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(54) Title: COMPUTER-IMPLEMENTED METHOD FOR SIMULATING CHEMICAL REACTIONS IN AN AGED CATALYTIC CONVERTER

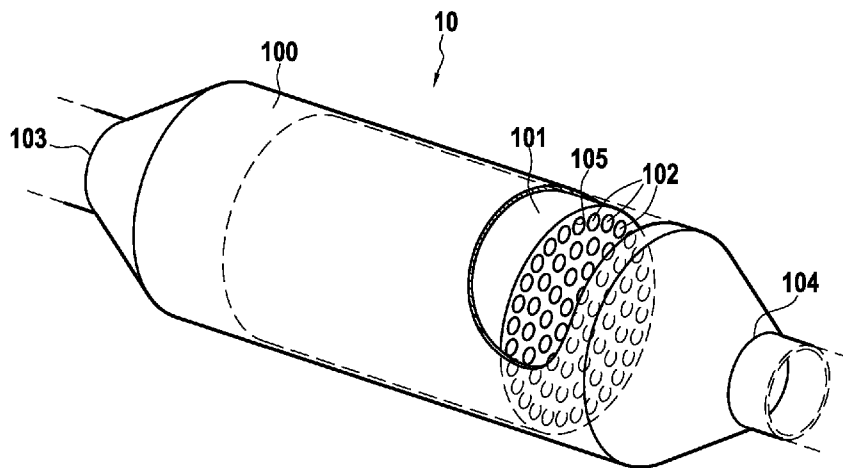


FIG.2

(57) Abstract: The present invention concerns a computer-implemented method for simulating chemical reactions in a catalytic converter (10) in an aged state. This method comprises the steps of applying, to a group of Arrhenius equations, a single corresponding common aging coefficient according to the aged state of the catalytic converter (10), calculating reaction rates for a group of chemical reactions using the group of Arrhenius equations with the corresponding common aging coefficient, and calculating a flowrate of one or more reagents and/or reaction products of the group of chemical reactions, out of the catalytic converter (10), by applying the reaction rates for the group of chemical reactions to an exhaust stream flowing through the catalytic converter (10). The corresponding common aging coefficient is applied to the group of Arrhenius equations by multiplying a pre-exponential factor of each Arrhenius equation of the group of Arrhenius equations by the corresponding common aging coefficient. Each Arrhenius equation from among the group of Arrhenius equations corresponds to a chemical reaction from among the group of chemical reactions with a catalyst in the catalytic converter (10).



(84) Designated States (*unless otherwise indicated, for every kind of regional protection available*): ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, KM, ML, MR, NE, SN, TD, TG).

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COMPUTER-IMPLEMENTED METHOD FOR SIMULATING CHEMICAL REACTIONS
IN AN AGED CATALYTIC CONVERTER

TECHNICAL FIELD

5 The disclosure relates to the field of emissions control, and in particular to a computer-implemented method for simulating a plurality of chemical reactions in an aged catalytic converter.

BACKGROUND

10 In order to restrain overall pollutant emissions, it is generally preferred to design the exhaust system of an IC engine-powered vehicle to be effective throughout the entire lifetime of the vehicle, and maintain low emissions even after aging and poisoning of the engine and the exhaust emissions control devices.

15

 It is well known, for example from P. S. Lambrou, C.N. Costa, S.Y. Christou, and A.M. Efstathiou in "Dynamics of oxygen storage and release on commercial aged Pd-Rh three-way catalysts and their characterization by transient experiments", Applied Catalysis B: Environmental 54 52004° 237-250, 20 A. Winkler, P. Dimopoulos, R. Hauert, C. Bach, and M. Aguirre in "Catalytic activity and aging phenomena of three-way catalysts in a compressed natural gas/gasoline powered passenger car", Applied Catalysis B: Environmental 84 (2008) 162-169, G. Koltsakis and A. Stamatelos in "Catalytic Automotive exhaust aftertreatment", Prog. Energy Combust. Sci. Vol. 23, pp. 1-39, 1997, or 25 S. K. Matam, E. H. Otal, M. H. Aguirre, A. Winkler, A. Ulrich, D. Rentsch, A. Weidenkaff, and D. Ferii in "Thermal and chemical aging of model three-way catalyst Pd/Al₂O₃ and its impact on the conversion of CNG vehicle exhaust", Catalysis Today 184 (2012) 237-244, that aging of catalytic converters, and in particular three-way catalytic converters (TWC), affects their performances and 30 that it can be advantageous to consider the consequences of this aging in advance during the design of the fresh catalyst. One of the consequences of aging is a decrease in redox properties of catalytic converters' oxygen storage components, leading to a decrease in oxygen storage capacity, as seen in the first abovementioned document, as well as in "An experimental and kinetic 35 modeling study of aging impact on surface and subsurface oxygen storage in three way catalysts", J. Gong, D. Wang, J. Li, K. Kamasamudram et al.,

