A general modular framework for the integrated optimal management of an industrial gases supply-chain and its production systems

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1. Introduction

Supply-chain management refers to the handling of raw material restocks and supplies, the delivery of final products to the customers and the mutually beneficial economic interactions between the company and its competitors. In simplest terms, the supply-chain can be considered as a coupling of material logistics and competitor-company interactions. The production level management refers to the determination of the operating conditions of the production sites. By looking at these two definitions, it is evident that these two operational levels are directly and strongly interconnected with each other and their main connection is through the product storage facilities.

Since the global profitability of any company strongly depends on the management policies adopted for both its supply-chain network and its production level, a number of authors have studied how these two areas can be optimized as a function of market factors, such as product demands, raw materials availability and cost, energy/utility prices fluctuation, other production costs and delivery expenses. Even though much research has been published in this area, especially in the last fifteen years, most papers only address specific cases. General methodologies have been studied but limited to certain classes of problems. For instance, several income-based scheduling strategies, for a single production plant, are analysed in (Busch et al., 2007; Floudas, 2005; Maravelias, 2012; Yue and You, 2013), some methods for the income-based opti-mization of the production subsystem at the corporate level are studied in (Grossmann, 2004, 2005; Manenti et al., 2013a,b; Varma et al., 2007) and a comprehensive knowledge on how to model and solve scheduling problems for single and multiple entities can be found in (Floudas and Lin, 2004; Méndez et al., 2006; Harjunkoski et al., 2014). Moreover, a few algorithms for the supply-chain net-work and alike optimal management are described in (Bansal et al., 2007; Neiro and Pinto, 2004; Ng and Lam, 2013; Park et al., 2006; Shah, 2005) while some applied studies, on the same topic, can be found in papers like (Bowling et al., 2011; Julka et al., 2002). Finally, planning approaches have been investigated in many papers such as (Kallrath, 2002; Timpe and Kallrath, 2000), with the additional aim of finding ways to quantify the impact of uncertainties on the achieved results (Cheng et al., 2003).

Within the last five years, new formulations and solution strategies, which integrate regulatory control and planning, have been

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conceptualized and developed. In these studies objective functions, similar to those used in planning problems, are employed within a model-predictive control scheme (MPC). However, all these strategies are highly computational demanding and thus they have only been applied to batch plants, modelled by means of low dimensional systems of linear equations (Subramanian et al., 2014).

All the above-mentioned supply-chain/production optimization approaches lead to very large-scale optimization problems which are linear or non-linear and might also include discrete variables, depending on the modelling strategies employed. However, generally some assumptions are introduced such that the resulting optimization problem is LP or MILP in order to be able to guarantee the global optimality and to keep CPU times at a feasible level. Since the logistics portion of the supply-chain networks can be typically modelled with linear equations, it is most convenient to use linear models to represent the operation of the production plants in the supply chain. As a consequence, some form of reduced order linear models must be used (Buzzi-Ferraris and Manenti, 2010a,b). The solution of the resulting large-scale optimization problem can then be attacked using several different direct or decomposition algorithms. The literature provides a considerable amount of information on this topic in many papers, such as (Biegler, 2007; Biegler and Grossmann, 2004).

While the problem of supply-chain/production level optimization has been and still is extensively studied in literature, fully-integrated strategies, which allow the simultaneous optimization of supply-chain and production levels, have only been reported in recent years (Maravelias and Sung, 2009; Muñoz et al., 2013; Grossmann et al., 2008; Phanden et al., 2011). In addition, the examples of these strategies that can be found in the literature often model the production facilities as a set of simple product sources, without incorporating the operational details of these sources. This simplification can lead to infeasibilities when it comes to applying the optimization-derived results in actual practical situations. It must be reported that the very recent tendency is to move towards a better (model-based) description of the production sites. Nev-ertheless, there is still no general strategy for the simultaneous optimization of supply-chain and production networks that fully realizes this goal.

Among the possible sectors where supply-chain/production optimization might be of relevance, the one involving the industrial gas producers (IGPs) is the focus of our interest since only a limited number of studies have been reported and none of them can be con-sidered to be sufficiently general (Ierapetritou et al., 2002; Mitra et al., 2012, 2014; Manenti et al., 2013a,b; Manenti and Rovaglio, 2013).

For these reasons, the current paper proposes an integrated approach for the simultaneous optimal management of both the supply-chain network and the production level of a generic IGP, at the entire company level. This novel approach consists of several main components:

- a general, hybrid modelling approach for the production plants (air separation units or ASU), which uses both first principles models and correlations developed from experimental data and/or rigorous simulations;
- a general model of the supply-chain network and storage system;
- a complete formulation of a cost-based objective function;
- a suite of numerical methods to reduce the resulting optimization problem dimensions and solve it efficiently.

The rolling horizon technique can also be easily employed in order to handle the uncertainties in the demands and make the method suitable for real industrial applications. The proposed methodology is implemented into a C++ tool, exploiting BzzMath classes (Buzzi-Ferraris and Manenti, 2012) in order to meet the needed efficiency requirements for online application. It is tested in a case study, based on a portion of the real supply-chain/production network of Linde Gas Italia S.r.l. (subsidiary of the Linde Group). This case study is employed to demonstrate the effectiveness of the proposed strategy and to compare it to the solution obtained using traditional supply-chain/production optimization methodologies.

The rest of the paper is divided into the following sections:

- The description of the supply-chain network modelling along with the description of the strategy employed for the treatment of the storage facilities;
- An outline of the approach applied for the modelling of the production sites and the production network;
- An explanation of the choices made to define a proper performance function for a whole IGP and the structure of the resulting supply-chain and production optimization problem;
- The presentation of the results of the case study;
- Some concluding remarks.

2. Supply-chain network and storage system modelling strategy

This section addresses both the description of the features of a generic IGP supply-chain plus the modelling approach adopted for it and the description of a typical IGP storage system. The spe-cific features of such a supply-chain are reported in Section 2.1, the adopted modelling approach and the resulting mathematical model are described in Section 2.2 and the storage system model is studied and reported in Section 2.3. All the equations, described in Sections 2.1–2.3, constitute the set of supply-chain and storage constraints in the IGP global optimization problem, i.e. the optimization problem whose solution consists in the optimal IGP operating condition.

2.1. Special features of IGPs supply-chain

The production and sale of industrial gases is a unique business from several viewpoints and thus the relating production sites (ASUs) and supply-chain networks have characteristic features that need to be reviewed. These specific features are listed below:

- The raw material, from which industrial gases are produced, is air that is free and always available in any required amount. Thus no raw materials restock and/or cost issues have to be taken into account;
- Industrial gases are stored in liquid phase at very low temperatures thus long haul transportation is unsuitable; as a consequence, products are typically either trucked in liquid phase or carried via pipeline in gas phase (at a short distance) from the production plants to the customers;
- Each IGP owns its own fleet of tankers that are used to deliver the products;
- IGPs and competitor companies draw-up commercial agreements that establish the option, for the IGPs, of buying products from competitor sites at low price. These volumes of purchased products are then typically employed to satisfy some of the demands of the IGPs customers (this restock method is named “shipment upon payment”);
- IGPs also draw up so-called SWAP contracts with their competitor companies. By means of these contracts an IGP can effectively treat its competitors’ production sites as its own production sites (competitors can do the same). As a result, an IGP can load product from a competitor site with its own tankers and carry it to its own customers (competitors can do the same). On a yearly basis the amount of each product that an IGP can load from a competitor

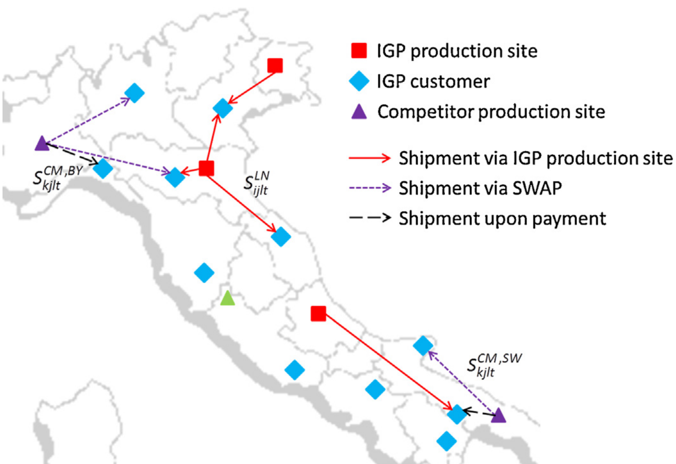

Fig. 1. Schematic supply-chain network of a generic IGP.

company is limited and a maximum for it is defined in the SWAP contract. Moreover, different products can also be swapped. For this reason, the SWAP contract provides a nominal price for each product in order to be able to define the relative economic value of each exchange of products. This is essential to define the relative amounts of each pair of products that correspond to the same economic value.

All of these features are incorporated, in the following section, in building the mathematical model of a generic IGP supply-chain network.

2.2. Supply-chain network modelling approach

Before introducing the mathematical model of a generic IGP supply-chain, some additional preliminary information must be provided.

The first key point that must be addressed is the description of a general scheme for the network, as shown in Fig. 1. Here the squares stand for the IGP production sites, the rhombuses symbol-ize the customers and the triangles represent the competitor sites. Moreover, it can be observed that customers can be supplied with products that come from either the IGP production sites (shipments via IGP sites, specified by solid arrows) or the competitor sites (ship-ments via SWAP, specified by dotted arrows, and shipment upon payment, specified by dashed arrows). Finally, the reader should notice that, in principle, a single customer demand can be satisfied with more than a single shipment and with shipments of different types.

The second key point that must be accommodated is the repre-sentation of time in the interval over which the dynamics of the IGP supply-chain network is to be captured. A planning horizon, appro-priate to the business planning cycle of the target company, has to be defined. This planning horizon is assumed to be divided into discrete intervals, whose length is determined and fixed a priori, based on the time constants characteristic for the critical decision activities of the supply chain.

Finally, the last key point that should be introduced and described is the adopted nomenclature. For the convenience of the reader, the commonly used variables and parameters and their def-initions are introduced and described just before they are used the first time.

Starting now with the detailed mathematical description of the IGP supply-chain model, the first set of equations are effectively the demand-supply balances which ensure that each customer is provided with the requested quantities of the requested products on time (Eq. (1)).

$$\sum_{i=1}^{N_S} PM_{il} S_{ijlt}^{LN} + \sum_{k=1}^{N_{cm}} S_{kjlt}^{CM,SW} + \sum_{k=1}^{N_{cm}} S_{kjlt}^{CM,BY} = R_{jlt} \quad \forall j, l, t \tag{1}$$

In terms of notation:

- S_{ijlt}^{LN} is the shipment of the lth product via the ith IGP site to the jth customer that leaves the IGP site by the end of the tth time interval;
- $S_{kjlt}^{CM,SW}$ is the shipment via SWAP of the lth product via the kth competitor site to the jth customer that leaves the competitor site by the end of the tth time interval;
- $S_{kjlt}^{CM,BY}$ is the shipment upon payment of the lth product via the kth competitor site to the jth customer that leaves the competitor site by the end of the tth time interval;
- PM_{il} is the generic element of the site-product boolean matrix that has a value of one if the ith IGP site is able to produce the lth product and a value of zero otherwise;
- R_{jlt} is the expected amount of the lth product requested by the jth customer in a time instant that belongs to the tth time interval;
- N_s is the number of IGP production sites;
- N_{cm} is the number of competitor sites.

Before going ahead, observe that Eq. (1) is a set of purely linear equations. Indeed, the site-product matrix is a structural property of the IGP supply-chain network, thus being a matrix of constants. Moreover, notice that customers' demands (R_{jlt}) are treated as hard constraints (each customer requests must be satisfied and no deliv-ery failure is tolerated), thus no backlog effects are present.

Two additional inequality sets are also required in order to limit the maximum amount of each product that can be used for ship-ments via SWAP and/or shipments upon payment, coming from all the competitor sites. Indeed, each competitor plant must satisfy its own customers' demands before supporting the IGP in making the same. The inequality set that relates to the limits in the shipments via SWAP is shown in Eq. (2) while the one that accounts for the limits in the shipments upon payment is given in Eq. (3).

$$\sum_{j=1}^{N_{cl}} S_{kjlt}^{CM,SW} \leq F_{klt}^{CM,MAX} \quad \forall k, l, t \tag{2}$$

$$\sum_{j=1}^{N_{cl}} S_{kjlt}^{CM,BY} \leq FBY_{klt}^{CM,MAX} \quad \forall k, l, t \tag{3}$$

In terms of notation:

- $F_{klt}^{CM,MAX}$ stands for the expected maximum amount of lth product that the kth competitor site can offer in the tth time interval for shipments via SWAP;
- $FBY_{klt}^{CM,MAX}$ is the expected maximum amount of lth product that the kth competitor site can offer in the tth time interval for ship-ments upon payment;
- N_{cl} is the number of IGP customers.

It is important to note that Eq. (2) relates to the limits in the shipments via SWAP for the single competitor site, not depending on the competitor company to which this site belongs. It is essential to bear this in mind to avoid confusions with the next inequality set.

The second to last inequality set, which must be introduced, is the one that translates in mathematical expressions the SWAP agreements between the IGP and the competitor companies. Since the formulation of these inequalities is less intuitive than that of the previous ones, a longer and more detailed description is required. The objective is to define a set of expressions that force the vol-umes of all the products, swapped via each competitor company inside the entire horizon within which the IGP supply-chain net-work is simulated, to be less than or equal to certain upper bounds. Of course these upper bounds are specific for the single competi-tor company and depend on the SWAP agreements. Moreover, the SWAP balances must also take into account that different prod-ucts can be swapped on the basis of specific nominal prices, once again defined in the SWAP agreements. The simplest solution is to initially compute the nominal economic values (i.e., the eco-nomic values based on nominal prices) relating to the volumes of the single products, swapped via each competitor company over the entire simulation horizon of the IGP supply-chain network. The next step is to combine them to derive the global nominal economic value of all the swapped products for each competitor company and force it to be less than or equal to a maximum threshold, evaluated by means of the SWAP agreements. Conversion of the aforemen-tioned concepts into a set of mathematical expressions results in the inequalities reported in Eq. (4).

$$\sum_{k=1}^{N_{cm}} CMSM_{hk} \sum_{l=1}^{N_p} MEV_l \sum_{t=1}^{N_g^{eq}} \sum_{j=1}^{N_{cl}} S_{kjlt}^{CM,SW} \leq \sum_{l=1}^{N_p} MEV_l FDCM_{hl} \quad \forall h \tag{4}$$

In terms of notation:

- $FDCM_{hl}$ is the first guess maximum amount of lth product that the hth competitor company can offer in the entire planning interval where the IGP supply-chain is simulated for shipments via SWAP;
- MEV_l is the nominal price for the lth product;
- $CMSM_{hk}$ is the generic element of the competitor site-competitor company boolean matrix that has a value of one if the kth competitor site belongs to the hth competitor company and a value of zero otherwise;
- N_p is the number of products in the IGP portfolio;
- N_g^{eq} is the number of time intervals in the planning horizon over which the IGP supply-chain is simulated.

One relevant remark relating to Eq. (4) is that there are infinite sets of $FDCM_{hl}$ values that, put in the expression, give the same set of inequalities. This may seem strange but it is consistent with the physical meaning of Eq. (4) (see the description in the previous lines).

