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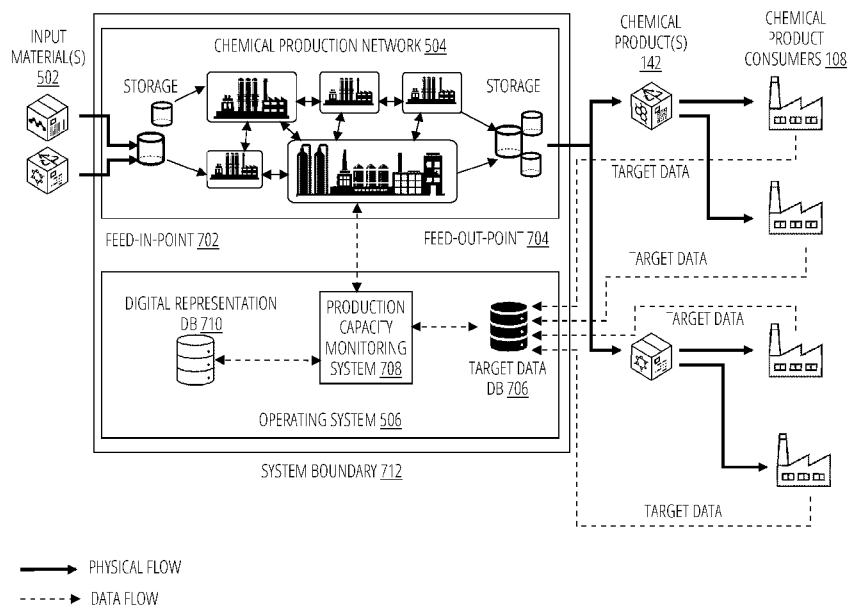


FIG. 7

(57) **Abstract:** Disclosed are methods, apparatuses and systems for monitoring and/or controlling a production of a chemical product based on a quantity (e.g. volume or amount) as requested by one or more downstream participant(s) of a chemical supply chain involving the chemical product and for generating mitigation data which may serve as a trigger to adopt the production such that capacity shortages are avoided and the chemical product can be produced in the quantity and for the time periods requested by the one or more downstream participant(s). Further disclosed is a chemical product produced by a chemical production network using said mitigation data and the use of the generated mitigation data to adapt the production of the chemical product.

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Capacity early warning systems

TECHNICAL FIELD

Disclosed are methods, apparatuses and systems for monitoring and/or controlling a production of a chemical product based on a quantity (e.g. volume or amount) as requested by one or more downstream participant(s) of a chemical supply chain involving the chemical product and for generating mitigation data which may serve as a trigger to adapt the production such that capacity shortages are avoided and the chemical product can be produced in the quantity and for the time periods requested by the one or more downstream participant(s). Further disclosed is a chemical product produced by a chemical production network using said mitigation data and the use of the generated mitigation data to adapt the production of the chemical product.

TECHNICAL BACKGROUND

Large supply chains involve many different layers and variables that may affect the timeliness of supply chain milestones. For example, large supply chains typically include raw material suppliers, chemical product producers, chemical product consumers, and end-product manufacturers. Each of these components may be associated with many different dimensions which may impact the demands of various supply chain participants and hence also the production volume(s) of upstream participants of such supply chain participants. For example, end-product consumer demand may directly influence the demand of the end-product producer and hence also the demand of each upstream participant of the end-product producer. Large fluctuations in the demand of downstream participants may give rise to idle capacity or, even more problematic, capacity shortages at upstream participants, such as chemical product producers. Capacity shortages of chemical product producers in turn may negatively impact production and delivery milestones of downstream participants of the supply chain.

Hence, there is a need to tailor production operations of chemical product producers to quantities to be produced for one or more downstream participant(s).

SUMMARY

In an aspect, the disclosure relates to a computer-implemented method for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, said method comprising:

(a) providing target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided via a peer-to-peer communication from computing node(s) of a decentral network, the computing node(s) being associated with the one or more downstream participant(s),

- (b) providing one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- (c) determining production capacity shortage(s) based on the provided target data and the provided digital representation(s),
- (d) if production capacity shortage(s) are determined, generating mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters,
- (e) providing the generated mitigation data for adapting the production of the chemical product according to the mitigation data
- (f) optionally generating a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

In an aspect, the disclosure relates to a computer-implemented method for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, said method comprising:

- (a) providing target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided by determining via a decentral network an endpoint address associated with a chemical product producer operating the chemical production network and providing the target data via the decentral network to the determined endpoint address,
- (b) providing one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- (c) determining production capacity shortage(s) based on the provided target data and the provided digital representation(s),
- (d) if production capacity shortage(s) are determined, generating mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters,

- (e) providing the generated mitigation data for adapting the production of the chemical product according to the mitigation data,
- (f) optionally generating a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

In a further aspect, the present invention relates to an apparatus for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, said apparatus comprising:

- (a) a target data provider configured to provide target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided via a peer-to-peer communication from computing node(s) of a decentral network, the computing node(s) being associated with the one or more downstream participant(s),
- (b) a data provider configured to provide one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain,
- (c) a production capacity shortage determinator configured to determine production capacity shortage(s) based on the provided target data and the provided digital representation(s), in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- (d) a capacity shortage mitigation data generator configured to
- generate mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters if production capacity shortage(s) are determined,
 - provide the generated mitigation data for adapting the production of the chemical product according to the mitigation data,
- (e) optionally a digital twin generator configured to generate a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

In a further aspect, the present invention relates to an apparatus for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, said apparatus comprising:

- 5 (a) a target data provider configured to provide target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided by determining via a decentral network an endpoint address associated with a chemical product producer operating the chemical production network and providing the target data via the decentral network to the determined
10 endpoint address,
- (b) a data provider configured to provide one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain,
- 15 (c) a production capacity shortage determinator configured to determine production capacity shortage(s) based on the provided target data and the provided digital representation(s) , in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- (d) a capacity shortage mitigation data generator configured to
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 - generate mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters if production capacity shortage(s) are determined,
 - provide the generated mitigation data for adapting the production of the chemical product according to the mitigation data
- 25 (e) optionally a digital twin generator configured to generate a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier
30 by the chemical product producer.

In a further aspect, the present invention relates to an apparatus for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, the apparatus comprising one or more computing node(s) and one or
35 more computer-readable media having thereon computer-executable instructions that are structured such that, when executed by the one or more computing node(s), cause the apparatus to perform the steps below:

- 5 (a) providing target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided via a peer-to-peer communication from computing node(s) of a decentral network, the computing node(s) being associated with the one or more downstream participant(s),
- 10 (b) providing one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- 15 (c) determining production capacity shortage(s) based on the provided target data and the provided digital representation(s),
- (d) if production capacity shortage(s) are determined, generating mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters,
- 20 (e) providing the generated mitigation data for adapting the production of the chemical product according to the mitigation data
- (f) optionally generating a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

25 In a further aspect, the present invention relates to an apparatus for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, the apparatus comprising one or more computing node(s) and one or more computer-readable media having thereon computer-executable instructions that are structured such that, when executed by the one or more computing node(s), cause the apparatus to perform the steps below:

- 30 (a) providing target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided by determining via a decentral network an endpoint address associated with a chemical product producer operating the chemical production network and providing the target data via the decentral network to the determined endpoint address,
- 35 (b) providing one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production

chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),

(c) determining production capacity shortage(s) based on the provided target data and the provided digital representation(s),

5 (d) if production capacity shortage(s) are determined, generating mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters,

(e) providing the generated mitigation data for adapting the production of the chemical product according to the mitigation data

10 (f) optionally generating a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

15 In a further aspect, the present invention relates to a system for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), said system comprising:

(a) an apparatus for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s) according to the methods disclosed herein,

20 and

(b) a chemical production network configured to

- receive the mitigation data or the monitor and/or control data as generated according to the methods disclosed herein, and
- produce the chemical product from one or more input material(s) via one or more chemical

25 intermediate(s),

(c) optionally a digital twin generator configured to generate a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

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In a further aspect, the present invention relates to a computer-implemented method for generating mitigation data for adapting a production of a chemical product to produce the chemical product a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, said method comprising:

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- (a) providing target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided via a peer-to-peer communication from computing node(s) of a decentral network, the computing node(s) being associated with the one or more downstream participant(s),
- (b) providing one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- (c) determining production capacity shortage(s) based on the provided target data and the provided digital representation(s),
- (d) if production capacity shortage(s) are determined, generating mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters,
- (e) providing the generated mitigation data for adapting the production of the chemical product according to the mitigation data,
- (f) optionally generating a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

In a further aspect, the present invention relates to a computer-implemented method for generating mitigation data for adapting a production of a chemical product to produce the chemical product a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, said method comprising:

- (a) providing target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided by determining via a decentral network an endpoint address associated with a chemical product producer operating the chemical production network and providing the target data via the decentral network to the determined endpoint address,
- (b) providing one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),

- (c) determining production capacity shortage(s) based on the provided target data and the provided digital representation(s),
- (d) if production capacity shortage(s) are determined, generating mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product
5 and/or production parameters,
- (e) providing the generated mitigation data for adapting the production of the chemical product according to the mitigation data,
- (f) optionally generating a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical
10 product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

In a further aspect, the present invention relates to an apparatus for generating mitigation data for adapting a production of a chemical product to produce the chemical product a quantity as requested
15 by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, apparatus comprising one or more computing node(s) and one or more computer-readable media having thereon computer-executable instructions that are structured such that, when executed by the one or more computing node(s), cause the apparatus to perform the steps below:

- (a) provide target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided via a peer-to-peer communication from computing node(s) of a decentral network, the computing node(s) being associated with the one or more downstream participant(s),
- (b) provide one or more digital representation(s) associated with production chain(s) used to produce
25 the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- (c) determine production capacity shortage(s) based on the provided target data and the provided
30 digital representation(s),
- (d) if production capacity shortage(s) are determined, generate mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters,
- (e) provide the generated mitigation data for adapting the production of the chemical product
35 according to the mitigation data
- (f) optionally generate a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical

product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

In a further aspect, the present invention relates to an apparatus for generating mitigation data for adapting a production of a chemical product to produce the chemical product a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, apparatus comprising one or more computing node(s) and one or more computer-readable media having thereon computer-executable instructions that are structured such that, when executed by the one or more computing node(s), cause the apparatus to perform the steps below:

- (a) provide target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided by determining via a decentral network an endpoint address associated with a chemical product producer operating the chemical production network and providing the target data via the decentral network to the determined endpoint address,
- (b) provide one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- (c) determine production capacity shortage(s) based on the provided target data and the provided digital representation(s),
- (d) if production capacity shortage(s) are determined, generate mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters,
- (e) provide the generated mitigation data for adapting the production of the chemical product according to the mitigation data
- (f) optionally generate a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

In a further aspect, the present invention relates to an apparatus for generating mitigation data for adapting a production of a chemical product to produce the chemical product a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, the apparatus comprising:

- 5 (a) a target data provider configured to provide target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided via a peer-to-peer communication from computing node(s) of a decentral network, the computing node(s) being associated with the one or more downstream participant(s),
- 10 (b) a data provider configured to provide one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),
- (c) a production capacity shortage determinator configured to determine production capacity shortage(s) based on the provided target data and the provided digital representation(s) ,
- (d) a capacity shortage mitigation data generator configured to
- 15 • generate mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters if production capacity shortage(s) are determined,
 - provide the generated mitigation data for adapting the production of the chemical product according to the mitigation data
- 20 (e) optionally a digital twin generator configured to generate a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.
- 25 In a further aspect, the present invention relates to an apparatus for generating mitigation data for adapting a production of a chemical product to produce the chemical product a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, the apparatus comprising:
- 30 (a) a target data provider configured to provide target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s), in particular wherein the target data is provided by determining via a decentral network an endpoint address associated with a chemical product producer operating the chemical production network and providing the target data via the decentral network to the determined endpoint address,
- 35 (b) a data provider configured to provide one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data associated with plant(s) forming the production chain(s) and capacity

threshold(s) per plant and/or production chain, in particular wherein the production chains are connected or interconnected via the chemical intermediate(s),

(c) a production capacity shortage determinator configured to determine production capacity shortage(s) based on the provided target data and the provided digital representation(s) ,

5 (d) a capacity shortage mitigation data generator configured to

- generate mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), the chemical product and/or production parameters if production capacity shortage(s) are determined,

10 • provide the generated mitigation data for adapting the production of the chemical product according to the mitigation data

(e) optionally a digital twin generator configured to generate a digital twin associated with the produced chemical product, wherein the digital twin includes a decentral identifier and chemical product data associated with the chemical product, wherein the digital twin is stored in a data storage associated with the chemical product producer for access by the downstream participant(s) and wherein access to the stored digital twin is controlled via the decentral identifier by the chemical product producer.

20 In a further aspect, the present invention relates to the use of mitigation data as generated by the computer-implemented methods disclosed herein or by the apparatuses disclosed herein to adapt the production of a chemical product to produce the chemical product in a quantity as requested by one or more downstream participant(s).

In a further aspect, the present invention relates to a chemical product produced by a chemical production network using the mitigation data as generated by the computer-implemented methods disclosed herein or by the apparatuses disclosed herein.

25 In a further aspect, the present disclosure relates to a computer element, such as a computer readable storage medium, a computer program or a computer program product, comprising instructions, which when executed by a computing node or a computing system, direct the computing node or computing system to carry out the steps of the computer-implemented methods disclosed herein.

30 In a further aspect, the present disclosure relates to a computer element, such as a computer readable storage medium, a computer program or a computer program product, comprising instructions, which when executed by the apparatuses or systems disclosed herein, direct the apparatuses or systems to carry out steps the apparatuses or systems disclosed herein are configured to execute.

35 Any disclosure, embodiments and examples described herein relate to the methods, the apparatuses, the systems, the chemical product(s), the uses and computer elements lined out above and below. Advantageously, the benefits provided by any of the embodiments and examples equally apply to all other embodiments and examples.

Embodiments

To avoid capacity shortages resulting in a negative impact of downstream participants up to the production of the end-product and hence to reliably produce chemical products based on quantities (e.g. volumes or amounts) as requested by such downstream participants, generation of mitigation data for adapting the production to avoid capacity shortage(s) in a data-driven manner is proposed.

By providing the target data via a decentral network, the target data can be provided in a secure yet reliable and standardized manner from the downstream participant to the product producer operating the chemical production network. By publishing an endpoint for providing target data within the decentral network by the chemical product producer, downstream participant(s) can reliably determine such an endpoint and provide respective target data in a secure, reliable and standardized manner to such endpoint without requiring the chemical product producer to request such data via the decentral network. This way, a reliable provision of target data in a secure and standardized manner can be achieved, allowing the chemical product producer to efficiently determine capacity shortages and to generate mitigation data upon determining such capacity shortage(s). This allows to avoid disruption of supply chains due to capacity bottlenecks, hence ensuring reliable and stable production of products by the downstream participants. By using a data-driven approach that incorporates digital representation(s) of production chain(s) related to the production of the chemical product, capacity shortage(s) occurring in one or more production chain(s) can be reliably identified. Specifically for chemical production networks that produce more than one chemical product from more than one input material via interconnected and connected production chains, the use of one or more digital representation(s) allows to flexibly route intermediates necessary to produce the chemical product from one production chain to another production chain such that the chemical product can be produced in the quantity requested by the downstream participant(s) while avoiding capacity shortage(s) within production chain(s) and/or a negative impact on a quantity of other chemical products produced by such production chain(s). For instance, the production of the chemical product may be adapted such that an intermediate necessary to produce the chemical product is routed from a first production chain to a second production chain such that the output of the second production chain (e.g. the chemical product) can be increased to fulfil the target quantity as requested by the downstream participant(s). The one or more digital representation(s) may be used to perform a virtual production process to identify capacity shortage(s) occurring in one or more of said production chain(s) upon virtually producing the chemical product in the quantity and for the future time period(s) requested by the one or more downstream participant(s). By using the identified capacity shortage(s), mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), chemical product, production time and/or production location may be generated that allow(s) to adapt the production such that the identified capacity shortage(s) are avoided while at the same time ensuring production of the chemical product in the quantity and for the future time period(s) as requested by the one or more downstream participant(s). Such capacity shortage mitigation data may be determined using data sets including candidate mitigation data associated with the determined capacity

shortage(s) and selecting the most suitable mitigation data to remedy the identified capacity shortage(s). By using one or more digital representation(s) of the production chain(s), the influence of candidate mitigation data on the production of other chemical products produced by such production chain(s) may be determined and considered during selection of suitable mitigation data to remedy the identified capacity shortage(s). This allows to reduce or eliminate balancing effects on a bottom level which may result in capacity shortage(s) for other chemical products produced by the chemical production network. The approach proposed herein allows to ensure reliable and timely production of chemical products based on quantities requested by downstream participant(s) and hence avoids capacity shortages negatively influencing the production of said downstream participants up to the end-product producer.

In the following, embodiments of the present disclosure will be outlined by ways of examples. It is to be understood that the present disclosure is not limited to said embodiments and/or examples.

Chemical product may include or be any material produced by the chemical production network using at least one input material. The chemical product may comprise or be any output product of the chemical production network (e.g. chemical intermediate(s) and chemical product(s)). The chemical product or output material may be produced from input materials via one or more chemical intermediate(s). The chemical product may be produced from the input material(s) via one or more chemical and/or physical processes. Chemical processes may include chemical reactions. Chemical reactions may include any chemical reaction commonly known in the state of the art in which the reactants are converted to one or more different chemical products. Chemical reactions may involve the use of catalysts, enzymes, bacteria, etc. to achieve the chemical reaction between the reactants. Physical processes may include mixing, separation and/or extrusion.

Requested chemical products or target chemical products may include chemical product(s) to be produced for use by downstream participant(s). Requested quantity or target quantity may include the quantity of the chemical product as requested by the one or more downstream participant(s).

The input material may comprise any indiscrete material, e.g., may be a continuous volume of solid or liquid material. The input material may include starting material used in any process performed in the chemical production network to produce the chemical product. The input material may be chemical intermediate product(s) (e.g. chemical intermediate(s)). The input material may be a chemical material, such as a natural, organic or inorganic chemical material. The input material may be a virgin material, e.g. an input material that has not undergone a previous production-and-use cycle, in particular, has not been processed and/or used. The input material may be a recycled material having undergone at least one recycling step. The input material may be selected from petrochemical feedstocks, such as naphtha crude oil, and natural gas, or intermediates from such feedstocks that in turn require a certain quantity of naphtha, crude oil, and natural gas. The input material may be

selected from natural feedstocks, such as vegetable oils, biologicals like enzymes, and/or naturally occurring inorganic or organic chemical materials, or intermediates from such natural feedstocks that in turn require a certain quantity of vegetable oils, biologicals and/or naturally occurring inorganic or organic chemical materials. The input material may comprise or be any input material entering the chemical production network and provided at any entry point of the chemical production network. The input material may be any material entering the system boundary of the chemical production network.

The produced chemical product may be provided or supplied to one or more downstream participant(s) of the chemical supply chain. The one or more downstream participant(s) may use the provided or supplied chemical product. The one or more downstream participant(s) may be downstream producers. The one or more downstream participant(s) may be downstream users. The one or more downstream participant(s) may operate a consumption location(s) configured to consume or use the supplied chemical product. The consumption location may be a further chemical production or a discrete product production. Discrete products may be any products associated with a distinct physical unit. Discrete manufacturing in contrast to process manufacturing uses such discrete products to assemble other discrete products. Chemical production in contrast uses process manufacturing where material(s) are mixed and chemically converted to chemical product(s). The supplied chemical product may be consumed at the consumption location (e.g. may be used in at least one production step performed within the consumption location).

The quantity to be produced for the one or more downstream participant(s) (e.g. the target quantity) may correspond to the use or the projected use of the chemical product. The use or projected use of the chemical product may be monitored and may be compared to chemical product available or planned to be available at storage locations associated with the one or more downstream participant(s). The target data may be generated based on the current or planned storage data associated with the chemical product and the current or planned use of the chemical product within a given future time period. The target data may be generated based on a request to trigger production of the chemical product. The target data may be generated based on a request to trigger production involving the use of the chemical product.

The digital representation(s) associated with production chain(s) related to the production of the chemical product may correspond to digital twin(s) of such production chain(s). The production chain(s) may produce one or more output product(s) including the chemical product as requested by the downstream participant(s). The production chain(s) may produce from one or more input material(s) one or more chemical intermediate(s) required to produce the requested chemical product. Different production chains may hence be interconnected via chemical intermediate(s) used to produce multiple output products including the requested chemical product. The digital representation(s) of the production chain(s) may correspond to digital twin(s) of such production chain(s). The digital twin of the production chain may be a digital representation of the physical entity

of the production chain with a defined semantic description of said physical entity of the production chain. The digital twin or digital representation of the physical entity of the production chain is hence a digital version of said physical entity. Once created, the digital twin may be used to represent the physical entity of the production chain in a digital representation of a real-world chemical production including said production chain. The digital twin may be uniquely linked to the physical entity of the production chain via an identifier. The digital twin may be created such that it is identical in form and behavior of the corresponding physical entity of the production chain. Additionally, the digital twin may mirror the properties of the physical entity of the production chain during its lifetime (e.g. existence). For example, sensors may capture real-time (or near real-time) data, such as production data and/or operating parameters, from the physical entity of the production chain to relay it back to a remote digital twin. The digital twin may then be updated to maintain its correspondence to the physical production chain. Hence, the digital twin may at any time represent the current state of the physical entity of the production chain. The digital twin may contain digital twins of one or more apparatus(es) or plant(s) used to perform a production step of the production chain. The digital twin may include a chemical product identifier such that the digital twin may be linked to a chemical product associated with the production chain (e.g. producible by the production chain). The digital twin may be linked to digital twins of one or more plants used to perform a product step of the production chain. For instance, the digital twin may contain identifiers associated with digital twins of said plants, hence allowing to gather said digital twins using said identifiers.

