

Claims

1. A computer-implemented method (300) of determining at least one recipe for a
5 production process to produce a chemical, pharmaceutical and/or biotechnological
product, wherein the production process is defined by a plurality of steps specified by
recipe parameter(s) controlling an execution of the production process and a recipe
comprises the plurality of steps defining the production process, the method
comprising:
- 10 - retrieving (310):
- one or more recipe template composites (200), wherein a recipe template
composite (200) comprises one or more recipe templates and a recipe template is a
recipe in which at least one of the recipe parameter(s) specifying the plurality of steps
is a variable recipe parameter being variable and having no predetermined value at
15 the outset;
 - process evolution information (210) that describes the time evolution of
process variable(s) that describe a state of the production process, wherein the
process evolution information (210) comprises evolution parameter(s) and at least one
of the evolution parameter(s) is a variable evolution parameter being variable and
20 having no predetermined value at the outset;
 - a likelihood function (220) for the evolution parameter(s), wherein the
likelihood function (220) provides a likelihood that value(s) for the evolution
parameter(s) are feasible for the production process;
 - a mapping (230) that maps the process variable(s) onto performance
25 indicator(s);
 - a utility function (240) for at least one of the performance indicator(s), wherein
the utility function provides a desirability value associated to the performance
indicator(s);
- selecting (320) a recipe template composite (200) and performing a first optimisation
30 step comprising:
- providing (410) a set of input values for the at least one variable recipe
parameter in the recipe template composite (200);
 - performing (415) a second optimisation step providing a utility score;

- repeating (420) the second optimisation step for at least another set of input values, thereby obtaining a plurality of utility scores;
- identifying (425) the optimal utility score from the plurality of utility scores;
- if only one recipe template composite (200) was retrieved, selecting (350) the set of
5 input values (280) that yields the optimal utility score (260) together with the one recipe template composite as the at least one recipe for the production process; or
- if more than one recipe template composite (200) was retrieved:
 - repeating (330) the first optimisation step for each recipe template composite (200), thereby obtaining a plurality of optimal utility scores;
 - 10 -- identifying (340) the best optimal utility score (260) among the plurality of optimal utility scores;
 - selecting (350) the recipe template composite (270) and the set of input values (280) that yield the best optimal utility score (260) as the at least one recipe for the production process;
- 15 wherein:
 - the second optimisation step comprises:
 - providing (430) a set of likely values for the at least one variable evolution parameter based on the likelihood function (220);
 - performing (435) a third optimisation step providing a utility tally;
 - 20 -- if there is at least another set of likely values that is suitable, repeating the third optimisation step for the at least another set of likely values, thereby obtaining a plurality of utility tallies;
 - computing (440) the utility score by weighting the utility tally(ies) by the likelihood function (220);
 - 25 - the third optimisation step comprises:
 - performing (445) a fourth optimisation step providing a utility value;
 - if a stochasticity flag is set, repeating the fourth optimisation step, thereby obtaining a plurality of utility values;
 - computing (450) the utility tally as the utility value or by compounding the
30 plurality of utility values;
 - the fourth optimisation step comprises:
 - generating (455) a simulation by simulating the execution of the production process using a recipe template in the recipe template composite (200) with the set of input values for the at least one variable recipe parameter, the process evolution

information (210) and the set of likely values for the at least one variable evolution parameter;

-- if the recipe template composite (200) comprises more than one recipe template, repeating the step of generating the simulation for each recipe template in the recipe template composite (200);

-- determining (460), from the one or more simulations, trajectory(ies) (250) for the process variable(s), wherein a trajectory (250) corresponds to a time-based profile of values recordable during the simulated execution of the production process;

-- computing (465) the utility value by evaluating the utility function (240) using the process variable(s) of the trajectory(ies) (250) and the mapping (230).

2. The method (300) of claim 1, wherein the chemical, pharmaceutical and/or biotechnological product is a first product and retrieving the likelihood function (220) comprises:

- retrieving akin data related to at least one akin production process to produce a second chemical, pharmaceutical and/or biotechnological product, wherein the at least one akin production process has been at least partially performed and wherein the at least one akin production process is different from the production process;
- retrieving relatedness information providing a quantitative indication of similarity between the production process and the akin production process;
- computing the likelihood function (220) based on the akin data and the relatedness information.

3. The method (300) of any one of the preceding claims, wherein retrieving the likelihood function (220) comprises:

- retrieving current data related to an ongoing run of the production process;
- computing the likelihood function (220) based on the current data.

4. The method (300) of any one of the preceding claims, wherein retrieving the likelihood function (220) comprises:

- retrieving historical data related to one or more past runs of the production process;
- computing the likelihood function (220) based on the historical data.

5. The method (300) of any one of the preceding claims, further comprising:

providing the at least one recipe to a control system (20);
executing, by the control system (20), the production process based on the at least one recipe.

5 6. The method (300) of claim 5, further comprising:
storing data from the executed production process as historical data and/or storing
data from the executing production process as current data.

7. The method (300) of any one of the preceding claims, further comprising
10 updating the likelihood function based on the trajectory(ies) and storing the updated
likelihood function.

8. A computer program product comprising computer-readable instructions, which,
when loaded and executed on a computer system, cause the computer system to
15 perform operations according to the method of any one of the preceding claims.