The last inequality set that needs to be added consists of the bound constraints on the product shipments of all kind. Indeed, all the shipments must be non-negative as reported in Eq. (5).

$$\begin{aligned} &S_{ijlt}^{LN} \geq 0 \quad \forall\, i, j, l, t : PM_{il} = 1 \\ &S_{kjlt}^{CM,SW}, S_{kjlt}^{CM,BY} \geq 0 \quad \forall\, k, j, l, t \end{aligned} \tag{5}$$

The complete supply-chain model consists of Eqs. (1)–(5). One last additional remark on this complete model is that its expressions have been derived under the assumption that no clustering techniques are employed (i.e., each customer is directly included in the network as a single entity). The same model can also be used, as it is, by replacing some or all customers with clusters because a cluster can be considered as a virtual customer. As a conclusion, the proposed IGP supply-chain model demonstrates to be general since it can be applied to every IGP but also very flexible because it is able to support both individual customers and customer clusters.

2.3. Storage system modelling approach

The storage system (Fig. 2) consists of all the storage tanks belonging to each production plant of the IGP. Each tank is refilled with fresh product coming from its corresponding IGP produc-tion site and is subject to product withdrawals of different nature. Indeed, the stored product can be either employed by some com-petitor sites for SWAP shipments and/or shipments upon payment or used in shipments via the IGP production site itself. Each tank of each storage system is also limited to a maximum and a min-imum capacity, where the minimum capacity is typically related to the need for a minimum liquid level that, in turn, may be essential to the correct operation of the refrigeration equipment (the reader should recall that all these storage units are cryogenic systems).

Therefore, the model of the storage system of an IGP production plant must include the material balances on all the tanks belonging to it (Eqs. (6) and (7)) along with the bound constraints on the products storage levels (Eq. (8)).

$$G_{il1} + \sum_{j=1}^{N_{cl}} S_{ijl1}^{LN} - MM_{i1} F_{il1}^{LN} - G_{il}^{0} = -(FP_{il1} + FNP_{il1}) \quad \forall\, i, l : PM_{il} = 1 \tag{6}$$

$$G_{ilt} + \sum_{j=1}^{N_{cl}} S_{ijlt}^{LN} - MM_{it} F_{ilt}^{LN} - G_{il(t-1)} = -(FP_{ilt} + FNP_{ilt}) \quad \forall\, i, l, t \neq 1 : PM_{il} = 1 \tag{7}$$

$$G_{il}^{MIN} \leq G_{ilt} \leq G_{il}^{MAX} \quad \forall\, i, l, t : PM_{il} = 1 \tag{8}$$

In terms of notation:

- G_{ilt} is the volume of lth product stored in the ith IGP plant storage system at the end of the tth time interval;
- G_{il}^{0} is the initial volume of lth product stored in the ith IGP plant storage system at the beginning of the first time interval;
- FP_{ilt} and FNP_{ilt} are the expected amounts of lth product with-drawn from the ith IGP site by all the competitor sites in the tth time interval for shipments via SWAP and shipments upon payment, respectively;
- F_{ilt}^{LN} is the amount of lth product produced by the ith IGP site in the tth time interval;
- MM_{it} is the generic element of the maintenance matrix that has a value of one if the ith IGP production site is active inside the tth time interval and a value of zero otherwise;
- G_{il}^{MIN} and G_{il}^{MAX} are the minimum and maximum storage capac-ities for the lth product in the ith IGP plant storage system, respectively.

Finally, by looking at Eqs. (6) and (7), it can be confirmed that the storage system plays the key role of the main interconnector between the supply-chain and the production networks. Indeed, both supply-chain-like variables $\left(S_{ijlt}^{LN}\right)$ and production-like variables $\left(F_{ilt}^{LN}\right)$ jointly belong to those two equation sets.

3. Production layer modelling strategy

An IGP production network includes all the ASUs belonging to the IGP itself. The models of these ASUs are essential for the effectiveness of the proposed integrated supply-chain and produc-tion optimization strategy and have to be accurately built. Since

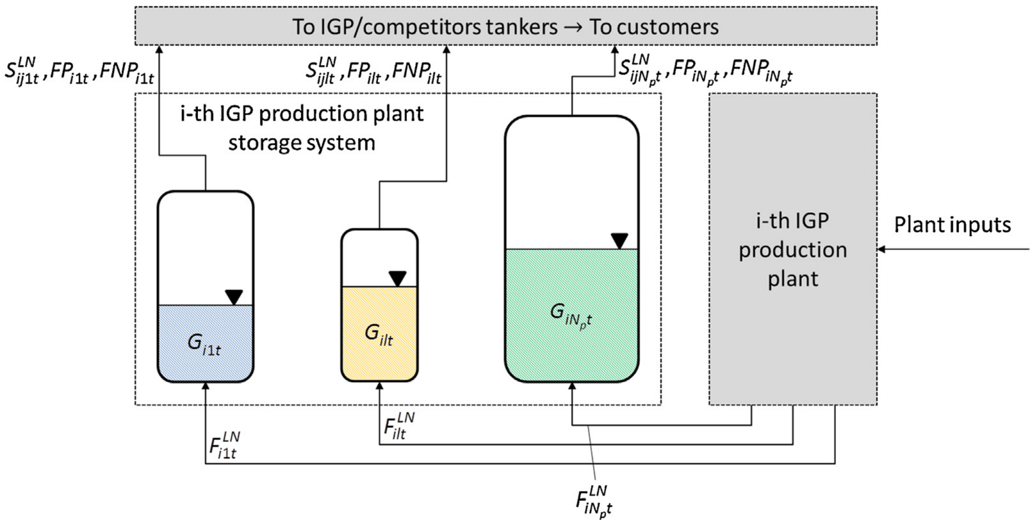

Fig. 2. Structure and interconnections of a generic IGP storage system.

the production of industrial gases is a well-established process, all the ASUs share almost the same layout (Fig. 3), thus a general modelling strategy can be developed. The theoretical guidelines of such a strategy are described in Section 3.1 while its practical application is reported in Section 5. Once the modelling approach employed for each single IGP ASU is clarified, Section 3.2 addresses the combination of these single site models to build the model of the overall IGP production network. The latter plays the role of the production constraints within the IGP global optimization problem.

3.1. *Single IGP ASU modelling approach*

We first note that the layout of each ASU plant can be well approximated with the block flow diagram (BFD) shown in Fig. 4.

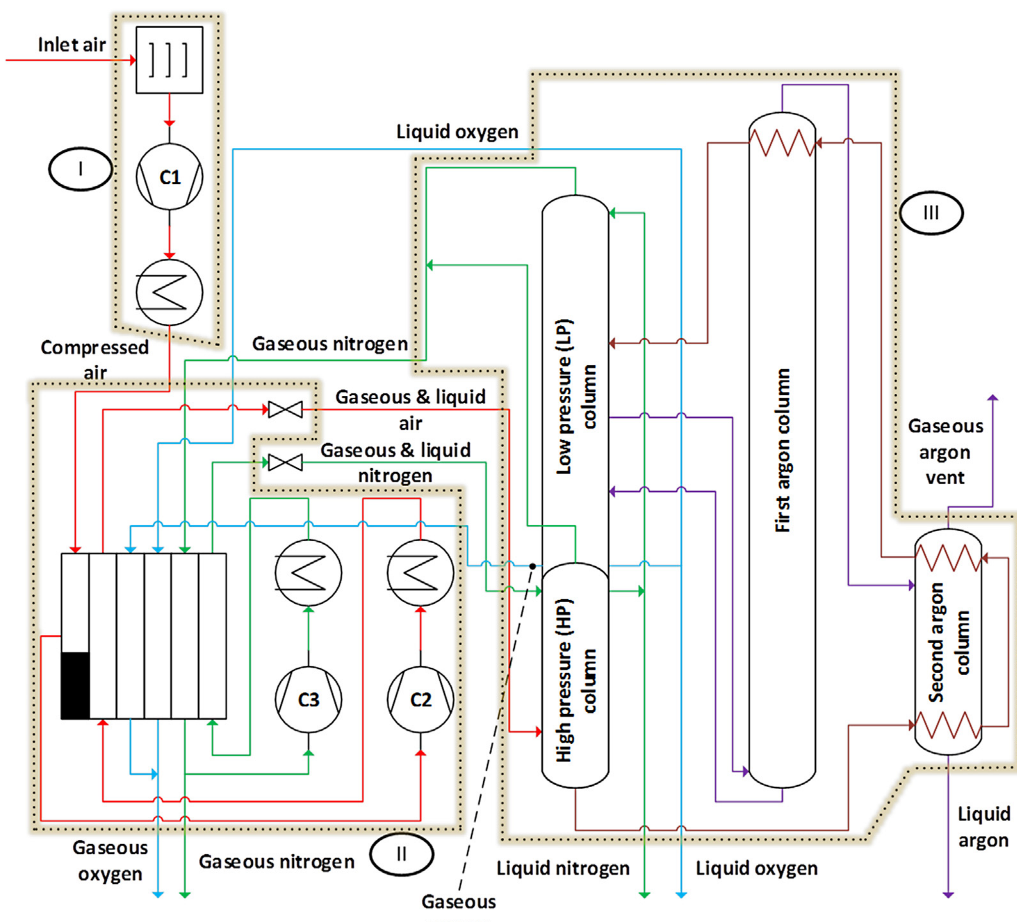

Fig. 3. ASU plant representative process flow diagram.

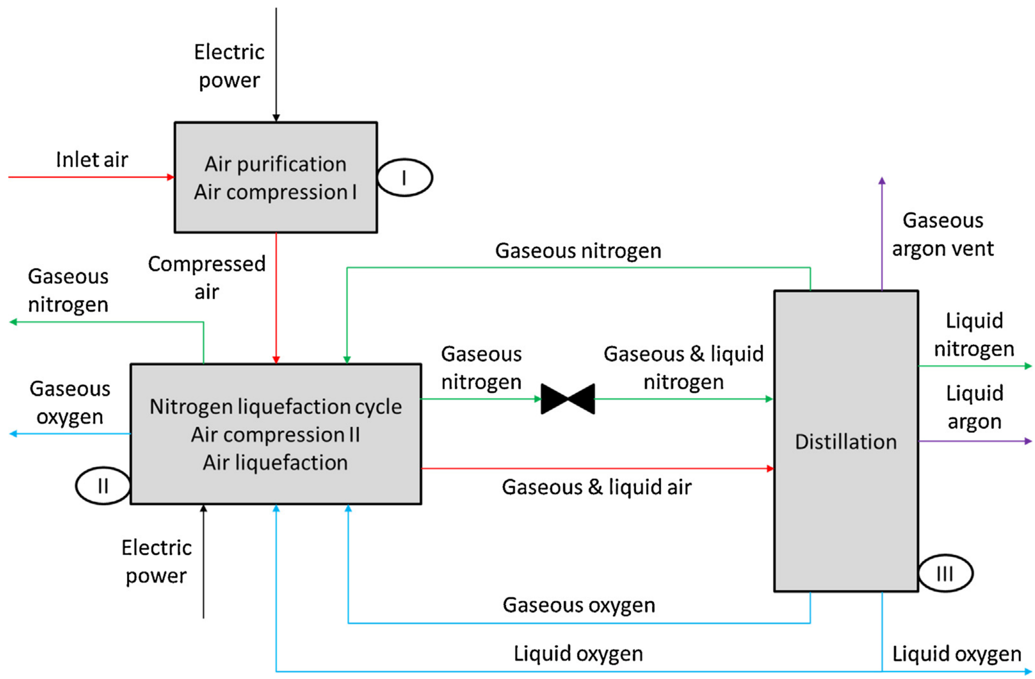

Fig. 4. ASU plant representative block flow diagram.

Indeed, all ASUs consist of the three main sections that are highlighted in yellow in Fig. 3 and represented as black-boxes in Fig. 4.

By approximating one single IGP site with the BFD shown in Fig. 4, the following mathematical expressions can be used to model its operation:

- one equation relating the power consumed by compressor $C1$ on the inlet air flowrate (black-box I);
- one equation connecting the total power consumed by compressors $C2$ and $C3$ on some or all the streams going in or out black-box II (black-box II);
- all the component material balances on black-box II (black-box II);
- all the component material balances on the whole plant (black-box I, II and III);
- one equation that characterizes the thermal integration between the *HP* and *LP* columns (black-box III);
- one equation describing the liquid to vapour ratio achieved in the *Gaseous* & *liquid nitrogen* stream as a consequence of the expansion in the preceding valve;
- one or more additional correlative/a priori expressions that are needed to make the number of independent variables of the analysed IGP site model equal the number of degrees of freedom of the real IGP site (typically these equations are used to account for some physical constraints that have been "lost" in the approximation of all the distillation columns as a single black-box);
- one maximum and one minimum constraint for each variable of the analysed IGP site.

All the above listed equations are written under the following assumptions that ensure the achieved system to be algebraic and linear:

- the ASU is assumed to operate in steady-state conditions;
- the efficiency and compression ratios of the turbo machinery are fixed;
- the temperature levels inside black-box II are constant;
- the inlet air dry composition and temperature are constant;
- the evaporation rate of the nitrogen expansion valve (black valve in Fig. 4) is set to a constant value;
- nitrogen/oxygen latent heat of vaporization is set to a constant value;
- the reflux ratios and boil-ups of the distillation columns are fixed;
- the compositions of all the streams do not vary.

Before proceeding, it should be noted that no thermal balances have been written, except for the one relating to the *HP-LP* columns thermal integration. The reasons of this choice will be explained later. Moreover, observe that all the listed equations are chosen as to provide a precise description of those phenomena that strongly affect ASUs operation. For instance, the accurate modelling of the thermal integration between *HP* and *LP* columns is essential to ensure the feasibility of the model predictions, the correct estimation of the liquid to vapour ratio in *Gaseous* & *liquid nitrogen* is fundamental to correctly predict the produced liquid nitrogen and so on. The aforementioned equations are also configured as to include all the variables that are commonly exploited to adjust ASUs operation:

- the inlet air flowrate (*Inlet air*) that is used to globally set the production level;
- the nitrogen flowrate to the nitrogen liquefaction cycle (*Gaseous nitrogen*) that can be changed to regulate the ratio of produced liquid nitrogen to the produced liquid oxygen;
- the gaseous oxygen flowrate to the nitrogen liquefaction cycle (*Gaseous oxygen*) that is employed to ensure the thermal feasibility in the multi-stream heat exchanger (Fig. 3);
- the gaseous nitrogen and oxygen flowrates leaving the nitrogen liquefaction cycle (*Gaseous nitrogen* and *Gaseous oxygen*) that define the production of gaseous products.

Finally, it is relevant to discuss some of the above listed assumptions that might appear unusual:

- The hypothesis of steady-state operation is acceptable since the characteristic time of the supply-chain network is typically much greater than the time constant of an ASU;
- All the assumptions relating to intrinsic properties of the ASUs equipment (efficiencies and compression ratios of the turbo machinery, temperature levels, reflux ratios and boil-ups of the distillation columns and so on) are acceptable because ASUs are very sensitive to the modification of these parameters. Therefore, the mentioned variables are never intentionally changed in operation in the industrial practice;
- The hypothesis of constant composition for all the streams is acceptable because of their nature of final products or vents (see Figs. 3 and 4).

