Patent claims

1. A method for controlling a chemical process, wherein the chemical process is one or more of the preparation of methanol, hydrogen sulfide, methyl mercaptan, hydrocyanic acid, acrolein, 3-methylthiopropionaldehyde, 5-(2-methylmercaptoethyl)-hydantoin, methionine, a salt of methionine, and a derivative of methionine, comprising the steps of

a) providing a training set TS1, wherein said training set TS1 comprises process values PV1 and process values PV2 being correlated to one another, and/or laboratory values LV1 and process values PV2 being correlated to one another,

b) training a processing unit on the training set TS1 of step a) to identify a pattern of correlation between one or more measured process variables and at least one process variable, and developing a calibration function CF1 for a calibrated soft sensor from the identified pattern of correlation,

c) predicting at least one operating parameter for the chemical process as approximation to LV1 and/or PV1, comprising the steps of

c1) requesting one or more process values corresponding to PV2 from the distributed control system (DCS) of the chemical process, and

c2) predicting an operating parameter with the value of step c1) by means of the calibrated soft sensor of step b),

d) calculating a deviation as being the difference between the operating parameter predicted in step c2) and the corresponding laboratory value LV1 and/or the processing value PV1 of the training set TS1 of step a),

e) proceeding with step f) if the deviation calculated in step d) exceeds a threshold value, otherwise proceeding with step g),

f) re-calibrating the soft sensor of step b), comprising the steps of

f1) augmenting the training set TS1 of step a) with further laboratory values LV1 and/or further process values PV1 or replacing at least a part of the training set TS1 with the further laboratory values LV1 and/or further process values PV1 to provide a training set TS2,

f2) training the processing unit of step b) on the augmented training set TS1 or on the training set TS2 of step f1) to revise the calibration function of step b),

f3) re-calibrating the soft sensor of step b) by means of the revised calibration function of step f2), and

f4) returning to step c) using the re-calibrated soft sensor of step f3),

g) writing the at least one operating parameter predicted in step c2) into the DCS, and

h) repeating the steps c) to g).

2. The method according to claim 1, wherein the steps a) and/or f1) further comprise the steps of

A1) collecting laboratory values LV1 and process values PV2, and/or process values PV1 and process values PV2,

A2) providing each value of step A1) with a time stencil indicating the point in time at which the value was recorded and/or the sample underlying said value was taken,

A3) providing each laboratory value LV1 and/or each process value PV1 with a time pattern, going back in time from the time stencil of LV1 and/or PV1 for a pre-defined time span, and

A4) linking a laboratory value LV1 and/or a process value PV1 to one or more process values PV2 having a time stencil matching the time pattern of the laboratory value LV1 and/or the time pattern of the process value PV1.

3. The method according to claim 1 or 2, wherein i) a process value PV1 and a process value PV2 are correlated to one another, when the process value PV1 is dependent or influenced by the process value PV2, or vice versa, and/or ii) a laboratory value LV1 and a process value PV2 are correlated to one another, when the laboratory value LV1 is dependent or influenced by the process value PV2, or vice versa.

4. The method according to any of claims 1 to 3, wherein the process values are current values or averaged values.

5. The method according to claim 4, wherein the averaged values are obtained by averaging aggregated process values over a pre-defined time span.

6. The method according to claim 4, wherein the averaged values are obtained by averaging aggregated process values over the pre-defined time span of step A4.

7. The method according to any of claims 1 to 6, wherein the measurement underlying a laboratory value LV1, a process value PV1 and/or a process PV2 value is repeated when the value in question has a variance of more than 2 sigma from its expected value.

8. The method according to any of claims 1 to 7, wherein the step f) is also performed periodically in pre-defined intervals or non-periodically in pre-defined stages of the chemical process or when changing from one stage to another.

9. The method according to any of claims 1 to 8, wherein the step f) is triggered whenever deemed necessary.

10. The method according to any of claims 1 to 9, wherein the training set TS1 is replaced in step f) at least partially or completely with the training set TS2.

11. The method according to claim 10, wherein the laboratory values LV1 and/or the process values PV1 having the oldest time stencils are replaced with laboratory values LV1 and/or the process values PV1 having current time stencils.

12. The method according to any of claims 1 to 11, wherein the training set TS1 is replaced at least partially or completely with the training set TS2 in pre-defined stages of the chemical process or when the number of performances of step f) within a pre-defined time period exceeds a defined threshold.

13. The method according to any of claims 1 to 12, wherein the processing unit is an artificial neural network.

14. The method according to claim 13, wherein the artificial neural network is a convolutional neural network.

15. A system for controlling a chemical process, comprising

i) a calibration branch (1) for generating a calibration function, comprising a laboratory information management system (LIMS) (2) for providing laboratory values LV1 (3), and a process information management system (PIMS) (5) for providing process values PV1 and/or PV2 (6),

ii) an operation loop (9) for requesting one or more process values (12) from the distributed control system (DCS) (10) of the chemical process, and

iii) a processing unit (13) adapted to carry out the method according to any of claims 1 to 14, wherein the processing unit is connected to the calibration branch (1) and the operation loop (9).