The one or more digital representation(s) may include plant data associated with plant(s) used within the production chain(s) and capacity threshold(s) per plant and/or per production chain. The one or more digital representation(s) may further be associated with chemical product identifier(s) of chemical product(s) or output product(s) produced by said production chain(s). The one or more digital representation(s) may be associated with input material identifier(s) of input material(s) consumed by said production chain(s). The one or more digital representation(s) may be associated with chemical intermediate identifier(s) associated with chemical intermediate(s) produced within said production chain and/or consumed within said production chain. The one or more digital representation of the chemical production chain(s) may be provided based on data contained in the provided target data. For instance, the chemical product identifier contained in the provided target data may be used to gather the digital representation(s) associated with production chain(s) used to produce the chemical product by matching the chemical product identifier contained in the provided target data with a chemical product identifier included in the one or more digital representation(s). A production capacity shortage may be determined for each production chain associated with a gathered digital representation. This allows to select production chain(s) associated with sufficient capacity. This allows to adapt the production in case production capacity shortage(s) are determined in one or more production chain(s). Adaption may include routing of chemical intermediate(s) to different production

chain(s) to achieve the quantity of output product (e.g. target chemical product) as requested by downstream participant(s).

A production chain may include one or more plant(s). A production chain may include one or more chemical and/or physical processes. The one or more chemical and/or physical processes may be performed by the one or more plant(s). A production chain may produce one or more output product(s) from input material(s) and/or chemical intermediate(s). The output product may be produced via one or more chemical and/or physical processes. A plant may include one or more apparatuses configured to perform one or more chemical and/or physical processes. Production chain(s) used to produce the target chemical product may include production chain(s) producing from one or more input material(s) and/or one or more chemical intermediate(s) the chemical product as output product. Production chain(s) used to produce the target chemical product may include production chain(s) producing from one or more input material(s) chemical intermediate(s) required to produce the target chemical product. The production chains may be connected via chemical intermediate(s) used within multiple production chains to produce multiple output products including the target chemical product.

The capacity threshold(s) may include or be associated with a maximum quantity of output product (e.g. chemical intermediate(s) and/or chemical product(s) including the target chemical product) which can be produced by a given plant or a given production chain within a given time period. The maximum quantity may be dependent on the chemical and/or physical process(es) performed at the given plant or within the given production chain and/or on parameters associated with the plant(s) and/or the production chain. Parameters may include men labor hours available within the given time period to operate the plant(s). The given time period may be associated with the time required to produce a defined quantity of output product. The capacity threshold(s) may include or be associated with a given percentage of the maximum quantity of output product (e.g. chemical intermediate(s) and/or chemical products including the target chemical product) which can be produced by a given plant or production chain within a given time period. For instance, the capacity threshold(s) may include or be associated with 80% of the maximum quantity. This allows to tailor the sensitivity of the warning system, for example to the time necessary to react to determined production capacity shortage(s). The capacity threshold may further include or be associated with a minimum quantity of input material(s) required to produce a defined quantity of output product. Using capacity threshold(s) per production chain and/or per plant allows to determine capacity shortages on a more granular level compared to the use of capacity threshold(s) per chemical production network. This more granular determination allows to mitigate such capacity shortages without negatively impacting other production processes performed within the chemical production network, for example production processes performed within the same production chain or plants and/or production processes using the same intermediate(s) that are used for the production of the chemical product.

Capacity shortages for the output material may be associated with the quantity of output material producible by plant(s) and/or production chain(s) used to produce the output material. The output material may include chemical intermediate(s) and/or chemical products including the target chemical product. Hence, capacity shortage(s) may be occurring if the quantity of chemical product as requested
5 by the one or more downstream participants for the one or more time period(s) is higher than the quantity of requested chemical product that can be produced by the chemical production network within said time period(s). The difference may be due to limitations of the input material(s) and/or chemical intermediate(s) (e.g. material shortages) and/or limitations of plant(s) and/or production chain(s) related to the production of output products associated with the target data (e.g. shortages in
10 production capacity).

Mitigation measures related to input material(s) may include measures related to input material usage. Measures related to input material usage may include adapting the allocation of input material to production chain(s) and/or plant(s). For instance, the quantity of input material allocated to production chain(s) related to the production of the requested chemical product may be adapted such that the
15 requested quantity of chemical product is producible by said production chain(s) for the one or more time period(s). Measures related to chemical intermediate(s) may include measures related to chemical intermediate usage. For instance, the allocation of chemical intermediate(s) to production chain(s) and/or plant(s) may be adapted. For instance, chemical intermediate(s) may be allocated to one or more production chain(s) related to the production of the requested chemical product such that
20 the requested quantity of chemical product is producible by said production chain(s) for the one or more time period(s). In another instance, an increased quantity of chemical intermediate(s) may be allocated to the one or more production chain(s). In yet another instance, chemical intermediate(s) may be reallocated, e.g. at least part of a produced quantity of chemical intermediate(s) may be routed to different production chain(s) such that the requested quantity of chemical product is producible by
25 said different production chain(s) for the one or more time period(s). Measures related to the chemical product may include measures related to chemical product usage. For instance, quantities of chemical product producible by one or more production chain(s) for a plurality of downstream participants may be allocated to one or more particular downstream participant(s) such that the quantity of chemical product producible for such downstream participant can be increased. Measures related to the
30 production parameters may include measures related to the production schedule, measures related to the production location and/or measures related to processing parameters. For instance, production of the requested or target chemical product may be scheduled earlier to allow production of a higher quantity of chemical product for the time period(s) provided by the one or more downstream participants. In another instance, at least part of the production may be allocated to a different
35 production location, such as a different production site. The different production location may have idle production capacity for such chemical product or may be able to produce at least part of the target quantity of the chemical product for the time period(s) provided by the one or more downstream

participant(s). In yet another instance, processing parameters used by one or more plant(s) may be adapted to increase the quantity of chemical product producible by said plant(s).

The chemical product producer producing the target chemical product (e.g. the entity operating the chemical production network producing the target chemical product) and the one or more downstream participant(s) may be part of a product ecosystem. The product ecosystem may include different stages including manufacturing, use and re-use. In these stages one or more ecosystem participant(s) may contribute to the manufacture, use or re-use of the product. For example, the manufacturing stage may include raw material manufacturers, intermediate material manufactures and/or end-product manufacturers. Further for example, the use stage may include product user, product maintainers and/or product distributors. Further for example, the re-use stage may include collectors, sorters, dismantlers, recyclers, restorers and/or re-furbishers.

The participants of the product ecosystem may be connected via a decentral network. The decentral network may include computing nodes associated with participants of the product ecosystem and may be configured to perform data transactions. The computing nodes associated with participants of the product ecosystem may be associated with producers, users or re-users of physical products, such as chemical product producers, intermediate product producers, end-product producers, end product users, used product users or product re-users. The data transactions may be based on a transaction protocol including authentication and/or authorization mechanism(s). Based on the authentication and/or authorization mechanism(s) a peer-to-peer communication between computing nodes associated with participants of the product ecosystem may be established. The respective nodes of the decentral network associated with the participants of the product ecosystem may be configured as decentral data consuming network node(s) and/or decentral data providing network node(s).

The one or more authentication mechanism(s) may be associated with or linked to a decentral identifier associated with the physical entity of the respective raw material, chemical product, intermediate product, end-product or end-of life product. The decentral identifier may uniquely identify the respective physical entity within the decentral network. The decentral identifier may connect the physical entity of the respective raw material, chemical product, intermediate product, end-product or end-of life product to respective raw material data, chemical product data, intermediate product data, end-product data, end-of-life product data, respectively. The decentral identifier may include one or more Universally Unique Identifier(s) (UUID(s)) and/or one or more Decentralized Identifier(s) (DID(s)). The one or more authentication mechanism(s) associated with the decentral identifier may be provided to participant node(s). The one or more authentication mechanism(s) associated with the decentral identifier may be accessible by the decentral data providing network node and/or the decentral data consuming network node. The decentral configuration allows for more efficient use of computing resources and strengthens control by the data owners of the decentral network.

The one or more authorization mechanism(s) may include at least one authorization rule for controlling access to data by the data owners. The computing nodes associated with participants of the product ecosystem may be configured to provide decentral data consuming network node(s) and/or decentral data providing network node(s). A decentral data providing network node may be configured to provide or send data to another participant node of the decentral network. A decentral data consuming network node may be configured to ingest or receive data from another participant node of the decentral network. Providing data to the decentral network for access by a decentral data consuming network node may include indirect or direct access of the decentral data consuming network node to the data. Indirect access may include access to the data via the decentral data providing network node associated with the data owner of the data.

The target data provided from or by the one or more downstream participant(s) may be associated with a target quantity of the chemical product and one or more time period(s). The one or more time period(s) may be associated with the target quantity of the chemical product, e.g. the target quantity of the target chemical product, that is to be supplied to the one or more downstream participant(s) for the one or more time period(s).

In an embodiment, the target data is provided via a peer-to-peer communication from computing node(s) of a decentral network, the computing node(s) being associated with the one or more downstream participant(s). The target data may be provided from decentral data providing network node(s) associated with the one or more downstream participant(s) to a decentral data consuming network node associated with the chemical product producer operating the chemical production network. The decentral data providing network node(s) and the decentral data consuming network node may be part of the decentral network. The target data may be generated by the one or more downstream participant(s). The target data may be generated on behalf of the one or more downstream participant(s). The decentral data consuming network node may be configured to transfer the received data to an application configured to perform the methods disclosed herein. The decentral data consuming network node may be configured to store the received data in a database associated with the operating system of the chemical production network.

The target data may correspond to a target data set having a defined semantic description of the target data. The target data may be generated by applying a data model having a defined semantic description to gathered target data. The data model may include a structure of at least a portion of the target data set, and/or properties of the target data set. The properties of the target data set may include data types. The properties of the target data set may include possible or allowable values and/or value ranges. The properties of the target data set may be a physical unit of parameter(s) described by values contained in the target data set. The properties of the target data set may include one or more attribute(s). Use of a target data set having a defined semantic description ensures that the target data is provided in a uniform and harmonized data format, hence allowing to efficiently

process the provided target data without requiring data transformations to harmonize the provided target data to a uniform data format to determine production capacity shortage(s) based on said provided demand data.

In an embodiment, the target data includes a decentral identifier, data associated with the chemical product, a target quantity of the chemical product and time period data.

The decentral identifier may uniquely identify the target data, in particular the target data set, within the decentral network. The decentral identifier may include one or more UUID(s) and/or DID(s) as previously described. The decentral identifier may be generated any time prior to providing the target data to the chemical product producer operating the chemical production network. For instance, the decentral identifier may be generated upon generation of the target data.

Data associated with the chemical product may include data being indicative of the chemical producer producing the target chemical product and/or location data associated with the location of the chemical production network. Data being indicative of the chemical producer producing the target chemical product may include a name of the chemical product producer, a decentral participant identifier associated with the chemical product producer or a combination thereof. The decentral participant identifier may uniquely identify the chemical product producer within the decentral network. The decentral participant identifier may include letters, numbers, symbols or a combination thereof.

Data associated with the chemical product may include data being indicative of the downstream participant(s) processing or using the target chemical product as produced and supplied by the chemical product producer. Data being indicative of the downstream participant(s) may include a name of the downstream participant(s), a decentral participant identifier(s) associated with the downstream participant(s) or a combination thereof. The decentral participant identifier may uniquely identify the respective downstream participant within the decentral network.

Data associated with the chemical product may include a target chemical product identifier associated with or used by the respective downstream participant and/or a chemical product identifier associated with or used by the chemical product producer. The chemical product identifier associated with or used by the chemical product producer and the target chemical product identifier associated with or used by the respective downstream participant may differ from each other. Hence, it may be necessary to include both identifiers to ensure unique identification of the target chemical product the provided target data is associated with.

Data associated with the chemical product may include data being indicative of the chemical producer producing the target chemical product and/or location data associated with the location of the chemical production network, data being indicative of the downstream participant(s), a target chemical product

identifier associated with or used by the respective downstream participant and/or a chemical product identifier associated with or used by the chemical product producer.

The target quantity of the chemical product may correspond to the use or projected use of chemical product at location(s) associated with the one or more downstream participants(s). The target quantity may hence refer to a target chemical product not yet having been received at the location associated with the one or more downstream participant(s), e.g. not yet having been produced and/or supplied by the chemical product producer.

The time period data may include the time period(s) associated with the target data. The time periods may correspond to future time periods, e.g. time periods lying in the future with respect the point in time associated with the provision of the target data. The time period may include a period of time more than 12 weeks in the future. The time period may include a period of time up to 12 month in the future. The time period may include a period of time up to 24 month in the future. The time period may include a period of time more than 12 weeks in the future and up to 12 month in the future. The time period may include a period of time more than 12 weeks in the future and up to 24 month in the future.

In an embodiment, the time period includes a period of time more than 12 weeks in the future. In an embodiment, the time period includes a period of time up to 12 month in the future. In another embodiment, the time period includes a period of time up to 24 month in the future. In an embodiment, the time period includes more than 12 weeks and up to 12 month. In another embodiment, the time period includes a period of time more than 12 weeks in the future and up to 24 month in the future.

Receipt of target data including time period(s) of more than 12 weeks in the future may allow to produce the target chemical product using the chemical production network for such time period while provided target data including shorter time period(s) may require to supply the one or more downstream participant(s) with chemical product available within a storage location associated with the chemical production network since production of the chemical product may take longer than the time period(s).

In an embodiment, the provided target data is aggregated. Aggregation may be performed prior to determining production capacity shortage(s). Aggregation may include aggregation of the quantity or quantities contained in the provided target data. The provided target data may be aggregated based on time period data contained in the provided target data. For instance, target data received for different time periods may be aggregated to obtain aggregated target data for an aggregated time period. The provided target data may be aggregated based on data associated with the chemical product contained in the provided target data. For instance, the target data provided for a particular target chemical product from a plurality of downstream participants may be aggregated to obtain aggregated target data for such target chemical product. The provided target data may be aggregated based on the downstream participant providing the target data. For instance, all target data provided

by a downstream participant may be aggregated. Aggregation may allow to determine the total quantity of target chemical product which needs to be produced for one or more time periods to fulfil the quantity requested by the one or more downstream participant(s) for one or more time period(s).

The one or more digital representation(s) may include plant data associated with plant(s) forming the production chain(s) and capacity threshold(s) per plant and/or production chain. In an embodiment, the plant data may include plant identifier(s) associated with plant(s) forming the production chain(s). The plant data may further include plant parameters. Plant parameters may include maintenance data, operation hours, size, identifier(s) associated with output product(s) producible by said plant(s), identifier(s) associated with input material(s) and/or chemical intermediate(s) used by said plant(s), recipe data associated with recipes used during production performed within said plant(s), construction data, operation parameters or a combination thereof. The recipe(s) may define input material(s) and/or chemical intermediate(s) and associated quantities(s). The recipe(s) may further define the associated output product. Operation parameters may include the yield (e.g. quantity) of output product(s) producible by said plant(s) and/or the current production capacity of said plant(s).

In an embodiment, the one or more digital representation(s) may be provided based on the provided target data. For instance, the one or more digital representation(s) may be selected from a plurality of digital representations associated with production chains of the chemical production network based on the data associated with the target chemical product contained in the provided target data. The data associated with the target chemical product may include a chemical product identifier associated with the target chemical product. Such chemical product identifier may be used to select such digital representation(s) associated with a matching chemical product identifier. Hence, the chemical product identifier contained in the provided target data may be mapped to chemical product identifier(s) contained in the plurality of digital representations and digital representation(s) including matching chemical product identifier(s) may be selected and provided. The plurality of digital representations may be stored on a data storage medium, such as a database associated with one or more operating system(s) operating the chemical production network.

In an embodiment, the digital representation(s) include(s) mapping data mapping quantities of input material(s) (e.g. raw materials and/or chemical intermediate(s)) to quantities of target output product(s) (e.g. chemical intermediate(s) and/or chemical product(s) including the target chemical product) for at least part of the plant(s). The mapping data may further include a chemical product identifier linking the mapping data to the chemical product the mapping data is associated with. The mapping data may be generated by a virtual production module.

In an embodiment, the digital representation(s) further include(s) mapping data mapping quantities of target chemical product(s) to target production data for at least part of the plant(s) and/or production chain(s) for given future time period(s). The mapping data may be generated by a virtual production

module. Use of mapping data allows to determine target production data quickly and reliably for at least part of the plant(s) and/or production chain(s) related to the production of the target chemical product based on the quantities contained in the mapping data.

The chemical production network may include multiple types of production processes for producing different chemical products or output products from input materials. The chemical production network may include a complex production network producing multiple chemical products (output products) in multiple production or value chains. A production or value chain may include one or more process(es) configured to produce one chemical product or chemical product class from one or more input material(s). The chemical production network may produce from input materials multiple output products. Output products may correspond to intermediates and/or chemical products. The chemical production network may produce from input materials multiple chemical intermediates and from said intermediates multiple output products. The chemical production network may include connected, interconnected and/or non-connected production chains. In an embodiment, the production chains may be connected or interconnected via chemical intermediate(s), e.g. chemical intermediates may be used within more than one production chain to produce multiple output products. Hence, produced chemical intermediates may be used in multiple production chains producing multiple output products. The production chains included in the chemical production network may be defined by the physical system boundary of the chemical production network. The system boundary may be defined by location or control over production processes. The system boundary may be defined by the site of the chemical production network. The system boundary may be defined by production processes controlled by one entity or multiple entities jointly. The system boundary may be defined by the value chain with staggered production processes to an end-product, which may be controlled by multiple entities jointly or separately. The chemical production network may include a waste collection and sorting step, a recycling step such as pyrolysis, a cracking step such as steam cracking, a production step to produce chemical products or intermediates from provided inbound material(s), a separation step to separate intermediates of one process step and further processing steps to convert such outputs to chemical product(s) leaving the system boundary of the chemical production network. Input material may enter the chemical production network at entry points. Chemical products may leave the production network at exit points (or feed-out points).

The chemical production network may comprise one or more entry points at which input materials are provided to the chemical production network. Input material may include raw materials, or chemical intermediate products. Input material may be provided to a plant performing the first production step of the production chain associated with the chemical product.

In an embodiment, determining production capacity shortage(s) includes

- determining target production data for production chain(s) and/or plant(s) associated with the provided digital representation(s) for the one or more time period(s) based on the provided target data or the aggregated data and the provided digital representation(s),
- comparing the determined target production data to the capacity threshold(s) associated with the production chain(s) and/or the plant(s).

The plant(s) may be determined prior to determining production capacity data based on plant data contained in provided digital representation(s). For instance, the plant identifier(s) contained in the provided digital representation(s) may be used to determine the respective plant(s). Production capacity shortage(s) may be determined if the determined target production data for at least one production chain and/or plant associated with the provided digital representation(s) is above at least one capacity threshold.

Determining the target production data may include

- determining target production data by determining the required quantity of output products for the production chain(s) and/or plant(s) for the one or more time period(s) based on provided digital representation(s) and the target data or the aggregated data,
- determining whether further output products are produced by the production chain(s) and/or plant(s),
- in accordance with the determination that further output product(s) are produced, determining further production data by determining the quantity of further output product(s) to be produced for the one or more time period(s) and summing up the target production data and further production data for the one or more time period(s).

The output products may correspond to chemical intermediate(s) associated with the target chemical product and the target chemical product. Further output product(s) may correspond to chemical intermediate(s) associated with further chemical products being different from the target chemical product, and further chemical products. Considering further output products produced by such production chain(s) ensures that capacity shortage(s) are reliably identified within the complex chemical production network producing multiple different chemical products from various input materials via one or more chemical intermediate(s).

The target production data may be determined based on storage data associated with available target chemical product present within a chemical product storage associated with the chemical production network. The target production data may be determined based on determined storage data associated with available target chemical product to be present within a chemical product storage associated within the chemical production network for the one or more time period(s). Storage data associated with available target chemical product may be considered during determination of the target production data. Hence, the quantity of target chemical product(s) to be produced may be reduced by the quantity

of available target chemical product present or to be present within a chemical product storage for the one or more time periods. Available target chemical product may refer to target chemical product not being assigned or allocated to a downstream participant.

In an embodiment, the production capacity shortage(s) is/are determined via a virtual production process using the provided digital representation(s) and the provided target data or the aggregated data. Virtual production may refer to receiving target data or the aggregated data for a target chemical product and the one or more digital representation(s) and virtually producing the quantities of output products necessary to produce the target quantity of the target chemical product. Output products may include chemical intermediate(s) required to produce the target chemical product and the target chemical product. The virtual production process may be performed by a virtual production module configured to receive target data or aggregated data and the provided digital representation(s) and to produce the input material(s) and output product(s) as well as respective quantities. The virtual production module may be configured to determine the production chain(s) and associated plant(s) related to the production of the target chemical product based on the provided digital representation(s). The virtual production module may be configured to determine data associated with the input material(s) and respective quantities used within the respective plant. Input material(s) may be materials entering the system boundary of the chemical production network and/or chemical intermediate(s) required to produce the target chemical product. The virtual production module may be configured to determine data associated with the output product(s) and respective quantities used within the respective plant. Output product(s) may be chemical intermediate(s) or the target chemical product. The virtual production module may be configured to determine the target production data from the determined production chain(s) and/or plant(s), the determined output products and respective associated quantities for the one or more time period(s). The virtual production module may be configured to determine the target production data based on production data associated with the production of further chemical products (output products) produced by said plant or production chain apart from the target chemical product. Hence, the target production data may correspond to the sum of target production data for each output product produced by said respective plant or production chain for the one or more time period(s).

The target production data may be determined for each time period contained in the provided target data or the aggregated data. This ensures a higher level of granularity since capacity shortages may be determined for all time periods contained in the provided target data or the aggregated data.

In an embodiment, generating mitigation data includes

- generating warning message data and/or
- generating monitoring and/or control data to adapt the production of the chemical product (e.g. the target chemical product).