Once the formal model of the single IGP site is available, it is finally needed to evaluate its parameters relating to either the features of the site-specific equipment (compressors, valves, distillation columns and so on) or some standard plant operation rules (vents composition, products purity and so on). These parameters can be partially assigned a priori but some of them have to be evaluated by means of a regression procedure based on experimental data sets or data coming from rigorous simulations (Aspen HYSYS, PRO/II, etc.). The usage of regression procedures ensures some relevant benefits:

- It allows reducing the mismatch between the linear model predictions and the real operation, depending on the non-linear behaviour of the real ASU;
- It guarantees thermal balances to be indirectly satisfied in orders of magnitude (this is why almost no thermal balances have been added to the previously described model equation list).

At this point, the model of a single IGP ASU has been fully detailed.

3.2. Integration of single ASU models into the IGP production network model

Once the modelling strategy described in Section 3.1 is applied to each of the IGP sites, all of the corporate production sources will have been represented. However, these individual IGP plant models must be employed, in turn, to build a model of the overall IGP production network, suitable for its simulation inside a certain time interval. As with the supply-chain modelling, addressed in Section 2, this simulation horizon is discretized into time intervals, whose length is defined a priori. In addition, the two time discretization grids, the one relating to the supply-chain network and the other referring to the production level, are chosen to be identical (N_g^{eq} and the time intervals are identical). Notice that, in principle, it might also be of interest to employ different time grids for the supply-chain network and the production level. Of course, the length of the discretization intervals belonging to the production level discretization grid must be much greater than the characteristic time required to complete an ASU transient (ASU models are steady-state models). The use of different discretization grids might help in considering the effect of the energy price fluctuation over a 24 h period. Moreover, it could also allow computing more detailed optimal operating conditions for the IGP production sites. The generalization of the proposed single-grid framework to a multi-grid framework will be addressed in future work.

The model of the overall IGP production network includes, at first, $N_g^{eq}N_s$ sets of equations and bounds, one for each time interval and IGP plant. The set of equations and bounds, referring to the ith IGP site and the tth discretization interval, simply is the model of the ith IGP site (already available) applied to the tth time interval. In this way, each IGP production plant is allowed to run in a potentially different steady-state operating condition in each time interval. The mathematical formulation of this first portion of the IGP production level model is reported in Eqs. (9) and (10).

$$\mathbf{E}_i\mathbf{w}_{it}^P = \mathbf{e}_i \quad \forall\, i, t : MM_{it} = 1 \tag{9}$$

$$\mathbf{w}_i^{MIN} \le \mathbf{w}_{it}^P \le \mathbf{w}_i^{MAX} \quad \forall\, i, t : MM_{it} = 1 \tag{10}$$

In terms of notation:

- $\mathbf{w}_{it}^P$ is the vector consisting of the variables of the ith IGP plant model applied inside the tth time interval;
- $\mathbf{w}_i^{MIN}$ and $\mathbf{w}_i^{MAX}$ are the minimum and maximum thresholds for the variables of the ith IGP site model, respectively;
- $\mathbf{E}_i$ is the coefficients matrix of the linear system constituting the model of the ith IGP site (already available);
- $\mathbf{e}_i$ is the right-hand terms vector of the same linear system mentioned in the previous bullet.

The remaining portion of the IGP production network model consists of the so-called anti-ringing constraints. The anti-ringing constraints are inequalities whose aim is to prevent the IGP sites from dramatically varying their operating conditions between two adjacent time intervals. They are essential since it is infeasible to impose severe changes in the ASUs operating conditions in consecutive time periods due to the subsequent mechanical stress on the equipment. These inequalities, which are described in Eqs. (11) and (12), are included in the model of the IGP production network only for those pairs of discretization intervals where the IGP sites are active. In detail, only if the ith IGP site is active at the beginning of the first discretization interval ($MV_i^0 = 1$) or in both the tth and the $(t-1)$th discretization intervals ($MM_{it} = MM_{i(t-1)} = 1$), the corresponding anti-ringing constraints will be imposed. Notice that $\mathbf{MV}^0$ is the initial maintenance vector, whose ith element has a value of one if the ith IGP plant is active at the beginning of the first discretization interval and a value of zero otherwise.

$$w_{im}^{P,0} - \mu_{im}^{AR}\left(w_{im}^{MAX} - w_{im}^{MIN}\right) \le w_{im1}^{P} \le w_{im}^{P,0} + \mu_{im}^{AR}\left(w_{im}^{MAX} - w_{im}^{MIN}\right)$$
$$\forall\, i, m : MM_{i1} = MV0_i = 1 \tag{11}$$

$$-\mu_{im}^{AR}\left(w_{im}^{MAX} - w_{im}^{MIN}\right) \le w_{imt}^{P} - w_{im(t-1)}^{P} \le \mu_{im}^{AR}\left(w_{im}^{MAX} - w_{im}^{MIN}\right)$$
$$\forall\, i, m, t \ne 1 : MM_{it} = MM_{i(t-1)} = 1 \tag{12}$$

In terms of notation:

- $w_{im}^{P,0}$ is the value of the mth independent variable of the ith IGP site model at the beginning of the first time interval;
- w_{im}^{MAX} and w_{im}^{MIN} are the maximum and minimum threshold for the mth independent variable of the ith IGP plant, respectively;
- w_{imt}^{P} represents the value of mth independent variable belonging the ith IGP production plant in the tth time interval;
- μ_{im}^{AR} are assigned coefficients that define the severity of the anti-ringing and vary in (0, 1].

The complete model of the IGP production network finally consists of Eqs. (9)–(12). It should be noted that the proposed production level model is much more accurate and reliable than that typically employed in the literature, where no anti-ringing is used and the production plants are often simply considered as product sources, characterized by a minimum and maximum production volume. This specific feature of the model developed for the IGP production network allows the proposed integrated supply-chain/production optimization strategy to be much more realistic than many of those advanced in the literature.

4. Objective function definition and optimization problem formulation and implementation

Once the models for the supply-chain network, storage system and production level of a generic IGP are complete, the inte-grated optimization strategy for the supply-chain and production networks still requires the definition of a proper objective function. The objective function formulation is detailed in Section 4.1. Finally, the IGP global optimization problem needs to be formulated and efficiently implemented into a numerical code. This is addressed in Section 4.2.

4.1. Objective function selection

The objective function plays the key role of global cost-based performance indicator measuring the profitability of an IGP business. Here it is formulated as the sum of all the relevant costs incurred by the IGP on a certain horizon. This time interval is managed via discretization as for the simulation horizon of the supply-chain network and production level. In detail, the employed discretization grid equals those detailed in Sections 2 and 3 (N_g^{eq} and the discretization intervals are identical). Of course, observe that if two different discretization grids were employed for the produc-tion and supply-chain network, then the supply-chain related costs should refer to the supply-chain related discretization grid while the production related costs should refer to the production related discretization grid. That is the subject of future work.

The costs that are considered in the detailed objective function formulation include:

- The total delivery expenses incurred by the IGP over the chosen planning horizon, including the shipments via IGP production sites (Eq. (13)) and the shipments via competitor sites (Eq. (14));
- The total costs incurred by the IGP over the chosen planning horizon, connected with the purchase of product needed for the shipments upon payment (Eq. (15));
- The total production expenses incurred by the IGP over the chosen production horizon (Eq. (16)).

Therefore, the mathematical expression for the objective function is given by Eq. (17).

$$TSC_{LN}^{STD} = \sum_{i=1}^{N_s} \sum_{j=1}^{N_{cl}} \alpha_{ij} d_{ij}^{LN} \sum_{l=1}^{N_p} C_l^{SP} \sum_{t=1}^{N_g^{eq}} \left(\frac{S_{ijlt}^{LN}}{cmc} \right) \quad (13)$$

$$TSC_{LN}^{SW,BY} = \sum_{k=1}^{N_{cm}} \sum_{j=1}^{N_{cl}} \varepsilon_{kj} d_{kj}^{CM} \sum_{l=1}^{N_p} C_l^{SP} \left[\sum_{t=1}^{N_g^{eq}} \left(\frac{S_{kjlt}^{CM,SW}}{cmc} \right) + \sum_{t=1}^{N_g^{eq}} \left(\frac{S_{kjlt}^{CM,BY}}{cmc} \right) \right] \quad (14)$$

$$TPC_{LN}^{BY} = \sum_{k=1}^{N_{cm}} \sum_{j=1}^{N_{cl}} \sum_{l=1}^{N_p} C_{lk}^{BY} \sum_{t=1}^{N_g^{eq}} S_{kjlt}^{CM,BY} \quad (15)$$

$$TPRC_{LN} = \sum_{i=1}^{N_s} C_i^{EN} \sum_{t=1}^{N_g^{eq}} W_{it}^{C,TOT} \quad (16)$$

$$f_{obj} = TSC_{LN}^{STD} + TSC_{LN}^{SW,BY} + TPC_{LN}^{BY} + TPRC_{LN} \quad (17)$$

In terms of notation:

- d_{ij}^{LN} and d_{kj}^{CM} are the average road distances between the jth IGP customer and either the ith IGP site or the kth competitor site;
- α_{ij} and ε_{kj} are adaptive coefficients that can be often (but not always) used to prevent some specific customer-site assignments;
- C_l^{SP} is the delivery cost per unit distance of a standard IGP tanker of lth product;
- C_{lk}^{BY} is the purchase cost per unit mass of the lth product from the kth competitor site;
- C_i^{EN} is the expected electric energy price per unit electric power for the ith IGP site;
- cmc is the average capacity of a standard IGP tanker;
- $W_{it}^{C,TOT}$ is the total compression power consumed by the ith IGP site in the tth discretization interval;
- TSC_{LN}^{STD} is the total cost incurred by the IGP over the selected horizon, relating to the shipments via IGP production sites;
- $TSC_{LN}^{SW,BY}$ is the total cost incurred by the IGP over the selected horizon, relating to the shipments via competitor sites;
- TPC_{LN}^{BY} is the total cost, incurred by the IGP over the selected horizon, connected with the purchase of product needed for the shipments upon payment;
- $TPRC_{LN}$ is the total production cost incurred by the IGP over the production horizon;
- f_{obj} is the objective function of the IGP global optimization problem.

Three final remarks are needed. First, notice that some cost sources, such as the expenses due to the cryogenic storages and the costs for the IGP plants' maintenance, are neglected due to their limited relevance. Indeed, since ASUs are very energy intensive, the only relevant production cost is that of energy (there is no raw material cost since air is free of charge). In addition, observe that the energy cost is considered constant over time even though future version of the methodology may implement a time-dependent energy cost. Secondly, observe the specific structure of TSC_{LN}^{STD} and $TSC_{LN}^{SW,BY}$ where each shipment is divided by the average capacity of a standard IGP tanker. This formulation is employed in order to account for the possibility of using a single tanker to restock several different customers. Indeed, thanks to this strategy, the delivery expenses are evaluated on the basis of the average number of tankers needed to satisfy all the customers' requests and not on the number of shipments to be performed (this last statement refers to each discretization interval of the horizon over which f_{obj} is evaluated). Finally, it is essential to highlight the importance of α_{ij} and ε_{kj} coefficients. These parameters, which are typically set to one, can be adjusted to force the supply-chain network to fulfil some specific external requirements. For instance, if it is needed that each customer is supplied by only one source, it is sufficient to iteratively rescale the proper α_{ij} and ε_{kj} coefficients to allow for this external constraint, without the need for adding integer variables. The iterative rescaling procedure that has to be followed in this case can be summarized in the following steps:

- Solution of the IGP global optimization problem with all α_{ij} and ε_{kj} coefficients set to one;
- Identification of all those customers whose demand is fulfilled by more than one production site and definition of the main and secondary customer-site assignments (the main customer-site assignments are those that cover most of the customers' demands);
- Rescaling of all the α_{ij} and ε_{kj} coefficients relating to secondary customer-site assignments and solution of a new IGP global optimization problem;
- Check of the residual presence of customers supplied by multiple sources and eventual reapplication of the steps discussed in the

last three bullets (typically this is not needed and convergence is reached after the first trial).

Notice that here only the use of α_{ij} and ε_{kj} coefficients for avoiding multiple customer-site assignments is shown but this is not the only way in which these coefficients can be employed. Therefore, α_{ij} and ε_{kj} can be considered as multi-purpose supply-chain network tuning coefficients.

4.2. Global IGP optimization problem formulation and implementation

At this point, the proposed integrated strategy for the optimal management of the supply-chain network and production level of a generic IGP can be formalized into an optimization problem, called the IGP global optimization problem (Eq. (18)).

$$\begin{cases} \underset{*}{Min}\{f_{obj}\} \\ \mathbf{s.t.} \\ \text{Eq. (1), Eq. (2), Eq. (3), Eq. (4), Eq. (5)} \\ \text{Eq. (6), Eq. (7), Eq. (8)} \\ \text{Eq. (9), Eq. (10), Eq. (11), Eq. (12)} \end{cases} \tag{18}$$

In terms of notation * stands for all the optimization variables, i.e., S_{ijlt}^{LN}, $S_{kjlt}^{CM,SW}$, $S_{kjlt}^{CM,BY}$, G_{ilt} and $\mathbf{w}_{it}^{P}$. Observe that F_{ilt}^{LN} and $W_{it}^{C,TOT}$ are not explicitly listed as optimization variables because they are already included as single elements or sum of elements into the $\mathbf{w}_{it}^{P}$ vectors. Moreover, MM_{it} variables are also not considered as optimization variables. This choice is reasonable since ASUs are typically not continuously switched on/off to avoid thermal and mechanical stress on the equipment. The maintenance matrix is only included to account for scheduled/emergency maintenance periods, occurring typically only few times a year.

The IGP global optimization problem (Eq. (18)) is clearly a very large-scale sparse LP, whose solution consists of the optimal operating condition of a generic IGP on a user-defined time interval. Its efficient solution is fundamental to ensure the online applicability of the proposed integrated supply-chain/production optimization approach. Moreover, when it comes to the numerical implementation, it is essential to preserve the strategy comprehensiveness. Indeed, to the authors' knowledge no such comprehensive and detailed approaches for IGPs have been implemented and published in the literature. Therefore, Eq. (18) is coded into a C++ software, named *ASUNetworkSupplyChain.exe*, that has some specific features detailed in the following lines.

At first, it employs BzzMath algorithms to ensure the highest efficiency. Indeed, especially BzzMath LP solver, based on the Attic Method (Buzzi-Ferraris, 2011; Manenti and Buzzi-Ferraris, 2012), is significantly more performing than the standard LP solution pack-ages based on simplex-like and/or interior point strategies.

Secondly, it uses ad-hoc pre-processing algorithms developed to reduce as much as possible the problem size by eliminating "useless" variables, thus decreasing the required computational effort. These methods, which are not described in detail for the sake of brevity, are able to identify variables, whose optimal value is known a priori, and eliminate them from the overall optimization problem. Their effectiveness is relevant because they typically manage to reduce the initial problem size by approximately 50% (the more R_{jlt} are zeroes, the better for the pre-processing method is).

Finally, *ASUNetworkSupplyChain.exe* is both a solver and an inter-preter that is not only able to efficiently solve Eq. (18) but also to read specific sets of .txt input files, containing the features of a generic IGP production and supply-chain network. This allows the software to be applied to every IGP and/or to support updates and changes into the IGP characteristics in the course of time.

As a result of these features of its implementation, C_{lk}^{BY} is able to solve problems of very large size, up to 1 million variables, in only some seconds while preserving all the comprehensive properties of the mathematical methodology (Eq. (18)), on which it is based. Consequently, it is well suitable for the online usage.

