is a discrete set of operating modes the plant can operate in, as shown in Fig. 5. Hence, a set of logic constraints that capture the transitional behavior between different modes of operation is required. Additionally, constraints related to mass balances and demand satisfaction need to be enforced. In the following, the associated constraints are described. Note that for all operations in the domain $h \in H$, the wrap-around operator (Shah, Pantelides and Sargent, 1993) is used to enforce cyclic schedules for each time period t and scenario s .

3.2.1 Feasible region

We assume that the feasible region of operation is known in the product space by using projection techniques in offline computations, e.g. steady-state simulations, empirical models based on plant data or analytical methods (Swaney and Grossmann, 1985; Grossmann and Floudas, 1987; Goyal

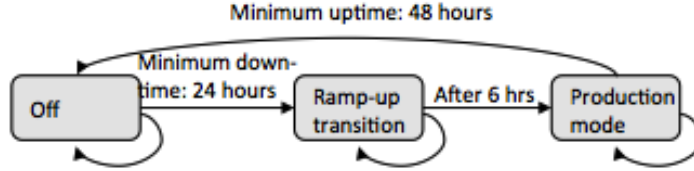


Figure 5: **Example of a state graph with operating modes (nodes) and transitions (arcs). Additionally, minimum up- and downtime constraints are indicated (from Mitra et al., 2012a).**

and Ierapetritou, 2002; Sung and Maravelias, 2007, 2009). Note that a plant has different modes $m \in M$ in which it can be operated, e.g. a mode is a state when only a subset of the plant equipment is running or when the plant is in transition, denoted by $y_m^{t,s,h}$ (see nomenclature section). The data for all modes and options is represented as a collection of operating points (slates), x , and defines the feasible region for the production levels $P_g^{t,s,h}$.

The representation of the feasible region by a set of disjoint convex polyhedra like in Fig. 4 also implies that available plant modifications have to be specified in the reduced space of products. Therefore, it is possible to specify alternative feasible regions for a given mode m , which we refer to as “options” $o \in O(m)$, with corresponding mode variables $\tilde{y}_{m,o}^{t,s,h}$. Later, these options will be linked to different investments. To represent the multiple feasible regions for a mode m , the disjunctions in (1) can be formulated as shown in chapter Mitra et al. (2012a).

$$\bigvee_{m \in M} \left(\bigvee_{o \in O(m)} \left(\begin{array}{l} \sum_{i \in I} \lambda_{m,o,i}^{t,s,h} x_{m,o,i,g} = P_g^{t,s,h} \quad \forall g \\ \sum_{i \in I} \lambda_{m,o,i}^{t,s,h} = 1 \\ 0 \leq \lambda_{m,o,i}^{t,s,h} \leq 1 \\ \tilde{y}_{m,o}^{t,s,h} = 1 \end{array} \right) \right) \quad \forall t \in T, s \in S, h \in H \quad (1)$$

The corresponding convex hull can be represented algebraically by a set of equations (2) - (7) in terms of disaggregated variables (Balas, 1985).

$$\sum_{i \in I} \lambda_{m,o,i}^{t,s,h} x_{m,o,i,g} = \bar{P}r_{m,o,g}^{t,s,h} \quad \forall m \in M, o \in O(m), g \in G, t \in T, s \in S, h \in H \quad (2)$$

$$\sum_{i \in I} \lambda_{m,o,i}^{t,s,h} = \tilde{y}_{m,o}^{t,s,h} \quad \forall m \in M, o \in O(m), t \in T, s \in S, h \in H \quad (3)$$

$$0 \leq \lambda_{m,o,i}^{t,s,h} \leq 1 \quad \forall m \in M, o \in O(m), i \in I, t \in T, s \in S, h \in H \quad (4)$$

$$Pr_g^{t,s,h} = \sum_{m \in M, o \in O(m)} \bar{P}r_{m,o,g}^{t,s,h} \quad \forall g \in G, t \in T, s \in S, h \in H \quad (5)$$

$$\sum_{m \in M} y_m^{t,s,h} = 1 \quad \forall t \in T, s \in S, h \in H \quad (6)$$

$$\sum_{o \in O(m)} \tilde{y}_{m,o}^{t,s,h} = y_m^{t,s,h} \quad \forall m \in M, t \in T, s \in S, h \in H \quad (7)$$

3.2.1.1 Rate of change constraints For transitions between operating points that belong to the same operating mode, the rate of change from hour h to $h + 1$ might be restricted. The maximum rate of change in production of product g (in $[mass/\Delta h]$) when operating in mode m (and option o) is denoted by $r_{m,o,g}$ and calculated according to the same time discretization Δh that is used to calculate the extreme points of the feasible region. The rate of change constraint is written as follows.

$$|\bar{P}r_{m,o,g}^{t,s,h+1} - \bar{P}r_{m,o,g}^{t,s,h}| \leq r_{m,o,g} \quad \forall m \in M, o \in O(m), g \in G, t \in T, s \in S, h \in H \quad (8)$$

3.2.2 Logic constraints

If the plant switches the mode of operation, logic constraints are required to enforce the feasible transitions that are implied by the state graph, which is shown in Fig. 5. For a detailed derivation of the logic constraints based on propositional logic (Raman and Grossmann, 1993), we refer to Mitra et al. (2012a, 2012b).

3.2.2.1 Switch variables constraints We introduce binary switching variables $z_{m,m'}^{t,s,h}$ that represent a transition from mode m to m' in hour h of time period t and scenario s and link the switching variables with the state variables $y_m^{t,s,h}$ in the following constraint:

$$\sum_{m' \in M} z_{m',m}^{t,s,h} - \sum_{m' \in M} z_{m,m'}^{t,s,h} = y_m^{t,s,h} - y_m^{t,s,h-1} \quad \forall t \in T, s \in S, h \in H, m \in M \quad (9)$$

3.2.2.2 Minimum Stay Constraint If the plant needs to stay a minimum number of hours $K_{m,m'}$ within a certain mode m' after a transition from mode m occurred, we can formulate constraint (10). It can be applied to minimum uptime (after a plant starts up), minimum downtime (after a plant shuts down) and minimum transition time (e.g. during startup procedures) constraints.

$$y_{m'}^{t,s,h} \geq \sum_{\theta=0}^{K_{m,m'}^{min}-1} z_{m,m'}^{t,s,h-\theta} \quad \forall (m, m') \in MS, \forall t \in T, s \in S, h \in H, \quad (10)$$

3.2.2.3 Transitional Mode Constraints For the case of a transitional mode m' , e.g. a startup mode, the plant has to stay $K_{m,m'}^{min}$ hours within mode m' after the transition from mode m (minimum stay, as described before). Afterwards the plant has another transition to mode m'' . Therefore, the two transitions (m to m' and m' to m'') are coupled, which can be expressed with constraint (11).

$$z_{m,m'}^{t,s,h-K_{m,m'}^{min}} - z_{m',m''}^{t,s,h} = 0 \quad \forall (m, m', m'') \in Trans, \forall t \in T, s \in S, h \in H \quad (11)$$

The set *Trans* summarizes all transitions, where a transitional mode constraint applies.