Catalysis Today, 302 (2019)51-60. The aging of a catalytic converter also impacts its platinum-group metal (PGM) reactions, leading to an increase of the tailpipe emissions of CO, HC and NO_x (see the second, third and fourth abovementioned documents, as well as "Effect of catalyst aging on the activity and selectivity of commercial three-way catalysts", J.H. Baik, H.J. Kwon, Y.T. Kwon, I-S Nam et al., Topics in Catalysis, Vols. 42-43, May 2007, DOI: 10.1007/s11244-007-0201-3).

Until now, exhaust system designs have generally been evaluated on the basis of actual tests for each vehicle, using exhaust lines aged on engine test benches or burner benches. This induces a high cost for car manufacturers as it requires many exhaust line prototypes and tests on engine test benches, chassis dynamometer benches and/or real road conditions. Moreover, such testing can normally only be carried out late in the development cycle.

15

Consequently, a Model Based Development (MBD) approach can be a powerful way to improve this process by allowing system evaluation under multiple aging conditions from an early development stage. Moreover, the use of MBD for a broad evaluation of routes and vehicles can help reduce the number of vehicle tests and the prototyping cost by optimizing the number of catalyst converter designs without prototypes. Computer-implemented catalyst converter modeling methods started a few decades ago, see for instance, "Development and application range of mathematical models for 3-way catalyst converters", G.C. Koltsakis, P.A. Konstantinidis, A.M. Stamatelos, Applied Catalysis B: Environmental 12 (1997) 161-191; "Modeling dynamic phenomena in 3-way catalytic converters", G.C. Koltsakis, A.M. Stamatelos Chemical Engineering Science 54 (1999) 4567-4578; "Mathematical modelling of catalytic exhaust systems for Euro-3 and Euro-4 emissions standards", G. Pontikakis, A. Stamatelos, Proc. Instn. Mech. Engrs., Vol. 215 Part D, 2001; "Three-Way-Catalyst Modeling – A comparison of 1D and 2D simulations", S. Tischer, Y. Jiang, K. W. Hughes, M. D. Patil, M. Murtagh, SAE International 2007-01-1071; "An attempt at modelling the activity of Pt—Rh/Al₂O₃ three way catalysts in the CO+NO reactions", P. Granger, J.J. Lecomte, L. Leclercq, G. Leclercq, Applied Catalysis A: General 208 (2001) 369-379, and "Oxygen Storage Modeling in Three-Way Catalytic Converters", D. N. Tsinoglou, G. C. Koltsakis and J. C. Peyton Jones, Ind. Eng. Chem. Res. 2002, 41, 1152-1165.

Several approaches have been proposed for such modelling of catalytic converters. For example, some researchers focused on the modeling of a few specific reactions in order to better understand their mechanisms, while other developed models are more complete, including heat and mass transfer calculations, heterogeneous chemical reactions, oxygen storage and release phenomena. In such models, Langmuir-Hinshelwood kinetics have been applied with various numbers of reactions depending on the modelling detail. Different approaches have also been presented for the consideration of radial temperature gradients within the catalytic converters: while some authors have proposed using 1D approach for modelling the temperature gradient throughout each individual channels within the catalytic converter, with possibly a 2D resolution for the monolith wherein those channels are formed, others have presented a more detailed (2D) modeling of the temperature gradient within each channel.

In any case, these models typically apply a set of Arrhenius equations, each corresponding to a chemical reaction set to happen within the catalytic converter, to calculate corresponding reaction rates within the catalytic converter. An Arrhenius equation has the following form:

$$R = Ae^{-E_a/RT}$$

wherein R is a reaction rate, A represents a so-called pre-exponential factor, E_a is the activation energy of the chemical reaction, T the temperature, and R the ideal gas constant.

A significant drawback of the abovementioned catalytic converter models and corresponding simulation methods is that individually adjusting each Arrhenius equation to the aging state of the catalyst converter requires a significant effort in terms of experimentation and manual model calibration.

SUMMARY

A first object of the disclosure is that of proposing a simpler, easier computer-implemented method for simulating chemical reactions in a catalytic

converter in an aged state, in order to calculate the flowrate of one or more reagents and/or reaction products out of the catalytic converter.