The online applicability ensures the possibility of coupling *ASUNetworkSupplyChain.exe* with a rolling horizon methodology, in order to reduce the effect of the long term uncertainties in the program input data (customers demand previsions $\left(R_{jlt}\right)$, competitors SWAP/purchase withdrawals (FP_{ilt} / FNP_{ilt}) and availabilities $\left(F_{klt}^{CM,MAX} / FBY_{klt}^{CM,MAX}\right)$ and so on). This also makes the coded software suitable for the real industrial applications.

5. Case study: Linde Gas Italia S.r.l.

The proposed integrated solution for the optimization of the supply-chain network and production level of a generic IGP is validated and tested on a case study derived from the real supply-chain and production network of Linde Gas Italia S.r.l. In order to demonstrate the benefits offered by the proposed methodology, its performance is compared to that of several conventional options that oversimplify the production level model, as it is typically done in the literature. The features of the simplified version of the real Linde Gas Italia S.r.l. supply-chain network, employed in the case study, are described in detail in Section 5.1. The structure of the production network, derived with the approach detailed in Section 3, is addressed in Section 5.2 and the production level conventional models, developed with literature-based approaches, are described in Section 5.3. Finally, the test case numerical results and their validity even in the case of uncertain input data are discussed in Sections 5.4 and 5.5, respectively.

5.1. Linde Gas Italia S.r.l.: the simplified supply-chain network

Linde Gas Italia S.r.l. supplies a large number of customers in Italy and competes with several world-class companies like Air Liquide S.p.a., Rivoira, Siad, Sapio, Sol and so on. Its supply-chain network is enormous and counts thousands of different entities. The proposed approach has been successfully tested also on large-scale case studies (not reported here) but the aim of the current paper is to highlight the benefits of this methodology compared to the conventional solutions. For this purpose, a small scale problem is much more meaningful. The features of the simplified small-scale supply-chain network, employed in the case study, are reported

in Table 1 (N_{cm}^{C} stands for the number of competitor companies included in the IGP supply-chain). The supply-chain model equations have already been described in Section 2.

It should be noted that all fifteen customers listed in Table 1 are real Linde Gas Italia S.r.l. customers and the same can be said for both the three production sites (Trieste, Bologna and Terni) and the two competitor sites (Ostuni and Grugliasco). In addition, notice that only three products, all in liquid phase, are included in the case study:

- liquid nitrogen at almost 100% purity on a molar basis (LIN);
- liquid oxygen at 99.95% purity on a molar basis ($LOX_{3.5}$);
- liquid argon at almost 100% purity on a molar basis (LAR).

This choice is justified since most of the cryogenic products are delivered in liquid phase via tankers while the market of gas phase pipeline-supplied products is much less important. However, an additional validation study (not reported here) including gaseous products has been successfully executed.

It is also relevant to highlight that the customers demand $\left(R_{jlt}\right)$, not reported here for the sake of brevity, is randomly generated as

Table 1
Simplified supply-chain network main features.

Supply-chain network size		Truck shipments cost (C_l^{SP}) [€/km]		Products purchase cost (C_{lk}^{BY}) [€/kg]		Products nominal economic prices (MEV_l) [–]	
N_s	3	LIN	1.5	LIN (Ostuni)	0.08	LIN	1
N_{cl}	15			$LOX_{3.5}$ (Ostuni)	0.16		
N_{cm}	2	$LOX_{3.5}$	1	LAR (Ostuni)	0.64	$LOX_{3.5}$	2
N_{cm}^C	1			LIN (Grugliasco)	0.08		
N_p	3	LAR	1	$LOX_{3.5}$ (Grugliasco)	0.16	LAR	8
N_g^{eq}	14			LAR (Grugliasco)	0.64		

α_{ij} and ε_{kj} parameters are all set to one.
d_{ij}^{LN} and d_{kj}^{CM} road distances are not reported for the sake of brevity.
The supply-chain discretization grid is made of discretization intervals lasting one day each.

to guarantee a global demand of LIN, $LOX_{3.5}$ and LAR that is comparable to the one that Linde Gas Italia S.r.l. has to fulfil in a typical two week period. In addition, the maximum availabilities for shipments via SWAP both for the single competitor sites $\left(F_{klt}^{CM,MAX}\right)$ and the competitor companies ($FDCM_{hl}$) and the maximum available volumes for shipments upon payment $\left(FBY_{klt}^{CM,MAX}\right)$ are derived from data provided by Linde Gas Italia S.r.l. The same approach is employed to compute the product withdrawals, performed by the competitor sites, for shipments via SWAP (FP_{ilt}) and upon payment (FNP_{ilt}).

Finally no uncertainty is considered in the reported input data in this current case study. This might seem not reasonable but it will be demonstrated in Section 5.4 that the results achieved in these ideal conditions, in terms of optimization approach and performance comparison results, can be immediately extended to the real case where uncertainties cannot be ignored.

5.2. *Linde Gas Italia S.r.l.: the production network*

Linde Gas Italia S.r.l. production network is made of three ASU plants, named Trieste, Bologna and Terni based on their geographic location. The model of the above-mentioned production network is essential for the execution of the current test case and is obviously addressed with the strategies described in Section 3. All the material needed in this stage, such as the plant process flow diagrams (PFDs) and typical operating conditions, has been provided by Linde Gas Italia S.r.l. The results coming from the application of the above-mentioned modelling strategy include:

- the block flow diagrams (BFDs) of Trieste, Bologna and Terni plants reported in Figs. 5–7;
- the corresponding single plant models reported in Eqs. (19)–(28), Eqs. (29)–(38) and Eqs. (39)–(49).

In detail, the equations constituting Trieste model are the following:

$$\omega_0^{C1161,TS} + F_A^{TS}\omega_1^{C1161,TS} - W_{C1161}^{TS} = 0 \tag{19}$$

$$\begin{aligned}&\omega_0^{C1361-2,TS} + \omega_1^{C1361-2,TS}\left(W_{N_2}^{LP,TS} - GAN_{LP}^{TS}\right)\\&+\omega_2^{C1361-2,TS}\left(W_{N_2}^{LP,TS} - GAN_{LP}^{TS} + W_{N_2}^{AP,TS}\right)\\&+\omega_3^{C1361-2,TS}\left(W_{N_2}^{LP,TS} - GAN_{LP}^{TS} + W_{N_2}^{AP,TS} - GAN_{HP}^{TS}\right) - W_{C1361}^{TS} = 0\end{aligned} \tag{20}$$

$$W_{N_2}^{LP,TS} + W_{N_2}^{AP,TS} - GAN_{LP}^{TS} - GAN_{HP}^{TS} - W_{N_2,L}^{RAP,TS} - W_{N_2,G}^{RAP,TS} = 0 \tag{21}$$

$$\left(1-\alpha_v^{TS}\right)W_{N_2,G}^{RAP,TS} - \alpha_v^{TS}W_{N_2,L}^{RAP,TS} = 0 \tag{22}$$

$$F_A^{TS}x_A^{N_2} - LIN^{TS} - GAN_{LP}^{TS} - GAN_{HP}^{TS} - V_{Ar}^{TS}x_V^{N_2} = 0 \tag{23}$$

$$F_A^{TS}x_A^{O_2} - \left(LOX_{3.5}^{TS} + GOX_{LP}^{TS} + GOX_{HP}^{TS}\right)x_{3.5}^{O_2} = 0 \tag{24}$$

$$F_A^{TS}x_A^{Ar} - LAR^{TS}\left(LOX_{3.5}^{TS} + GOX_{LP}^{TS} + GOX_{HP}^{TS}\right)x_{3.5}^{Ar} - V_{Ar}^{TS}x_V^{Ar} = 0 \tag{25}$$

$$\begin{aligned}&W_{N_2,L}^{RAP,TS} - \mathrm{RR}_{AP}^{TS}W_{N_2,G}^{RAP,TS} - \mathrm{RR}_{BP}^{TS}W_{N_2}^{LP,TS} - LIN^{TS} - \gamma_{REF}GAN_{LP}^{TS}\\&+\left(1-\mathrm{RR}_{AP}^{TS}\right)BU_{BP}^{TS}\frac{\Delta h_{ev}^{O_2}}{\Delta h_{ev}^{N_2}}\left(LOX_{3.5}^{TS} + GOX_{LP}^{TS} + GOX_{HP}^{TS}\right) = 0\end{aligned} \tag{26}$$

$$V_{Ar}^{TS} - \alpha_{Ar}^{TS}LAR^{TS} - \beta_{Ar}^{TS} = 0 \tag{27}$$

$$\phi_{BAP}\left(LOX_{3.5}^{TS} + GOX_{LP}^{TS} + GOX_{HP}^{TS}\right) - \left(1-RR_{BP}^{TS}\right)W_{N_2}^{LP,TS} - V_{Ar}^{TS}x_V^{N_2} = 0 \tag{28}$$

The equalities included in Bologna model are:

$$\omega_0^{C1161,BO} + F_A^{BO}\omega_1^{C1161,BO} - W_{C1161}^{BO} = 0 \tag{29}$$

$$\omega_0^{C1461,BO} + W_{N_2}^{AP,BO}\omega_1^{C1461,BO} - W_{C1461}^{BO} = 0 \tag{30}$$

$$W_{N_2}^{AP,BO} - W_{N_2,L}^{RAP,BO} - W_{N_2,G}^{RAP,BO} = 0 \tag{31}$$

$$\left(1-\alpha_v^{BO}\right)W_{N_2,G}^{RAP,BO} - \alpha_v^{BO}W_{N_2,L}^{RAP,BO} = 0 \tag{32}$$

$$F_A^{BO}x_A^{N_2} - GAN^{BO} - LIN^{BO} - V_{Ar}^{BO}x_V^{N_2} = 0 \tag{33}$$

$$F_A^{BO}x_A^{O_2} - LOX_{2.5}^{BO}x_{2.5}^{O_2} - LOX_{3.5}^{BO}x_{3.5}^{O_2} - GOX^{BO}x_{3.5}^{O_2} = 0 \tag{34}$$

$$F_A^{BO}x_A^{Ar} - LOX_{2.5}^{BO}x_{2.5}^{Ar} - LOX_{3.5}^{BO}x_{3.5}^{Ar} - GOX^{BO}x_{3.5}^{Ar} - V_{Ar}^{BO}x_V^{Ar} - LAR^{BO} = 0 \tag{35}$$

$$\begin{aligned}&W_{N_2,L}^{RAP,BO} + \left(1-\mathrm{RR}_{AP}^{BO}\right)BU_{BP}^{BO}\frac{\Delta h_{ev}^{O_2}}{\Delta h_{ev}^{N_2}}\left(LOX_{2.5}^{BO} + LOX_{3.5}^{BO}\right)\\&-LIN^{BO} - \mathrm{RR}_{AP}^{BO}W_{N_2}^{AP,BO} - \mathrm{RR}_{BP}^{BO}GAN^{BO} = 0\end{aligned} \tag{36}$$

$$V_{Ar}^{BO} - \alpha_{Ar}^{BO}LAR^{BO} - \beta_{Ar}^{BO} = 0 \tag{37}$$

$$GOX^{BO} - \alpha_{O_2}^{BO}LIN^{BO} - \beta_{O_2}^{BO} = 0 \tag{38}$$

Finally, the equations representing Terni model are as follows:

$$F_A^{TR}\omega^{C01,TR} - W_{C01}^{TR} = 0 \tag{39}$$

$$\begin{aligned}&\omega_1^{C20-1,TR}\left(W_{N_2}^{LP,TR} - GAN^{TR}\right)\\&+\omega_2^{C20-1,TR}\left(W_{N_2}^{AP,TR} + W_{N_2}^{LP,TR} - GAN^{TR}\right) - W_{C20-1}^{TR} = 0\end{aligned} \tag{40}$$

$$W_{N_2}^{AP,TR} + W_{N_2}^{LP,TR} - GAN^{TR} - W_{N_2,L}^{RAP,TR} - W_{N_2,G}^{RAP,TR} = 0 \tag{41}$$

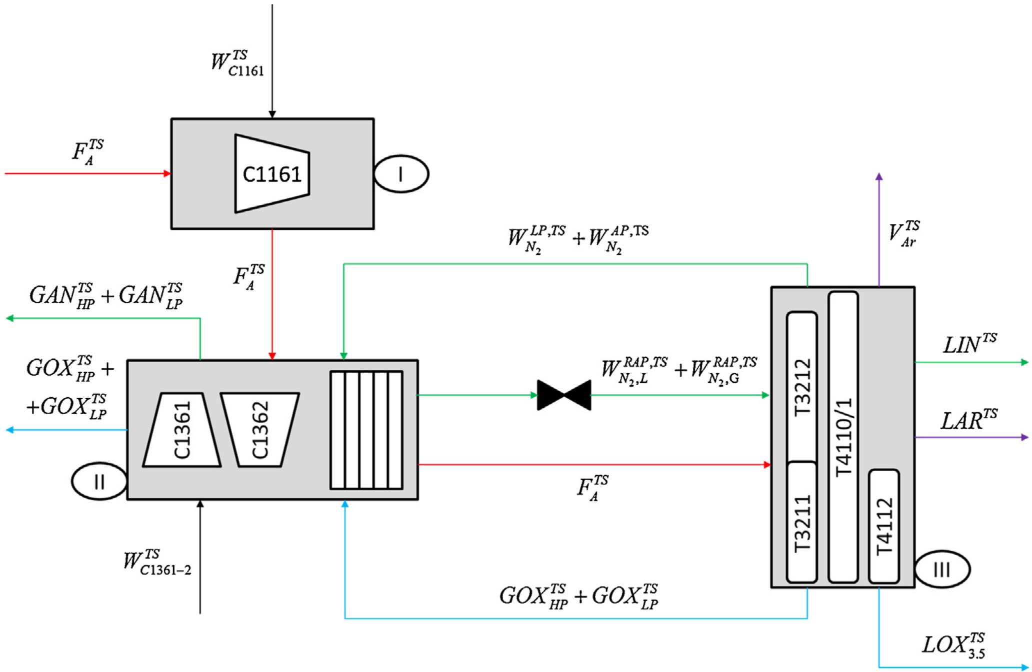

Fig. 5. Trieste representative block flow diagram.