- The warning message data may include data being indicative of the chemical product and data being indicative of the determined production capacity shortage(s). Data being indicative of the chemical product may include a chemical product name, a chemical product ID, an order number associated with the production of the chemical product, data being indicative of the one or more downstream participants associated with the provided target data, or a combination thereof. Data being indicative of the determined capacity shortage(s) may include data associated with the plant(s) and/or production chain(s) where the determined production capacity data reached or exceeded the capacity threshold(s). Data associated with the plant(s) may include plant identifier(s). Data associated with the production chain(s) may include production chain identifier(s).
- 5 The production may be adapted such that the target quantity of the target chemical product is producible for the one or more time period(s) associated with the provided target data or the aggregated data. Adaption of the production may include performing mitigation measure(s) related to input material(s), intermediate product(s), target chemical product and/or production parameters as previously described.
- 10 In an embodiment, generating mitigation data includes
- identifying one or more data set(s) including candidate mitigation data associated with the determined production capacity shortage(s),
 - for each candidate mitigation data within the data set, determining an estimated impact on the mitigation data based on the candidate mitigation data, the provided target data or the aggregated data and the provided digital representation(s),
 - identifying a target mitigation data from the data set(s) based on a comparison of the estimated impacts on the mitigation data.
- 20 The candidate mitigation data may include instructions to reduce the production (e.g. the produced quantity) of further chemical product(s) for plant(s) and/or production chain(s) related to the production of the target chemical product for the one or more time period(s). The instructions may include one or more conditions constraining respective quantity reductions. The constraints may be related to minimum quantities of further output products which must not be fallen short of. This may allow to avoid an overly negative influence of the reduction on the production of further chemical product(s). Reduction of the production of further output product(s) may allow to increase the production capacity for the output products (e.g. chemical intermediate(s) and/or target chemical product) associated with the provided target data.
- 30 The candidate mitigation data may include instructions to allocate the production of output products (e.g. chemical intermediate(s) and/or target chemical product) associated with the provided target data. Allocating the production may include allocating the production of output products associated with the provided target data to a different chemical production or chemical production network located
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at a different geographic location than the chemical production used to determine the production capacity data. This may allow to shift production to a different chemical production or chemical production network, thus circumventing production capacity shortage(s) at the chemical production network while having idle production capacity at another chemical production or chemical production network. The instructions may include one or more conditions constraining respective allocations. The constraints may be related to certification data associated with the production of the target chemical product. Such certification data may be indicative of certifications required or requested by one or more downstream participant(s) of the chemical product producer. Use of such constraints allows to ensure that allocation of the production still fulfils certifications related to the production of the target chemical product as required or requested by the one or more downstream participant(s). Allocation of the production may include allocating the production of further output products produced by the production chain(s) and/or plant(s) related with the production of the target chemical product to a further chemical production. This may allow to increase the production capacity to produce the target chemical product for production chain(s) and/or plant(s) by shifting production capacities for further output products to other chemical production(s) or chemical production network(s). The instructions may include one or more rules that indicate priorities associated with respective allocations. Allocation of the production may include allocating the production of output product(s) associated with the provided target data with respect to time. This may include changing the production order for output product(s) to be produced by said production chain(s) and/or plant(s).

The candidate mitigation data may include instructions to consider storage data associated with available target chemical product present within a chemical product storage associated with the chemical production network and/or storage data associated with available target chemical product to be present within a chemical product storage associated within the chemical production network for the one or more time period(s). The instructions may include rules that indicate under which conditions such storage amounts may be considered.

Determining an estimated impact may include

- determining target production data for production chain(s) and/or plant(s) based on the candidate mitigation data, the provided target data or the aggregated data and the provided digital representation(s),
- determining an estimated impact by comparing at least part of the determined target production data to the capacity threshold(s).

Determining target production data may include recalculating previously determined target production data considering (e.g. using) the respective candidate mitigation data. For instance, previously determined target production data may be recalculated using instructions to reduce the production of further output product(s). Recalculation may include determining the target production data using one or more conditions (or constraints) included in the candidate mitigation data to avoid production

capacity shortage(s) for further output products or at chemical productions/chemical production networks present at different geographic locations. This way, the influence of candidate mitigation data on the production of other chemical products produced by such production chain(s) may be considered during selection of suitable mitigation data to remedy the identified capacity shortage(s).

- 5 This allows to reduce or eliminate balancing effects on a bottom level which may result in capacity shortage(s) for other chemical products produced by the chemical production network.

The estimated impact may correspond to a score. The score may be based on a deviation of the target production data to the capacity threshold(s). The score may indicate how good the candidate mitigation data remedies the determined production capacity shortage(s). The estimated impact may be a classifier classifying whether the candidate mitigation data is suitable to remove or eliminate the determined production capacity shortage(s). The classifier may be "suitable" or "unsuitable". The classifier may be associated with the determination that the determined target production data is below capacity threshold(s). For instance, the classifier "suitable" may be assigned as estimated impact if the determined target production data is below at least a part of the capacity threshold(s).

- 15 Identification of the target mitigation data may include selecting the candidate mitigation data associated with the best estimated impact. For example, the candidate mitigation data associated with the classifier "suitable" may be selected. In another example, the candidate mitigation data associated with the best impact score may be selected. The best impact score may refer to the score being associated with the candidate mitigation data remedying the determined production capacity shortage(s) the best.

In an embodiment, the method further includes a step of generating monitor and/or control data to monitor and/or control production of the quantity of the target chemical product as requested by the one or more downstream participant(s) based on the provided target data or the aggregated data and the provided digital representation(s) if no production capacity shortage(s) are determined. The monitor and/or control data may include production data associated with the production of the target chemical product according to the provided target data or according to the determined aggregated data. The monitor and/or control data may be used by the chemical production network to produce the target chemical product in quantities contained in the provided target data or the determined aggregated data. The monitor and/or control data may include a chemical product identifier. The monitor and/or control data may include quantities of input material(s) necessary to produce the target chemical product in the quantities contained in the provided target data or the determined aggregated data. The monitor and/or control data may include production chain(s) and/or plant(s) related to the production of the target chemical product.

- 35 The generated monitor and/or control data may be provided to the chemical production network for producing the target chemical product in the quantities contained within the provided target data or

the aggregated data. The chemical production network may be configured to produce the target chemical product based on the received monitor and/or control data.

BRIEF DESCRIPTION OF THE SEVERAL VIEWS OF THE DRAWINGS

In the following, the present disclosure is further described with reference to the enclosed figures. The same reference numbers in the drawings and this disclosure are intended to refer to the same or like elements, components, and/or parts.

FIG. 1 illustrates an example embodiment of a decentral network environment including decentral participant network nodes associated with participants of a product ecosystem involving chemical products.

FIG. 2 shows a schematic illustration of providing access via a decentral data providing network node associated with a data owner to chemical product data associated with a chemical product using a decentral data consuming network node associated with a data user.

FIG. 3 illustrates an example of a digital access element including DID owner data, DID document data and decentral identity infrastructure.

FIG. 4 illustrates an example data model structure for generating target data associated with a target chemical product.

FIG. 5 illustrates an example of a chemical production network producing one or more chemical product(s) from one or more input material(s) in connection with an operating system including a production capacity monitoring system.

FIG. 6 illustrates an example of a chemical production network producing multiple output products from multiple input materials and comprising production chains interconnected or connected by chemical intermediates.

FIG. 7 illustrates an example of a chemical production network producing one or more chemical product(s) from one or more input material(s) in connection with an operating system including a production capacity monitoring system controlling and/or monitoring the production of a chemical product based on target data provided by downstream participant(s).

FIG. 8 shows a schematic illustration of a virtual production system for determining production capacity shortage(s) by producing quantities of output products necessary to produce the target chemical product.

- FIG. 9 shows a schematic illustration of processing target data provided from downstream participant(s) by the production capacity monitoring system described in the context of FIG. 5 and FIG. 7.
- 5 FIG. 10 shows a schematic illustration of providing target data via a decentral data providing network node associated with a downstream participant to a chemical product producer producing the target chemical product by a chemical production network via a decentral network.
- 10 FIG. 11 shows a schematic illustration of a digital representation of a production chain related to the production of a target chemical product including several plants involved in the production of the target chemical product.
- FIG. 12 illustrates an example method for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s).
- FIG. 13 illustrates an example for generating mitigation data associated with mitigation measure(s) according to an embodiment of the present disclosure.
- 15 FIG. 14 illustrates an example for determining target production data for plant(s) and/or production chain(s) related to the production of the target chemical product according to an embodiment of the present disclosure.

DETAILED DESCRIPTION

20 The following embodiments are mere examples for implementing the method, the system or application device disclosed herein and shall not be considered limiting.

FIG. 1 illustrates an example embodiment of a decentral network environment. The decentral network environment may include a decentral participant network 134. The decentral participant network 134 may include one or more decentral network participants 102 to 112. The decentral network participants may be part of a product ecosystem including chemical products. The product ecosystem may include
25 production chains to produce an end-product. The product ecosystem may include recycling chains to recycle at least part of end-of-life products. The product ecosystem may include a chemical product producer 102, a chemical product consumer 108, an OEM 112, an end-product user 114, an EOL product collector 116 and a recycler 118. The product ecosystem may include further participants, such as raw material suppliers 106. The product ecosystem may allow to use materials resulting from
30 recycling of end-of-life product to produce new end-products. The product ecosystem may be associated with the production of chemical products and the use of the produced chemical products to produce further chemical products or discrete products.

The participant(s) of the decentral participant network 134 may be associated with the production end-products and/or recycling of end-of-life end products. The decentral network participant 102 to 118 may refer to a manufacturer of physical products, such as chemical product producer 102, chemical product consumer 108, OEM 112, end-product user 114, EOL product collector 116 and recycler 118.

- 5 The decentral network participant may be associated with a decentral participant identifier. The decentral participant identifier may uniquely identify the decentral network participant within the decentral participant network 134.

- 10 The participant(s) of the decentral participant network 134 may be connected via material flow 140. The material flow 140 may correspond to the flow of product from an upstream participant of the decentral participant network 134 to the downstream participant of the decentral participant network 134. The material flow 140 may refer to a continuous or a discontinuous flow of product. The flow of product may include any means of transportation suitable to transport the product from a participant to the downstream participant. The means of transportation may include pipes, containers, barrels, packages. The material flow 140 may be associated with raw materials, chemical products, chemical
15 intermediate products, parts, part assemblies, end-products, end-of-life products, recycled material, etc..

- The data flow 136 between decentral network participant nodes may be directly or indirectly associated with the material flow 140 between the decentral network participants. For instance, data flow 136 may be directly associated with material flow 140 if chemical product data associated with a physical
20 entity of a chemical product provided from chemical product producer 102 to chemical product consumer 108 is accessed by a decentral data consuming network node associated with said chemical product consumer 108. For instance, data flow 136 may be indirectly associated with material flow 140 if data associated with a chemical product produced by chemical product producer 102 is accessed by a decentral data consuming network node associated with end-product user 114 or
25 recycler 118.

- At least part of the participants of the decentral participant network 134 may be associated with decentral participant network nodes 120, 122, 124, 126, 128, 130, 132. The decentral participant nodes 120 to 132 may be under control of the respective decentral participant associated with the respective decentral participant node. The decentral participant nodes 120 to 132 may form decentral
30 network 138. The decentral network 138 may be a peer-to-peer communication network. The decentral network 138 may be configured to perform data transactions 136. The data transactions 136 may be based on a transaction protocol including authentication and/or authorization mechanism(s). Based on the authentication and/or authorization mechanism(s) a peer-to-peer communication between decentral network nodes 120 to 132 associated with decentral network participants 102 to 118 may
35 be established. The one or more authentication mechanism(s) may be associated with or linked to a decentral identifier as described in the context of FIG. 2. The one or more authentication mechanism(s)

associated with the decentral identifier may be accessible by a decentral data providing network node and/or a decentral data consuming network node as described in the context of FIG. 2. The decentral configuration allows for more efficient use of computing resources and strengthens control by the data owners of the decentral network.

5 Data transactions between decentral network participant nodes may be based on a decentral identifier associated with the product data to be accessed and/or decentral identifier(s) associated with material(s) used to produce the respective product. The decentral identifier may be uniquely associated with the physical entity of the product and associated product data. The product may be any raw material, chemical product, part, part assembly, end-product, end-of-life product or recycled
10 material. The decentral identifier may uniquely identify the respective product within the decentral network. The decentral identifier may be associated with further decentral identifier(s), such as decentral material identifier(s) of material(s) used to produce the product. This may allow to track the materials(s) used to produce the product. The decentral identifier may be included in a digital access element associated with the respective product, for example as described in the context of FIG. 2 and
15 FIG. 3.

The decentral participant nodes 120 to 132 may be decentral computing nodes. The decentral computing node may be any device or system that includes at least one physical and tangible processor, and a physical and tangible memory capable of having thereon computer-executable instructions that are executed by a processor. The memory may take any form and depends on the
20 nature and form of the computing node.

At least part of the decentral participant nodes 120 to 132 may be decentral data providing network nodes. At least part of the participant nodes 120 to 132 may be decentral data consuming network nodes. A participant of the decentral participant network 134 may be associated with a decentral data providing network node and/or a decentral data consuming network node depending on whether data
25 is provided to downstream participants and/or consumed from upstream participants. For instance, chemical product producer 102 may be associated with a decentral data providing network node configured to provide chemical product data and/or target production data (e.g. capacity data) to a downstream participant (e.g. chemical product consumer 108) for example as described in the context of FIG. 2. In addition to or alternatively, chemical product consumer 108 may be associated with a
30 decentral data consuming network node configured to receive target data associated with a target quantity requested by chemical product consumer 108 via a decentral data providing network node associated with said chemical product consumer 108, for example as described in the context of FIG. 7.

The decentral network 138 may include further decentral network nodes. The further decentral network
35 nodes may be decentral infrastructure service nodes (not shown in FIG. 1). The decentral

infrastructure service nodes may not be associated with a participant of the product ecosystem. The decentral infrastructure service nodes may provide services for decentral participant nodes 120 to 132, such as verifying the identity of the decentral network participant nodes 120 to 132 prior to performing a data exchange. The decentral network participant nodes 120 to 132 may be associated with or include certificate(s), such as X.509 certificate(s). The certificate(s) may be associated with decentral infrastructure service node(s) including e.g. a certificate issuing service and/or a dynamic provisioning service providing dynamic attribute tokens (e.g. OAuth Access Tokens). This way the decentral network participant nodes 120 to 132 possess a unique identifier embedded in a X.509 certificate that identifies the respective decentral network participant node 120 to 132. The information required to verify the certificate may be provided via an authentication registry associated with the certificate issuing service and/or a dynamic provisioning service. For instance, in the IDSA Reference Architecture Model, Version 3.0 of April 2019, a decentral data providing network node associated with a data owner, a Certification Authority (CA), a Dynamic Attribute Provisioning Service (DAPS) and a decentral data consuming network node associated with a data consumer are used to verify the identity prior to performing a data exchange (not shown).

FIG. 2 shows a schematic illustration of providing access via a decentral data providing network node associated with a data owner to chemical product data associated with a chemical product using a decentral data consuming network node associated with a data user. The system shown in FIG. 2 may be used to exchange product data, such as product data associated with products produced by participants of the product ecosystem, within a decentral participant network, such as described in the context of FIG. 1.

The chemical product may be associated with a digital twin. The digital twin of the chemical product may include a decentral identifier and the chemical product data. The chemical product data may include at least one measured chemical and/or physical property of the chemical product and/or at least one physical and/or chemical property determined from collected data associated with the production and/or the use of the chemical product. The chemical product data may include determined target production data (see for example FIG. 12). The digital twin may be generated by the data owner of the chemical product data, such as chemical product producer 102. The digital twin may be generated on behalf of the data owner of the chemical product data. The digital twin may be generated by gathering chemical product data and applying one or more data models to the chemical product data to generate digital twin data set(s). The digital twin may include the decentral identifier. The decentral identifier may comprise any unique identifier uniquely associated with the digital twin and/or digital twin data set(s), and optionally the data owner. The decentral identifier may connect the physical entity of the chemical product to the digital twin. The decentral identifier may include one or more Universally Unique Identifier(s) (UUID(s)) or Digital Identifier(s) (DID(s)). The one or more DID(s) and/or UUID(s) may be associated with the digital twin and/or the digital twin data set. The one or more DID(s) and/or UUID(s) may further be associated with the chemical product. The decentral

identifier may be generated by the data owner or on behalf of the data owner of the digital twin data. The decentral identifier may include authentication information. Via the decentral identifier and its unique association with the digital twin (and hence with the chemical product) and optionally the data owner, access to the digital twin or access to parts of the digital twin, such as digital twin data set(s) contained in the digital twin, may be controlled by the data owner. This contrasts with central authority schemes, where identifiers are provided by such central authority and access to data is controlled by such central authority. Decentral in this context refers to the usage of the decentral identifier(s) in implementations as controlled by the data owner of the data associated with the decentral identifier, e.g. the chemical product data. The decentral identifier may include or be associated with one or more identifier(s) used in the decentral network and allowing for data exchange via the decentral network. For instance, the decentral identifier may include or be associated with digital twin data set identifier(s) of digital twin data sets, such as UUID(s) of digital twin data set(s). Any combination of UUID(s) and DID(s) may be possible. For instance, the decentral identifier may be a DID while the digital twin data set identifier(s) may be UUID(s). In another instance, the decentral identifier, and the digital twin set data identifier(s) may be UUIDs. Data exchange may include discovery of the decentral identifier and optionally identifier(s) associated with said decentral identifier for participant nodes of the decentral network, authentication of participant nodes of the decentral network and/or authorization of data transfers via a peer-to-peer communication between participant nodes of the decentral network.

The digital twin may be stored in a database 220 associated with the data owner, such as chemical product producer 102. Access to the database 220 and digital twins stored in such database 220 may be controlled by the data owner. Access to the database 220 and stored digital twins may be controlled via the decentral data providing network node 122 associated with the data owner. The digital twin may be stored in database 220 for access by downstream participants, such as chemical product users.

The decentral identifier may be linked to other decentral identifier(s) according to a physical relation of the chemical product entity with other physical entities e.g. those produced using the chemical product or those produced from the chemical product. This way decentral participant node(s) of the decentral network may be able to interpret the relation of the decentral identifier corresponding to the physical relation of the physical chemical product entity to other physical entities. The linking of the decentral digital twin identifier with other decentral product identifier(s) allows to determine the decentral participant node(s) storing the collected data associated with the use of the chemical product or the determined physical and/or chemical property. The collected data and/or the determined chemical and/or physical property may be provided by said decentral participant node(s) and may be stored within the digital twin. For instance, a new data set may be generated by applying an aspect model associated with the use of the chemical product and said new data set may be used to update the digital twin. The decentral identifier may be digital or virtual identifier(s), e.g. may not correspond to physical identifier(s) physically attached to the chemical product.

The decentral identifier may or may be assigned to a physical identifier connected to the chemical product. The connection of the physical identifier with the chemical product may be provided by means of physical connection to the physical chemical product or physical entity. For instance, the physical identifier may be connected with the physical entity of the chemical product. The physical identifier may have one-to-one correspondence to a virtual identity or to a physical identity by means of a physical connection to the physical entity. The physical identifier may be physically attached to the chemical product via an identifier element. Physical identifier or physical identifier element may refer to any virtual or physical arrangement that associates the decentral identifier with the chemical product. The physical identifier may be any identifier for the produced chemical product, such as a batch number or a part number. The physical identifier element may comprise a passive or active element, e.g. QR-code, RFID-tag, but is not limited thereto. The physical identifier element may be a physical identifier physically connected to the product. The identifier element may include markers embedded in materials, a bar code, a QR-Code, a tag like a RFID tag or similar physical arrangement that allows to digitally identify the product.

A digital access element may be generated for the produced chemical product 142. The digital access element may include a decentral passport identifier and access data. The decentral access element identifier may be associated with the decentral identifier. The decentral access element identifier may correspond to the decentral identifier. The access data may include a digital representation pointing to the decentral data providing network node associated with the digital twin. The access data may include a digital representation for accessing the digital twin or parts thereof. Examples of digital access elements are illustrated in FIG. 3. The digital access element may further include or relate to authentication and/or authorization information linked to the decentral access element identifier. The authentication and/or authorization information may be provided for authentication and/or authorization of the decentral network node/decentral data consuming network nodes and decentral data providing network nodes. The digital access element may be provided to a decentral registry node, for example as described in the context of FIG. 2. The decentral registry node may store decentral access element identifier(s) and associated access data.

The physical entity of the chemical product 142 as produced from one or more input materials by a chemical production associated with chemical product producer 102 (not shown, see for example FIG. 5) may be physically provided from the chemical product producer 102 to the chemical product consumer 108. The chemical product may be provided in association with the digital access element to chemical product consumer 108. The chemical product consumer 108 may use the supplied chemical product to produce further chemical products or discrete products. The chemical product 142 may be connected to a code, such as a bar code or QR-code, having encoded the decentral access element identifier or the chemical product identifier. The chemical product consumer 108 receiving chemical product 142 may read the code through code reader 202. The code reader 202 may be a smartphone running a code reading application, such as a QR code reader app. The data obtained by

the code reading application may be used to determine the decentral access element identifier. For instance, the chemical product identifier may be used by decentral data consuming network node 124 to gather endpoint(s) of the decentral data providing network node(s) 122 associated with chemical product data associated with such chemical product identifier. The endpoint may be gathered from
5 decentral infrastructure node(s) based on the chemical product identifier (not shown in FIG. 2). Based on the chemical product identifier, the decentral participant identifier associated with the data owner of the chemical product data may be gathered from decentral infrastructure node(s) by decentral data consuming network node 122. Based on the decentral participant identifier, endpoint(s) of decentral data providing network node(s) associated with such decentral participant identifier may be gathered
10 from decentral infrastructure node(s) by decentral data consuming network node 122. The data obtained by the code reading application may be used to determine the decentral identifier. The data obtained by the code reading application may be used to determine the chemical product identifier. The data obtained by the code reading application may be used to determine the access data. The decentral passport identifier, decentral identifier, chemical product identifier and access data may be
15 determined by code reader 202. For instance, the decentral passport identifier determined by the code reader 202 may be a DID and the code reader 202 may be configured to retrieve the associated DID document containing the decentral identifier and the access data, for example using a DID resolver (see also FIG. 3). In another instance, the chemical product identifier is determined by code reader 202 and used to retrieve the decentral passport identifier and associated access data, for example
20 from a database, such as decentral registry node 208. Hence, code reader 202 may be configured to retrieve the digital access element containing the decentral passport identifier and access data from decentral registry node 208. Code reader 202 may be configured to provide the decentral passport identifier and/or the decentral identifier to a database 206 associated with chemical product consumer 108. Code reader 202 may be configured to provide the determined decentral passport identifier,
25 decentral identifier and access data to decentral data consuming network node 124.