For this purpose, this computer-implemented method may comprise the steps of applying, to a group of Arrhenius equations, a single corresponding common aging coefficient according to the aged state of the catalytic converter, by multiplying a pre-exponential factor of each Arrhenius equation of the group of Arrhenius equations by the corresponding common aging coefficient, wherein each Arrhenius equation from among the group of Arrhenius equations corresponds to a chemical reaction from among a group of chemical reactions with a catalyst in the aged catalytic converter; calculating reaction rates for the group of chemical reactions using the group of Arrhenius equations with the corresponding common aging coefficient; and calculating a flowrate of one or more reagents and/or reaction products of the group of chemical reactions, out of the catalytic converter, by applying the reaction rates for the group of chemical reactions to an exhaust stream flowing through the catalytic converter.

Because the aged state of the catalytic converter mainly affects the number, quality and accessibility of available reaction sites within the catalytic converter, it will normally only be reflected in the pre-exponential factors of the Arrhenius equations, and not in their activation energies. However, the inventors have also found out that the aged state can surprisingly affect the pre-exponential factors of a whole group of Arrhenius equations, each corresponding to a different chemical reaction with the same catalyst, in a similar manner, so that, instead of applying a different aging coefficient to each individual Arrhenius equation, a single common aging coefficient can be applied to the whole group of Arrhenius equations while maintaining significant accuracy in the calculation of each reaction rate. Consequently, by this approach, the calibration of the Arrhenius equations according to the aged state of the catalytic converter, and thus the simulation of the chemical reactions, can be significantly facilitated without affecting the accuracy of the resulting estimation of the flowrate of one or more reagents and/or reaction products out of the catalytic converter.

In particular, all chemical reactions within the group of chemical reactions may involve a common chemical substance as reagent and/or reaction product, so that individual divergences from the corresponding common aging coefficient may balance each other out, especially if the step of calculating a flowrate of one or more reagents and/or reaction products out of the catalytic converter includes calculating a flowrate of the common chemical substance out of the catalytic converter.

The corresponding common aging coefficient may be, for instance, an average of individual aging coefficients, each corresponding to an individual chemical reaction from among the group of chemical reactions, wherein each individual aging coefficient may be a quotient of a pre-exponential factor of an Arrhenius equation determined for the corresponding individual chemical reaction in a reference catalytic converter in said aged state, divided by a pre-exponential factor of an Arrhenius equation determined for the corresponding individual chemical reaction in the reference catalytic converter in a fresh state, wherein the Arrhenius equations determined for each individual chemical reaction in the reference catalytic converter in the aging and fresh states may be determined from experimental data. The corresponding common aging coefficient for the aged state may be interpolated from common aging coefficients for different aged states. Measurements and/or estimations from a reference catalytic converter may thus be easily generalized to the simulation of other catalytic converters.

While a single corresponding common aging coefficient may be applied to a first group of Arrhenius equations corresponding to a first group of chemical reactions with a first catalyst, other chemical reactions and catalysts may be affected differently. Consequently, to take this into account, the computer-implemented method may further comprise the steps of applying, to one or more other groups of Arrhenius equations, one or more other corresponding common aging coefficients, all also according to the aging state of the catalytic converter, by multiplying a pre-exponential factor of each Arrhenius equation of the one or more other groups of Arrhenius equations by another corresponding aging coefficient from among the one or more other corresponding common aging coefficients, wherein each Arrhenius equation from each one or more other group of Arrhenius equations corresponds to a chemical reaction from

among one or more other groups of chemical reactions with a catalyst in the catalytic converter; calculating reaction rates for the one or more other groups of chemical reactions using the one or more other group of Arrhenius equations with the one or more other common aging coefficients; and calculating a
5 flowrate of one or more reagents and/or reaction products of the one or more other groups of chemical reactions, out of the catalytic converter, by applying the reaction rates for the one or more other groups of chemical reactions to an exhaust stream flowing through the catalytic converter.

10 In order to simulate the chemical reactions over the whole catalytic converter, the reaction rates may be calculated for multiple positions within a grid representing the catalytic converter.

In order to verify performance of the catalytic converter, the computer-
15 implemented method may comprise a further step of comparing, with a predetermined flowrate threshold, the flowrate of the one or more reagents and/or reaction products out of the catalytic converter.