$$\left(1-\alpha_v^{TR}\right) W_{N_2,G}^{RAP,TR} - \alpha_v^{BO} W_{N_2,L}^{RAP,TR} = 0 \tag{42}$$

$$F_A^{TR} x_A^{N_2} - LIN^{TR} - GAN^{TR} - \hat{W}_{Ar}^{TR} \hat{x}_{N_2} - GAN_{WT}^{TR} = 0 \tag{43}$$

$$F_A^{TR} x_A^{O_2} - \left(LOX_{3.5}^{TR} + GOX^{TR}\right) x_{3.5}^{O_2} - \hat{W}_{Ar}^{TR} \hat{x}_{O_2} = 0 \tag{44}$$

$$F_A^{TR} x_A^{Ar} - \left(LOX_{3.5}^{TR} + GOX^{TR}\right) x_{3.5}^{Ar} - \hat{W}_{Ar}^{TR} \hat{x}_{Ar} = 0 \tag{45}$$

$$W_{N_2,L}^{RAP,TR} - \mathrm{RR}_{AP}^{TR} W_{N_2,G}^{RAP,TR} - \mathrm{RR}_{BP}^{TR} W_{N_2}^{LP,TR} - LIN^{TR} + \left(1-\mathrm{RR}_{AP}^{TR}\right) BU_{BP}^{TR} \frac{\Delta h_{ev}^{O_2}}{\Delta h_{ev}^{N_2}} \left(LOX_{3.5}^{TR} + GOX^{TR}\right) = 0 \tag{46}$$

$$F_A^{TR} x_A^{O_2} \frac{x_{N_2}^{\circ}}{x_{O_2}^{\circ}} - \left(1 - RR_{BP}^{TR}\right) W_{N_2}^{LP,TR} - \hat{W}_{Ar}^{TR} \hat{x}_{N_2} = 0 \tag{47}$$

$$GAN_{WT}^{TR} - \alpha_G GAN^{TR} = 0 \tag{48}$$

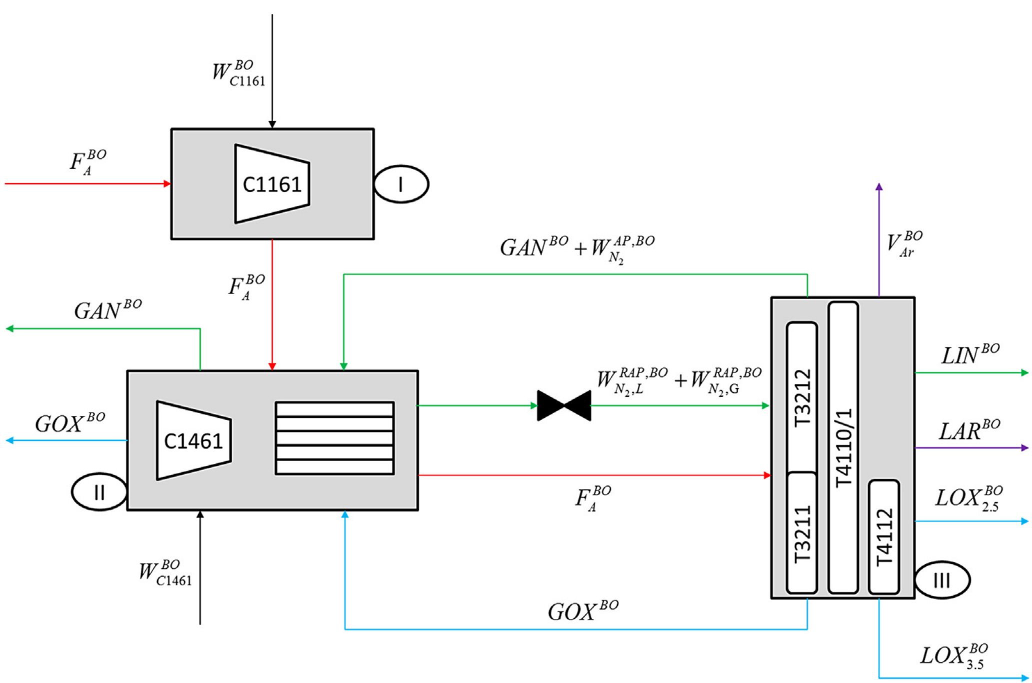

Fig. 6. Bologna representative block flow diagram.

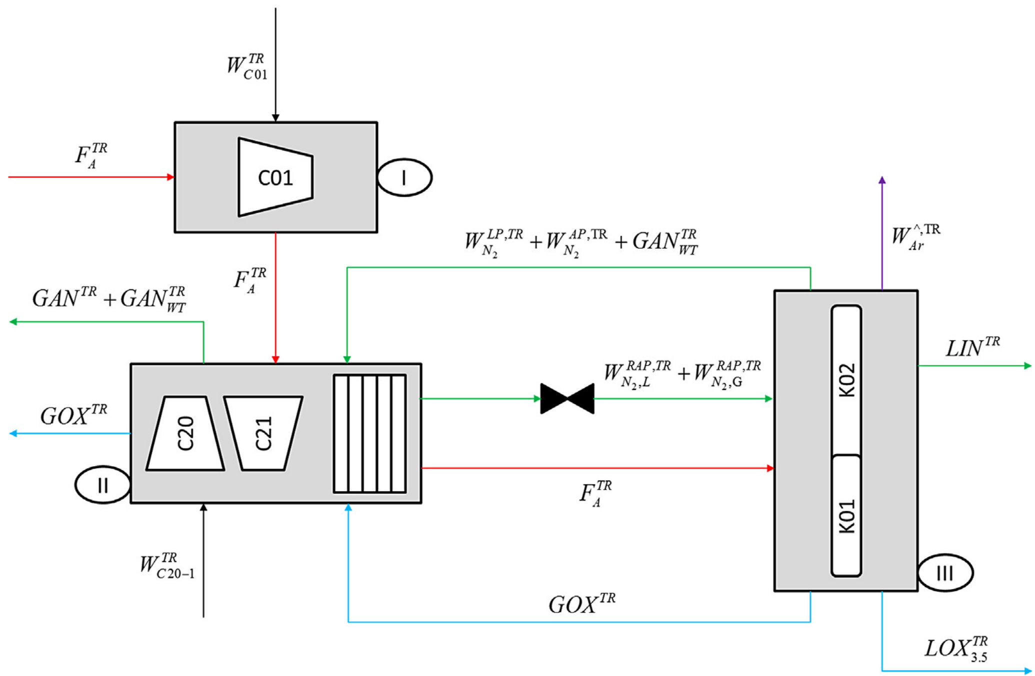

Fig. 7. Terni representative block flow diagram.

$$GOX^{TR} - \alpha_{O_2}^{TR} LIN^{TR} - \beta_{O_2}^{TR} = 0 \tag{49}$$

Notice that no bound constraints, relating to the three plant models, are described in the above for the sake of brevity. In addition, the anti-ringing constraints formulation for the entire production level has been already addressed in Section 3 and is not repeated here.

For both the above-mentioned figures and equations the employed notation is the following:

- F_A^{TS}, F_A^{BO} and F_A^{TR} are the inlet air flowrates for Trieste, Bologna and Terni plants, respectively;
- W_{C1161}^{TS}, $W_{C1361-2}^{TS}$, W_{C1161}^{BO}, W_{C1461}^{BO}, W_{C01}^{TR} and W_{C20-1}^{TR} are the power consumptions of the inlet air and refrigeration cycle compressors for Trieste, Bologna and Terni plants, respectively;
- LIN^{TS}, LIN^{BO} and LIN^{TR} are the liquid nitrogen flowrates produced in Trieste, Bologna and Terni plants, respectively;
- $LOX_{3.5}^{TS}$, $LOX_{3.5}^{BO}$, $LOX_{2.5}^{BO}$ and $LOX_{3.5}^{TR}$ are the liquid oxygen flowrates produced in Trieste, Bologna and Terni plants, respectively (subscripts "3.5" and "2.5" refer to a purity of 99.95% and 99.5% on a molar basis, respectively);
- LAR^{TS} and LAR^{BO} are the liquid argon flowrates produced in Trieste and Bologna plants, respectively;
- GAN_{HP}^{TS}, GAN_{LP}^{TS}, GAN^{BO}, GAN^{TR} and GAN_{WT}^{TR} are the gaseous nitrogen flowrates produced in Trieste, Bologna and Terni plants, respectively (subscripts "*HP*" and "*LP*" refer to high pressure and low pressure nitrogen while subscript "*WT*" stands for waste nitrogen);
- GOX_{HP}^{TS}, GOX_{LP}^{TS}, GOX^{BO} and GOX^{TR} are the gaseous oxygen flowrates produced in Trieste, Bologna and Terni plants, respectively (once again, subscripts "*HP*" and "*LP*" refer to high pressure and low pressure oxygen);
- V_{Ar}^{TS} and V_{Ar}^{BO} are the second argon column vents in Trieste and Bologna plants, respectively;
- $W_{\hat{Ar}}^{TR}$ is the overhead of the first argon column in Terni plant (see the descriptions below for further information);
- $W_{N_2}^{LP,TS}$, $W_{N_2}^{AP,TS}$, $W_{N_2}^{AP,BO}$, $W_{N_2}^{LP,TR}$ and $W_{N_2}^{AP,TR}$ are the gaseous nitrogen flows going from the distillation section back to the nitrogen refrigeration cycle in Trieste, Bologna and Terni plants, respectively;
- $W_{N_2,L}^{RAP,TS}$, $W_{N_2,G}^{RAP,TS}$, $W_{N_2,L}^{RAP,BO}$, $W_{N_2,G}^{RAP,BO}$, $W_{N_2,L}^{RAP,TR}$, $W_{N_2,G}^{RAP,TR}$ are the gaseous and liquid nitrogen flows going from the nitrogen refrigeration cycle back to the distillation section (subscript "G" and "L" refer to gaseous and liquid nitrogen, respectively);
- $x_A^{N_2}, x_A^{O_2}, x_A^{Ar}$ represents the inlet air composition in nitrogen, oxygen and argon;
- $x_V^{N_2}, x_V^{Ar}$ represents the composition, in nitrogen and argon, of the second argon columns vent in both Trieste and Bologna plants;
- $\hat{x}_{N_2}, \hat{x}_{O_2}, \hat{x}_{Ar}$ represents the composition in nitrogen, oxygen and argon of the overhead of the first argon column in Terni plant;
- $x_{3.5}^{O_2}$, $x_{3.5}^{Ar}$ and $x_{2.5}^{O_2}$, $x_{2.5}^{Ar}$ represent the composition, in oxygen and argon, of the 99.95% and 99.5% liquid oxygen flowrates, respectively;
- $\Delta h_{ev}^{O_2}$ and $\Delta h_{ev}^{N_2}$ are the latent heat of vaporization for oxygen and nitrogen, respectively;
- all the non-listed symbols identify the adaptive parameters of the three production sites.

Some remarks on both the simplified plant BFDs and the corresponding models are appropriate.

First, notice that the block flow diagrams in Figs. 5–7 are almost identical to the one reported in Fig. 4, thus proving that the ASUs general layout is standardized and the modelling methodology pro-posed in Section 3 is reasonable. Of course, some minor differences between Figs. 5–7 and Fig. 4 can be found. The most relevant of them are detailed in Table 2. However, these unavoidable, intrinsic, minor differences are not enough to invalidate the comprehensiveness of the proposed modelling approach.

Secondly, notice that the equations constituting the three Linde Gas Italia S.r.l. plant models are fully compliant with the theoretical modelling guidelines listed in Section 3.1. This can be easily understood by analysing the information included in Table 3, where each equation of Trieste, Bologna and Terni model is organized based on its type and/or function (the notation used in Table 3 is consistent with that employed in Section 3.1 for the sake of clarity). The compliance among the theoretical modelling guidelines explained

Table 2
Comparison in terms of process layout of the three Linde Gas Italia S.r.l. plants.

Air separation unit (ASU)		Generic (Fig. 4)	Trieste (Fig. 5)	Bologna (Fig. 6)	Terni (Fig. 7)
Saleable products					
Gaseous nitrogen (GAN)	Low pressure (LP)	YES	YES	NO	NO
	High pressure (HP)	YES	YES	NO	NO
Gaseous oxygen (GOX)	Low pressure (LP)	YES	YES	NO	NO
	High pressure (HP)	YES	YES	NO	NO
Liquid nitrogen (LIN)	–	YES	YES	YES	YES
Liquid oxygen (LOX)	99.95% molar purity (3.5)	YES	YES	YES	YES
	99.5% molar purity (2.5)	YES	NO	YES	NO
Liquid argon (LAR)	–	YES	YES	YES	NO[a]
Number of compressors in the nitrogen liquefaction cycle (black-box II)		–	2	1	2
Oxygen recycle stream (black-box III to black-box II)	Gaseous	YES	YES	YES	YES
	Liquid	YES	NO	NO	NO

[a] Terni plant is supposed not to produce deliverable liquid argon (LAR).

in Section 3.1 and the equations of the three Linde Gas Italia S.r.l. plant models is a further indication that the proposed production level modelling strategy is general and reliable.

One more interesting point is the analysis of the independent variables (DOFs) for the models of the three Linde Gas Italia S.r.l. sites:

- Trieste DOFs are GAN_{HP}^{TS}, LIN^{TS}, $LOX_{3.5}^{TS}$, GOX_{HP}^{TS} and GOX_{LP}^{TS};
- Bologna DOFs are LIN^{BO}, $LOX_{3.5}^{BO}$ and $LOX_{2.5}^{BO}$;
- Terni DOFs are LIN^{TR} and $LOX_{3.5}^{TR}$.

Notice that, as it is expected, all the independent variables represent product streams produced by the ASUs but not all of them are included into the supply-chain, i.e., requested by the customers and supplied to them. Moreover, liquid argon (LAR) is not an independent variable, i.e., it cannot be produced independently of the other products. The importance of this information will become clear especially in Sections 5.3 and 5.4.

Finally, it is relevant to observe that most of the three sites adaptive parameters have a clear physical meaning. For instance, RR-like and BU-like parameters represent reflux ratios and boil-ups of the ASUs distillation columns, α_v-like parameters stand for the vaporization rates of the expansion valves belonging to the nitrogen liquefaction cycles, ω-like parameters identify structural features of the ASUs compressors and so on. Therefore, even though all these adaptive parameters have been estimated via regression based on data sets provided by Linde Gas Italia S.r.l., their resulting values retain their physical identity. This allows both the proposed ASU models being an accurate and feasible representation of the real ASU plants and the results of a careful extrapolation of them being still reasonable.

Once the results of the application of the production level modelling strategy proposed in Section 3 have been discussed, it is needed to convey the most relevant quantitative information about the production network. Table 4, which reports all these information, ends this section.

5.3. *Linde Gas Italia S.r.l.: the production network based on conventional modelling strategies*

Different and simpler approaches can be used to model the Linde Gas Italia S.r.l. production network. Here a couple of them, conven-tionally employed in literature, are reported, discussed and applied. A third one is only reported and discussed since it is very recent and cannot be considered state-of-the-art. Observe that anti-ringing constraints are not included in all of these strategies. Therefore, when the first two of them are applied to the Linde Gas Italia S.r.l. production network, the modelling of the network practically collapses into the modelling of its single ASU plants (the same would apply to the third strategy). Also, note that the single ASU models reported in the following relate to a single discretization interval over which the Linde Gas Italia S.r.l. production network must be simulated, i.e., the presentation of these models is consis-tent with the presentation logics used in Section 5.2.

The first option is to consider each ASU plant simply as a source of products. This approach is conceptually very similar to those mentioned in (Bowling et al., 2011; Julka et al., 2002; Timpe and Kallrath, 2000; Ng and Lam, 2013). It means that, for the single

Table 3
Description of the equations constituting the three Linde Gas Italia S.r.l. plants models by function and/or type.

Air separation unit (ASU)	Trieste (Fig. 5)	Bologna (Fig. 6)	Terni (Fig. 7)
Equations type or function			
Power consumption of the main air compressor (black-box I)	Eq. (19)	Eq. (29)	Eq. (39)
Power consumption of the nitrogen liquefaction cycle compressors (black-box II)	Eq. (20)	Eq. (30)	Eq. (40)
Component material balances on black-box II	Eq. (21)	Eq. (31)	Eq. (41)
Component material balances on the whole plant (black-box I, II and III)	Eqs. (23)–(25)	Eqs. (33)–(35)	Eqs. (43)–(45)
Thermal integration between *HP* and *LP* columns (black-box III)	Eq. (26)	Eq. (36)	Eq. (46)
Liquid to vapour ratio in the nitrogen stream connecting black-box II and black-box III downstream the thermal expansion valve	Eq. (22)	Eq. (32)	Eq. (42)
Additional correlative/a priori expressions to adjust the number of degrees of freedom	Eqs. (27) and (28)	Eqs. (37) and (38)	Eqs. (47)–(49)

No bound constraints are mentioned for the sake of brevity.