Code reader 202 may be configured to display determined/retrieved data on a user interface as illustrated by reference sign 204. The user interface may display the determined decentral passport identifier (PP identifier), the determined decentral identifier (DT identifier) and the determined access data (DT location). In this embodiment, the decentral passport identifier and the decentral identifier
30 differ from each other. In another embodiment, the decentral passport identifier is equal to the decentral identifier. The user interface may further display the determined chemical product identifier (CP identifier). The user interface may also allow to initiate retrieval of the chemical product data based on the decentral passport identifier and the access data as described in the following. This process may be initiated by the button denoted "Access DT". Upon pressing said button, code reader
35 202 may send a request to access the chemical product data or a part thereof to decentral data consuming network node 124.

Decentral data consuming network node 124 may generate a request to access the chemical product data or a part thereof stored in database 220. Decentral data consuming network node 124 may generate the request based on the data received from code reader 202 or gathered from decentral infrastructure node(s). For instance, decentral data consuming network node 124 may generate the request based on the decentral identifier received from code reader 202 or the gathered endpoint(s). Decentral data consuming network node 124 may generate the request based on the decentral identifier provided to database 206. The request generated by decentral data consuming network node 124 may include the decentral identifier and the decentral participant identifier of the chemical product consumer 108 associated with decentral data consuming network node 124. The request generated by decentral data consuming network node 124 may include the chemical product identifier and the decentral participant identifier of the chemical product consumer 108 associated with decentral data consuming network node 124. Decentral data consuming network node 124 may be configured to determine the decentral data providing network node 122 associated with the chemical product data based on the access data provided by code reader 202 or retrieved from decentral registry node 208 or based on the chemical product identifier .

Decentral data consuming network node 124 may send the request to access the chemical product data or the part thereof to the determined decentral data providing network node 122 as signified by arrow 210. The decentral data providing network node 122 may be associated with the chemical product producer 102. The decentral data providing network node 122 may be associated with the chemical production network producing the chemical product. The decentral data providing network node 122 may be associated with the data owner of the chemical product data. The decentral data providing network node may be associated with the entity operating the chemical production network producing chemical product 142. In addition to the request, authentication and/or authorization information may be provided by decentral data consuming network node 124.

The request may be authenticated. Access to the chemical product data or the part thereof may be authorized based on access policy data associated with the chemical product data. The access policy data may define decentral participant identifier(s) permitted to access the chemical product data. The access policy data may define one or more authorization rule(s) associated with the usage of the chemical product data. The access policy data may define one or more action(s) permitted to be performed on data set(s) present within the chemical product data by decentral data consuming network nodes. This allows to filter decentral data consuming network nodes requesting access based on the decentral participant identifier(s) associated with said network nodes and requested actions to be performed on the accessed chemical product data. If the request is not authorized, e.g. if decentral data consuming network node 124 is not authorized to access the chemical product data, the peer-to-peer communication channel will be terminated by decentral data providing network node 122 and no chemical product data or a part thereof will be provided.

If the request is authorized, decentral data providing network node 122 may initiate contract negotiations with decentral data consuming network node 124 prior to providing the chemical product data or a part thereof. Decentral data providing network node 122 may provide an electronic contract to decentral data consuming network node 124. The electronic contract may include one or more
5 authorization rule(s) associated with the decentral identifier. This allows the data consumer to determine usage conditions associated with the provided chemical product data. Decentral data providing network node 122 and decentral data consuming network node 124 may be configured to negotiate an electronic contract and to sign the negotiated electronic contract. Use of the electronic contract ensures that the decentral data consuming network node and further systems handling the
10 chemical product data or a part thereof are complying to at least one authorization rule associated with the chemical product data. Upon signature of the electronic contract, decentral data consuming network node 124 may request the access element associated with the decentral identifier from decentral data providing network node 122. Decentral data providing network node 122 may gather,
15 based on the decentral identifier contained in the received request, the access element from decentral registry node 208 and may provide the access element to decentral data consuming network node 124. Decentral data consuming network node 124 may be configured to request access to the chemical product data based on the decentral identifier and the access data contained in the received access
20 element.. the chemical product data may be gathered by decentral data providing network node 122 from database 220 based on the provided decentral identifier and access policy data may be applied to the gathered data as signified by arrows 212 and 214. The chemical product data resulting from applying access policy data to the gathered chemical product data may be provided by decentral data
providing network node 122 to decentral data consuming network node 124 as signified by arrow 216.

The chemical product data provided by decentral data providing network node 122 may be stored in
25 database storage 206 associated with the decentral data consuming network node 124 according to the access policy data as signified by arrow 218.

Through the decentral identifier, the chemical product data can be uniquely associated with the chemical product. Through the decentral network, the chemical product data or a part thereof may be transferred between a chemical product producer and a chemical product consumer in a standardized and secure way, allowing the chemical product producer to control access to the chemical product
30 data by multiple decentral data consuming network nodes existing within the decentral network. This way, the chemical product data can be shared with unique association to the chemical product and without central intermediary directly between the participants of the product ecosystem.

FIG. 3 shows an example of a digital access element including DID owner data, DID document data and decentral identity infrastructure.

The decentral identifier may include a Decentralized Identifier (DID). The decentral identifier-based digital access element may in this case be a DID document 304 associated with the DID. Besides the DID document 304 serving as digital access element, FIG. 3 shows a DID owner data element 302 including decentral identifier-based owner data. Generally, the decentral identifier-based owner data may include the decentral identifier associated with a subject such as chemical product data set(s) and may include one or more authentication mechanism(s). The decentral identifier-based owner data 302 may include owner data that is electronically owned and controlled by the DID owner. In this context electronically owned may refer to data that is stored in an owner repository or wallet. Such data may be securely stored and/or managed on an organizational server or client device.

10 The decentral identifier-based owner data 302 may include a DID, a private key and a public key. The DID owner may own and control the DID that represents an identity associated with the DID subject, a private key and public key pair that are associated with the DID. DID may be understood as an identifier and authentication information associated with or uniquely linked to the identifier.

The DID subject may be a raw material, a basic substance, a chemical intermediate, a chemical product, a component, a component assembly or an end product. The DID subject may be a machine, a system, or a device used for producing the raw material, the basic substance, the chemical intermediate, the chemical product, the component, the component assembly or the end product, or a collection of such machine(s), device(s) and/or system(s). The DID owner may be a supply chain participant or a manufacturer such as a chemical producer producing chemical intermediate(s) and/or chemical product(s). The DID owner may be an upstream participant of chemical product producer 102 such as a supplier that supplies raw chemical products or precursors to produce the chemical product. The DID owner may be a downstream participant of the chemical product producer 102 such as chemical product consumer using the supplied chemical product(s) to produce a component, a component assembly or an end product. The DID owner may be any participant of the product ecosystem including raw chemical product supplier, intermediate chemical products manufacturer, chemical product manufacturer, component manufacturer, component assembly manufacturer, end product manufacturer, end product user, EOL collector/sorter or recycler.

The DID may be any identifier that is associated with the DID subject and/or the DID owner. Preferably, the identifier is unique to the DID subject and/or DID owner. The identifier may be unique at least within the scope in which the DID is anticipated to be in use. The identifier may be a locally or globally unique identifier for the raw material, the precursor, the basic substance, the chemical product, the intermediate product, the component, the component assembly, the vehicle, the recycled material or a collection thereof; the machine, the system, or the device used for producing the raw material, the basic substance, the chemical intermediate(s), the chemical product, the component, the component assembly, the end product, the recycled material, or the collection of such machine(s), device(s) and/or system(s); the chemical manufacturer producing chemicals, the upstream participant of the chemical manufacturer, the downstream participant of the chemical manufacturer or a collection

thereof; any participant of the product ecosystem including raw chemical product supplier, intermediate chemical products manufacturer, chemical products manufacturer, component manufacturer, component assembly manufacturer, end product manufacturer, end product user, EOL collector and/or sorter, recycler or a collection thereof.

- 5 The DID may be any identifier that is associated with the DID subject and the DID owner. Preferably, the DID is unique to the DID subject and/or DID owner. The DID may be unique at least within the scope in which the DID is anticipated to be in use. The DID may be a locally or globally unique identifier for any of the above mentioned possible DID subjects. The DID may also be a Uniform Resource Identifier (URI) such as a Uniform Resource Locator (URL). Moreover, the DID may be an
- 10 Internationalized Resource Identifier (IRI). The DID may be a Uniform Resource Identifier (URI) such as a Uniform Resource Locator (URL). The DID may be an Internationalized Resource Identifier (IRI). The DID may be a random string of numbers and letters for increased security. In one embodiment, the DID may be a string of 128 letters and numbers e.g. according to the scheme did:method name:method specific-did such as did:example:ebfeb1f712ebc6f1c276e12ec21. The DID may be
- 15 decentralized ID independent of a centralized, third-party management system and under the control of the DID owner.

- The digital access element as DID document data 304 may be associated with the DID, i.e. the DID included in the decentral identifier-based owner data 302. Accordingly, the digital access element may include a reference to the DID, which is associated with the DID subject that is described by the DID
- 20 document 304 . The DID document 304 may also include an authentication information such as the public key. The public key may be used by third-party entities that are given permission by the DID owner/subject to access information and data owned by the DID owner/subject. The public key may also be used for verifying that the DID owner, in fact, owns or controls the DID. The DID document may include authentication information, authorization information e.g. to authorize third party entities
- 25 to read the DID document or some part of the DID document e.g. without giving the third party the right to prove ownership of the DID.

- The digital access element 304 may include one or more representations that digitally link to digital twin data structure included in the digital twin the digital access element is associated with, e.g. by way of service endpoints. A service endpoint may include a network address at which a service
- 30 operates on behalf of the DID owner. In particular, the service endpoints may refer to services, such as data providing services, of the DID owner that give access to digital twin data. Such services may include services to read or analyze data contained in the digital twin data. Data contained in the digital twin data may include chemical product data.

- The digital access element 304 may include further identifiers, such as digital twin data identifier(s)
- 35 and a chemical product identifier.

The digital access element 304 may include various other information such as metadata specifying when the digital access element was created, when it was last modified and/or when it expires.

The DID and digital access element 304 may be associated with a data registry node such as a centralized data service system or a decentralized data service system 306, e.g. a distributed ledger or blockchain or a decentralized file system. The distributed ledger or blockchain may be used to store a representation of the DID that points to the digital access element 304. A representation of the DID may be stored on distributed computing nodes of the distributed ledger or blockchain 1906. For example, DID hash may be stored on multiple computing nodes of the distributed ledger and point to the location of the digital access element 304. In some embodiments, the digital access element 304 may be stored on the distributed ledger 306. Each of the computing nodes may store a copy of the distributed ledger 306. In this way, each DID hash can be stored redundantly, thereby allowing for an increased data safety. DIDs associated with a plurality of different digital access element 304 may be included in the distributed ledger 306.

In some embodiments, the digital access element 304 may be stored on the distributed ledger 306, i.e. either additionally or alternatively to the associated DID representation being stored on the distributed ledger 306. In other embodiments, the digital access element 304 may be stored in a data storage (not illustrated) that is associated with the distributed ledger or blockchain or decentralized file system.

The distributed ledger or blockchain 306 may be any decentralized, distributed network that includes various computing nodes that are in communication with each other. For example, the distributed ledger 306 may include a first distributed computing node, a second distributed computing node, a third distributed computing node, and any number of additional distributed computing nodes (not shown). The distributed ledger or blockchain 1806 may include known technology stacks like Bitcoin (see e.g. Bitcoin documentation of November 11, 2022 published https://en.bitcoin.it/wiki/Protocol_documentation), Ethereum (see e.g. Ethereum documentation of August 15, 2022 published on <https://ethereum.org/en/developers/docs/>), Solana (see e.g. Solana documentation of November 11, 2022 published on <https://spl.solana.com/>), Polygon (see e.g. Polygon documentation of November 11, 2022 published on <https://wiki.polygon.technology/>) or other implementations with varying degree of data transactions performed on the distributed ledger. The description of the example framework is only for illustrative purposes and shall not be considered limiting.

FIG. 4 illustrates an example data model structure for generating target data associated with a target chemical product. The target data may be generated by the downstream participant(s) by applying the data model shown in FIG. 4 to gathered target data.

The exemplary data model may include the following properties: chemical product producer data 404, downstream participant data 406, target data ID 408, chemical product data 410, unit data 412 and target data 414. The demand data may include further properties such as quantity data 416 and time period data 418. Each property may be associated with one or more attributes. Each attribute may be associated with a corresponding data type. The data type may correspond to allowable data types, such as strings, numbers, Booleans.

Chemical product producer data 404 may include the following attributes: chemical product producer name, production location, chemical product producer ID. The chemical product producer ID may correspond to a decentral participant identifier uniquely associated with the chemical product producer within the decentral network (see for example FIG. 1). The decentral participant identifier may include letters, numbers, symbols or a combination thereof.

Downstream participant data 406 may include the following attributes: downstream participant name, downstream participant ID, downstream participant location or site where target chemical product is to be used. The downstream participant ID may correspond to a decentral participant identifier uniquely associated with the downstream participant within the decentral network (see for example FIG. 1).

Target data ID 408 may include a decentral identifier as attribute. The decentral identifier may uniquely identify the target data, in particular the target data set, within the decentral network. The decentral identifier may include one or more UUID(s) and/or DID(s) as previously described.

Chemical product data 410 may include the following attributes: chemical product identifier used by the downstream participant, chemical product identifier used by the chemical product producer. The chemical product identifier used by the chemical product producer and by the downstream participant may differ from each other. Hence, it may be beneficial to include both identifiers to ensure unique identification of the target chemical product the provided target data is associated with.

Unit data 412 may include the corresponding unit as attribute. This ensures, that the quantity data does not have to be entered with a unit and avoids incorrect data entries.

Quantity data 416 may include the target quantity of the target chemical product as attribute. The quantity may be given as dimensionless number since the unit is already defined by the unit property 412. The quantity may correspond to the target quantity of chemical product (e.g. the quantity of the target chemical product to be produced by chemical product producer 102 and to be delivered to downstream participant 108 for one or more time period(s)).

Time period data 418 may include as attribute one or more time period(s). The time period(s) may include future time period(s). The time period may include week(s) and/or month(s) lying in the future.

Use of a data model having a defined semantic description ensures that the target data is generated and provided in a uniform and harmonized data format, hence allowing to efficiently process the provided target data by chemical product producer 102 without requiring data transformations to harmonize the target data provided from a plurality of downstream participants to a uniform data format to prior to determining production capacity shortage(s) using said provided target data.

FIG. 5 illustrates an example of a chemical production network producing one or more chemical product(s) from one or more input material(s) in connection with an operating system including a production capacity monitoring system. For producing one or more chemical product(s) 142 different input materials (feedstocks) 502 may be provided as physical inputs from material providers or suppliers (see also FIG. 1). The chemical products 142 produced from the input materials may be supplied to chemical product consumer 108, for example as described in the context of FIG. 6. The chemical production network 504 may include multiple interlinked processing steps. The chemical production network 504 may be an integrated chemical production network with connected or interconnected production chains. The chemical production network 504 may include multiple different production chains that have at least one chemical intermediate in common. The chemical production network 504 may include multiple stages of the chemical value chain. The chemical production network 504 may include the producing, refining, processing and/or purification of chemical products. The chemical production network 504 may include multiple production chains that produce from one or more input material(s) via chemical intermediate(s) multiple chemical products that exit the chemical production network 504. The chemical production network 504 may include multiple tiers of a chemical value chain. The chemical production network 504 may include physically connected or interconnected supply chains and/or production sites. The production sites may be at the same location or at different locations. In the latter case, the production sites may be connected or interconnected by means of dedicated transportation systems such as pipelines, supply chain vehicles, like trucks, ships or other cargo transportation means.

The chemical production network 504 may chemically convert input materials 502 via chemical intermediates to one or more chemical product(s) 142 that exit the chemical production network 504. The chemical production network 504 may convert input material(s) by way of chemical conversion to one or more chemical product(s).

The input material(s) may be fed into the chemical production network 504 at any entry point. The input material(s) may be fed into the chemical production network 504 at the start of the chemical production network 504. Input materials may for example make up the feedstock of the plant performing the first production step of the production chain associated with the chemical product.

The chemical production network 504 may produce the chemical product 142 via multiple production steps. The production steps may be defined by the system boundary of the chemical production

network 504. The system boundary may be defined by location or control over production processes. The system boundary may be defined by the site of the chemical production network 504. The system boundary may be defined by production processes controlled by one entity or multiple entities jointly. The system boundary may be defined by a value chain with staggered production processes to an end product, which may be controlled by multiple entities separately. The chemical production network 504 may include a waste collection and sorting step, a recycling step such as pyrolysis, a cracking step such as steam cracking, a chemical reaction step, a separation step to separate outputs of one process step and further processing steps to convert such outputs to a chemical product leaving the system boundary of the chemical production network 504.

The operating system 506 of the chemical production network 504 may monitor and/or control the chemical production network 504 based on operating parameters of the different processes. One process step monitored and/or controlled may be the feed of input materials and/or the discharge of chemical products. Another process step monitored and/or controlled may be the aggregation of provided target data. Yet another process step monitored and/or controlled may be the determination of production capacity shortage(s) for one or more time period(s) based on the provided target data. Yet another process step monitored and/or controlled may be the generation of mitigation data relating to mitigation measure(s). Yet another process step monitored and/or controlled may be the adaption of the production of the target chemical product according to the mitigation data.

The operating system may be configured to perform the method described in the context of FIG. 12 to FIG. 14. The operating system may be configured to perform at least part of the steps described in the context of FIG. 12 to FIG. 14.

FIG. 6 illustrates an example of a chemical production network producing multiple output products from multiple input materials and comprising production chains interconnected or connected by chemical intermediates. In the example illustrated in FIG. 6, the chemical production network 504 comprises three production chains 610, 618, 622. The chemical production network 504 illustrated in FIG. 6 serves as a mere example to explain the concept of interconnected or connected production chains and hence, the chemical production network may comprise more or less production chains than illustrated in FIG. 6.

Each production chain may comprise one or more plants. Each production chain 610, 618, 622 may produce one or more output products, such as output products 1 to 3, from one or more input material(s), such as input material(s) 1 to 3. Each production chain may comprise one or more plants, such as plants 602, 604, 606, 608, 612, 613, 614, 620. Each plant may perform one or more physical and/or chemical processes on input material(s) and/or chemical intermediate(s). Each plant may produce output product(s). The output product(s) may be chemical intermediate(s) and/or chemical products. Within a production chain, such as 610, 618, 622, the output product(s) produced by a plant

may correspond to at least part of the input material(s) for the following plant of said production chain as illustrated in FIG. 6.

Production chain(s) may be connected or interconnected via chemical intermediate(s), e.g. chemical intermediate(s) produced by a first production chain, such as production chain 2 618, may be used as input material(s) for a plant (e.g. plant 2 604) of a second production chain, e.g. production chain 1 610. Likewise output product(s) (e.g. chemical intermediate(s)) produced by a plant of the second production chain, e.g. production chain 1 610, may be used as input material(s) for a plant (e.g. plant 3 616) of the first production chain, e.g. production chain 2 618.

Such connection or interconnection of production chains needs to be considered when determining the production capacity shortage(s), since more than one production chain may be involved in the production of the target chemical product, for example by producing chemical intermediate(s) required as input material(s) in the production chain producing the target chemical product.

FIG. 7 illustrates an example of a chemical production network producing one or more chemical product(s) from one or more input material(s) in connection with an operating system including a production capacity monitoring system for controlling and/or monitoring the production of a chemical product based on target data provided by downstream participants. Chemical production network 504 is described above with reference to FIG. 5 and FIG. 6.

Operating system 506 may be a digital operating system configured to collect, store, manage and interpret a wide range of production and/or business data for chemical production network 504. Operating system 506 may be part of an Enterprise Resource Planning (ERP) system. Alternatively, operating system 506 may be partly implemented in an ERP system and partly implemented in one or more additional systems coupled with an ERP system. Operating system 506 may also be implemented in one or more systems outside of an ERP system.

Input materials 502 may be provided to chemical production network 504 at the feed-in-point 702. The input materials may include raw material(s). The input materials may include chemical intermediate(s). After they are delivered to chemical production network 504, the input materials may be stored into input material storage(s), such as tanks, as they enter the chemical production process.

Chemical products 142 produced by chemical production network 504 may be stored in chemical product storage(s), such as tanks, prior to providing such produced chemical products 142 to the feed-out-point 704. At the feed-out-point 704, the produced chemical products 142 may be provided to one or more downstream participants, such as chemical product consumers 108. The chemical product consumers 108 may use the supplied chemical products 142 to produce further chemical products or discrete products, such as parts or components. The chemical product consumers 108 may generate target data associated with a quantity of chemical product required during one or more future time

period(s). The target data may be generated using the data model illustrated in FIG. 4. The target data may be provided to the chemical product producer producing the target chemical product. Target data received from chemical product consumers 108 may be stored in database 706 of operating system 506. Operating system 506 may receive the target data through any computing system or apparatus,
5 such as a decentralized computing system. Operating system 506 may receive target data via a decentral network, such as described in the context of FIG. 10.

Production capacity monitoring system 708 may aggregate provided target data. Aggregation may be performed as described in the context of FIG. 12. Data aggregation may be triggered by receipt of new target data in database 706. Data aggregation may be triggered by operating system 506 prior to
10 or upon determining production capacity shortage(s) for chemical production network 504 for one or more time period(s) contained in the received target data. Production capacity monitoring system 708 may gather the received target data from database 706 and may parse the gathered data to determine the aggregated target data. Data aggregation may include addition of quantity data included in the gathered target data. Data aggregation may be based on the chemical product identifier included in
15 the gathered target data. Data aggregation may be performed for one or more defined time period(s). For instance, production capacity monitoring system 708 may be configured to gather target data associated with a given chemical product for a given time period and may sum up the quantity data included in the gathered target data. The target data may be gathered based on the chemical product identifier associated with the target chemical product. The aggregated target data may be stored in
20 database 706 or in a database included in production capacity monitoring system 708 (not shown).