9. A computer system (10) operable to determine at least one recipe for a
production process to produce a chemical, pharmaceutical and/or biotechnological
product, wherein the production process is defined by a plurality of steps specified by
20 recipe parameter(s) controlling an execution of the production process and a recipe
comprises the plurality of steps defining the production process, the computer system
(10) comprising:

- a retrieving module configured to retrieve:

-- one or more recipe template composites (200), wherein a recipe template
25 composite (200) comprises one or more recipe templates and a recipe template is a
recipe in which at least one of the recipe parameter(s) specifying the plurality of steps
is a variable recipe parameter being variable and having no predetermined value at
the outset;

-- process evolution information (210) that describes the time evolution of
30 process variable(s) that describe a state of the production process, wherein the
process evolution information (210) comprises evolution parameter(s) and at least one
of the evolution parameter(s) is a variable evolution parameter being variable and
having no predetermined value at the outset;

- a likelihood function (220) for the evolution parameter(s), wherein the likelihood function (220) provides a likelihood that value(s) for the evolution parameter(s) are feasible for the production process;
- a mapping (230) that maps the process variable(s) onto performance indicator(s);
- a utility function (240) for at least one of the performance indicator(s), wherein the utility function (240) provides a desirability value associated to the performance indicator(s);
- a computing module configured to select (320) a recipe template composite (200) and perform a first optimisation step comprising:
 - providing (410) a set of input values for the at least one variable recipe parameter in the recipe template composite (200);
 - performing (415) a second optimisation step providing a utility score;
 - repeating (420) the second optimisation step for at least another set of input values, thereby obtaining a plurality of utility scores;
 - identifying (425) the optimal utility score from the plurality of utility scores;wherein the computing module is further configured, if only one recipe template composite (200) was retrieved, to select (350) the set of input values (280) that yields the optimal utility score (260) together with the one recipe template composite as the at least one recipe for the production process;
- or the computing module is further configured, if more than one recipe template composite (200) was retrieved, to:
 - repeat (330) the first optimisation step for each recipe template composite (200), thereby obtaining a plurality of optimal utility scores;
 - identify (340) the best optimal utility score (260) among the plurality of optimal utility scores;
 - select the recipe template composite (270) and the set of input values (280) that yield the best optimal utility score (260) as the at least one recipe for the production process;
- and wherein:
 - the second optimisation step comprises:
 - providing (430) a set of likely values for the at least one variable evolution parameter based on the likelihood function (220);
 - performing (435) a third optimisation step providing a utility tally;

- if there is at least another set of likely values that is suitable, repeating the third optimisation step for the at least another set of likely values, thereby obtaining a plurality of utility tallies;
 - computing (440) the utility score by weighting the utility tally(ies) by the likelihood function (220);
 - the third optimisation step comprises:
 - performing (445) a fourth optimisation step providing a utility value;
 - if a stochasticity flag is set, repeating the fourth optimisation step, thereby obtaining a plurality of utility values;
 - computing (450) the utility tally as the utility value or by compounding the plurality of utility values;
 - the fourth optimisation step comprises:
 - generating (455) a simulation by simulating the execution of the production process using a recipe template in the recipe template composite (200) with the set of input values for the at least one variable recipe parameter, the process evolution information (210) and the set of likely values for the at least one variable evolution parameter;
 - if the recipe template composite (200) comprises more than one recipe template, repeating the step of generating the simulation for each recipe template in the recipe template composite (200);
 - determining (460), from the one or more simulations, trajectory(ies) (250) for the process variable(s), wherein a trajectory (250) corresponds to a time-based profile of values recordable during the simulated execution of the production process;
 - computing (465) the utility value by evaluating the utility function (240) using the process variable(s) of the trajectory(ies) (250) and the mapping (230).
10. The computer system (10) of claim 9, wherein the chemical, pharmaceutical and/or biotechnological product is a first product and the retrieving module is further configured to:
- retrieve akin data related to at least one akin production process to produce a second chemical, pharmaceutical and/or biotechnological product, wherein the at least one akin production process has been at least partially performed and wherein the at least one akin production process is different from the production process;

- retrieve relatedness information providing a quantitative indication of similarity between the production process and the akin production process;
and the computing module is further configured to compute the likelihood function (220) based on the akin data and the relatedness information.

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11. The computer system (10) of claim 9 or 10, wherein the retrieving module is further configured to retrieve current data related to an ongoing run of the production process and the computing module is further configured to compute the likelihood function (220) based on the current data.

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12. The computer system (10) of any one of claims 9 to 11, wherein the retrieving module is further configured to retrieve historical data related to one or more past runs of the production process and the computing module is further configured to compute the likelihood function (220) based on the historical data.

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13. The computer system (10) of any one of claims 9 to 12, further configured to be interfaced with a control system (20) for controlling a production process equipment (30), wherein:

the computer system (10) is configured to provide the at least one recipe to the control system (20); and

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the control system (20) is configured to execute the production process based on the at least one recipe.

14. The computer system (10) of claim 13, further configured to store data from the executed production process as historical data and/or to store data from the executing production process as current data.

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15. The computer system (10) of any one of claims 9 to 14, wherein:
the computing module is further configured to update the likelihood function based on the trajectory(ies).

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