Table 4
Production network main features.

Initial product storages (G_{il}^{0}) [kg]			Energy costs (C_i^{EN}) [€/kW]		Linde Gas Italia S.r.l. ASUs operation (MM_{it}; MV_i^0)	
Trieste	LIN $LOX_{3.5}$ LAR	0 0 0	Trieste	1.8	Trieste	Always active
Bologna	LIN $LOX_{3.5}$ LAR	0 0 0	Bologna	1.8	Bologna	Always active
Terni	LIN $LOX_{3.5}$ LAR	0 0 –	Terni	1.8	Terni	Always active

Terni plant is supposed not to produce deliverable liquid argon (LAR).
C_i^{EN} depends on the discretization grid employed for the production network and on the standard energy cost in [€/kWh].
The discretization grid of the production network is made of discretization intervals lasting one day each and equals that of the supply-chain.

ASU, the flowrates of the produced products, in each discretization interval of the discretization grid employed for the network (in the current situation the same employed for the supply-chain), can be freely varied in between a lower and upper bound. Moreover, the single ASU is supposed to produce only those products that are included in the supply-chain (LIN, $LOX_{3.5}$ and LAR). Finally the production costs related to the whole production network can be estimated based on the products average production cost per unit mass (Eq. (50)).

$$TPRC_{LN} = \sum_{t=1}^{N_g^{eq}} \sum_{i=1}^{N_s} \sum_{l=1}^{N_p} C_{il}^{PROD} F_{ilt}^{LN} \tag{50}$$

In terms of notation, C_{il}^{PROD} is the production cost per unit mass of the lth product in the ith IGP production site.

By applying this first strategy, Trieste, Bologna and Terni models are simply reduced to bound constraints. These bounds are chosen to equal those imposed in the detailed models developed in Section 5.2. Moreover, the C_{il}^{PROD} values for the three Linde Gas Italia S.r.l. plants are computed based on the same data employed for the evaluation of the parameters belonging to the detailed ASU models (Section 5.2). Unfortunately, it is impossible to mention them in the paper since they come from restricted data.

This first production network modelling option is the simplest one and also the one that can be more commonly found in the literature.

The second option for the production network modelling is a compromise between the pure source alternative, described above, and the detailed models alternative (Section 5.2). This option can be thought as an adaptation of the methods proposed in (Manenti and Rovaglio, 2013). Here, the single ASU is modelled with only two equations plus a set of bound constraints. The first equation is used to estimate the total power consumption as a function of the pro-duced products flowrate, the second equation is used to try to force the liquid argon to fulfil the material balances (liquid argon is not a degree of freedom for a real ASU plant). These two equations are purely mathematical relations, with no direct physical meaning and include some parameters that need to be evaluated via regression. Finally, observe that here all the produced products, even those not included in the supply-chain network, are considered inside the variables pool.

When this second modelling strategy is applied to the case of Linde Gas Italia S.r.l., the resulting Trieste and Bologna models consist of two equations each, plus the lower and upper bounds while the resulting Terni model consists of only one equation, plus the lower and upper bounds (recall that Terni cannot produce deliverable liquid argon as shown in Table 2). The equations relating to the Trieste plant are reported in Eqs. (51) and (52), those relating to the Bologna plant are described in Eqs. (53) and (54) and the one referring to the Terni plant is shown in Eq. (55).

$$\lambda_0^{TS} + \lambda_1^{TS} LIN^{TS} + \lambda_2^{TS} GAN_{HP}^{TS} + \lambda_3^{TS} \left(LOX_{3.5}^{TS} + GOX_{HP}^{TS} + GOX_{LP}^{TS} \right) - W_c^{TOT,TS} = 0 \tag{51}$$

$${}^{TS} \left(LOX_{3.5}^{TS} + GOX_{HP}^{TS} + GOX_{LP}^{TS} \right) - LAR^{TS} = 0 \tag{52}$$

$$\lambda_0^{BO} + \lambda_1^{BO} LIN^{BO} + \lambda_2^{BO} \left(LOX_{2.5}^{BO} + LOX_{3.5}^{BO} \right) - W_c^{TOT,BO} = 0 \tag{53}$$

$${}_{2.5}^{BO} LOX_{2.5}^{BO} + {}_{3.5}^{BO} LOX_{3.5}^{BO} - LAR^{BO} = 0 \tag{54}$$

$$\lambda_0^{TR} + \lambda_1^{TR} LIN^{TR} + \lambda_2^{TR} LOX_{3.5}^{TR} - W_c^{TOT,TR} = 0 \tag{55}$$

The bound constraints are not reported for the sake of brevity and are chosen to equal those employed for the detailed ASU models described in Section 5.2.

In terms of notation:

- $W_c^{TOT,TS}$, $W_c^{TOT,BO}$ and $W_c^{TOT,BO}$ are the total compression powers consumed by Trieste, Bologna and Terni plants, respectively;
- all the remaining symbols are the models adaptive parameters.

One last remark, which has to be added, deals with the determination of the fitting parameters included in Eqs. (51)–(55). These parameters are estimated via regression based, once again, on the data sets provided by Linde Gas Italia S.r.l. and employed for the tuning of both the detailed plant models (Section 5.2) and the pure-source-hypothesis-based plant models (see the description above).

This second production network modelling approach is less commonly found in the literature but is relevant to the purposes of this paper. Therefore, the authors have chosen to mention and apply it.

The third and last option for the production level modelling discussed in this work consists of an adaptation of that proposed in (Mitra et al., 2012, 2014). Remind that this option is not applied in the current case study. Briefly, it builds each ASU model through a two-step procedure:

- a set of feasible operating conditions for the single ASU is evaluated based on rigorous simulations or historical plant data;
- the convex hull of this set, miming the feasible operating space of the ASU, is built and formally converted into a set of equalities and/or inequalities and/or bounds that represent the ASU simplified model.

Notice that this third production network modelling strategy is certainly more accurate than the first two but probably not as accurate as that proposed in Section 3, especially when the mapping, described in the first bullet of the previous list, contains a limited number of points. Indeed, in this case, the convexification would probably take to an overestimation of the ASUs feasible oper-ating regions, thus leading to poor accuracy. Further comparisons and analyses on this third production level modelling strategy as opposed to the one proposed in Section 3 is material for future work.

Now the two more common conventional methodologies employed for an IGP production network modelling have been briefly described and applied to the case of Linde Gas Italia S.r.l.(a third strategy has only been described and discussed). There-fore, we can next proceed with the presentation of the results of the case study.

5.4. Numerical results and performance comparison

Before describing the numerical results of the case study, it is relevant to convey some information on how the case study itself is practically executed. Three different models for the overall Linde Gas Italia S.r.l. corporate can be derived from the supply-chain model (Section 5.1) and the three applied production network models (Sections 5.2 and 5.3). All these three corporate models share the same supply-chain network model and differ in the detail given to the production network modelling. In detail:

- the minimal model (MINM) describes the production level through the first modelling strategy reported in Section 5.3;
- the average model (AVEM) describes the production level through the second modelling strategy proposed in Section 5.3;
- the advanced model (ADVM) describes the production level through the detailed approach mentioned in Section 5.2.

The MINM, AVEM and ADVM models are used to construct three different global IGP optimization problems (Eq. (18)), named MIN-MGOP, AVEMGOP and ADVMGOP, that are subsequently solved over a two week planning horizon, discretized in one day long time intervals (see Tables 1 and 4). Recall that a single time grid is used for the supply-chain network, the production level and the objec-tive function evaluation. The first of these optimization problems needs an ad-hoc implementation since its objective function has to evaluate the $TPRC_{LN}$ term with Eq. (50) and not Eq. (16). However, the two remaining problems are easily solved with *ASUNetwork-SupplyChain.exe* program. The reader should recall that uncertainty is not considered for now on the input data, thus the rolling hori-zon methodology is not needed and the optimal Linde Gas Italia S.r.l. operating condition, on the two weeks period, can be found through one-shot optimizations.

The results, achieved in the three optimizations, include a huge amount of data that cannot be completely reported and discussed in detail. Therefore, the authors have chosen to include only those output data that are essential to convey the distinctions between the solutions obtained. Moreover, all the outputs referring to the operating regions of the Linde Gas Italia S.r.l. plants have been made dimensionless in order to avoid the release of restricted material.

The sequence of Figs. 8–10 shows a view of the Trieste, Bologna and Terni plants optimal operating conditions over the entire planning horizon (fourteen days). In detail, the optimal production rates of the only products included in the supply-chain and the optimal inlet air flow are reported for each plant and each of the three addressed global IGP optimization problems. The notation employed here is consistent with that already used in the rest of the paper, except for three aspects:

- the * symbol is added to all the dimensionless stream names in order to distinguish them from their dimensional counterparts;
- the subscript “3.5” is not added to the liquid oxygen streams at 99.95% purity on a molar basis since all the oxygen that is mentioned in the results (reported in this section) is of the “3.5” type;
- the “lb” and “ub” acronyms are added to a symbol to indicate its lower and upper bound, respectively.

Moreover, in order to distinguish among assignments arising from the solution of different global IGP optimization problems, the following notation is used:

- if the acronym “adv” is added to a certain symbol, it means that the corresponding assignment derives from the solution of ADVMGOP;
- if the acronym “ave” is added to a certain symbol, it means that the corresponding assignment derives from the solution of AVEMGOP;
- if the acronym “min” is added to a certain symbol, it means that the corresponding assignment derives from the solution of MINMGOP.

Liquid argon charts are an exception to the previous rule. Indeed, the produced argon flowrate is not a degree of freedom for a real ASU plant. Therefore, the LAR assignments directly coming from the solution of MINMGOP and AVEMGOP are denoted with the acronyms “min/pri” and “ave/pri”, respectively. The LAR assign-ments evaluated by substituting the optimal DOF profiles, coming from the solution of MINMGOP and AVEMGOP, into the detailed ASU models (Section 5.2) are denoted with the acronyms “min/adj” and “ave/adj”. Notice that the “adj” LAR profiles are an accurate approximation of those that would be achieved if the optimal oper-ating condition of Linde Gas Italia S.r.l. corporate, derived from the solution of MINMGOP or AVEMGOP, was applied in the real world.

The inlet air flow charts are a small exception too. In this case, the profiles identified with “min” and “ave” acronyms are evaluated with the same method used for the “min/adj” and “ave/adj” LAR assignments. Here the abbreviation “adj” is not added since the inlet air flows are not a direct result of the solution of AVEMGOP or MINMGOP, thus only the “adj” inlet air flows are available.

Once all the data included in Figs. 8–10 have been mentioned and the required explanations on the employed notation have been provided, a couple of remarks can be expanded.

First of all, notice that the “min/adj” LAR assignments often violate the maximum or minimum bound constraints. It happens in both Trieste and Bologna. Similar observations, extended to all the three Linde Gas Italia S.r.l. plants, can be made for the “ave” and “min” inlet air flowrate profiles. This means that the solutions arising from AVEMGOP and MINMGOP may be infeasible and this is a direct consequence of using simplified models for the produc-tion network. Indeed, no infeasibilities are observed in the solution of ADVMGOP, i.e., if the detailed models for the IGP production network, described in Section 5.2, are chosen.

Secondly, observe that the ASU operating conditions deriving from the solution of AVEMGOP and MINMGOP are characterized by extreme and repeated oscillations in the time space. It means that it is not uncommon for the LIN assignments or the inlet air flow profiles to move from the lower bound to the upper bound in only one day. This is clearly infeasible since such ASU management policy would lead to likely repeated failures in the inlet air compressor and the nitrogen liquefaction cycle compressors. By contrast, the ASU operating conditions deriving from the solution of ADVMGOP are characterized by a smooth variation in the time domain, thus leading to feasible and safe ASU management policies. This is a direct consequence of the anti-ringing constraints (Eqs.(11) and (12)) that are typically not employed in the supply-chain and production optimization strategies proposed in literature.

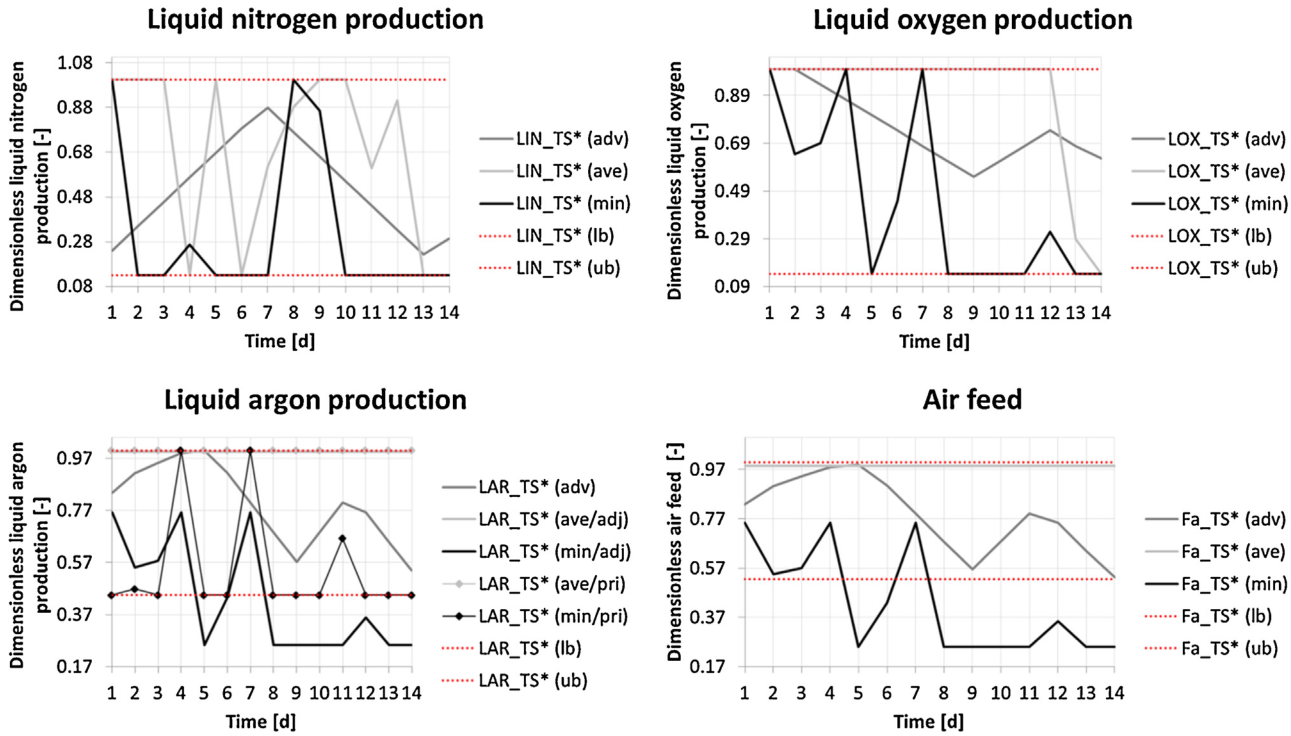

Fig. 8. Trieste plant operating conditions in the two weeks time period.

Based on these results it is evident that the integrated strategy for the supply-chain and production networks optimization proposed in this paper seems to be more robust and feasible than those typically employed in literature. Once again, this is a consequence of the plant details included in the modelling of the IGP production network.