Production capacity monitoring system 708 may gather or select digital representation(s) associated with production chain(s) related to the production of the target chemical product (e.g. the chemical product associated with the provided or received target data), for example as described in the context of FIG. 12. The digital representation(s) may be gathered from database 710. Database 710 may store
25 digital representations of production chains associated with chemical products produced by chemical production network 504. Each production chain may be associated with a digital representation. The digital representation(s) may be gathered based on the chemical product identifier contained within the provided target data. For instance, production capacity monitoring system 708 may be configured to select digital representation(s) 1102 associated with the target chemical product by selecting digital
30 representation(s) 1102 containing chemical product identifier(s) matching the chemical product identifier included in the target data. The production capacity monitoring system 708 may be configured to determine production chain(s) and/or associated plant(s) based on the selected digital representation(s). With reference to FIG. 11 and continued reference to FIG. 7, the digital representation(s) of production chain(s) related to the production of the target chemical product may
35 include plant data and capacity threshold(s) per production chain and/or plant. Production chain(s) related to the production of the target chemical product may include production chain(s) producing the target chemical product as output product. Such production chain(s) may include one or more plant(s)

related to the production of the target chemical product. Plant(s) related to the production of the target chemical product may include plant(s) producing chemical intermediate(s) necessary to produce the target chemical product as output product(s). Plant(s) related to the production of the target chemical product may include plant(s) producing the target chemical product as output product. Each plant may perform chemical reaction(s) and/or physical process(es). Each plant may be associated with input material(s) and output product(s). The output product(s) may correspond to chemical intermediate(s) (see also FIG. 6). The output products may correspond to the target chemical product. The output product(s) of one plant may correspond to input material(s) of a subsequent plant of the production chain. The plant(s) may be associated with input material(s) used as feed and/or produced output product(s) via identifier(s) associated with said input material(s) and/or output product(s). For instance, the plant data associated with plant(s) of the chemical production network 504 may include chemical product identifier(s) associated with chemical product(s) (e.g. output products) produced by said plant(s). The plant data may further include material identifier(s) associated with input material(s) (e.g. raw materials and/or chemical intermediate(s)) used within the plant(s) to produce the output product(s). Based on said identifier(s), the plant(s) and associated production chain(s) may be determined.

In the example illustrated in FIG. 11, the production chain 610 may include a first plant 602 performing production of a chemical intermediate, such as monomer, via a chemical reaction. The obtained reaction mixture may correspond to the output product of plant 1 602. The production chain may further include a second plant 604 performing physical processing of the resulting reaction mixture, such as separation of the monomer from the reaction mixture. The separated monomer may correspond to the output product of plant 2 604. The production chain may further include a third plant 606 performing production of the target chemical product from chemical intermediates (e.g. the monomer) produced by plant 2 604 and further chemical monomer(s) produced by different production chain(s) (not shown, see FIG. 6) via a chemical reaction. The reaction mixture may correspond to the output product of plant 3 606. The production chain may further include a fourth plant 608 performing separation of the target chemical product from the reaction mixture and packaging of the target chemical product. The target chemical product may correspond to the output product of plant 4 608. The produced target chemical product may be stored in a chemical product storage, such as tanks, prior to providing the produced target chemical product to the respective downstream participant, such as chemical product consumer 108, for example via tank trucks and or transporting the packaging units containing the target chemical product to the respective downstream participant.

In the example illustrated in FIG. 11, plant 1 602 to plant 4 608 may form the production chain 610 associated with the production of the target chemical product 142. The example illustrated in FIG. 11 shall not be considered limiting with respect to the plant(s) required to produce a specific chemical product. Likewise, production chain 610 may include more or less plant(s).

Plant(s) may be associated with a chemical production network. The chemical production network may include one or more production chain(s) include the one or more plant(s) producing multiple output products. Plant(s) may include any apparatus configured to perform chemical reaction(s) and/or a physical reaction(s). The plant(s) may have at least one feed line to allow feed of input material(s) (e.g. raw material(s) and/or chemical intermediate(s)). The plant may have at least one discharge line configured to discharge output product (e.g. chemical intermediate(s) or chemical product(s) including the target chemical product). Examples of plants may include steam cracker(s), chemical reactor(s), distillation apparatus(es), disperser(s), mill(s), mixer(s), extruder(s) or the like.

Each plant of the production chain may be associated with plant data. The plant data may correspond to a digital twin of the respective plant. The plant data may be related to identifier(s) associated with the target chemical product and associated intermediate chemical(s). The plant data may include plant identifier(s) associated with the respective plant(s). The plant data may include capacity threshold(s) for the respective plant. The plant data may further include plant parameters. Plant parameters may include maintenance data, operation hours, size, output product(s) producible by said plant(s), input material(s) and/or chemical intermediate(s) used by said plant(s), recipe(s) used by said plant(s), construction data, operation parameters or a combination thereof. The identifier(s) allow(s) to determine the respective digital representation(s) associated with the production of the target chemical product. The recipe(s) may define input material(s) and/or chemical intermediate(s) and associated quantities. The recipe(s) may further define the associated output product. Operation parameters may include the yield (e.g. quantity) of output product(s) producible by said plant(s) and/or current production capacity of said plant(s).

The current production capacity of a given plant or of a given production chain may be determined by comparing the quantity of output product(s) currently produced by the plant or production chain per defined time period to the capacity threshold(s) associated with the given plant or given production chain.

The digital representation 1102 of production chain 610 may include the plant data 1104 and capacity threshold(s) per plant and/or production chain. The digital representation 1102 may further include identifier(s) associated with the target chemical product and/or chemical intermediate(s) used to produce the target chemical product. This may allow to gather the digital representation(s) associated with the target chemical product based on chemical product data contained within the provided target data.

The plant data 1104 and/or the digital representation(s) may be used to generate mapping data, mapping quantities of required input material(s) (e.g. raw materials and/or chemical intermediate(s)) to quantities of target output product(s) (e.g. chemical intermediate(s) and/or chemical product(s) including the target chemical product) for at least part of the plant(s). The mapping data may be

included in the digital representation 1102. The digital representation 1102 may include a pointer to the mapping data. The mapping data may further include a chemical product identifier linking the mapping data to the chemical product the mapping data is associated with. The mapping data may be generated by a virtual production module.

- 5 The plant data 1104 and/or the digital representation(s) may be used to generate mapping data mapping quantities of target chemical product(s) to target production data for at least part of the plant(s) of the production chain(s) for given time period(s). The mapping data may further include a chemical product identifier linking the mapping data to the target chemical product the mapping data is associated with. The mapping data may be included in the digital representation 1102. The digital
10 representation 1102 may include a pointer to the mapping data. Use of mapping data allows to determine target production capacity data quickly and reliably for at least part of the plant(s) and/or production chain(s) related to the production of the target chemical product based on the quantities contained in the mapping data.

- Referring back to FIG. 7 and with continued reference to FIG. 9, production capacity monitoring system
15 708 may be configured to determine whether the target chemical product is producible for the one or more time period(s) contained in the provided target data/aggregated data. With reference to FIG. 9, production capacity monitoring system 708 may be configured to parse the target data to determine the time period(s) contained therein. The determined time period(s) may be compared to production times required to produce the target chemical product. If the determined time period(s) are less than
20 the required production time, such as less than 12 weeks, production capacity monitoring system 708 may be configured to compare the target quantity to storage data stored in database 904 or to projected storage data (e.g. data associated with the storage of target chemical product being present within the chemical product storage at the time period(s) given in the provided target data). Such comparison may be performed by storage monitoring system 902. This may allow to determine
25 whether the quantity of the target chemical product requested by the one or more downstream participant(s) is available within a chemical product material storage associated with the chemical production network 504. If the determined time period(s) are higher than the required production time, such as more than 12 weeks, production capacity monitoring system 708 may be configured to determine production capacity shortage(s). The production capacity shortage(s) may be determined
30 by production capacity shortage determinator 906, for example as described in the context of FIG. 12 to FIG. 14.

- Production capacity monitoring system 708 may be configured to determine production capacity shortage(s) based on the provided target data/aggregated data, the selected digital representation(s) and the capacity threshold(s), for example as described in the context of FIG. 12. The production
35 capacity shortage(s) may be determined by production capacity monitoring system 708 via a virtual production process using the provided digital representation(s) and the provided target

data/aggregated data. The virtual production process may be performed by a virtual production module of production capacity monitoring system 708.

With reference to FIG. 8 and continued reference to FIG. 7 and FIG. 9, the virtual production module 802 may be configured to gather target data and the respective digital representation(s) based on chemical product identifier(s) contained in the target data and to produce required quantities of chemical intermediate(s) 804 and target quantities of target chemical product 806 for given future time period(s). The virtual production module may further be configured to produce required quantities of further output products 808 (e.g. chemical intermediate(s) and/or chemical product(s) produced by plant(s) associated with the production chain(s) related to the production of the target chemical product). The virtual production module may further be configured to produce required quantities of input material(s). Input material(s) may include raw material(s) required to produce the target chemical product. The required quantities may correspond to the quantities necessary to produce the quantity of target chemical product corresponding to the target quantity contained in the target data provided by downstream participants, such as the chemical product consumer 108, or corresponding to aggregated quantities. The virtual production module 802 may be configured to determine whether sufficient input material is available within the chemical production network 504 based on the determined required quantities and input material storage data or projected input material storage data. The virtual production module 802 may be configured to determine target production data 810 based on the required quantities of chemical intermediate(s), target chemical product and optionally further output product(s) for given time period(s) (e.g. time period(s) included in the provided target data). The virtual production module 802 may be configured to determine target production data based on the mapping data included in the selected digital representation(s). The target production data 810 determined by the virtual production module 802 may correspond to the sum of the target production data for the target chemical product and further production data associated with further output products produced by said respective plant for the given time period(s).

Returning to FIG. 7 and with continued reference to FIG. 9, production capacity monitoring system 708 may be configured to determine capacity shortage(s) by comparing the determined target production data with capacity threshold(s) per production chain and/or per plant. The capacity threshold(s) may be included in the digital representation(s), such as digital representation 1102 illustrated in FIG. 11, associated with the respective production chain(s). The capacity threshold(s) may include or be associated with a maximum quantity of output product(s) (e.g. chemical intermediate(s) and/or chemical product(s)) producible by a respective plant or production chain for a given time period. The capacity threshold(s) may include or be associated with a given percentage of the maximum quantity of output product (e.g. chemical intermediate(s) and/or chemical product(s)) producible by a respective plant or production chain for a given time period. Production capacity shortage(s) may be determined if target production data is above at least one capacity threshold included in the provided digital representation(s).

Production capacity monitoring system 708 may be configured to generate mitigation data related to mitigation measure(s) associated with input material(s), chemical intermediate(s), target chemical product and/or production parameters if production capacity shortage(s) are determined, for example as described in the context of FIG. 12. Production capacity monitoring system 708 may be configured to provide the generated mitigation data to operating system 506. Operating system 506 may be configured to adapt the production of the target chemical product, such that the target quantity of the target chemical product is produced for the one or more time period(s) contained within the provided target data. Production capacity monitoring system 708 may be configured to generate monitoring and/or control data if no production capacity shortage is determined. Production capacity monitoring system 708 may be configured to provide the generated monitoring and/or control data to operating system 506. Operating system 506 may be configured to monitor and/or control production of the target chemical product by chemical production network 504 based on the provided monitoring and/or control data.

FIG. 10 shows a schematic illustration of providing target data via a decentral data providing network node associated with a downstream participant via a decentral network to a chemical product producer producing the target chemical product by a chemical production network. The target data received by chemical product producer 102 as described in the context of FIG. 10 may be used to monitor and/or control the chemical production network 504 as described in the context of FIG. 7. The target data received by chemical product producer 102 as described in the context of FIG. 10 may be used to generate mitigation data to adapt the production of the target chemical product by the chemical production network 504 as described in the context of FIG. 7.

Chemical product producer 102 may generate a data set including an endpoint address associated with decentral data consuming network node 122 and data being indicative that this is the endpoint to receive target data associated with target chemical product(s) from one or more downstream participant(s). The data set (hereinafter denoted as asset) may be provided to decentral registry node 208 or to decentral data consuming network node 122. Decentral registry node 208 may be configured to store assets and to provide access to the stored assets upon request from decentral data providing network node(s) associated with participants of a decentral network, such as decentral network 138 described in the context of FIG. 1. Decentral data consuming network node 122 may be configured to provide target data received from a decentral data providing network node 124 associated with a downstream participant, such as chemical product consumer 108, to target data database 706.

A downstream participant, such as chemical product consumer 108, may generate target data for a target chemical product, for example as described in the context of FIG. 7 and FIG. 12. The generated target data may be stored in target data storage 1008 associated with a decentral data providing network node 124 of chemical product consumer 108. Upon request, for example from an application being in communication with the decentral data providing network node 124, decentral data providing

network node 124 may be configured to retrieve the asset registered by chemical product producer 102 from decentral registry node 208 or decentral data consuming node 122. The asset may be retrieved by identifying the asset catalog (e.g. the list of available assets) associated with the chemical product producer 102 based on the decentral participant identifier of chemical product producer 102.

5 The asset may be identified in the catalog by searching for an asset containing a property being indicative of endpoint data to receive demand data.

Upon identifying the respective endpoint, decentral data providing network node 124 may establish a connection to decentral data consuming network node 122 using the data contained in the retrieved asset. Decentral data providing network node 124 and decentral data consuming network node 122
10 may perform authentication steps, for example as described in the context of FIG. 2. Upon successful authentication, electronic contract negotiations may be performed as described in the context of FIG. 2. Upon successful electronic contract negotiations, decentral data providing network node 124 may provide the generated target data to decentral data consuming network node 122 and decentral data consuming network node 122 may store the received target data in database 706.

15 The target data can be provided in a secure yet reliable and standardized manner via the decentral network from the downstream participant to the product producer operating the chemical production network. By publishing an endpoint for providing target data within the decentral network by the chemical product producer, downstream participant(s) can reliably determine such an endpoint and provide respective target data in a secure, reliable and standardized manner to such endpoint without
20 requiring the chemical product producer to request such data via the decentral network. This way, a reliable provision of target data in a secure and standardized manner can be achieved, allowing the chemical product producer to efficiently determine capacity shortages and to generate mitigation data upon determining such capacity shortage(s). This allows to avoid disruption of supply chains due to capacity bottlenecks, hence ensuring reliable and stable production of products by the downstream
25 participants.

FIG. 12 illustrates an example method for monitoring and/or controlling a production of a target chemical product in a quantity as requested by one or more downstream participant(s). FIG. 12 also illustrates an example method for generating mitigation data related to mitigation measure(s) for adapting the production of the target chemical product according to the provided target data. At least
30 parts of the example method illustrated in FIG. 12 may be performed by an operating system of a chemical production network, such as operating system 506 of chemical production network 504 illustrated in FIG. 5. At least parts of the example method may be performed by production capacity monitoring system 708 described in the context of FIG. 7. The target chemical product as produced according to the target data provided by the one or more downstream participant(s) may be supplied
35 to said downstream participant(s), such as chemical product consumers 108 as described in the context of FIG. 1 and FIG. 2. The chemical product consumers 108 may consume or use the chemical

product (e.g. may produce further chemical products or discrete products using the supplied chemical product). To ensure reliable production of the further products or discrete products, the chemical product consumers may require recurring supply of target quantities of the target chemical product. To ensure the recurrent supply of such target quantities, the chemical product consumers may generate target data for one or more time period(s) and provide the target data to the target chemical product producer. The target quantity of the target chemical product contained within said target data may be associated with the projected consumption of the target chemical product at production site(s) of the chemical product consumers. The chemical product producer may produce the target chemical product via the chemical production network based on the target data provided by the one or more downstream participants. This may avoid extensive storage capacities, hence reducing the overall costs associated with the production of the target chemical product. However, this also requires monitoring and/or controlling of production capacities to avoid production capacity shortage(s) and hence delayed supply of the target chemical product to the downstream participant(s). Delayed supply may in turn result in production shortages of downstream participants of the product ecosystem which may be undesirable and should hence be avoided.

In block 1202, target data associated with a target quantity of the target chemical product to be processed at plant(s) associated with the one or more downstream participant(s) may be provided from the one or more downstream participant(s) for one or more time period(s). The target data may be provided as described in the context of FIG. 10. The target data may be generated as described in the context of FIG. 4 and FIG. 7. Use of a data model to generate the target data ensures a uniform data format of the target data, hence making data transformations prior to processing the received target data redundant. The target data may be received by the operating system 506 of the chemical production network 504. The received target data may be stored in a database, such as database 706 illustrated in FIG. 7, associated with the operating system 506.

The target data may include a decentral identifier, data associated with the chemical product, a target quantity of the chemical product and time period data. Data associated with the chemical product may include data being indicative of the chemical producer producing the target chemical product and/or location data associated with the location of the chemical production network. Data associated with the chemical product may include data being indicative of the downstream participant(s) processing or using the target chemical product as produced and supplied by the chemical product producer. Data associated with the chemical product may include a target chemical product identifier used by the respective downstream participant and/or a chemical product identifier used by the chemical product producer. The time period data may include the time period(s) associated with the target data. The time periods may be future time periods, e.g. time periods lying in the future with respect the point in time associated with the provision of the target data. The time period may include a period of time more than 12 weeks in the future. The time period may include a period of time up to 12 month in the future. The time period may include a period of time up to 24 month in the future. The time period may

include a period of time more than 12 weeks in the future and up to 12 month in the future. The time period may include a period of time more than 12 weeks in the future and up to 24 month in the future.

In block 1204, the target demand data may be aggregated, for example as described in the context of FIG. 7, this block being generally optional. The received target data may be aggregated per target chemical product. Aggregation may be performed by the operating system 506. Aggregation may be triggered by the operating system for a predefined time period. Aggregation may be performed by production capacity monitoring system 708 upon receiving an indication from operating system 506. Aggregation may include aggregation of the quantity or quantities contained in the provided target data. The provided target data may be aggregated based on time period data contained in the provided target data. For instance, target data received for different time periods may be aggregated to obtain aggregated target data for an aggregated time period. The provided target data may be aggregated based on data associated with the chemical product contained in the provided target data. For instance, the target data provided for a particular target chemical product from a plurality of downstream participants may be aggregated to obtain aggregated target data for such target chemical product. The provided target data may be aggregated based on the downstream participant providing the target data. For instance, all target data provided by a downstream participant may be aggregated. Aggregation may allow to determine the total quantity of target chemical product which needs to be produced for one or more time period(s) to fulfil the quantity requested by the one or more downstream participant(s) for one or more time period(s). In block 1206, digital representation(s) of the production chain(s) associated with the production of the target chemical product may be provided. An example of such a digital representation is illustrated in FIG. 11. The digital representation(s) may be provided based on the provided target data. For instance, the one or more digital representation(s) may be selected from a plurality of digital representations associated with the production chains of the chemical production network based on the data associated with the target chemical product contained in the provided target data. The data associated with the target chemical product may include a chemical product identifier associated with the target chemical product. Such chemical product identifier may be used to select such digital representation(s) associated with a matching chemical product identifier. Hence, the chemical product identifier contained in the provided target data may be mapped to chemical product identifier(s) contained in the plurality of digital representations and digital representation(s) including matching chemical product identifier(s) may be selected and provided. The plurality of digital representations may be stored on a data storage medium, such as a database associated with one or more operating system(s) operating the chemical production network. The digital representation(s) may include plant data and capacity threshold(s) per production chain and/or plant. The digital representation may further include mapping data as described in the context of FIG. 7. Based on the provided digital representation(s), the received target data and the capacity threshold(s), production capacity shortage(s) may be determined. In block 1208, production target data for the production chain(s) and/or plant(s) for the one or more time period(s) may be determined

based on the target data/aggregated data and the provided digital representation(s). The plant(s) may be determined prior to determining production capacity data based on plant data contained in provided digital representation(s). For instance, the plant identifier(s) contained in the provided digital representation(s) may be used to determine the respective plant(s). Production capacity shortage(s) may be determined if the determined target production data for at least one production chain and/or plant associated with the provided digital representation(s) is above at least one capacity threshold. Block 1206 to block 1208 may be performed by a virtual production module of production capacity monitoring system 708 described in the context of FIG. 7.

With reference to FIG. 14, target production data may be determined by determining the required quantity of output products for the production chain(s) and/or plant(s) for the one or more time period(s) based on provided digital representation(s) and the target data or the aggregated data (see block 1402). The output products may correspond to chemical intermediate(s) associated with the target chemical product and the target chemical product. The required quantity of output products may include the quantity contained in the provided target data or the quantity contained in the aggregated data determined in block 1204.

The target production data may be determined based on storage data associated with available target chemical product present within a chemical product storage associated with the chemical production network. The target production data may be determined based on determined storage data associated with available target chemical product to be present within a chemical product storage associated within the chemical production network for the one or more time period(s). Storage data associated with available target chemical product may be considered during determination of the target production data. Hence, the quantity of target chemical product(s) to be produced may be reduced by the quantity of available target chemical product present or to be present within a chemical product storage for the one or more time periods. Available target chemical product may refer to target chemical product not being assigned or allocated to a downstream participant.

With continued reference to FIG. 14, it may be determined in decision block 1404 whether further output product(s) are produced by the production chain(s) and/or plant(s). Further output product(s) may include chemical product(s) and chemical intermediate(s) being different from the target chemical product and associated chemical intermediate(s). Such different output products may, for example, differ in chemical structure and/or in chemical composition. If this is not the case, e.g. if the production chain(s) and/or plant(s) are exclusively used to produce the target chemical product, the data determined in block 1402 may correspond to the target production data. If this is not the case, e.g. if at least part of the production chain(s) and/or plant(s) are used to produce further output products, the further output products to be produced for the one or more time period(s) may be determined in block 1406. The further output products may be determined using the provided digital representation(s). For instance, the plant data included in the digital representation(s) may include data being indicative of

output product(s) produced by said plant and/or production chain. The data being indicative of output product(s) produced by said production chain(s) and/or plant(s) may include respective output product identifier(s).

Further production data may be determined by determining the quantity of further output material(s) to be produced for the one or more time period(s) (see block 1408). The quantities may be determined based on target data or aggregated data associated with said further output products as described in FIG. 7.

The target production data may be determined by summing up the target production data and the further production data, e.g. by summing up the required quantity of output products determined in block 1402 and the quantity of further output product(s) determined in block 1408 for the one or more time period(s). The target production data may be determined for the production chain(s) and/or for one or more plant(s) of the production chain(s).