3.2.2.4 Forbidden Transitions For transitions from mode m to mode m' that are not allowed (summarized in set *DAL*), the corresponding transitional variables $z_{m,m'}^{t,s,h}$ are set to zero, i.e. they do not exist in the model:

$$z_{m,m'}^{t,s,h} = 0 \quad \forall (m, m') \in DAL, \forall t \in T, s \in S, h \in H \quad (12)$$

3.2.3 Mass balances and demand satisfaction constraints

Mass balance (13) describes the relationship between current production levels $Pr_g^{t,s,h}$, inventory levels $INV_g^{t,s,h}$ and sales $S_g^{t,s,h}$ for each product g . If product g cannot be stored (e.g. gas) the upper and lower bounds of the inventory level are zero.

$$INV_g^{t,s,h} + Pr_g^{t,s,h} = INV_g^{t,s,h+1} + S_g^{t,s,h} \quad \forall g \in G, t \in T, s \in S, h \in H \quad (13)$$

In constraint (14), the product demand $d_g^{t,s,h}$ is met on an hourly level by either own production or external product purchases, $B_g^{t,s,h}$, for each time period t and scenario s . In the particular case of an air separation plant, liquid oxygen and nitrogen are commodity products that can also

be shipped from a different plant or be procured from a competitor if the plant is not able to meet demand. The latter case is covered by so-called product-swap agreements that allow to pick up product at a competitor's plant for a pre-set price. On a long-term horizon, shipping product from a different plant or product-swap agreements might be attractive in certain high-demand scenarios for which it might not be reasonable to expand the plant's capacity.

$$S_g^{t,s,h} + B_g^{t,s,h} \geq d_g^{t,s,h} \quad \forall g \in G, t \in T, s \in S, h \in H \quad (14)$$

3.3 Strategic capacity planning constraints

In the following, we describe the constraints related to strategic capacity planning decisions: process equipment upgrades, addition of new process equipment and addition of storage tanks.

3.3.1 Process equipment upgrades

We assume that replacing existing equipment does not impact the existence of the modes the plant initially has. It only changes the polyhedral representation of the modes that are affected by the equipment upgrade. Hence, the corresponding state variables $\tilde{y}_{m,o}^{t,s,h}$ are linked with binary decisions on upgrades VU_u^t according to the set *Upgrade*:

$$\tilde{y}_{m,o}^{t,s,h} \leq \sum_{t' \in T_{invest}, t' \leq t} VU_u^{t'} \quad \forall (m, o, u) \in Upgrade, t \in T, s \in S, h \in H \quad (15)$$

In case of an equipment upgrade u that activates option o for mode m , the state variables $\tilde{y}_{m,o'}^{t,s,h}$ for the other options o' of mode m , are forced to zero in the current and subsequent time periods.

$$\tilde{y}_{m,o'}^{t,s,h} \leq 1 - VU_u^{t'} \quad \forall (m, o, u) \in Upgrade, o' \in O(m), o' \neq o, \quad (16)$$

$$t \in T, t' \in T_{invest}, t' \leq t, s \in S, h \in H$$

Furthermore, we assume that only one equipment upgrade u can be made over the given time horizon:

$$\sum_{t \in T_{invest}} VU_u^t \leq 1 \quad \forall u \in U \quad (17)$$

3.3.2 Addition of new process equipment

If a new equipment $n \in N$ is added without removing previously installed equipment, several modes (production and transitional modes) might be

introduced. These relations are given by the set $NewEq$. The state variables $\tilde{y}_{m,o}^{t,s,h}$ and $y_m^{t,s,h}$ are linked with binary decisions on new equipment VN_n^t in (18) and (19).

$$\tilde{y}_{m,o}^{t,s,h} \leq \sum_{t' \in T_{invest}, t' \leq t} VN_n^t \quad \forall (m, n) \in NewEq, o \in O(m), t \in T, s \in S, h \in H \quad (18)$$

$$y_m^{t,s,h} \leq \sum_{t' \in T_{invest}, t' \leq t} VN_n^t \quad \forall (m, n) \in NewEq, t \in T, s \in S, h \in H \quad (19)$$

Each investment can be made only once over the given time horizon as per constraint (20).

$$\sum_{t \in T_{invest}} VN_n^t \leq 1 \quad \forall n \in N \quad (20)$$

3.3.3 Addition of product storage tanks

Adding storage capacity of pre-defined size $Tank_{st,g}$ for the final products g , which is indicated by the binary decision variables $VS_{st,g}^t$, does not change the polyhedral representation of a mode, it only affects the upper bound of inventory:

$$INV_g^{t,s,h} \leq INV_g^U + \sum_{st \in ST, t' \in T_{invest}, t' \leq t} Tank_{st,g} VS_{st,g}^{t'} \quad \forall t \in T, s \in S, h \in H, g \in G \quad (21)$$

3.4 Objective function

The objective function minimizes the total cost TC , which is the sum of capital expenses ($CAPEX^t$) and operating expenses ($OPEX^{t,s}$) across all time periods t and scenarios s :

$$TC = \sum_{t \in T_{invest}} CAPEX^t + \sum_{t \in T, s \in S} \tau^{t,s} OPEX^{t,s} \quad (22)$$

3.4.1 Capital expenses (CAPEX)

The capital expenses for time period $t \in T_{invest}$ are defined by the sum of all investments: new storage tanks (cost coefficient $Cs_{st,g}^t$), new process equipment (cost coefficient Cn_n^t) and process equipment upgrades (cost coefficient Cu_u^t). We assume that all associated cost coefficients are discounted appropriately.

$$CAPEX^t = \sum_{st \in ST, g \in G} C s_{st,g}^t V S_{st,g}^t + \sum_{n \in N} C n_n^t V N_n^t + \sum_{u \in U} C u_u^t V U_u^t \quad \forall t \in T_{invest} \quad (23)$$

3.4.2 Operating expenses (OPEX)

The operating expenses for time period t and scenario s consist of four terms, as shown in equation (24): electricity cost related to production, product procured from competitors, inventory cost and transition cost. It is assumed that the power consumption is known as a linear correlation with the production levels, where $\Phi_{m,o,g}$ are the correlation parameters. The cost of electricity is given by $e^{t,s,h}$ for each season t , scenario s and hour h . The cost for product procured from a competitor is given by $\rho_g^{t,s}$, the cost for inventory holding and the cost for transitions are δ_g and $\zeta_{m,m'}$ respectively. All original cost parameters are multiplied by 13 to match OPEX with CAPEX since we represent one season by a week.