Patent claims

1. A method for controlling a chemical process, wherein the chemical process is one or more of the preparation of methanol, hydrogen sulfide, methyl mercaptan, hydrocyanic acid, acrolein, 3-methylthiopropionaldehyde, 5-(2-methylmercaptoethyl)-hydantoin, methionine, a salt of methionine, and a derivative of methionine, comprising the steps of

a) providing a training set TS1, wherein said training set TS1 comprises laboratory values LV1 and process values PV2 being correlated to one another,

b) training a processing unit on the training set TS1 of step a) to identify a pattern of correlation between one or more measured process variables and at least one process variable, and developing a calibration function CF1 for a calibrated soft sensor from the identified pattern of correlation,

c) predicting at least one operating parameter for the chemical process as approximation to LV1, comprising the steps of

c1) requesting one or more process values corresponding to PV2 from the distributed control system (DCS) of the chemical process, and

c2) predicting an operating parameter with the value of step c1) by means of the calibrated soft sensor of step b),

d) calculating a deviation as being the difference between the operating parameter predicted in step c2) and the corresponding laboratory value LV1 of the training set TS1 of step a),

e) proceeding with step f) if the deviation calculated in step d) exceeds a threshold value, otherwise proceeding with step g),

f) re-calibrating the soft sensor of step b), comprising the steps of

f1) augmenting the training set TS1 of step a) with further laboratory values LV1 and/or further process values PV1 or replacing at least a part of the training set TS1 with the further laboratory values LV1 and/or further process values PV1 to provide a training set TS2,

f2) training the processing unit of step b) on the augmented training set TS1 or on the training set TS2 of step f1) to revise the calibration function of step b),

f3) re-calibrating the soft sensor of step b) by means of the revised calibration function of step f2), and

f4) returning to step c) using the re-calibrated soft sensor of step f3).

g) writing the at least one operating parameter predicted in step c2) into the DCS, and

h) repeating the steps c) to g).

2. The method according to claim 1, wherein the steps a) and/or f1) further comprise the steps of

A1) collecting laboratory values LV1 and process values PV2, ,

A2) providing each value of step A1) with a time stencil indicating the point in time at which the value was recorded and/or the sample underlying said value was taken,

A3) providing each laboratory value LV1 with a time pattern, going back in time from the time stencil of LV1 for a pre-defined time span, and

A4) linking a laboratory value LV1 to one or more process values PV2 having a time stencil matching the time pattern of the laboratory value LV1.

3. The method according to claim 1 or 2, wherein i) a laboratory value LV1 and a process value PV2 are correlated to one another, when the laboratory value LV1 is dependent or influenced by the process value PV2, or vice versa.

4. The method according to any of claims 1 to 3, wherein the process values are current values or averaged values.

5. The method according to claim 4, wherein the averaged values are obtained by averaging aggregated process values over a pre-defined time span.

6. The method according to claim 4, wherein the averaged values are obtained by averaging aggregated process values over the pre-defined time span of step A4.

7. The method according to any of claims 1 to 6, wherein the measurement underlying a laboratory value LV1, and/or a process PV2 value is repeated when the value in question has a variance of more than 2 sigma from its expected value.

8. The method according to any of claims 1 to 7, wherein the step f) is also performed periodically in pre-defined intervals or non-periodically in pre-defined stages of the chemical process or when changing from one stage to another.

9. The method according to any of claims 1 to 8, wherein the step f) is triggered whenever deemed necessary.

10. The method according to any of claims 1 to 9, wherein the training set TS1 is replaced in step f) at least partially or completely with the training set TS2.

11. The method according to claim 10, wherein the laboratory values LV1 having the oldest time stencils are replaced with laboratory values LV1 and/or the process values PV1 having current time stencils.

12. The method according to any of claims 1 to 11, wherein the training set TS1 is replaced at least partially or completely with the training set TS2 in pre-defined stages of the chemical process or when the number of performances of step f) within a pre-defined time period exceeds a defined threshold.

13. The method according to any of claims 1 to 12, wherein the processing unit is an artificial neural network.

14. The method according to claim 13, wherein the artificial neural network is a convolutional neural network.

15. A system for controlling a chemical process, comprising

i) a calibration branch (1) for generating a calibration function, comprising a laboratory information management system (LIMS) (2) for providing laboratory values LV1 (3), and a process information management system (PIMS) (5) for providing process values PV2 (6),

ii) an operation loop (9) for requesting one or more process values (12) from the distributed control system (DCS) (10) of the chemical process, and

iii) a processing unit (13) adapted to carry out the method according to any of claims 1 to 14, wherein the processing unit is connected to the calibration branch (1) and the operation loop (9).