Referring back to FIG. 12, production capacity shortage(s) may be determined by comparing the determined target production data to capacity threshold(s) (see block 1210). The target production data per plant may be compared to capacity threshold(s) per plant. The target production data per production chain may be compared to capacity threshold(s) per production chain. The capacity threshold(s) may be contained in the provided digital representation(s). The capacity threshold(s) may correspond to maximum quantities of output product(s) producible by the respective plant and/or production chain for a given time period. The capacity threshold(s) may correspond to a percentage of the maximum quantities of output product(s) producible by the respective plant and/or production chain within a for time period. Prior to comparison, the determined target production data may be normalized to the time period(s) associated with the capacity threshold(s).

In decision block 1212, it may be determined whether capacity threshold(s) may be reached or surpassed. The determination may be performed based on the result of the comparison performed in block 1210. In accordance with the determination, that the capacity threshold(s) are not reached or surpassed, monitoring and/or control data for the production of the target quantity of the target chemical product may be generated based on the provided target data and the generated monitoring and/or control data may be provided (see block 1214). The monitoring and/or control data may be generated by the operating system 506 of the chemical production network 504. Production capacity monitoring system 708 may be configured to provide an indication to operating system 506 that no production capacity shortage has been identified and operating system 506 may be configured to generate the monitoring and/or control data and to monitor and/or control the chemical production network 504 based on the generated monitoring and/or control data as described in the context of FIG. 7.

In accordance with the determination, that capacity threshold(s) is/are reached or surpassed, mitigation data related to the input material(s), chemical intermediate(s), target chemical product and/or production parameters may be generated in block 1216. Mitigation measures related to input material(s) may include measures related to input material usage. Measures related to input material usage may include adapting the allocation of input material to production chain(s) and/or plant(s). For instance, the quantity of input material allocated to production chain(s) related to the production of the requested chemical product may be adapted such that the requested quantity of chemical product is producible by said production chain(s). Measures related to chemical intermediate(s) may include measures related to chemical intermediate usage. For instance, the allocation of chemical intermediate(s) to production chain(s) and/or plant(s) may be adapted. For instance, chemical intermediate(s) may be allocated to one or more production chain(s) related to the production of the requested chemical product such that the requested quantity of chemical product is producible by said production chain(s). In another instance, an increased quantity of chemical intermediate(s) may be allocated to the one or more production chain(s). In yet another instance, chemical intermediate(s) may be reallocated, e.g. at least part of a produced quantity of chemical intermediate(s) may be routed to different production chain(s) such that the requested quantity of chemical product is producible by said production chain(s). Measures related to the chemical product may include measures related to chemical product usage. For instance, quantities of chemical product producible by one or more production chain(s) for a plurality of downstream participants may be allocated to one or more particular downstream participant(s) such that the quantity of chemical product producible for such downstream participant can be increased. Measures related to the production parameters may include measures related to the production schedule, measures related to the production location and/or measures related to processing parameters. For instance, production of the requested or target chemical product may be scheduled earlier to allow production of a higher quantity of chemical product for the time period(s) provided by the one or more downstream participants. In another instance, at least part of the production may be allocated to a different production location, such as a different production site. The different production location may have idle production capacity for such chemical product or may be able to produce at least part of the target quantity of the chemical product for the time period(s) provided by the one or more downstream participant(s). In yet another instance, processing parameters used by one or more plant(s) may be adapted to increase the quantity of chemical product producible by said plant(s).

With reference to FIG. 13, mitigation data may be generated using one of more data sets including candidate mitigation data. In a first step (see block 1302), one or more data sets including candidate mitigation data associated with determined capacity shortage(s) may be identified. The mitigation data may be generated by production capacity monitoring system 708.

The candidate mitigation data may include instructions to reduce the production (e.g. the produced quantity) of further output product(s) for one or more plant(s) and/or production chain(s) associated

with the production of the target chemical product for the one or more time period(s). The instructions may include one or more conditions constraining respective quantity reductions. The constraints may be related to minimum quantities of further output products which must not be fallen short of. This may allow to avoid an overly negative influence of the reduction on the production of further output product(s). Reduction of the production of further output product(s) may allow to increase the production capacity for the output products (e.g. chemical intermediate(s) and/or the target chemical product) associated with the provided target data. Considering further output products produced by such production chain(s) ensures that capacity shortage(s) are reliably identified within the complex chemical production network producing multiple different chemical products from various input materials via one or more chemical intermediate(s).

The candidate mitigation data may include instructions to allocate the production of output products (e.g. chemical intermediate(s) and/or target chemical product) associated with the provided target data. Allocating the production may include allocating the production of output products associated with the provided target data to a different chemical production or chemical production network located at a different geographic location than the chemical production used to determine the production capacity data. This may allow to shift production to a different chemical production or chemical production network, thus circumventing capacity shortage(s) at one chemical production while having idle production capacity at another chemical production. The instructions may include one or more conditions constraining respective allocations. The constraints may be related to certification data associated with the production of the target chemical product. Such certification data may be indicative of certifications required or requested by one or more downstream participant(s) of the chemical product producer. Use of such constraints allows to ensure that allocation of the production still fulfils certifications related to the production of the target chemical product as required or requested by the one or more downstream participant(s). Allocation of the production may include allocating the production of further output products produced by the production chain(s) and/or plant(s) related with the production of the target chemical product to a further chemical production. This may allow to increase the production capacity to produce the target chemical product for production chain(s) and/or plant(s) by shifting production capacities for further chemical products to other chemical production(s) or chemical production network(s). The instructions may include one or more rules that indicate priorities associated with respective allocations. Allocation of the production may include allocating the production of output product(s) associated with the provided target data with respect to time. This may include changing the production order for output product(s) to be produced by said production chain(s) and/or plant(s).

The candidate mitigation data may include instructions to consider storage data associated with available target chemical product present within a chemical product storage associated with the chemical production network and/or storage data associated with available target chemical product to be present within a chemical product storage associated within the chemical production network for

the one or more time period(s). The instructions may include rules that indicate under which conditions such storage amounts may be considered.

In block 1304, an estimated impact of the mitigation data may be determined for each candidate mitigation data within the data set based on the respective candidate mitigation data, the provided target data/aggregated data and the provided digital representation(s). Determining an estimated impact may include

- determining target production data for production chain(s) and/or plant(s) based on the candidate mitigation data, the provided target data/aggregated data and the provided digital representation(s),
- determining an estimated impact by comparing at least part of the determined target production data to the capacity threshold(s).

Determining target production data may include recalculating previously determined target production data considering (e.g. using) the respective candidate mitigation data. For instance, previously determined target production data may be recalculated using instructions to reduce the production of further output product(s). Recalculation may include determining the target production data using one or more conditions (or constraints) included in the candidate mitigation data to avoid production capacity shortage(s) for further output products or at chemical productions/chemical production networks present at different geographic locations. This way, the influence of candidate mitigation data on the production of other chemical products produced by such production chain(s) may be considered during selection of suitable mitigation data to remedy the identified capacity shortage(s). This allows to reduce or eliminate balancing effects on a bottom level which may result in capacity shortage(s) for other chemical products produced by the chemical production network.

The estimated impact may correspond to a score. The score may be based on a deviation of the target production data to the capacity threshold(s). The score may indicate how good the candidate mitigation data remedies the determined production capacity shortage(s). The estimated impact may be a classifier classifying whether the candidate mitigation data is suitable to remove or eliminate the determined production capacity shortage(s). The classifier may be "suitable" or "unsuitable". The classifier may be associated with the determination that the determined target production data is below capacity threshold(s). For instance, the classifier "suitable" may be assigned as estimated impact if the determined target production data is below at least part of the applicable capacity threshold(s).

In block 1306, target mitigation data may be identified from the one or more data sets based on a comparison of the estimated impacts of the candidate mitigation data. Identification of the target mitigation data may include selecting the candidate mitigation data associated with the best estimated impact. For example, the candidate mitigation data associated with the classifier "suitable" may be selected. In another example, the candidate mitigation action associated with the best impact score

may be selected. The best impact score may refer to the score being associated with the candidate mitigation data remedying the determined production capacity shortage(s) the best.

Returning to FIG. 12, the generated mitigation data may be provided. Production capacity monitoring system 708 may provide the generated mitigation data to operating system 506 and operating system 506 may be configured to generate monitoring and/or control data to adapt the production using the generated mitigation data. The production may be adapted such that the target quantity of the target chemical product is producible by the chemical production network for the one or more time period(s) associated with the target data.

A digital twin associated with the chemical product produced according to the provided mitigation data may be generated, this step being generally optional (see optional block 1220). The digital twin may include a decentral identifier and chemical product data associated with the chemical product, for example as described in the context of FIG. 2. The digital twin may be stored in a data storage associated with the chemical product producer for access by the downstream participant(s), such as chemical product consumers. The access to the stored digital twin may be controlled via the decentral identifier by the data owner of the digital twin, such as the chemical product producer, for example as described in the context of FIG. 2.

By using a digital representation(s) of production chain(s) related to the production of the target chemical product, production capacity shortage(s) occurring in production chain(s) and/or associated plant(s) can be reliably identified and mitigation data related to mitigation measures may be generated that allows to adapt the production such that the determined production capacity shortages are avoided while at the same time ensuring production of the target quantity of the target chemical product for the one or more time period(s). Specifically for chemical production networks that produce more than one chemical product from more than one input material via interconnected, connected and non-connected production chains, the use of one or more digital representation(s) allows to flexibly route intermediates necessary to produce the chemical product from one production chain to another production chain such that the chemical product can be produced in the quantity requested by the downstream participant(s) while avoiding capacity shortage(s). For instance, the production of the chemical product may be adapted such that an intermediate necessary to produce the chemical product is routed from a first production chain to a second production chain such that the output of the second production chain (e.g. the chemical product) can be produced in the quantity as requested by the downstream participant(s). The mitigation data may be determined using a data sets including candidate mitigation control data associated with the determined production capacity shortage(s) and selecting the most suitable control data to remedy the determined production capacity shortage(s). By using digital representation(s) of production chain(s), the influence of candidate mitigation data on the production of other output products to be produced by production chain(s) associated with the target chemical product may be determined and considered during selection of suitable candidate mitigation

data to remedy the determined production capacity shortage(s). This allows to reduce or eliminate balancing effects on a bottom level which may result in production capacity shortage(s) for other output products to be produced by said production chain(s) for the one or more time period(s). The approach proposed herein allows to ensure reliable and timely production of target chemical products based on target data provided from one or more downstream participant(s) and hence avoids production capacity shortage(s) negatively influencing the downstream participants of the supply chain up to the end-product producer.

The present disclosure has been described in conjunction with preferred embodiments and examples as well. However, other variations can be understood and effected by those persons skilled in the art and practicing the claimed invention, from the studies of the drawings, this disclosure and the claims.

Any steps presented herein can be performed in any order. The methods disclosed herein are not limited to a specific order of these steps. It is also not required that the different steps are performed at a certain place or in a certain computing node of a distributed system, i.e. each of the steps may be performed at different computing nodes using different equipment/data processing.

As used herein „determining“ also includes „initiating or causing to determine“, „generating“ also includes „initiating and/or causing to generate“ and „providing“ also includes „initiating or causing to determine, generate, select, send and/or receive“. „Initiating or causing to perform an action“ includes any processing signal that triggers a computing node or device to perform the respective action.

In the claims as well as in the description the word „comprising“ does not exclude other elements or steps and the indefinite article „a“ or „an“ does not exclude a plurality. A single element or other unit may fulfill the functions of several entities or items recited in the claims. The mere fact that certain measures are recited in the mutual different dependent claims does not indicate that a combination of these measures cannot be used in an advantageous implementation. In the claims as well as in the description the word „comprising“ or „including“ or similar wording does not exclude other elements or steps and shall not be construed limiting to the elements or steps lined out. The indefinite article „a“ or „an“ does not exclude a plurality. A single element or other unit may fulfill the functions of several entities or items recited in the claims. The mere fact that certain measures are recited in the mutual different dependent claims does not indicate that a combination of these measures cannot be used in an advantageous implementation or further elements may be included.

Providing in the scope of this disclosure may include any interface configured to provide data. This may include an application programming interface, a human-machine interface such as a display and/or a software module interface. Providing may include communication of data or submission of data to the interface, in particular display to a user or use of the data by the receiving entity.

All terms and definitions used herein are understood broadly and have their general meaning.

CLAIMS

1. A computer-implemented method for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, said method comprising:
- 5 (a) providing target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s),
- (b) providing one or more digital representation(s) associated with production chain(s) related with the production of the chemical product, wherein the digital representation includes plant data and capacity threshold(s) per plant and/or production chain,
- 10 (c) determining production capacity shortage(s) based on the provided target data, the provided digital representation(s) and the capacity threshold(s),
- (d) if production capacity shortage(s) are determined, generating mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), chemical product and/or production parameters,
- 15 (e) providing the generated mitigation data for adapting the production of the chemical product according to the mitigation data.
2. The method of claim 1, wherein the target data is provided via a peer-to-peer communication from computing node(s) of a decentral network, the computing node(s) being associated with the one or more downstream participant(s).
- 20 3. The method of claim 1 or 2, wherein the target data includes a decentral identifier, data associated with the chemical product, a quantity of the chemical product and time period data.
4. The method of any one of claims 1 to 3, wherein the plant data includes plant identifier(s) associated with plant(s) forming the production chain(s).
- 25 5. The method of any one of claims 1 to 4, wherein the production chains are connected or interconnected via the chemical intermediate(s).
6. The method of any one of claims 1 to 5, wherein determining production capacity shortage(s) includes
- 30 • determining target production data for production chain(s) and/or plant(s) associated with the provided digital representation(s) for the one or more time period(s) based on the provided target data and the provided digital representation(s),
- comparing the determined target production data to the capacity threshold(s) associated with the production chain(s) and/or the plant(s),

7. The method of any one of claims 1 to 6, wherein the production capacity shortage(s) is/are determined via a virtual production process using the provided digital representation(s) and the target data.
8. The method of any one of claims 1 to 7, wherein generating mitigation data includes
- 5 - generating warning message data and/or
- generating monitoring and/or control data to adapt the production of the chemical product.
9. The method of any one of claims 1 to 8, further including a step of generating monitor and/or control data to monitor and/or control production of the quantity of the chemical product as requested by the one or more downstream participant(s) based on the provided target data and
- 10 digital representation(s) if no production capacity shortage(s) are determined.
10. An apparatus for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediates by a chemical production network, said apparatus comprising:
- 15 (a) a target data provider configured to provide target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s),
- (b) a data provider configured to provide one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital
- 20 representation includes plant data and capacity threshold(s) per plant and/or production chain,
- (c) a production capacity shortage determinator configured to determine production capacity shortage(s) based on the provided target data, the provided digital representation(s) and the capacity threshold(s)
- 25 (d) a mitigation data generator configured to
- generate mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), chemical product and/or production parameters if production capacity shortage(s) are determined,
- provide the generated mitigation data for adapting the production of the chemical product
- 30 according to the mitigation data.
11. A system for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s), said system comprising:
- (a) an apparatus for monitoring and/or controlling a production of a chemical product in a quantity as requested by one or more downstream participant(s) as claimed according to
- 35 claim 10, and

- (b) a chemical production network configured to
- receive the mitigation data or the monitor and/or control data as generated according to the computer-implemented method claimed according to any one of claims 1 to 9, and
 - produce the chemical product from one or more input material(s) via one or more chemical intermediate(s) according to the received data.

12. A computer-implemented method for generating mitigation data for adapting a production of a chemical product to produce the chemical product quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, said method comprising:

- (a) providing target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s),
- (b) providing one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data and capacity threshold(s) per plant and/or production chain,
- (c) determining production capacity shortage(s) based on the provided target data, the provided digital representation(s) and the capacity threshold(s),
- (d) if production capacity shortage(s) are determined, generating mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), chemical product and/or production parameters,
- (e) providing the generated mitigation data for adapting the production of the chemical product according to the mitigation data.

13. An apparatus for generating mitigation data for adapting a production of a chemical product to produce the chemical product quantity as requested by one or more downstream participant(s), wherein the chemical product is produced from input material(s) via chemical intermediate(s) by a chemical production network, the apparatus comprising one or more computing node(s) and one or more computer-readable media having thereon computer-executable instructions that are structured such that, when executed by the one or more computing node(s), cause the apparatus to perform the steps below:

- (a) provide target data from the one or more downstream participant(s) for the chemical product to be provided to the downstream participant(s) for one or more time period(s),
- (b) provide one or more digital representation(s) associated with production chain(s) used to produce the chemical product, wherein the digital representation includes plant data and capacity threshold(s) per plant and/or production chain,
- (c) determine production capacity shortage(s) based on the provided target data, the provided digital representation(s) and the capacity threshold(s),

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- (d) if production capacity shortage(s) are determined, generate mitigation data associated with mitigation measure(s) related to input material(s), intermediate product(s), chemical product and/or production parameters,
- (e) provide the generated mitigation data for adapting the production of the chemical product according to the mitigation data.

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14. Use of the mitigation data as generated by the computer-implemented method of claim 12 or by the apparatus of claim 13 to adapt the production of a chemical product to produce the chemical product in a quantity as requested by one or more downstream participant(s).

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15. Chemical product produced by a chemical production network using the mitigation data as generated by the computer-implemented method of any one of claims 1 to 9 or by the apparatus of claim 10.