$$\begin{aligned} OPEX^{t,s} = & \sum_{h \in H} e^{t,s,h} \left(\sum_{m \in M, o \in O(m), g \in G} \Phi_{m,o,g} \bar{P}_{m,o,g}^{t,s,h} \right) \\ & + \sum_{g \in G} \rho_g^{t,s} \sum_{h \in H} B_g^{t,s,h} \\ & + \sum_{g \in G} \delta_g \sum_{h \in H} INV_g^{t,s,h} \\ & + \sum_{m,m' \in M} \zeta_{m,m'} \sum_{h \in H} z_{m,m'}^{t,s,h} \quad \forall t \in T, s \in S \end{aligned} \quad (24)$$

4 Case Study

One process for which production planning based on time-sensitive pricing can have significant potential for economic savings is cryogenic air separation, where electricity costs represent 40-50% of overall production costs, which adds \$3-5 to the cost of 1 m^3 of liquid product. The electricity consumption is largely due to the high-pressure compression of air that is required for the cryogenic separation of its components. Electricity is also required for further compression in order to obtain liquid argon, oxygen and nitrogen.

4.1 Model formulation

In the following, we apply the previously developed modeling framework to an air separation plant, which is illustrated in Fig. 6. The three different investment options are shown that potentially increase the operational

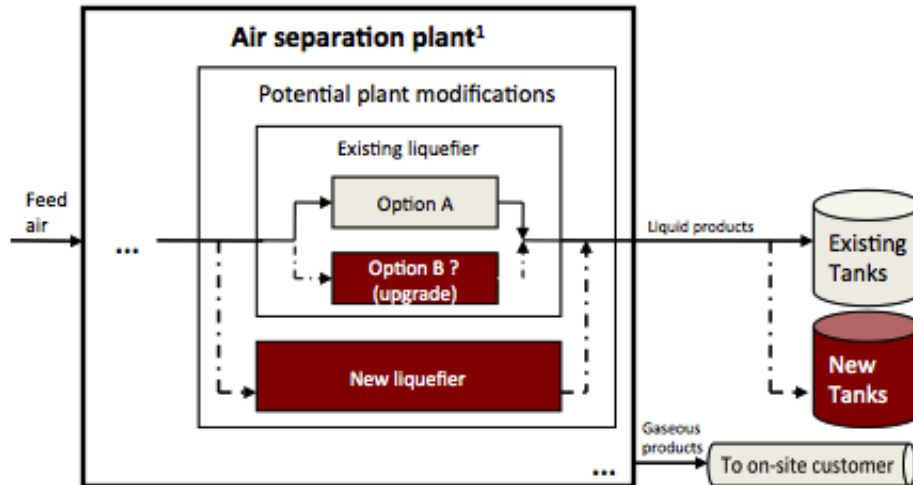


Figure 6: Superstructure of air separation plant with potential plant modifications: 1. Upgrade existing liquefier (option A) with option B. 2. Add new liquefier, 3. Add storage tanks for liquid products. ¹ Simplified scheme.

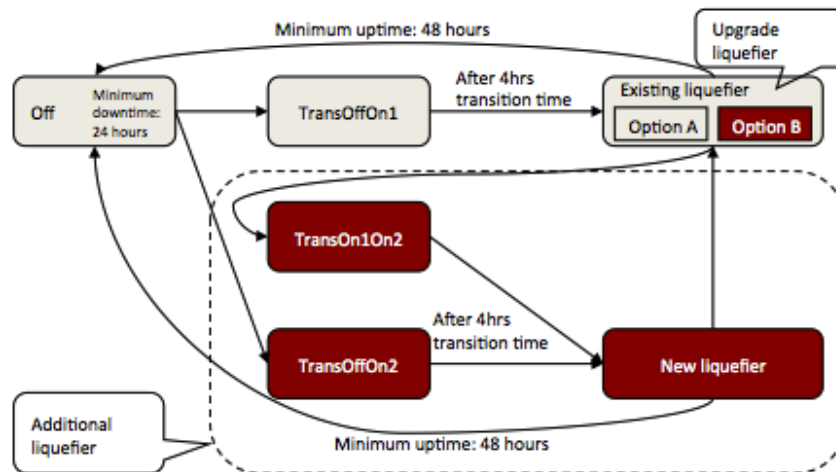


Figure 7: Operational superstructure in terms of modes: An upgrade of the existing liquefier with “option B”, the polyhedral structure of mode “existing liquefier” would be replaced. If the second liquefier is added, a set of modes is added.

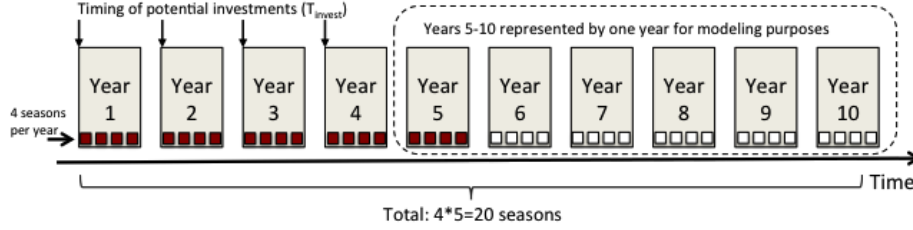


Figure 8: **The time horizon of ten years is represented by 5 years with 4 seasons each. Years 5-10 are aggregated in one year in order to maintain a manageable problem size.**

flexibility for the air separation plant, which has one liquefier pre-installed (option A). First, it is possible to upgrade the existing liquefier with a different liquefier (option B). Second, one additional liquefier can be purchased and installed in parallel. Third, additional storage tanks can be bought to increase the storage capacity for all three liquid products: oxygen, nitrogen and argon.

The superstructure of plant equipment in Fig. 6 can be translated into a superstructure of modes, as shown in Fig. 7. The replacement of the existing liquefier with option B does not affect the existence of the mode “existing liquefier”, as it just changes the polyhedral structure of the mode. If the second liquefier is added, the second production mode “new liquefier” as well as corresponding transitional modes are introduced. Adding storage capacity for the liquid products does not change the superstructure of modes, it only affects the upper bound of inventory variables.

Typically, a time horizon of multiple years is considered to justify investment decisions. In our case, we would like to study the trade-off between capital expenditures (CAPEX) and operating expenditures (OPEX) over a horizon of 10 years. The first four years are all modeled with four seasons, the operation of each represented by a cyclic schedule as described in section 3. For computational reasons that we will explain later in detail, years 5 to 10 are represented by one year with four seasons with operating costs that are weighted appropriately. Investments are allowed at the beginning of each of the first four years. We illustrate the temporal representation in Fig. 8.