Continuing with a further discussion of the results of the case study in terms of supply-chain network optimal configurations, it is relevant to highlight that the amount of information describing the optimal solution is quite large. Therefore, only a small portion of the results is reported in Figs. 11–13. Specifically, Fig. 11 reports the three optimal liquid oxygen supply-chain network configurations,

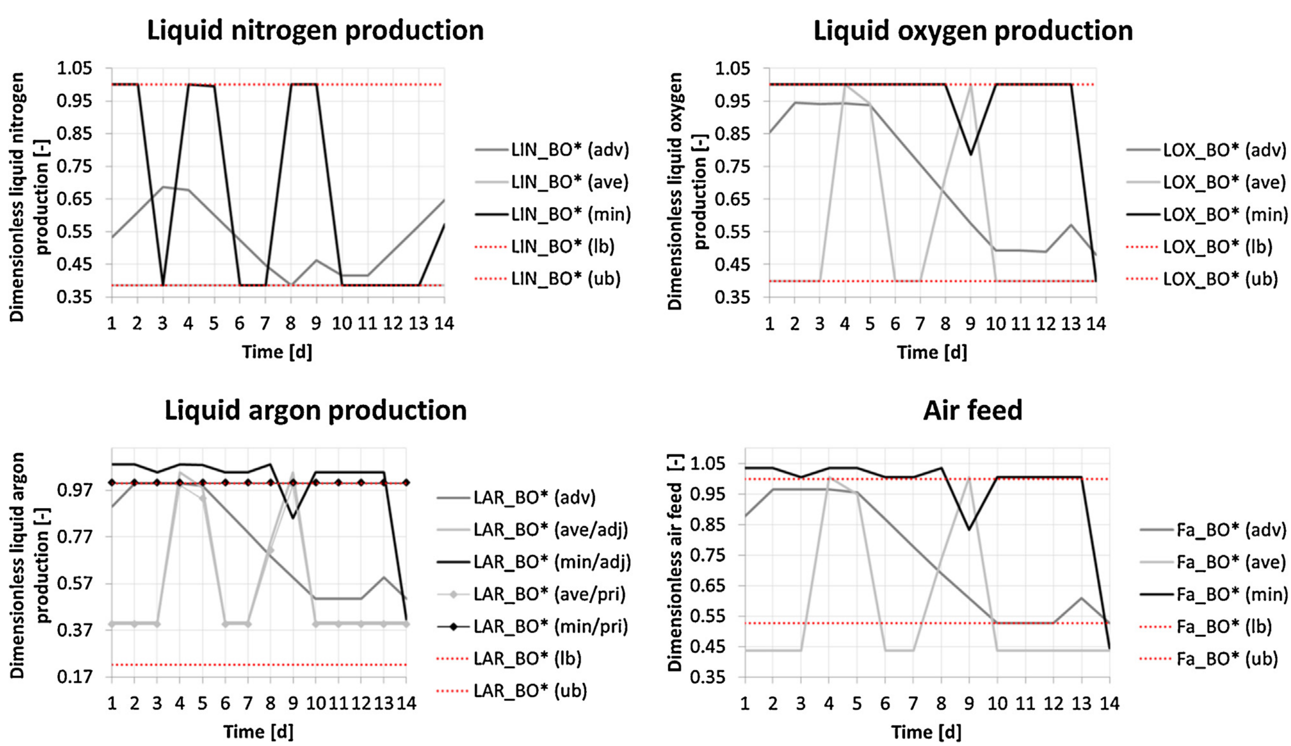

Fig. 9. Bologna plant operating conditions in the two weeks time period.

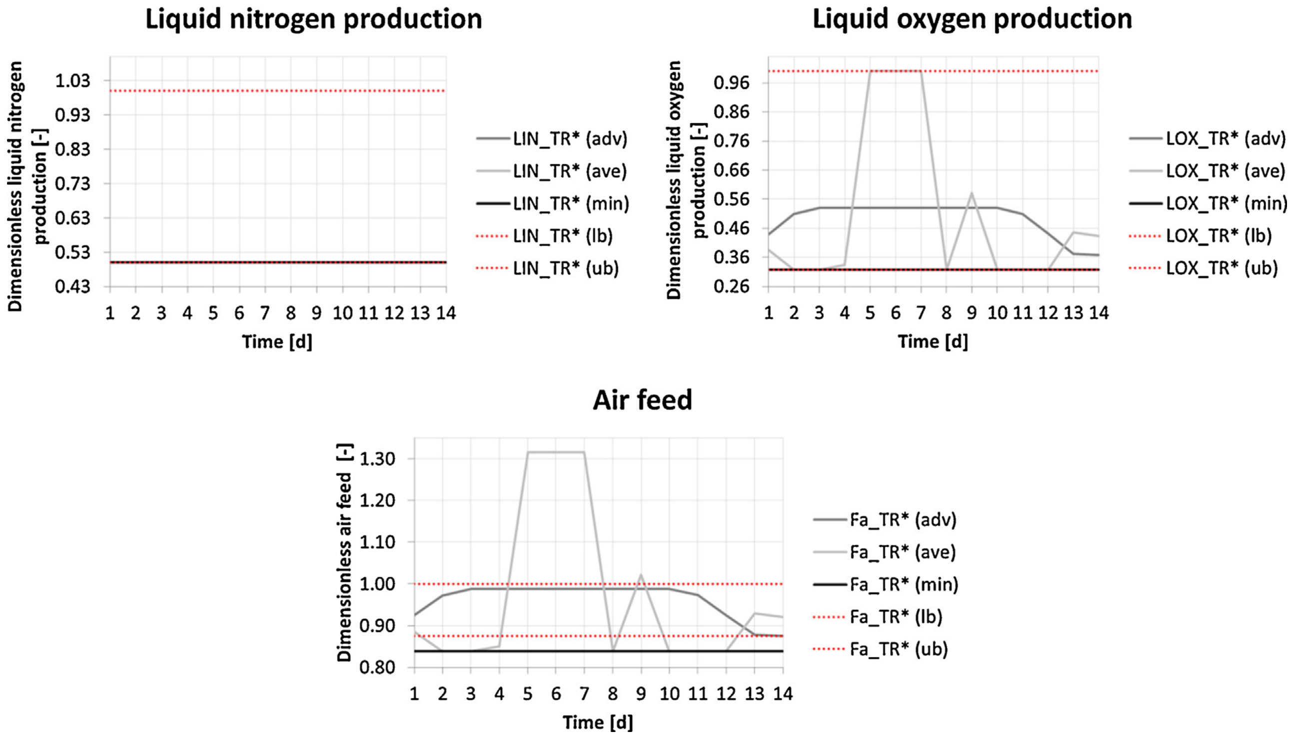

Fig. 10. Terni plant operating conditions in the two weeks time period.

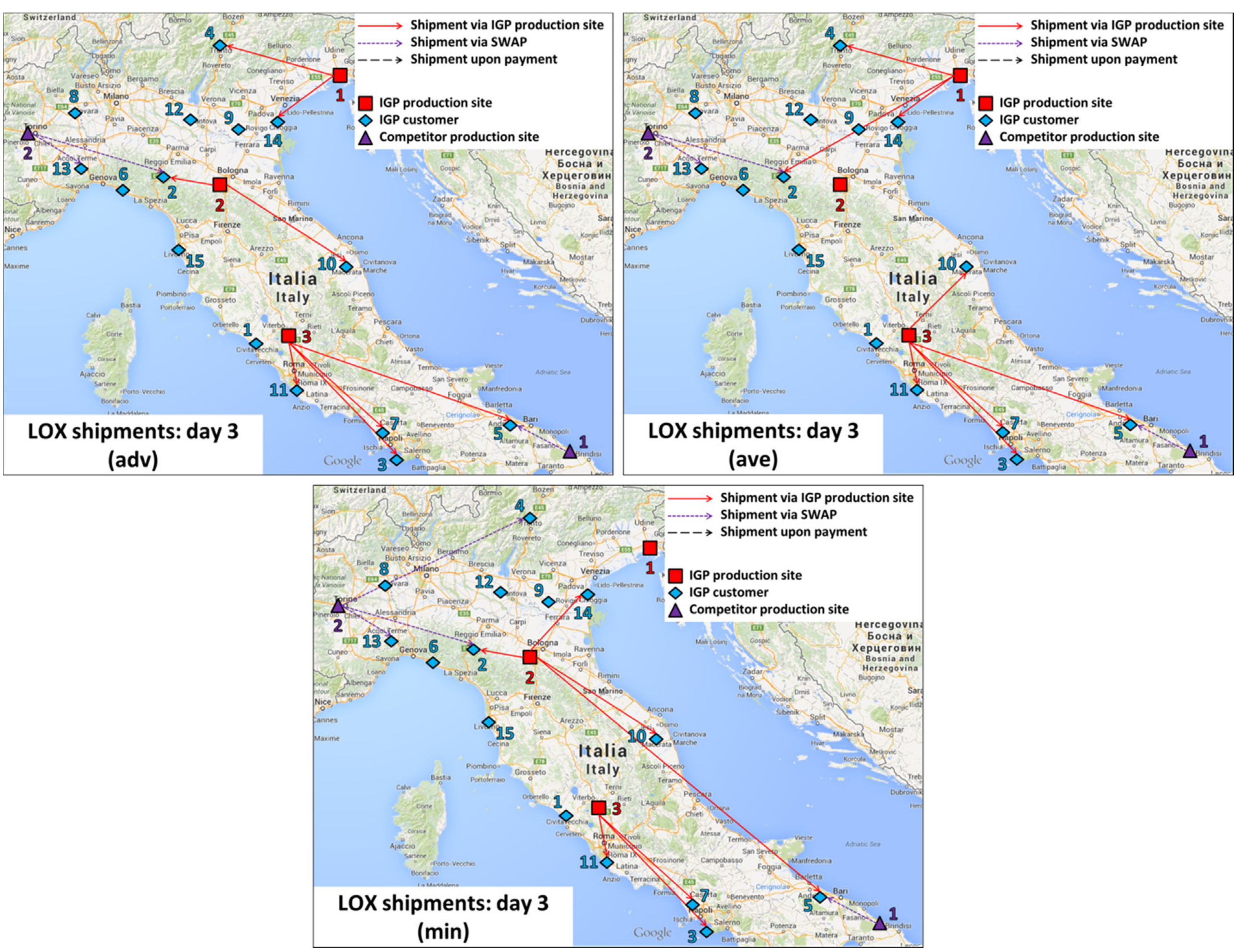

Fig. 11. Liquid oxygen supply-chain optimal configuration in day three.

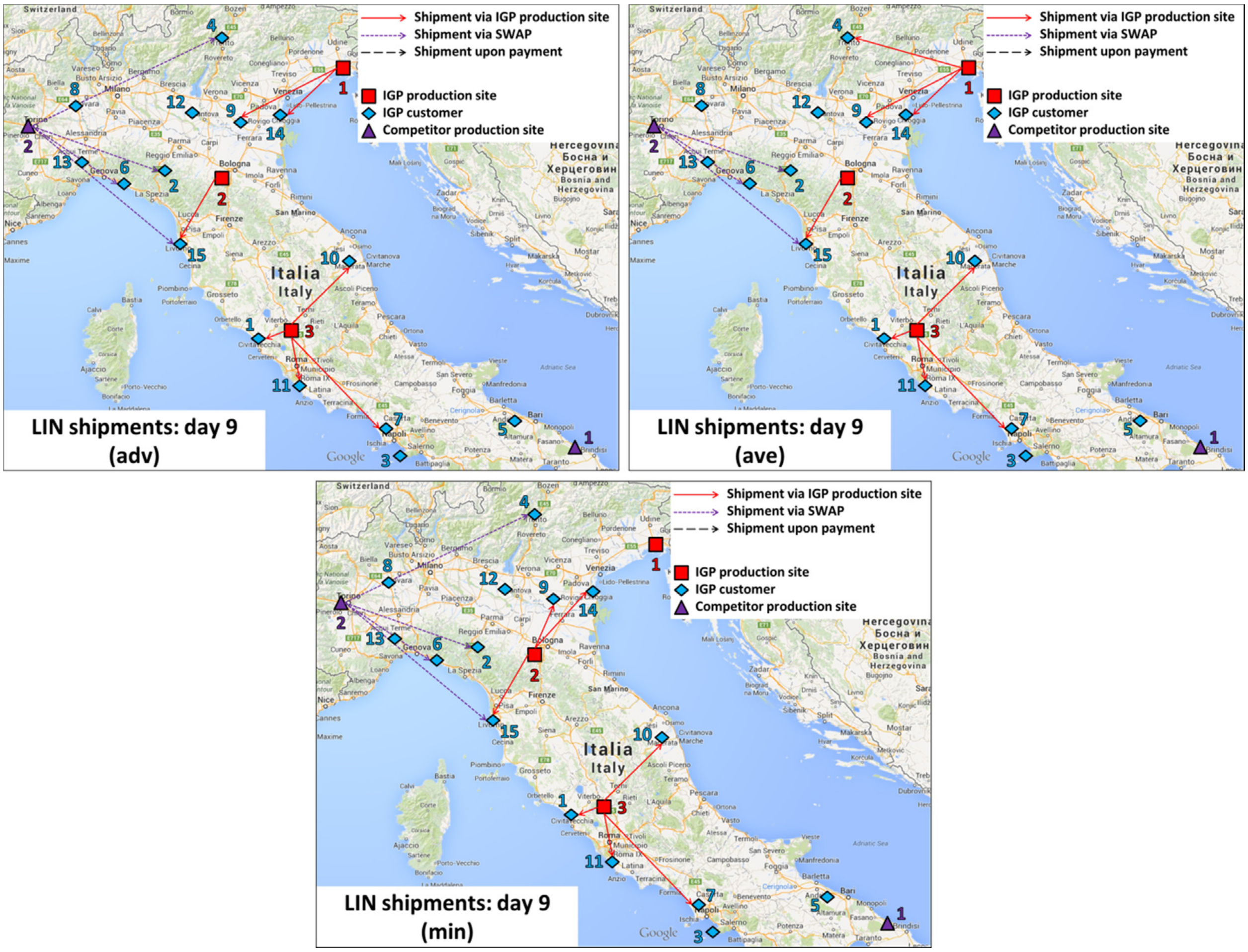

Fig. 12. Liquid nitrogen supply-chain optimal configuration in day nine.

for day three, deriving from the solution of MINMGOP, AVEMGOP and ADVMGOP. Fig. 12 is the equivalent of Fig. 11 for liquid nitrogen and day nine. Finally, Fig. 13 is the equivalent of Fig. 12 for liquid argon and day fourteen. The acronyms "adv", "ave" and "min" have the same meaning that is assigned to them in the above-mentioned production charts. In addition, in all the above-mentioned figures, IGP site one is Trieste, IGP site two is Bologna and IGP site three is Terni while competitor site one is Ostuni and competitor site two is Grugliasco.