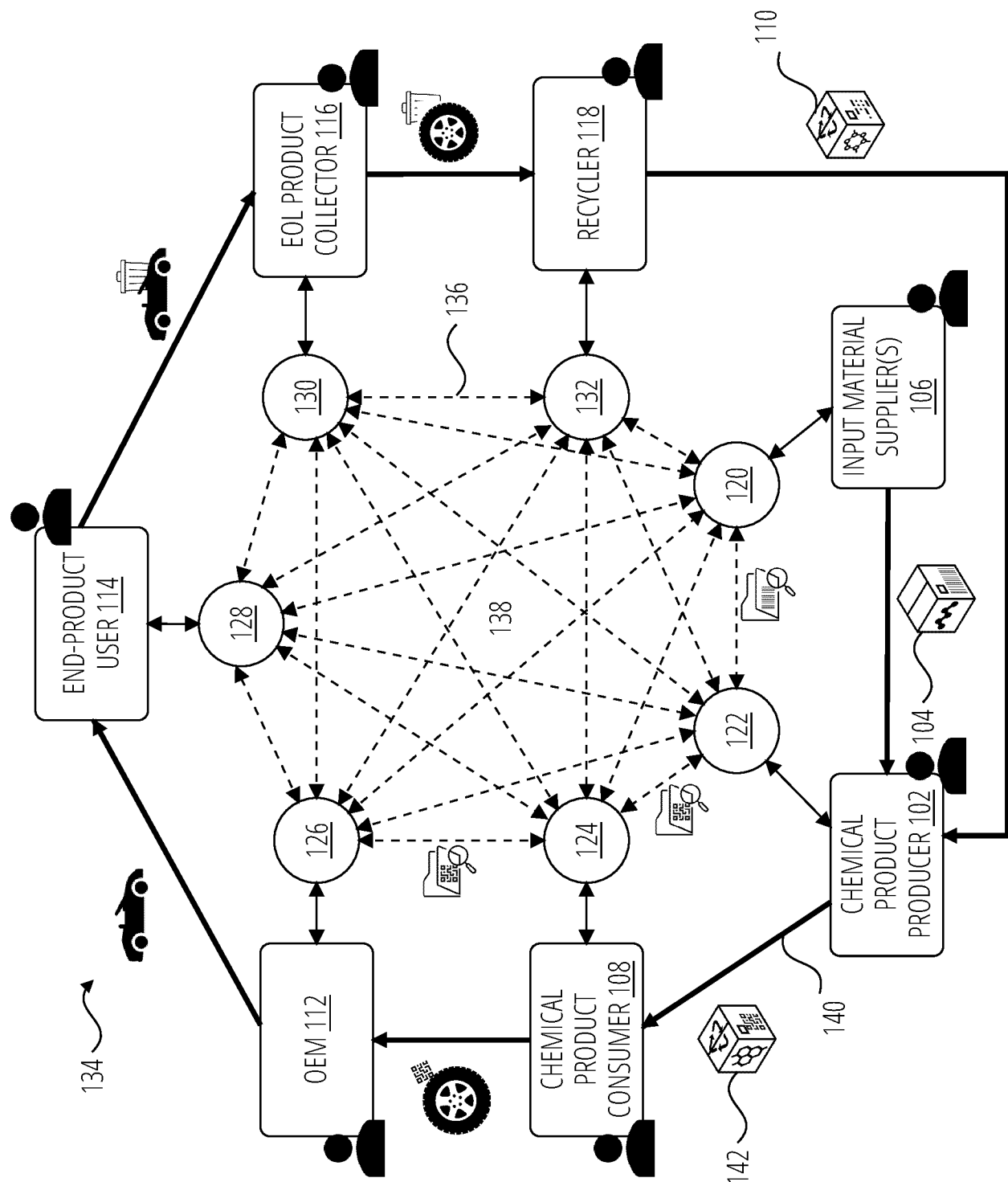


FIG. 1

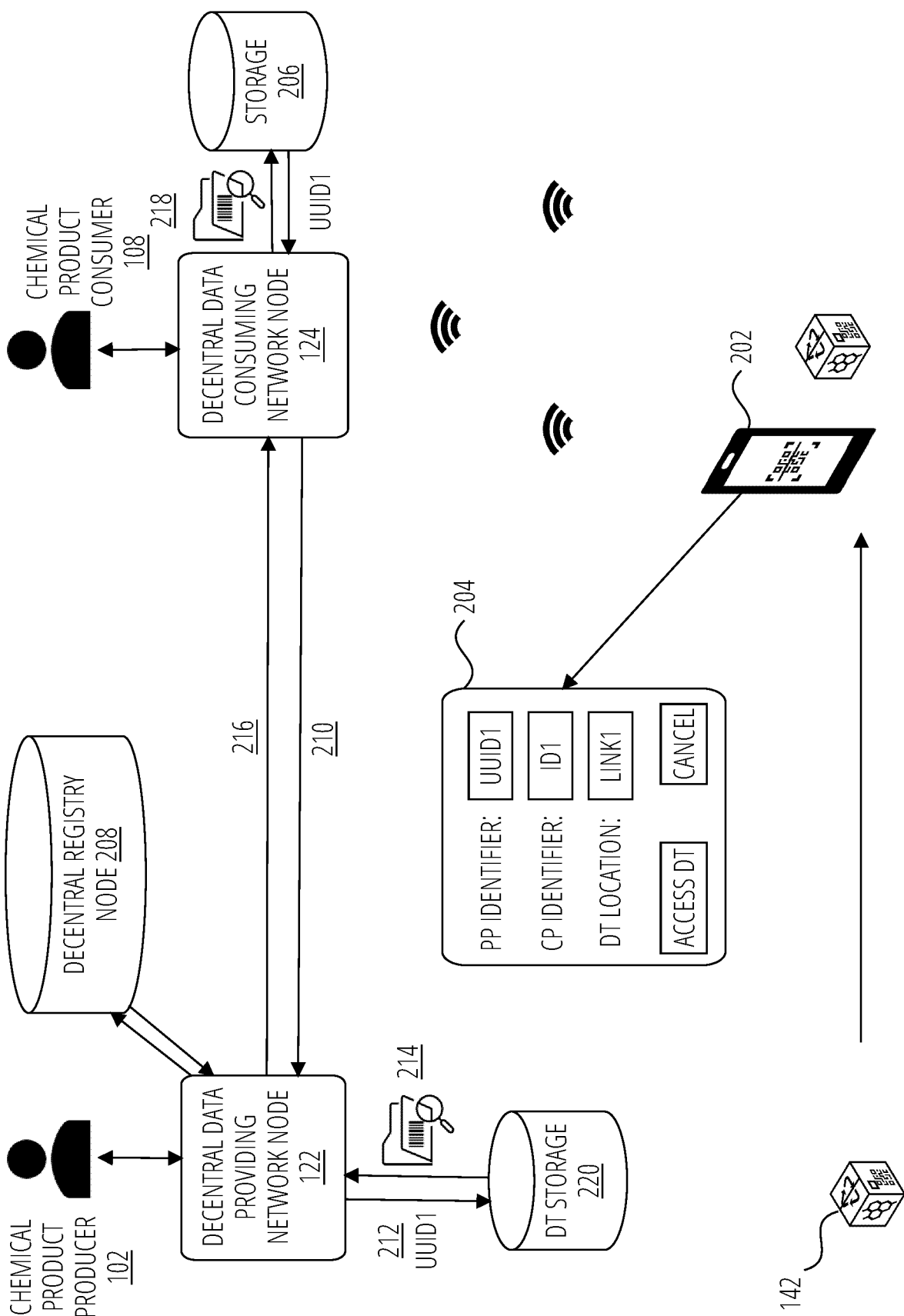


FIG. 2

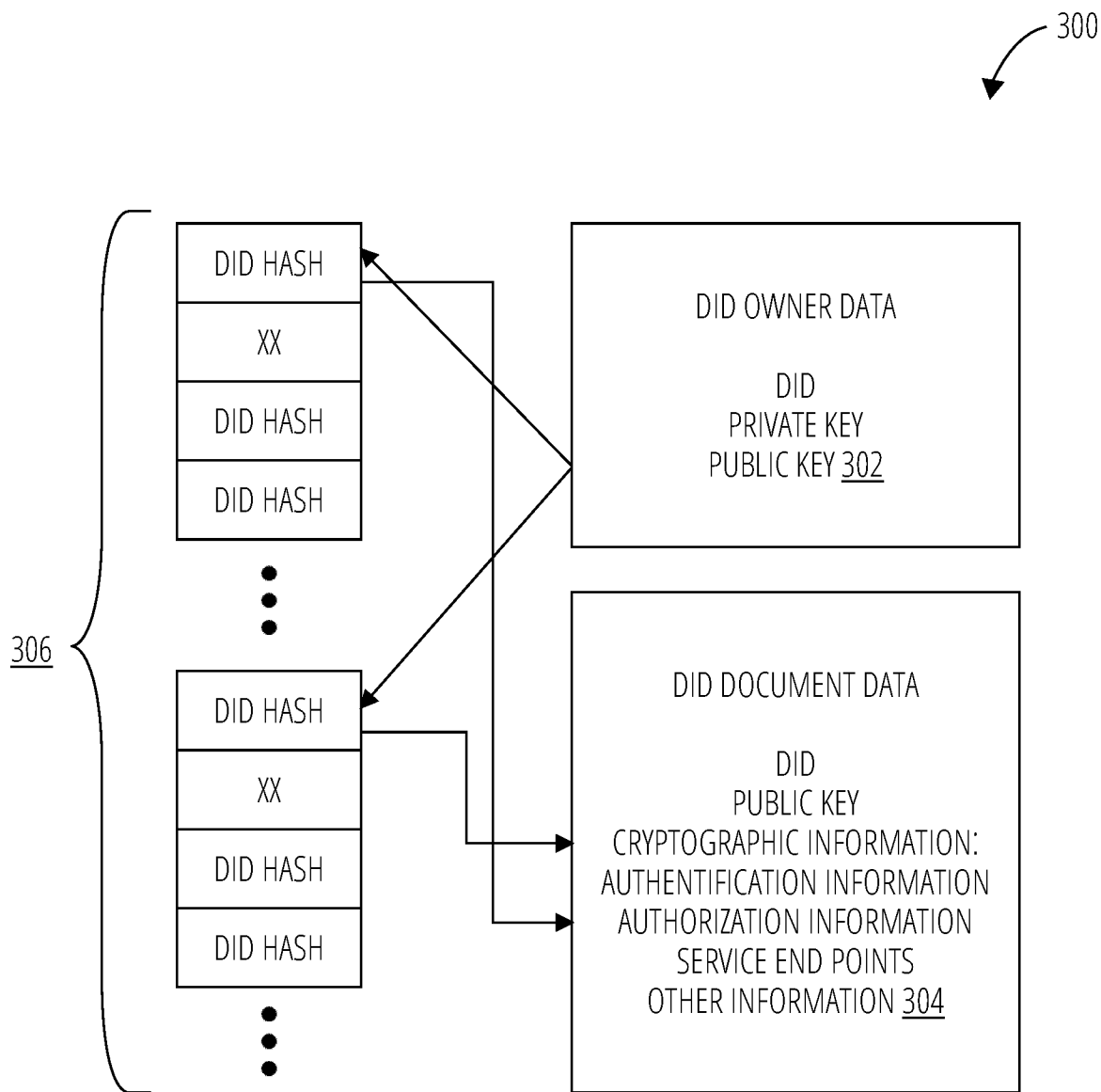


FIG. 3

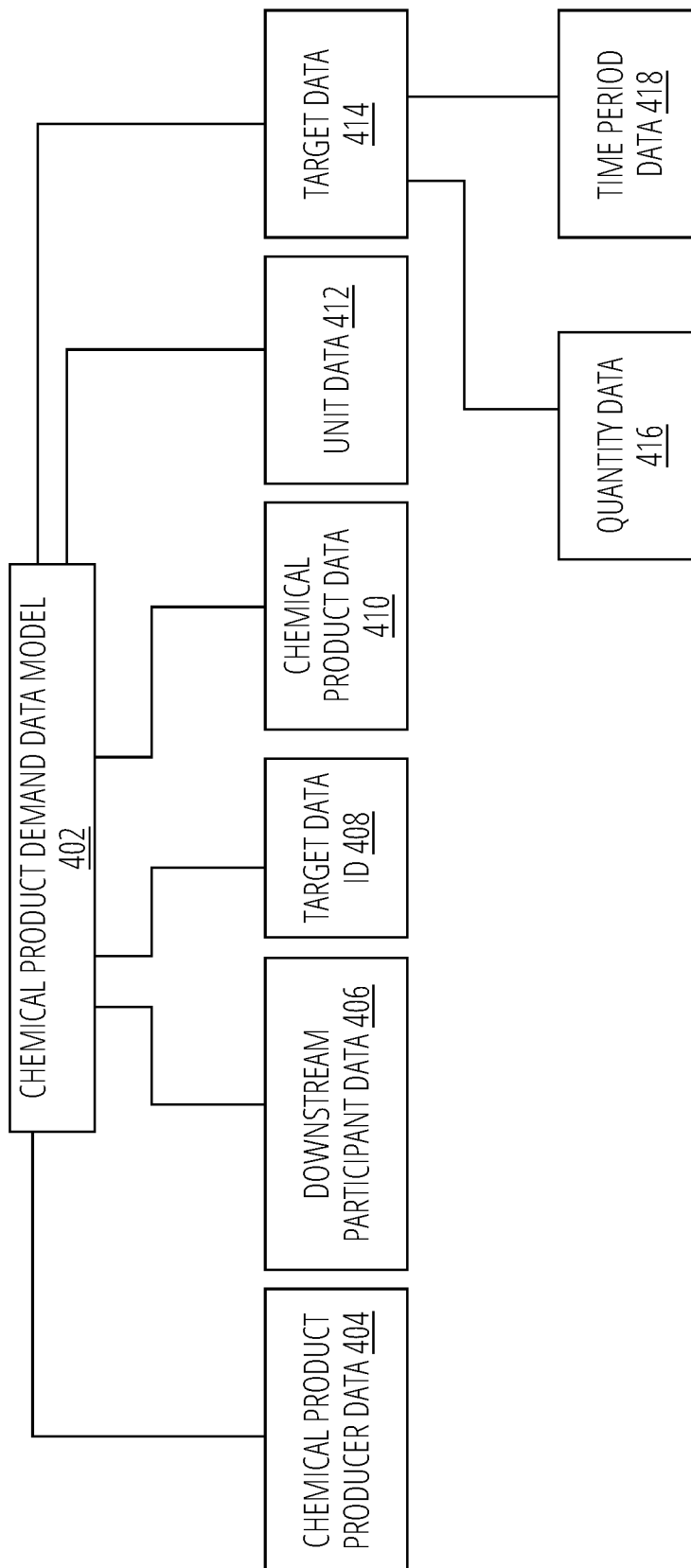


FIG. 4

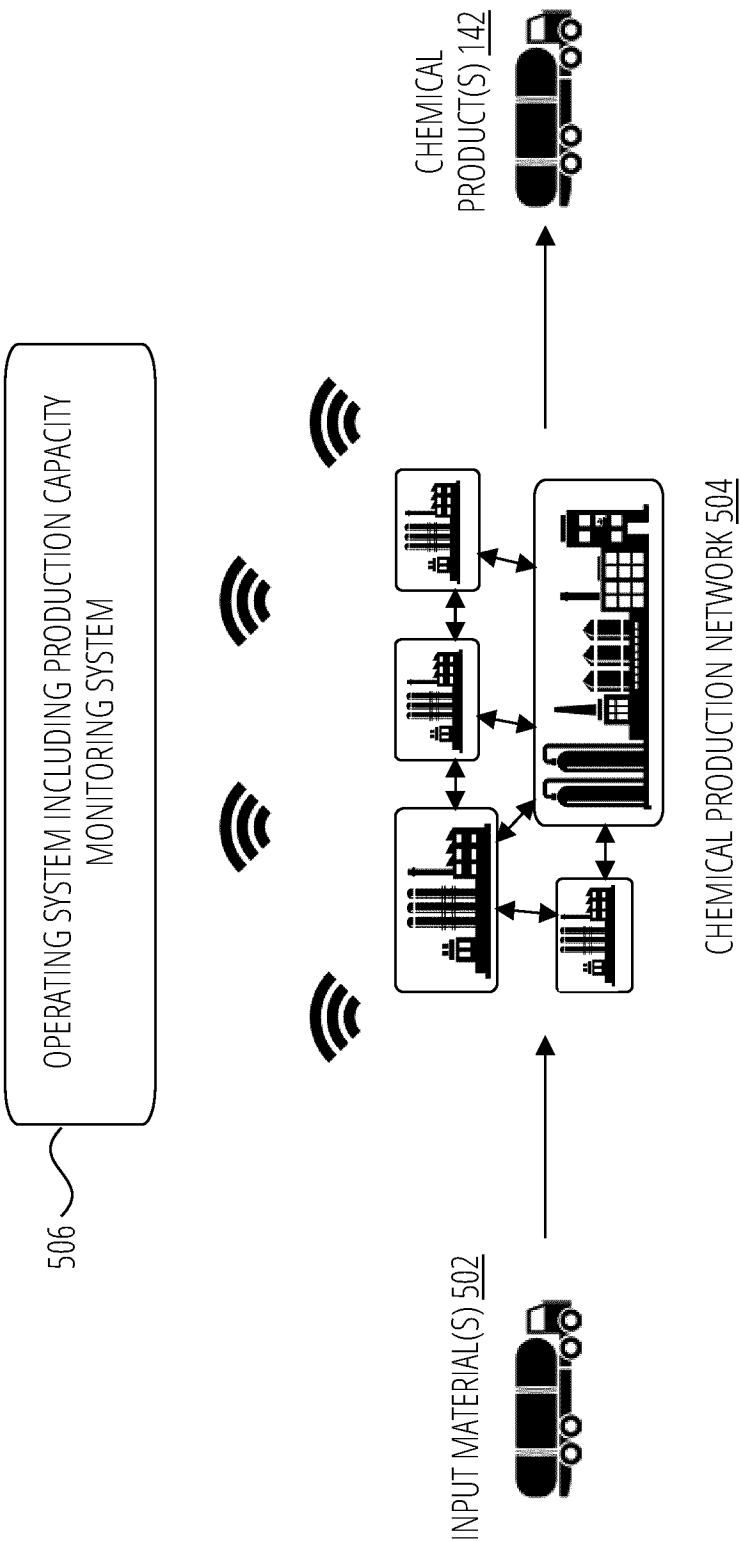


FIG. 5

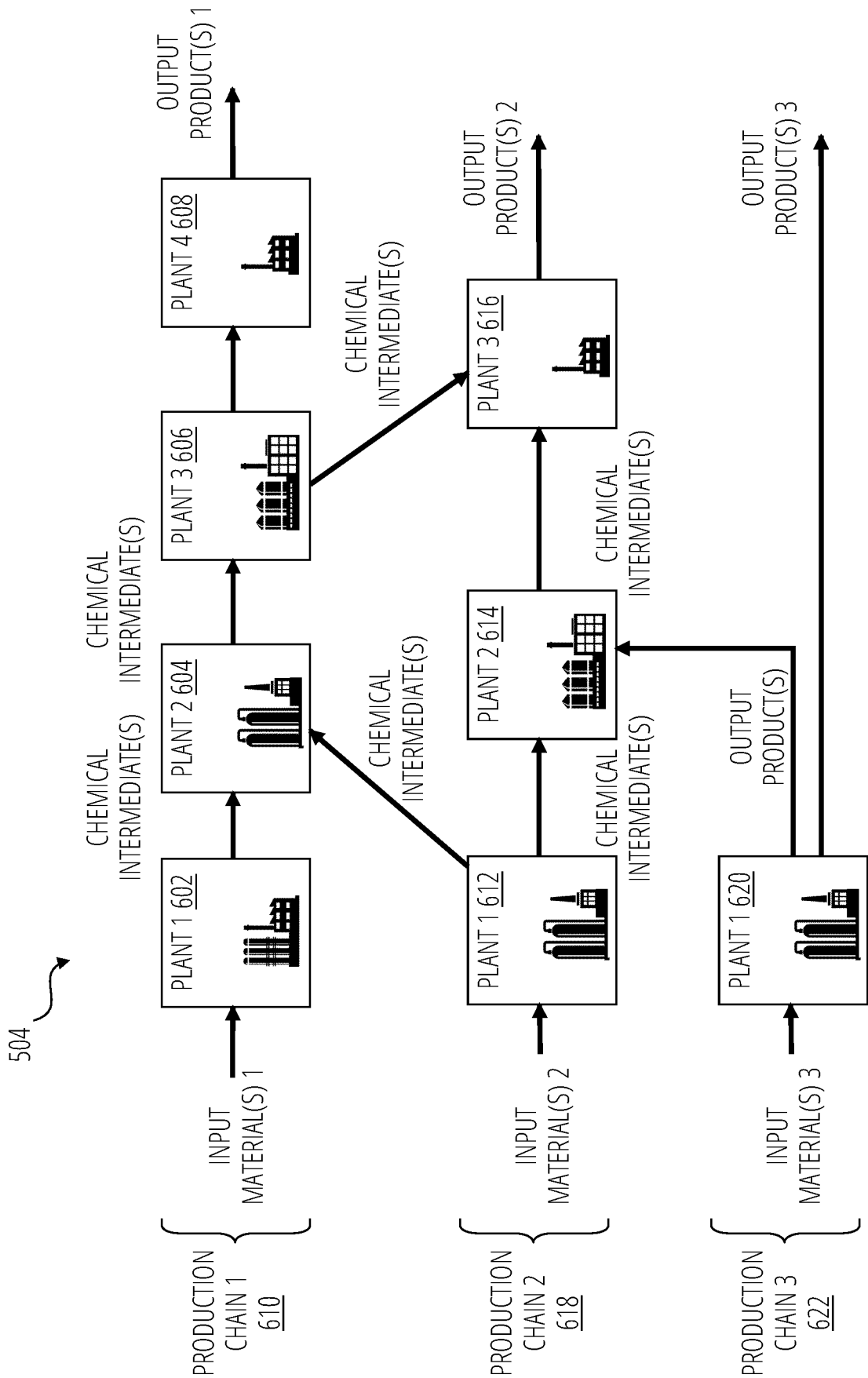


FIG. 6

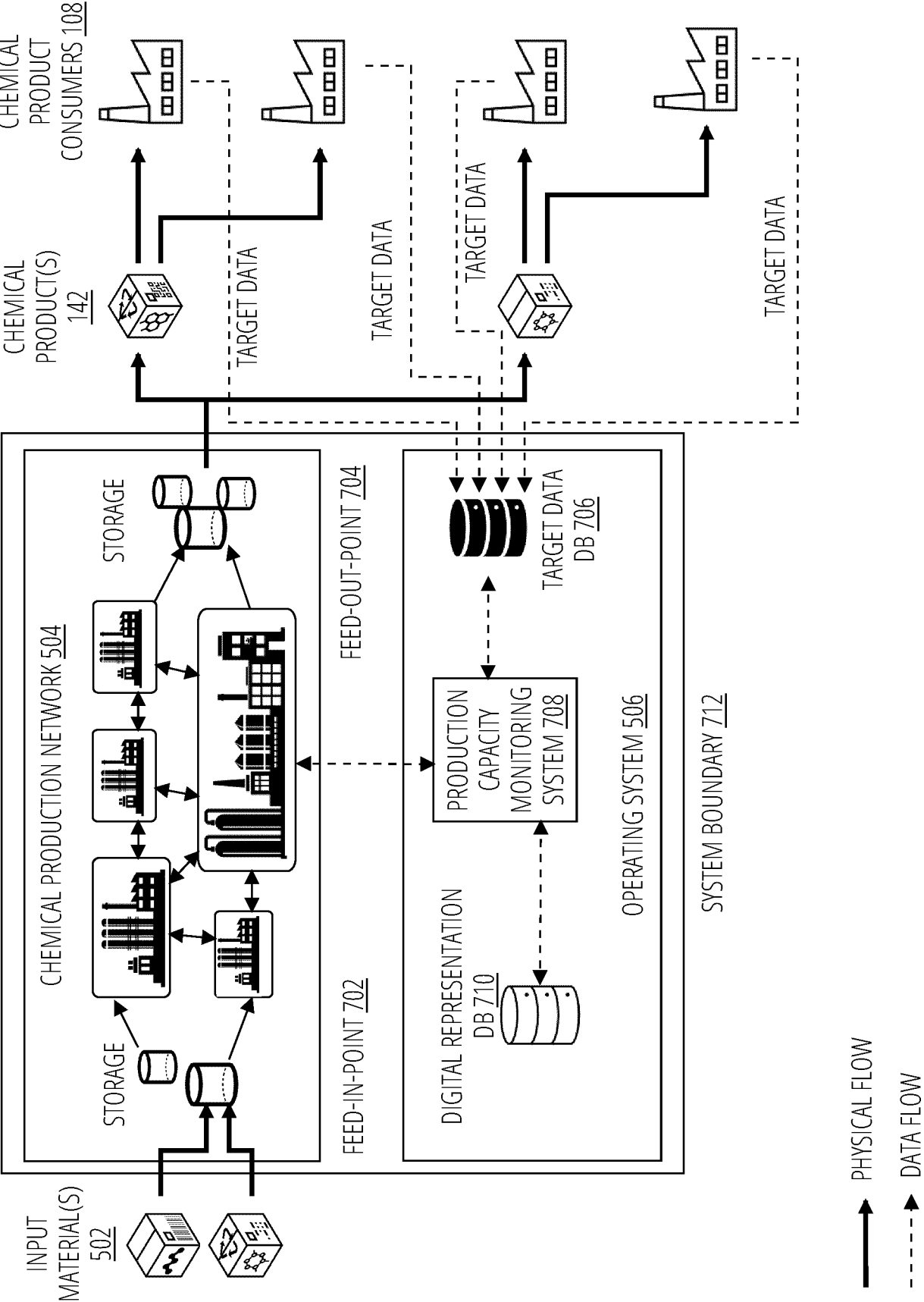


FIG. 7

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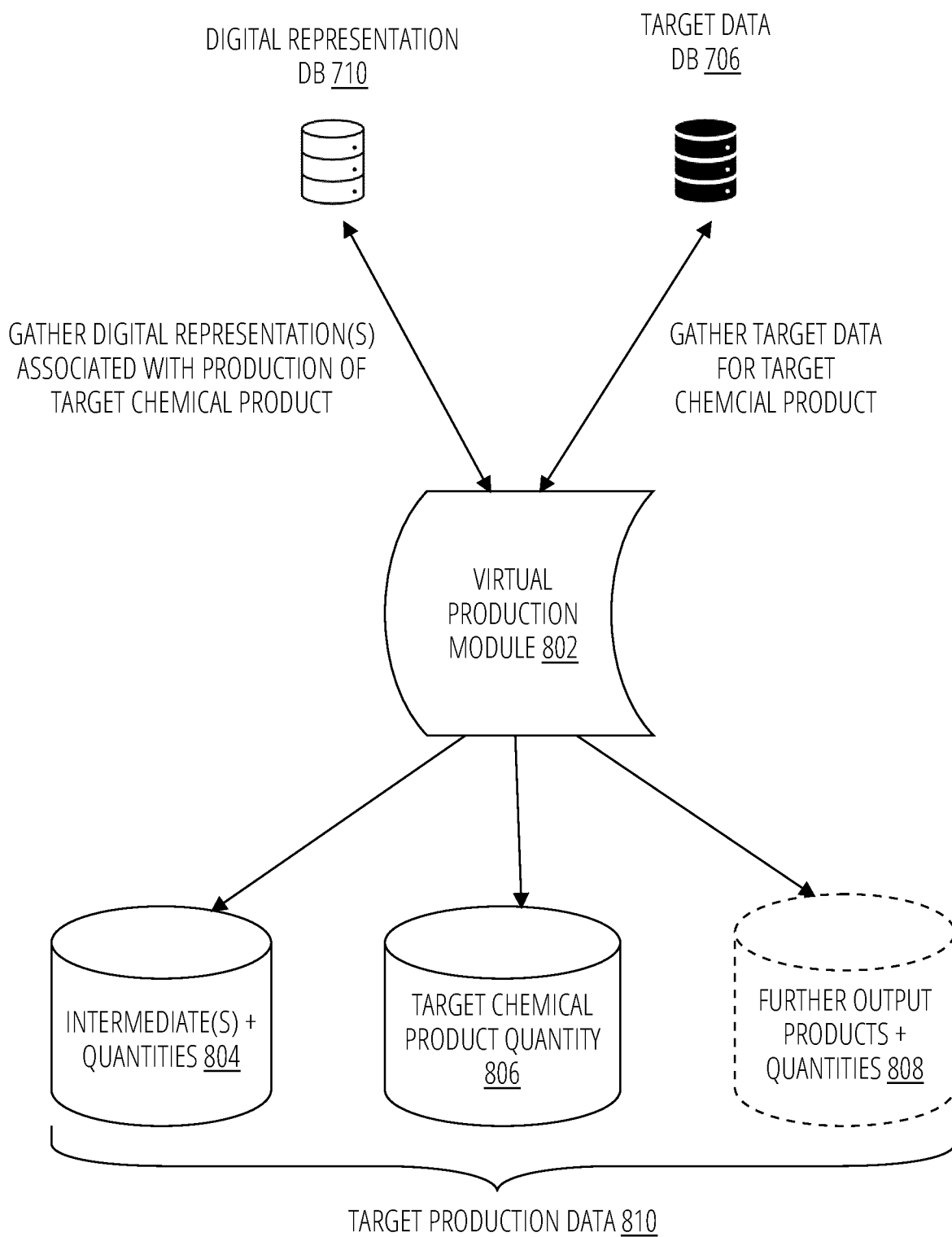