In summary, the model minimizes the total cost (TC), consisting of CAPEX and OPEX according to equations (22)-(24). The strategic constraints (15)-(17) represent decisions regarding the upgrade of the existing liquefier, and constraints (18)-(20) model the potential addition of the second liquefier. The addition of storage tanks is considered with constraint (21). The operation of the air separation plant in each season is modeled with constraints (2)-(14).

4.2 Input data

4.2.1 Demand modeling

One of the main drivers, which determines whether an investment should be made or not, is the forecast of the product demand in time period t , D^t , which is a random variable with expected value $\mathbb{E}(D^t) = \mu^t$ and associated standard deviation σ^t . As shown in Fig. 9, the annual demand growth rate a , which defines the trajectory of the future demand μ^t (medium profile), is usually calculated with a regression model that correlates expectations for external market factors (e.g. GDP growth) with product demand based on historical data. In the following, we refer to the demand of the first year (μ^1) as “baseline demand”.

Once the overall demand level is set for a given season, the hourly demand $d_g^{t,s,h}$ has to be determined. There is a mapping $f(\mu^t, \sigma^t) \rightarrow d_g^{t,s,h}$, which translates the plant demand into a weekly pattern on an hourly basis. The mapping f is based on historical data. It explains how much product is withdrawn by the trucks that arrive at the plant during the week, and also specifies the ratio of product demands.

In this paper, we investigate the differences in the solutions of the associated optimization problem for two demand models: a deterministic version and a stochastic model version that addresses the uncertainty in the forecast.

4.2.1.1 Deterministic demand In the deterministic demand model, for each time period t there is just one demand scenario ($|S| = 1$) with probability $\tau^{t,1} = 1$. The demand pattern is based on the expected value μ^t . Hence, the demand profile corresponds to the medium demand profile in Fig. 9, and the number of operational subproblems is $4 \times 5 = 20$ due to the aggregation of years 5-10.

Table 1: **Data that characterizes the distributions DI-DIII (see also Fig. 10), from which demand scenarios are generated for the stochastic demand model.**

Distribution	μ^t	σ^t	b	$\tau^{t,1}$ (low)	$\tau^{t,2}$ (medium)	$\tau^{t,3}$ (high)
DI	1	0.065	1.15	25%	50%	25%
DII	1	0.185	1.15	25%	50%	25%
DIII	1	0.23	$b_{low} = 1.087$ $b_{high} = 1.652$	30%	50%	20%

4.2.1.2 Stochastic demand In the stochastic demand model, we additionally include information that is available regarding the uncertainty in

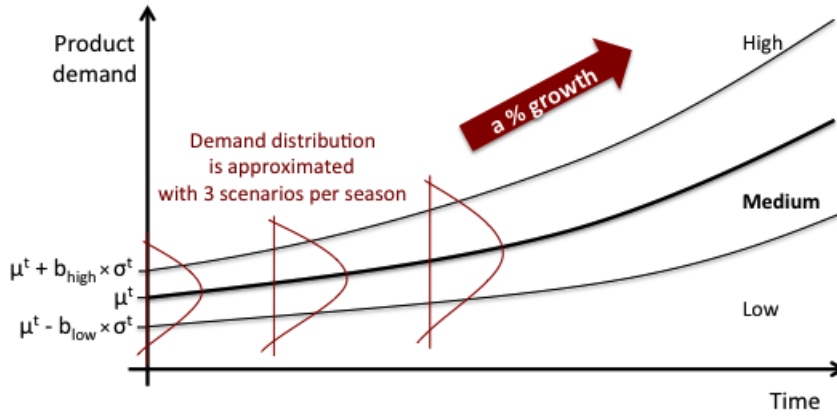


Figure 9: Qualitative illustration of the degrees of freedom in product demand trajectories and associated scenarios. μ^t is the expected demand in time period (season) t . σ^t is the standard deviation in time period t . a is the growth rate in demand and b_{low} , b_{high} are factors chosen according to the percentile where the low and high scenarios are centered at.

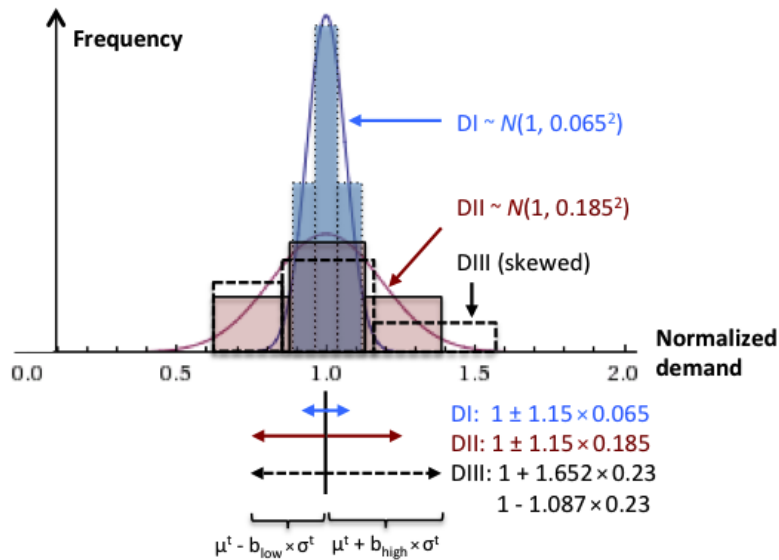


Figure 10: Distributions DI-DIII and their approximations with 3 scenarios that were used in the case study. For DI and DII, the low and high demand scenarios were centered at the 12.5 and 87.5 percentile respectively, and weighted with 25%. The medium scenario is weighted with 50%. DI and DII are normal distributions, whereas DIII is skewed.

the forecast. First, the distribution of historic demand data is analyzed to determine the underlying distribution. Second, based on the analysis, demand scenarios are generated.

In this paper, we investigate the impact of different demand distributions, such as normal distributions and skewed distributions. Fig. 10 shows the three distributions DI-DIII, which are used in the case study. All distributions are scaled and centered at 1, as reported in Table 1. DI and DII are normal distributions, i.e. $D^t \sim \mathcal{N}(\mu^t, (\sigma^t)^2)$, where $3\sigma_{DI}^t \approx \sigma_{DII}^t$. DIII is a skewed distribution with $\sigma_{DIII}^t > \sigma_{DII}^t$.