Comparing the different optimal configurations of the supply-chain network (for the same product) derived from the solution of MINMGOP, AVEMGOP and ADVMGOP is not very interesting in itself. However, Figs. 11–13 suggest that all the three IGP global optimization problems lead to similar and reasonable results in terms of supply-chain. This confirms that the modelling strategy employed for the supply-chain is accurate but does not add anything in terms of performance comparison between the proposed integrated strategy for the supply-chain and production optimization and its literature counterparts. However, by looking at the "adv" supply-chain configurations, it can be clearly seen that some of the shipments do not follow the universal logistic paradigm "resupply a customer from the closest available source of product". This confirms that *ASUNetworkSupplyChain.exe* is able to efficiently find the optimum balance between production and supply-chain needs, i.e., the global corporate scale optimum. Moreover, notice that no shipments upon payment are executed in Figs. 11–13 (this is true in general for all the days and products over the planning horizon). This is reasonable since the products purchase costs (C^{BY}_{lk}) are relatively high in this case study, thus it is always more cost-effective to produce a product in Linde Gas Italia S.r.l. own sites than purchasing it from a competitor site, providing that sufficient production capacity is available. Indeed, it is the expectation in practice that the shipment upon payment option would only be exercised in exceptional situations. Finally, observe from Figs. 11–13 that the optimal supply-chain network configuration shows some customers to be simultaneously supplied from several sources. It is possible to force only single customer-single source assignments by changing the α_{ij} and ε_{kj} values. Here this procedure has been avoided because it generates extra costs. However, the additional cost of single source assignments might be acceptable if the resulting simplification in the logistics is deemed desirable from a corporate perspective.

One last point that has to be addressed is the economic comparison of the results of the solution of MINMGOP, AVEMGOP and ADVMGOP alternatives. This comparison can be made on the basis of the global costs incurred, in each of three cases, by Linde Gas Italia S.r.l. over the two week planning horizon. These costs summary is reported in Table 5. It can be clearly seen that the solution corresponding to ADVMGOP ensures the lowest global costs. Specifically, its costs are about 1.75% lower than those resulting from the solution corresponding to AVEMGOP and about 10.5% lower than those resulting from the solution of MINMGOP. This suggests that the proposed integrated optimization strategy for supply-chain/production is not only more robust and feasible than its literature counterparts but seems to be also more economical. However, two additional remarks must be added to this first

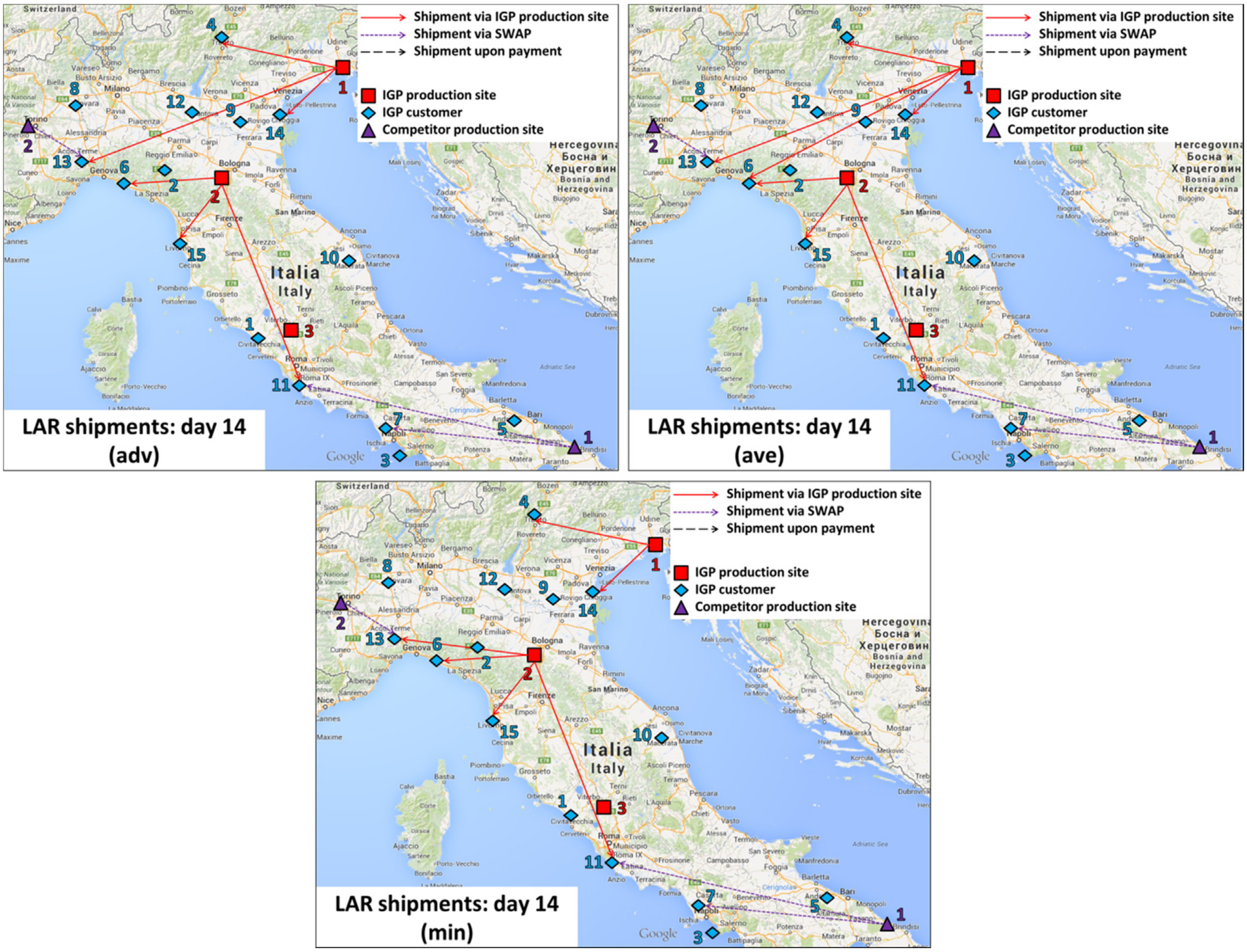

Fig. 13. Liquid argon supply-chain optimal configuration in day fourteen.

analysis. First, it should be noted that the total costs relating to the solution of MINMGOP are only an estimate of the true costs since this solution is infeasible. Nevertheless, it can be assumed that if feasibility were enforced the economics of the MINMGOP solution would be even less favourable. Second, MINMGOP and AVEMGOP might seem to the reader mathematical relaxations of ADVMGOP and this might lead to think that the global costs trend observed in Table 5 is unusual or incorrect. However, MINMGOP and AVEMGOP are not mathematical relaxations of ADVMGOP. Indeed, these three optimization problems rely on different constraints and, sometimes, different formulations of the objective function and are not mathematical subsets one of another. Therefore, the global costs trend shown in Table 5 is perfectly feasible. In conclusion, the abovementioned remark, claiming that the proposed integrated optimization strategy for supply-chain/production is more economically convenient than many other literature approaches, still holds.

Table 5
Total costs incurred by Linde Gas Italia S.r.l. relating to three different solutions of the global IGP optimization problem.

Time [d]	ADVMGOP case total costs [€]	AVEMGOP case total costs [€]	MINMGOP case total costs [€]
1	52,503.62	49,294.71	77,031.39
2	57,907.22	52,039.23	66,500.88
3	61,903.78	54,504.73	63,531.01
4	60,371.56	59,942.57	75,834.43
5	64,155.12	68,274.48	61,497.63
6	61,258.97	57,007.70	61,117.85
7	75,494.57	77,770.57	87,112.37
8	54,828.98	59,796.27	67,147.74
9	50,284.31	62,670.70	59,490.11
10	53,108.40	54,970.00	55,153.80
11	62,535.69	66,517.50	65,118.19
12	54,048.37	58,370.26	59,830.71
13	54,385.27	54,186.69	56,828.03
14	55,456.70	57,399.12	49,484.47
All days	**818,242.55**	**832,744.52**	**905,678.60**

5.5. Extension to uncertain input data

Section 5.4 has demonstrated that the proposed integrated strategy for the supply-chain and production network optimization is typically superior to its literature counterparts in terms of robustness, feasibility of the outputs and costs. However, this has been checked only in the case of no uncertainty on the input data. The hypothesis of deterministic input data is not realistic but the trends shown in the previous section can be extrapolated to the case of uncertain input data, at least on a qualitative level. Indeed, the results achieved in Section 5.4 correspond to a single step of a rolling horizon methodology that can be easily applied in the case of uncertain inputs. In the spirit of the MPC strategy, it can be assumed that a rolling horizon approach, coupled with the proposed integrated optimization strategy, will offer the most appropriate and practical approach to dealing with supply chain uncertainty and will ensure similar economical results, at least on a relative basis. However, this needs to be tested against using a robust solution approach in which uncertainty is taken into account directly in the integrated problem formulation. Future works will be aimed at investigating in detail these considerations.

6. Conclusions

In this paper, a general modular methodology for the simultaneous optimization of the supply-chain network and the production subsystem of a generic IGP has been developed and implemented in a C++ program, called *ASUNetworkSupplyChain.exe*. The methodology consists of several blocks: a general IGP supply-chain and storage system model, a specific approach for the modelling of the IGP production subsystem, the definition of a comprehensive cost-based objective function and a suitable set of numerical algorithms. The *ASUNetworkSupplyChain.exe* software, which implements the above-mentioned methodology, is based on the BzzMath library numerical algorithms and employs ad-hoc preprocessing methods to ensure the online feasibility of the approach. The proposed strategy for the integrated optimization of supply-chain/production is an advance over the alternatives reported in the literature in both the details of the production subsystem modelling and in its generality that allows it to be applied for any IGP. The performance of the proposed methodology has been demonstrated and compared to that of two common literature alternatives in a case study based on Linde Gas Italia S.r.l. data. The results of the performance comparison have shown that the proposed strategy for the integrated supply-chain and production level optimization is superior to its literature counterparts in terms of robustness, feasibility of the outputs and economics. While the study assumes deterministic inputs (customers demand, costs, etc.), the formulation can readily accommodate uncertainties through the use of the rolling horizon strategy. A more detailed comparison of this strategy against a robust stochastic optimization strategy is subject for future work.

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References

Bansal M, Karimi IA, Srinivasan R. Optimal contract selection for the global supply and distribution of raw materials. Ind Eng Chem Res 2007;46:6522–39.

Biegler LT, Grossmann IE. Retrospective on optimization. Comput Chem Eng 2004;28:1169–92.

Biegler LT. Large-scale nonlinear programming: an integrating framework for enterprise-wide dynamic optimization. Comput Aided Chem Eng 2007;24:575–82.

Bowling IM, Ponce-Ortega JM, El-Halwagi MM. Facility location and supply chain optimization for a biorefinery. Ind Eng Chem Res 2011;50:6276–86.

Busch J, Oldenburg J, Santos M, Cruse A, Marquardt W. Dynamic predictive scheduling of operational strategies for continuous processes using mixed-logic dynamic optimization. Comput Chem Eng 2007;31:574–87.

Buzzi-Ferraris G, Manenti F. Fundamentals and linear algebra for the chemical engineer. Wiley-VCH; 2010a.

Buzzi-Ferraris G, Manenti F. Interpolation and regression models for the chemical engineer. Wiley-VCH; 2010b.

Buzzi-Ferraris G. Linear programming with the attic method. Ind Eng Chem Res 2011;50:4858–78.

Buzzi-Ferraris G, Manenti F. BzzMath: library overview and recent advances in numerical methods. Comput Aided Chem Eng 2012;30:1312–6.

Cheng L, Subrahmanian E, Westerberg AW. Design and planning under uncertainty: issues on problem formulation and solution. Comput Chem Eng 2003;27:781–801.

Floudas CA, Lin X. Continuous-time versus discrete-time approaches for scheduling of chemical processes: a review. Comput Chem Eng 2004;28:2109–29.

Floudas CA. Mixed integer linear programming in process scheduling: modeling, algorithms, and applications. Ann Oper Res 2005;139:131–62.

Grossmann IE. Challenges in the new millennium: product discovery and design, enterprise and supply chain optimization, global life cycle assessment. Comput Chem Eng 2004;29:29–39.

Grossmann I. Enterprise-wide optimization: a new frontier in process systems engineering. AIChE J 2005;51:1846–57.

Grossmann I, Erdirik-Dogan M, Karuppiah R. Overview of planning and scheduling for enterprise-wide optimization of process industries. At-Automatisierungstechnik 2008;56:64–79.

Harjunkoski I, Maravelias CT, Bongers P, Castro PM, Engell S, Grossmann IE, et al. Scope for industrial applications of production scheduling models and solution methods. Comput Chem Eng 2014;62:161–93.

Ierapetritou MG, Wu D, Vin J, Sweeney P, Chigirinskiy M. Cost minimization in an energy-intensive plant using mathematical programming approaches. Ind Eng Chem Res 2002;41:5262–77.

Julka N, Karimi I, Srinivasan R. Agent-based supply chain management – 2: a refinery application. Comput Chem Eng 2002;26:1771–81.

Kallrath J. Planning and scheduling in the process industry. OR Spectrum 2002;24:219–50.

Timpe CH, Kallrath J. Optimal planning in large multi-site production networks. Eur J Oper Res 2000;126:422–35.

Manenti F, Buzzi-Ferraris G. Comparing Attic method with the existing techniques for linear programming. Chem Eng Trans 2012;29:271–6.

Manenti F, Bozzano G, D'Isanto M, Lima NMN, Linan LZ. Raising the decision-making level to improve the enterprise-wide production flexibility. AIChE J 2013a;59:1588–98.

Manenti F, Rossi F, Croce G, Grottoli MG, Altavilla M. Intensifying air separation units. Chem Eng Trans 2013b;35:1249–54.

Manenti F, Rovaglio M. Market-driven operational optimization of industrial gas supply chains. Comput Chem Eng 2013;56:128–41.

Maravelias CT, Sung C. Integration of production planning and scheduling: overview, challenges and opportunities. Comput Chem Eng 2009;33:1919–30.

Maravelias CT. General framework and modeling approach classification for chemical production scheduling. AIChE J 2012;58:1812–28.

Méndez CA, Cerdá J, Grossmann IE, Harjunkoski I, Fahl M. State-of-the-art review of optimization methods for short-term scheduling of batch processes. Comput Chem Eng 2006;30:913–46.

Muñoz E, Capón-García E, Laínez JM, Espu ña A, Puigjaner L. Integration of enterprise levels based on an ontological framework. Chem Eng Res Des 2013;91:1542–56.

Mitra S, Grossmann IE, Pinto JM, Arora N. Optimal production planning under time-sensitive electricity prices for continuous power-intensive processes. Comput Chem Eng 2012;38:171–84.

Mitra S, Pinto JM, Grossmann IE. Optimal multi-scale capacity planning for power-intensive continuous processes under time-sensitive electricity prices and demand uncertainty Part I: Modeling. Comput Chem Eng 2014;65:89–101.

Neiro SMS, Pinto JM. A general modeling framework for the operational planning of petroleum supply chains. Comput Chem Eng 2004;28:871–96.

Ng WPQ, Lam HL. Sustainable supply network design through optimisation with clustering technique integration. Chem Eng Trans 2013;35:661–6.

Park M, Park S, Mele FD, Grossmann IE. Modeling of purchase and sales contracts in supply chain optimization. Ind Eng Chem Res 2006;45:5013–26.

Phanden RK, Jain A, Verma R. Integration of process planning and scheduling: a state-of-the-art review. Int J Comput Integr Manuf 2011;24:517–34.
Shah N. Process industry supply chains: advances and challenges. Comput Chem Eng 2005;29:1225–35.
Subramanian K, Rawlings JB, Maravelias CT. Economic model predictive control for inventory management in supply chains. Comput Chem Eng 2014;64:71–80.
Varma VA, Reklaitis GV, Blau GE, Pekny JF. Enterprise-wide modeling and optimization: an overview of emerging research challenges and opportunities. Comput Chem Eng 2007;31:692–711.
Yue D, You F. Sustainable scheduling of batch processes under economic and environmental criteria with MINLP models and algorithms. Comput Chem Eng 2013;54:44–59.