FIG. 8

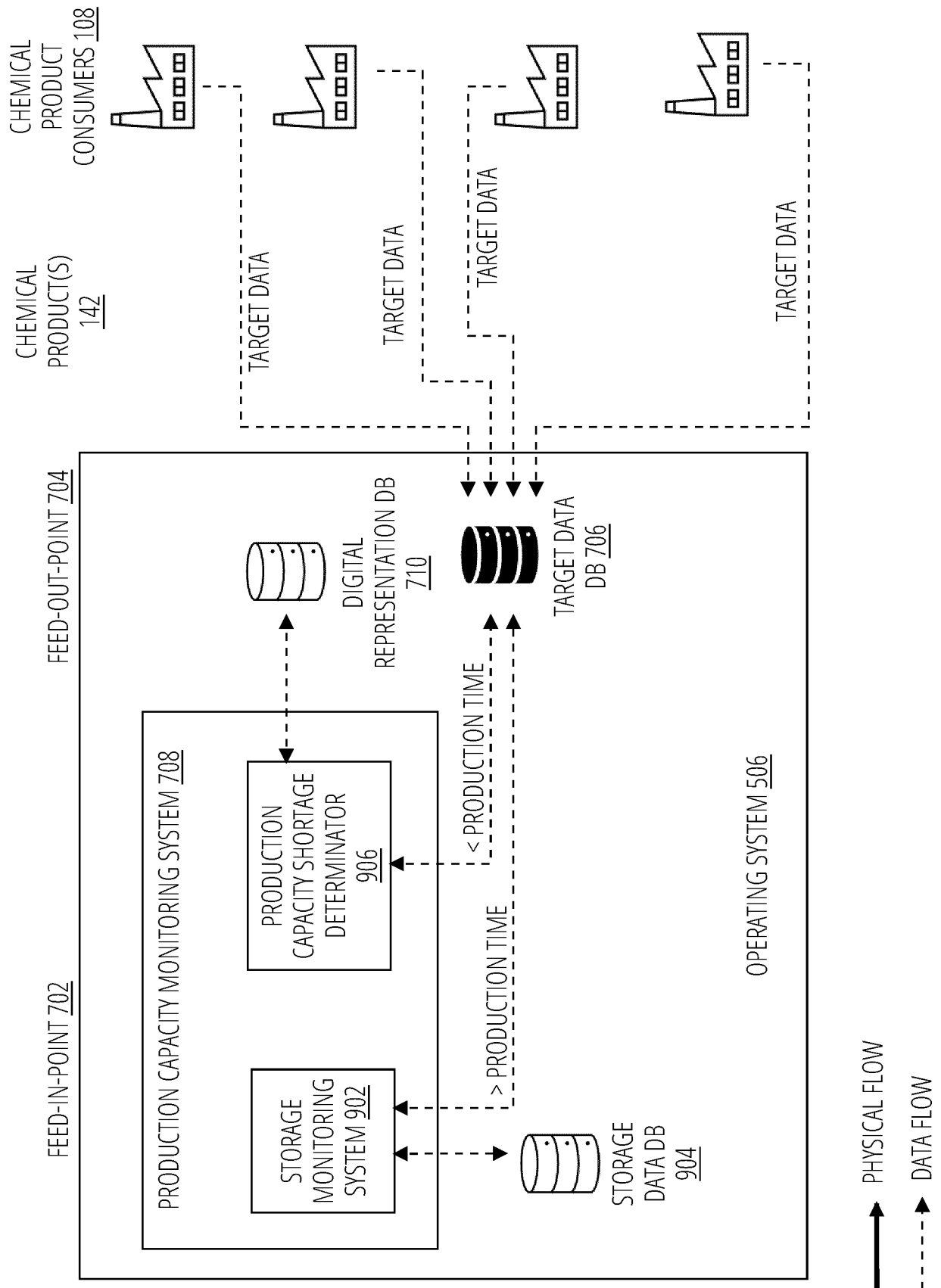


FIG. 9

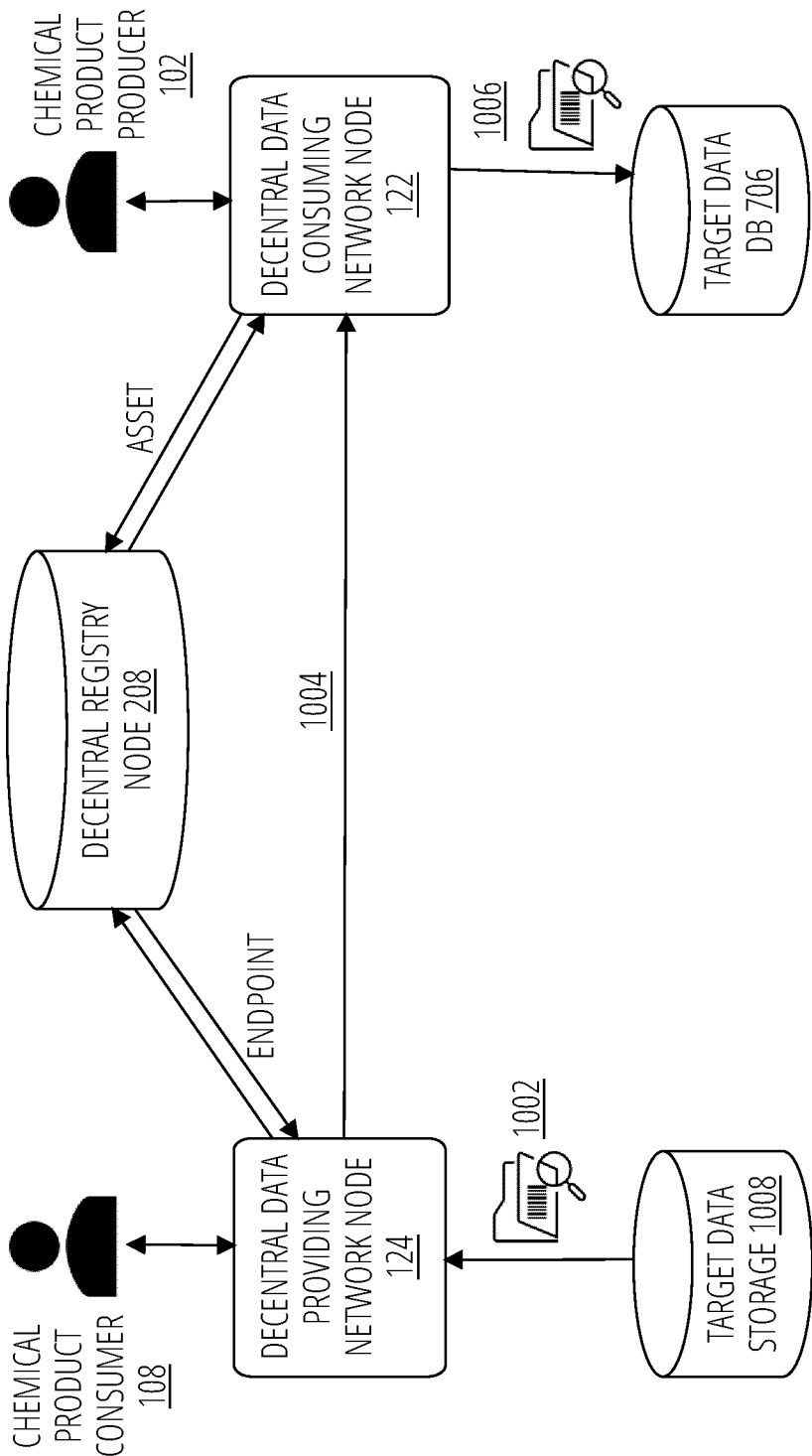
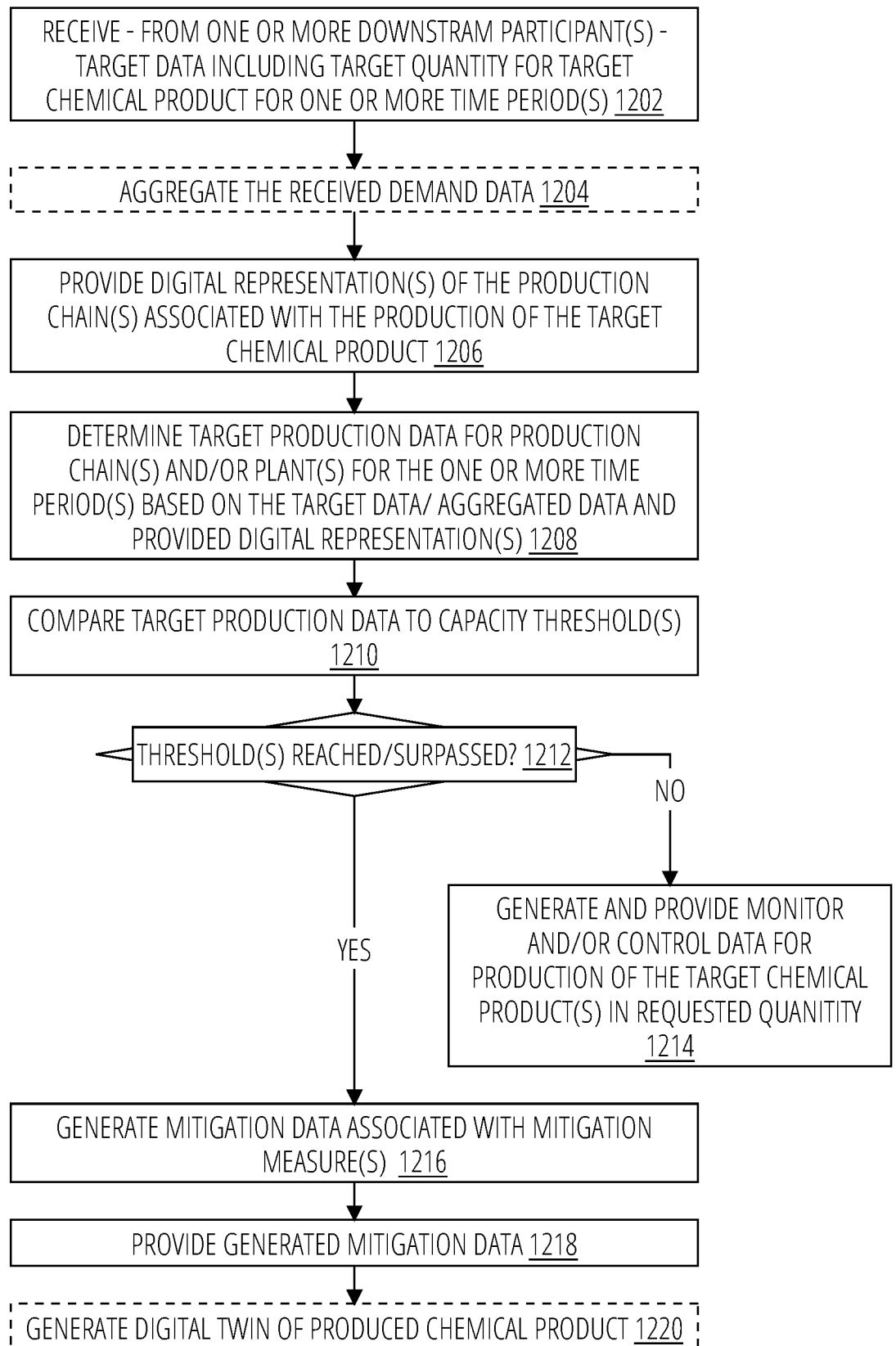
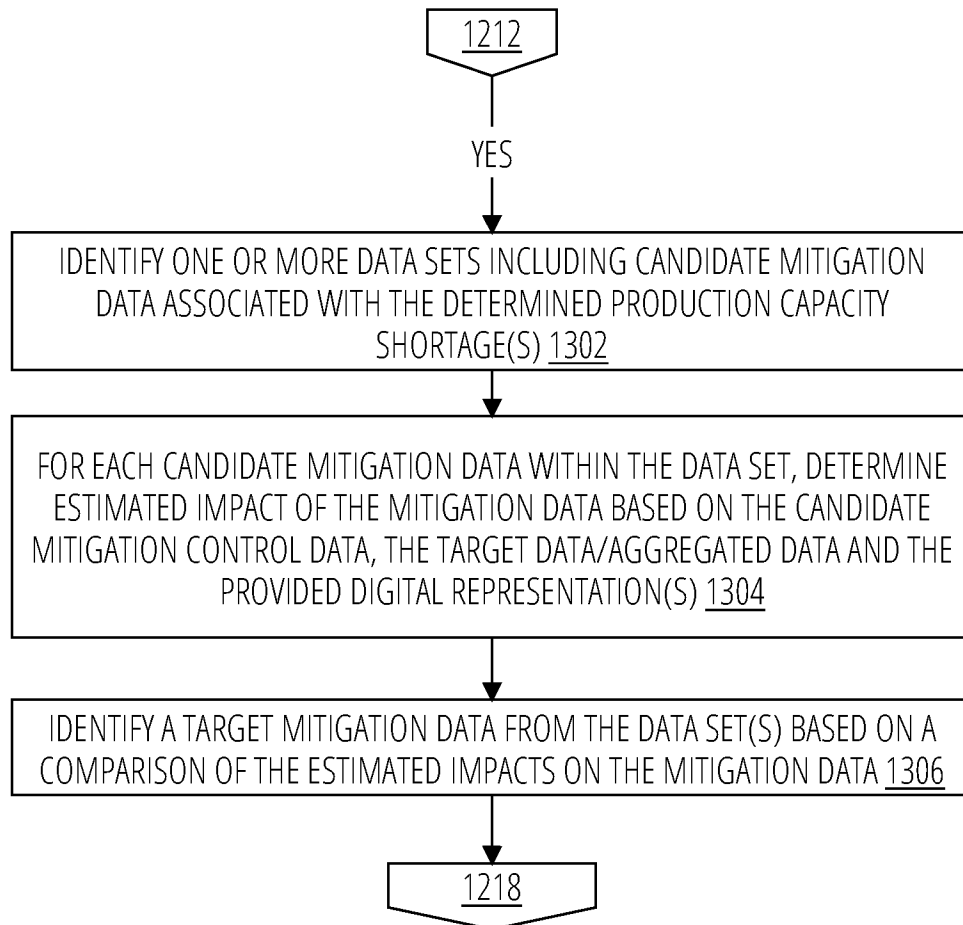


FIG. 10

12/14**FIG. 12**

13/14**FIG. 13**

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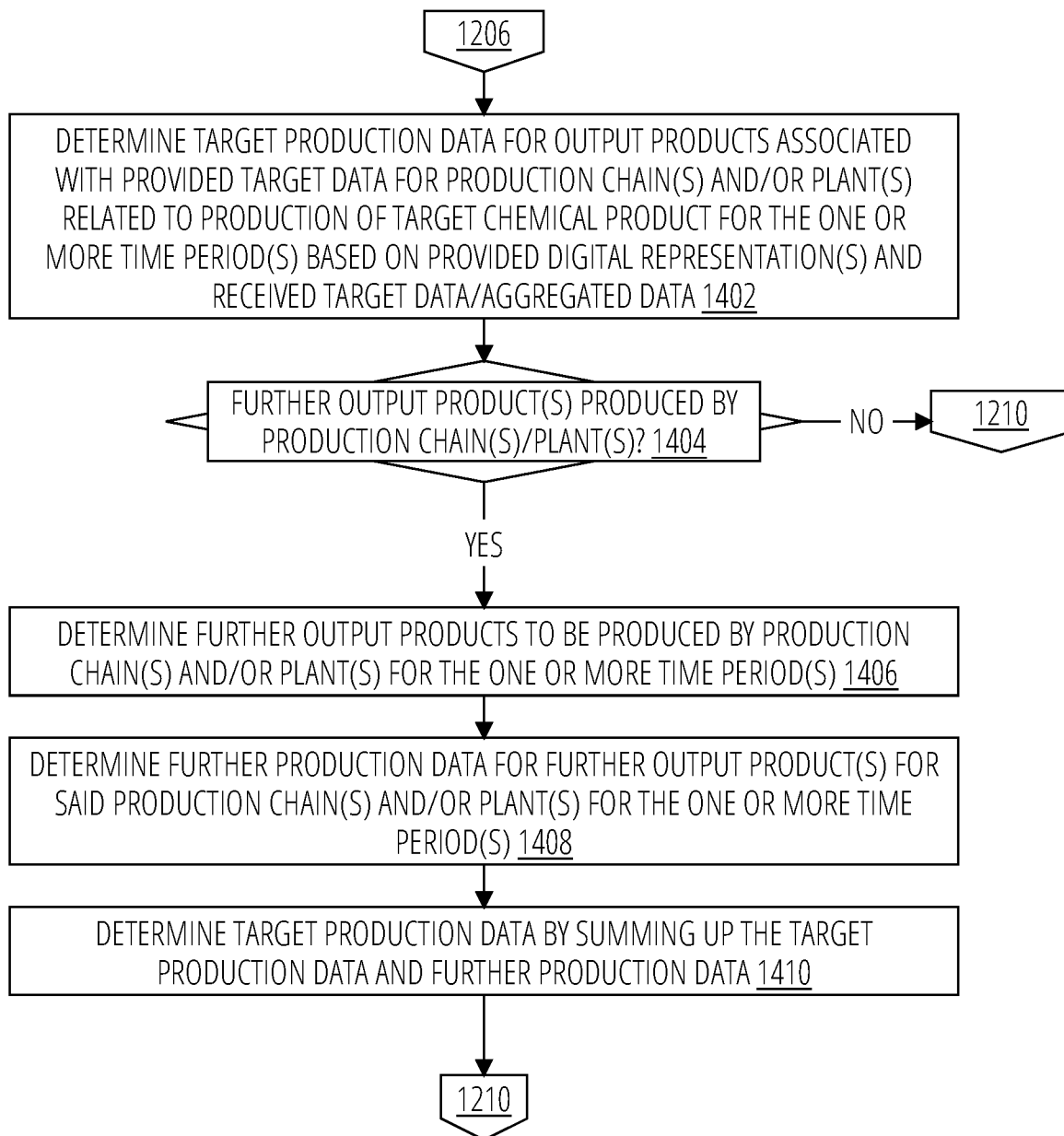


FIG. 14

INTERNATIONAL SEARCH REPORT

International application No
PCT/EP2024/068458

A. CLASSIFICATION OF SUBJECT MATTER INV. G06Q10/0635 G06Q10/06 G06Q50/04 H04L9/00 H04L9/32 ADD.		
According to International Patent Classification (IPC) or to both national classification and IPC		
B. FIELDS SEARCHED Minimum documentation searched (classification system followed by classification symbols) G06Q H04L Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) EPO-Internal		
C. DOCUMENTS CONSIDERED TO BE RELEVANT		
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	US 2023/161326 A1 (WIEGERT ERIK [DE]) 25 May 2023 (2023-05-25) the whole document -----	1 - 15
X	US 2003/208389 A1 (KURIHARA HIDESHI [JP] ET AL) 6 November 2003 (2003-11-06) figures 1-3, 6 paragraph [0060] - paragraph [0063] paragraph [0070] paragraph [0079] paragraph [0091] - paragraph [0106] paragraph [0115] -----	1 - 15
X	EP 3 211 572 A1 (HITACHI SOLUTIONS LTD [JP]) 30 August 2017 (2017-08-30) figures 9, 12 paragraph [0019] - paragraph [0022] paragraph [0035] - paragraph [0036] paragraph [0048] - paragraph [0054] -----	1 - 15
☐ Further documents are listed in the continuation of Box C. ☒ See patent family annex.		
* Special categories of cited documents : "A" document defining the general state of the art which is not considered to be of particular relevance "E" earlier application or patent but published on or after the international filing date "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) "O" document referring to an oral disclosure, use, exhibition or other means "P" document published prior to the international filing date but later than the priority date claimed "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention "X" document of particular relevance;; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone "Y" document of particular relevance;; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art "&" document member of the same patent family		
Date of the actual completion of the international search 3 September 2024		Date of mailing of the international search report 17/09/2024
Name and mailing address of the ISA/ European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Fax: (+31-70) 340-3016		Authorized officer Komnios, Ioannis

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No

PCT/EP2024/068458

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