The number of scenarios is limited to three (low, medium, high) per time period t due to the resulting large size of the optimization problem. Therefore, the number of operational subproblems is $3 \times 4 \times 5 = 60$. As shown in Fig. 10 and as summarized in Table 1, for DI and DII, the low and high demand scenarios are centered at the 12.5 and 87.5 percentile respectively ($b = 1.15$), and each one is weighted with 25%. The medium scenario is weighted with 50%, such that $\sum_{s \in S} \tau^{t,s} = 1, \forall t$. For DIII, the low demand scenario is closer to the medium demand scenario than the high demand scenario, since the distribution is skewed. The two different values for b are also reported in Table 1.

4.2.2 Electricity price modeling

The other main influence factor for an investment decision, is electricity cost and in particular the variability in electricity pricing. As mentioned in section 3, the introduction of time periods t , which represent different seasons of a year, is driven by different typical profiles in electricity prices. We use a weighted average over multiple years of data from PJM (2011) to determine the baseline price profiles for year one. Based on data published by the Energy Information Administration (EIA, 2011), a long-term price projection is used to forecast future electricity price levels, while assuming that the same average pattern will be present in future years as well.

4.2.3 NPV cost modeling

All cost factors in OPEX and CAPEX need to be discounted to consider the time value of money. We adjust for inflation and use the weighted average cost of capital (WACC) to discount the cost accordingly.

4.2.4 Summary of the investigated cases

We investigate four cases, in which we vary the baseline demand, the annual growth rate, the demand distribution (see section 4.2.1.2) and the price for external product purchases. The cases are reported in Table 2. As described earlier, we solve the cases for deterministic and stochastic demand. In the deterministic case, the information about the demand distribution is not

used. In the stochastic case, the distributions are centered ($\equiv 1$) at the baseline demand μ^1 for year one and at increasing demand values, which grow according to the annual growth rate a , for subsequent years.

Table 2: **List of investigated cases, for which baseline demand, annual growth, the demand distribution and the price for external purchases are varied.**

case	baseline demand (μ^1)	Annual growth (a)	Demand distribution	Scaled prices for external purchases (ρ)
1	65%	3%	DI	1.0
2	91%	6.5%	DI	1.0
3	81%	4.5%	DII	1.0
4	81%	5%	DIII	1.33

4.3 Results

4.3.1 Value of current and additional flexibility

For each case, we would like to understand the value of the current flexibility (without new investments) and the value of additional flexibility that can be achieved by retrofitting the air separation plant. Therefore, we investigate three setups for both, deterministic demand and stochastic demand: (1) constant operation with the currently installed equipment, (2) flexible operation with the currently installed equipment, and (3) the joint optimization of investment and operational decisions. The difference in total cost between (1) and (2) is the value of the current flexibility. The difference in total cost between (2) and (3) is the value of additional flexibility. These values may differ for the deterministic demand model and the stochastic demand model, which we discuss in the following.

4.3.1.1 Deterministic demand model As one can see in Fig. 11 in which total costs are reported for all four cases, the value of current flexibility depends on plant utilization. If utilization is relatively low, as in case 1 (65% utilization for the existing liquefier in terms of baseline demand and an annual growth rate of 3%), the plant already has a significant amount of flexibility to react to variability in electricity prices with temporary shutdowns and flowrate adjustments during hours of high electricity prices. Therefore, the value of current flexibility is equivalent to a reduction in total costs of 13.3% in case 1. In contrast, if the utilization is very high, e.g. in case 2 (93% utilization for baseline demand with an annual growth rate of 6%), the value of current flexibility to shift production to periods with low electricity

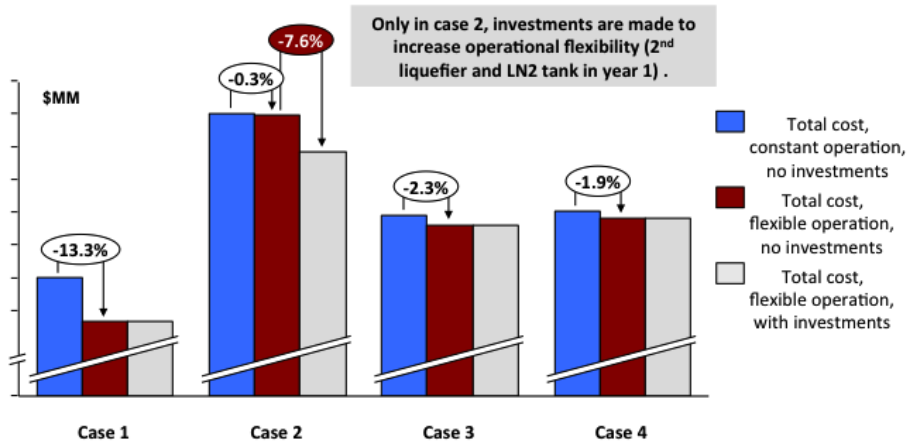


Figure 11: Deterministic demand model: Value of current and additional flexibility. For each case, the value of current flexibility is the difference between the first two columns; the value of additional flexibility is the difference between the second and the third column.

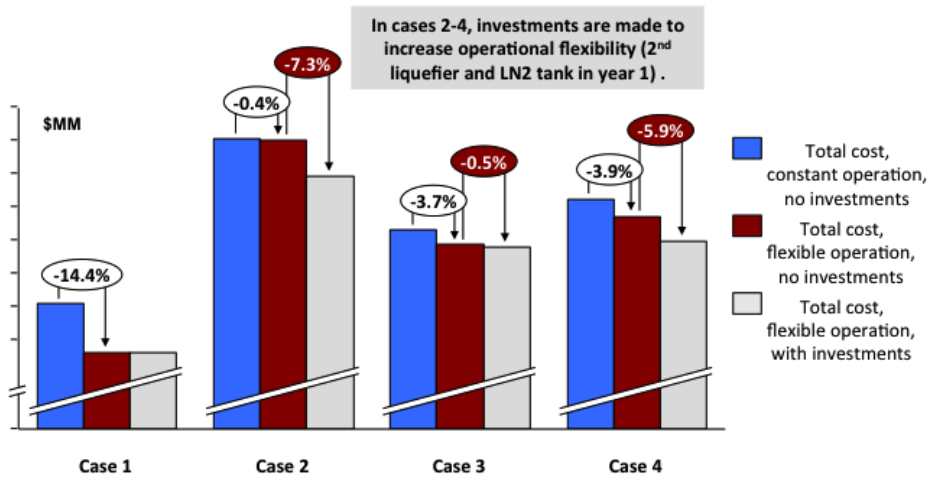


Figure 12: Stochastic demand model: Value of current and additional flexibility. For each case, the value of current flexibility is the difference between the first two columns; the value of additional flexibility is the difference between the second and the third column.

prices is low. Hence, the cost savings are relatively small (0.3%). Consequently, the value of current flexibility is intermediate if the utilization is also within a medium range as one can see in cases 3 and 4. Case 3 has a medium baseline demand of 81% utilization and a growth rate of 4.5%, case 4 has the same baseline demand and a growth rate of 5%. The realized values of current flexibility are equivalent to cost reductions of 2.3% and 1.9% respectively.

Only in case 2 investments are made to increase operational flexibility, driven by the higher demand. In the first time period, the second liquefier and an additional storage tank for LN2 are installed. The existing liquefier is not replaced; neither, additional storage tanks for LO2 or LAr are purchased. The realized cost savings, i.e. the value of additional flexibility, are 7.6%. In all other cases, the joint optimization of investments and operational decisions lead to no investments.

4.3.1.2 Stochastic demand model In Fig. 12, the total costs for all cases using the stochastic demand model are reported. As in the deterministic case, the value of existing flexibility is also a function of utilization. While the absolute total cost values as well as the relative cost savings are slightly different compared to the deterministic solution due to the set of demand scenarios, the overall trend is still the same.

In cases 1 and 2, the value of additional flexibility is also similar to the deterministic solution. While there are no investments made in case 1, the second liquefier and one LN2 tank are installed in the first year in case 2, which leads to 7.3% cost savings.

However, in cases 3 and 4, the stochastic solutions suggest a very different investment strategy compared to the deterministic solution. In both cases, the second liquefier and one LN2 tank are installed in the first year. The associated values of additional flexibility are 0.5% and 5.9% respectively. In the next section, we discuss the origin of the differences and the value of the stochastic solution.

An additional interesting observation is that the investments are always made during the first time period. Hence, the yearly cost savings due to improved operational schedules are larger than the potentially lower investment costs due to deferred investments (after inflation and discounting).

4.3.2 Value of the stochastic solution (VSS)

In Fig. 13, one can observe how the additional production capacity of the second liquefier increases operational flexibility and allows the plant to adjust for swings in electricity prices. Furthermore, costs for external product purchases can be avoided.

In cases 3 and 4, one can observe that the deterministic and the stochastic solutions propose different investment strategies. While the deterministic

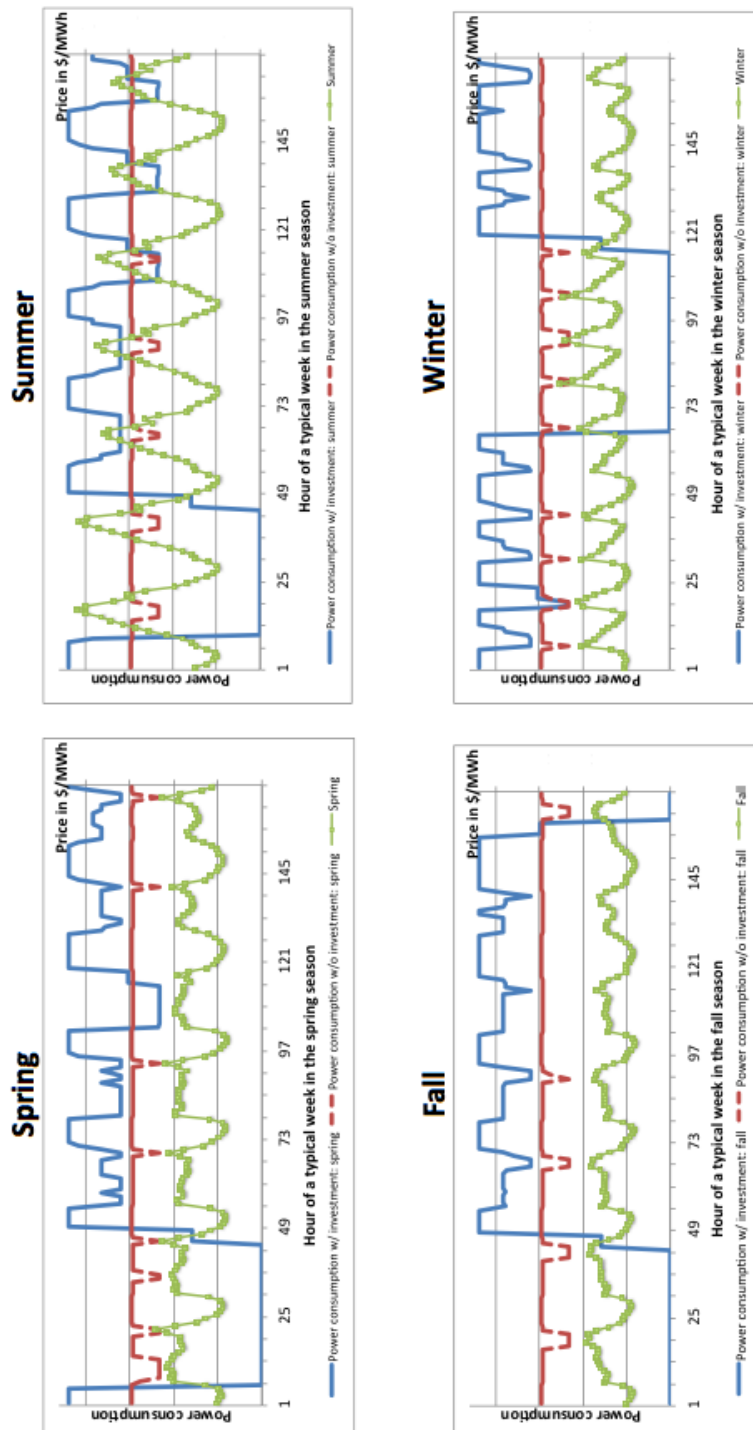


Figure 13: Characteristic operating profiles with and without investments for scenarios at high utilization. Additional production capacity of the second liquefier increases operational flexibility and allows the plant to adjust for swings in electricity prices.

solutions do not suggest to invest, the stochastic solutions recommend buying the second liquefier and one LN2 tank in the first year. Hence, in Fig. 14, we analyze the cost breakdown for the two different investment strategies under stochastic demand for cases 3 and 4.

In both cases, the underlying distributions (DII and DIII) have a high standard deviation from the expected value. Therefore, there are more scenarios with higher demand that potentially have higher cost due to external product purchases, if no investments are made. Note that the additional liquefier provides sufficient production capacity to meet the demand in these scenarios, such that costs due to external product purchases are practically eliminated. Furthermore, the combination of the liquefier with the additional LN2 tanks allows to reduce electricity cost by means of more flexible production schedules. In case 3, the cost difference is 0.5%. In case 4, the cost difference is higher (5.9%) mostly due to the skewed distribution DIII, which generates scenarios with higher deviations from the expected demand, and due to the 33% higher price for external product purchases.

The cost difference we described for cases 3 and 4 is also known as the **Value of the Stochastic Solution (VSS)**. More formally, it can be determined by solving the stochastic version of the problem with the investment decisions fixed to the values of the deterministic solution (Birge and Louveaux, 2011). If the deterministic and the stochastic solutions suggest the same investment strategy, the VSS is equal to zero, as in cases 1 and 2.

In Fig. 15, we summarize the drivers behind different investment strategies for the deterministic and the stochastic solution with a matrix structure, and classify the investigated cases. Small deviations from the expected demand are in favor for similar behavior in both solutions. For cases with low utilization (low baseline demand and small growth), the deterministic as well as the stochastic solutions suggest no investments. For cases with high utilization (high baseline demand and high growth) both solutions propose new investments. However, if the setup is unclear, i.e. if there are large deviations from the expected demand, potentially skewed distributions and a high prices for external product purchases, the deterministic and the stochastic solution behave differently. For those cases, the VSS is greater than zero.

4.3.3 Discussion of computational performance

We solved all test cases within GAMS 23.9.1 (Brooke et al., 2012) on a Intel i7-2600 (3.40 GHz) machine with 8 processors and 8 GB RAM. The commercial solver CPLEX 12.4.0.1 was employed using a termination criterion of 0.5% optimality gap. We specified branching priorities on the investment variables VN_n^t , VU_u^t and $VS_{st,g}^t$. Additionally, we used the parallel computing capabilities of CPLEX by setting `threads=8`.

As one can see from Table 3, the problem sizes for the deterministic and the stochastic model are very large due to the multi-scale nature of the

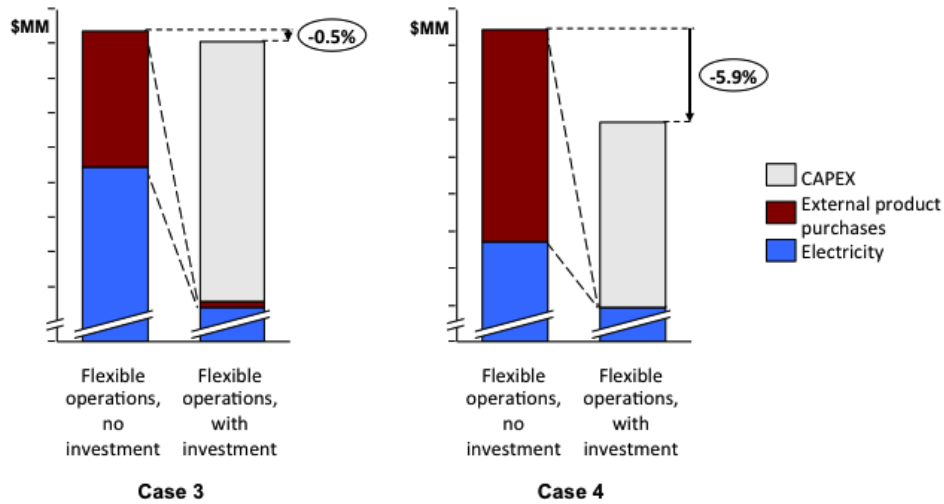


Figure 14: Analysis of the value of the stochastic solution (VSS). The flexibility gained from the second liquefier and the additional LN2 tank reduces electricity cost by means of flexible production and helps avoiding costs for external product purchases.

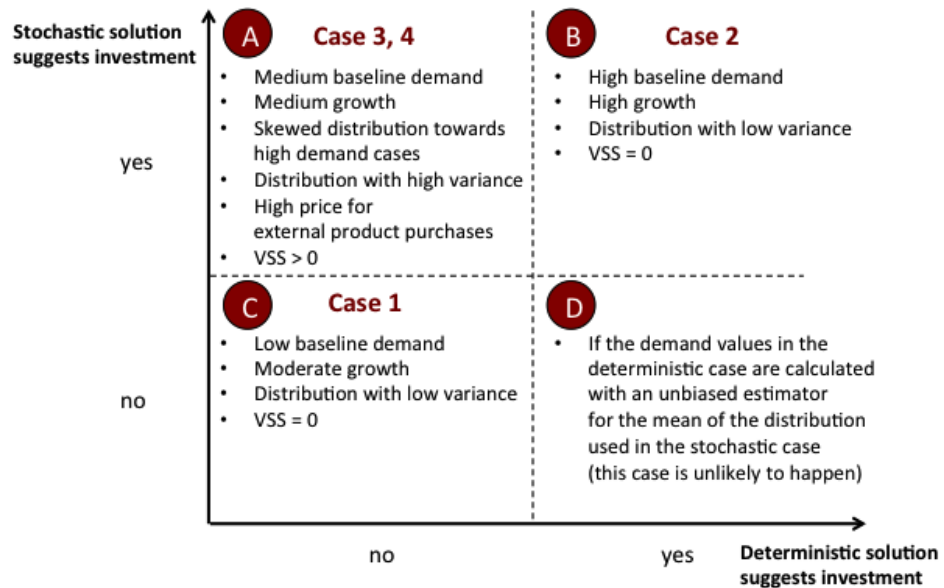


Figure 15: Qualitative analysis of VSS (value of stochastic solution) for capacity planning: Stochastic programming helps analyzing unclear demand scenarios.

Table 3: **Sizes of the resulting optimization problems in terms of constraints and variables for the deterministic and the stochastic demand model.**

	Deterministic model	Stochastic model
Number of operational problems	20	60
Constraints	305,094	915,270
Variables	796,344	2,388,984
Binary Variables	73,940	221,780

optimization problem. In Table 4, we report the computational times and the corresponding final gaps for deterministic and stochastic demand with the distinction whether investments are jointly optimized or not.

In 10 out of 16 reported cases, we can converge to the required accuracy of 0.50% final gap. In 5 out of the 6 cases, which do not achieve that accuracy, the solver runs out of memory, but converges within 1.5% accuracy. Only in one case, the solution process is terminated due to a time limit of 80 hours with a final gap of 3.23%. Case 1 is especially difficult to solve because the high flexibility leads to a large solution space (3 runs do not converge to the required accuracy). As expected, the deterministic cases as well as the cases, in which investments are not optimized, are comparably easier to solve due to a smaller solution space.

Since there is a final gap in some cases, it is interesting to understand whether the obtained solutions are mathematically optimal in terms of investments. In fact, as we will explain in part II of this paper, this question is one motivating factor for additional research on decomposition methods, which confirms the optimality of the obtained investments for all cases.

5 Conclusion

In this paper, we have described a multi-scale model for the integrated optimization of investments and operations for continuous power-intensive processes under time-sensitive electricity prices and demand uncertainty. We applied the model to an industrial case study of an air separation plant for deterministic demand as well as stochastic demand.

For different baseline demands, annual growth rates and demand distributions, we investigated the current flexibility of the plant and the additional flexibility due to retrofitting. If the underlying demand distribution has a low standard deviation, the deterministic and the stochastic solution yield the same investment strategy. For cases with low utilization, no additional flexibility needs to be incorporated. For cases with high utilization, the

Table 4: **Computational times for the investigated cases with flexible operations. Allowed gap: 0.50%.** ^a: out of memory; ^b: terminated after 80 hours of computation

case	det./ stoch.	investments optimized?	Wall time (s)	Final gap (%)
1	det.	no	9963	0.50%
1	stoch.	no	5877	1.25% ^a
1	det.	yes	20128	0.51% ^a
1	stoch.	yes	78810	1.32% ^a
2	det.	no	26	0.09%
2	stoch.	no	2151	0.38%
2	det.	yes	1657	0.50%
2	stoch.	yes	67137	0.50%
3	det.	no	37	0.47%
3	stoch.	no	1190	0.50%
3	det.	yes	4546	0.50%
3	stoch.	yes	288000	3.23% ^b
4	det.	no	111	0.46%
4	stoch.	no	5237	0.55% ^a
4	det.	yes	4814	0.50%
4	stoch.	yes	154312	0.63% ^a

current flexibility is low and additional flexibility is desirable. However, in unclear demand setups, e.g. medium baseline demand and annual growth rate, with a (potentially skewed) demand distribution that has a large standard deviation, the deterministic and the stochastic solution suggest different investment strategies. For those case, we showed that the value of the stochastic solution can be significant.

Due to the multi-scale nature of the problem, the resulting MILP problems are large-scale and hard to solve. While most of the investigated problem instances could be solved within at most three days, there is a clear demand for an efficient algorithm that can solve the problem faster with a higher numerical accuracy, and can potentially solve instances with a larger number of scenarios, which would reduce the need for the described aggregation of seasons. Therefore, we outline a decomposition algorithm in part II of the paper.

Acknowledgments

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Nomenclature

Sets

- $DAL(m, m')$: The set of disallowed transitions from mode m to m'
- G (index g): The set of products. For air separation plants it is $\{LO_2, LN_2, LAr, GO_2, GN_2\}$.
- H (index h): The set of hours of a week in the operational representation
- $I(m, o)$ (index i), abbreviated as I : The set of extreme points that relate to option o of mode m
- M (index m): The set of operating modes
- $MS(m, m')$ characterizes all minimum stay relationships that hold once a transition from mode m to mode m' occurs. Examples include minimum uptimes, minimum downtimes and minimum transition times.
- N : The set of available new equipment to be added to the plant
- $NewEq(m, n)$, abbreviated as NewEq: The set captures the links between the addition of equipment n with modes m that would be introduced to the state graph

- $O(m)$ (index o), abbreviated as O : The set of options for mode m depending on how the plant is modified
- S (index s): The set of demand scenarios
- ST : The set of available storage tanks
- T (index t): The set of time periods related to seasons (four per year); each one's operation is represented by a cyclic scheduling problem
- $T_{invest} \subset T$: The set of time periods, in which investments can take place
- $Trans(m, m', m'')$: The set of possible transitions from mode m to a production mode m'' with the transitional mode m' in between
- U : The set of equipment upgrades available
- $Upgrade(m, o, u)$, abbreviated as $Upgrade$: The set captures the links between the equipment upgrade u and the options o of mode m that would be changed in their polyhedral representation

Variables

Binary investment variables

- VU_u^t : Indicates whether upgrade u is performed in time period t
- VN_n^t : Describes whether the new equipment n is added in time period t
- $VS_{st,g}^t$: Indicates whether storage tank st for product g is purchased in time period t

Binary operational variables

- $y_m^{t,s,h}$: Determines whether the plant operates in mode m in hour h (of time period t and scenario s)
- $\tilde{y}_{m,o}^{t,s,h}$: Determines whether the plant operates in option o for mode m in hour h (of time period t and scenario s)
- $z_{m,m'}^{t,s,h}$: Indicates whether there is a transition from mode m to mode m' from hour $h - 1$ to h (of time period t and scenario s)

Continuous (operational) variables

- $\bar{P}_{m,o,g}^{t,s,h}$: Production amount of product g in option o of mode m in hour h (of time period t and scenario s)
- $P_g^{t,s,h}$: Total production of product g in hour h (of time period t and scenario s)
- $\lambda_{m,o,i}^{t,s,h}$: Variable for the convex combination of slates i to describe the feasible region of option o of mode m in hour h (of time period t and scenario s)
- $INV_g^{t,s,h}$: Inventory level of product g in hour h (of time period t and scenario s)
- $S_g^{t,s,h}$: Sales of product g in hour h (of time period t and scenario s)
- $B_g^{t,s,h}$: External product purchases in hour h (of time period t and scenario s)
- $CAPEX^t$: Capital spent due to investments in time period t
- $OPEX^{t,s}$: Operating expenses in scenario s of time period t
- TC : Objective function variable that represents total cost

Parameters

- $e^{t,s,h}$: Electricity price in hour h in time period t and scenario s
- $\Phi_{m,o,g}$: Coefficient that correlates production level of product g for option o of mode m with power consumption, in [power/volume]
- $\rho_g^{t,s}$: Cost for product g shipped from another plant or procured from a competitor in time period t and scenario s , in [\$/volume]
- δ_g : Cost coefficient for inventory of product g , in [\$/volume]
- $\zeta_{m,m'}$: Cost coefficient for transitions from mode m to m' , in [\$/]
- $\tau^{t,s}$: Probability of scenario s in time period t
- $x_{m,o,i,g}$: Extreme points of the convex hull of the feasible regions
- $K_{m,m'}$: Number of hours the plant has to stay in mode m' after a transition from mode m
- $r_{m,o,g}$: Maximum rate of change for product g in option o of mode m

- $d_g^{t,s,h}$: Hourly demand for the products g in hour h (in time period t and scenario s).
- INV_g^U : Current tank capacity for product g
- $Tank_{st,g}$: Tank size for new storage tank st for product g
- $CS_{st,g}^t$: Cost for purchasing storage tank st for product g in time period t
- Cn_n^t : Cost for investing in new equipment n in time period t
- Cu_u^t : Cost for investing in the equipment upgrade u in time period t

Other symbols

- D^t : Random variable for the overall product demand in time period t
- μ^t : The expected demand in time period t , i.e. $\mu^t = \mathbb{E}(D^t)$
- σ^t : The standard deviation for the demand in time period t
- a : Annual growth rate for product demand
- b_{low}, b_{high} : Scaling factors

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