However, alternatively or in combination with this comparison with an
20 instantaneous flowrate threshold, the flowrate of one or more reagents and/or reaction products of the group of chemical reactions, out of the catalytic converter, may be calculated for multiple time steps within a period of time, and the computer-implemented method may further comprise a step of calculating a cumulated flow of the one or more reagents and/or reaction
25 products of the group of chemical reactions out of the catalytic converter over the period of time, as well as another step of comparing the cumulated outflow with a predetermined cumulated outflow threshold to verify performance of the catalytic converter, especially if the exhaust stream flowing through the catalytic converter varies in flowrate, composition and/or temperature during
30 the period of time.

This computer-implemented method may for instance be applied for catalytic converter production, wherein a process for producing catalytic converters, may comprise the steps of simulating, in a computer system,
35 chemical reactions within a catalytic converter according to a predefined set of specifications by using the abovementioned computer-implemented method,

and fabricating catalytic converters according to the predefined set of specifications, especially if the performance of the catalytic converter is successfully verified in the simulation step.

5 It may however also be applied in engine emissions control, wherein a process for controlling a combustion engine may comprise the steps of simulating, in a computer system, using the abovementioned computer-implemented method, chemical reactions within a catalytic converter incorporated in the exhaust system of the combustion engine, with an exhaust
10 stream corresponding to a given set of engine control parameters, adjusting the engine control parameters so that the calculated flowrate of the one or more reagents and/or reaction products out of the catalytic converter does not exceed a predetermined threshold, and applying the adjusted control parameters to control the combustion engine.

15 The present disclosure also concerns a computer program product and/or computer-readable storage medium comprising instructions which, when executed by a computer, cause it to carry out the abovementioned computer-implemented method.

20 The above summary of some example embodiments is not intended to describe each disclosed embodiment or every implementation of the invention. In particular, selected features of any illustrative embodiment within this specification may be incorporated into an additional embodiment unless clearly
25 stated to the contrary.

BRIEF DESCRIPTION OF THE DRAWINGS

The invention may be more completely understood in consideration of the following detailed description of various embodiments in connection with the
30 accompanying drawings, in which :

- FIG. 1 is a schematic drawing of a motor vehicle comprising a combustion engine with an exhaust system comprising two catalytic converters arranged in series.
- FIG. 2 is a schematic cutout drawing of a catalytic converter.
- 35 – FIG. 3A is a schematic representation of a first channel wall configuration within a catalytic converter.

– FIG. 3B is a schematic representation of a second channel wall configuration within a catalytic converter.

– FIGS. 4A, 4B and 4C are graphs illustrating the evolution of CO, HC and NO_x cumulative emissions out of a fresh-state catalytic converter, according to both experimental and computer-implemented simulation results.

– FIGS. 5A, 5B and 5C are graphs illustrating the evolution of CO, HC and NO_x cumulative emissions out of an aged-state catalytic converter, according to both experimental and computer-implemented simulation results using individually calibrated Arrhenius equations.

– FIGS. 6A to 6H are graphs comparing simulated and real, cold start and final CO, HC and NO_x cumulative emissions for the same catalytic converter in a fresh state, as well as in three different aged states.

– FIG. 7 is a graph illustrating individual aging coefficients for a group of three chemical reactions at three different aged states, together with a single corresponding aging coefficient, averaged from the individual aging coefficients, at each of the three aged states, with interpolated values in between.

– FIGS. 8A, 8B and 8C are graphs illustrating the evolution of CO, HC and NO_x cumulative emissions out of an aged-state catalytic converter, according to both experimental and computer-implemented simulation results using both individually calibrated Arrhenius equations, and groups of Arrhenius equations sharing common aging coefficients.

– FIGS. 9A to 9D are graphs comparing cold start and final CO, HC and NO_x cumulative emissions for the same catalytic converter in a two different aged states, according to experimental results as well as experiments using both individually calibrated Arrhenius equations, and groups of Arrhenius equations sharing common aging coefficients.

– FIGS. 10A, 10B and 10C are graphs illustrating the evolution of CO, HC and NO_x cumulative emissions according to both experimental results as well as computer-implemented simulation results for a fresh-state catalytic converter, and for an aged-state catalytic converter, wherein the simulation uses groups of Arrhenius equations with common aging coefficients.

While the invention is amenable to various modifications and alternative forms, specifics thereof have been shown by way of example in the drawings and will be described in detail. It should be understood, however, that the intention is not to limit aspects of the invention to the particular embodiments

described. On the contrary, the intention is to cover all modifications, equivalents, and alternatives falling within the scope of the invention.

DETAILED DESCRIPTION

5 For the following defined terms, these definitions shall be applied, unless a different definition is given in the claims or elsewhere in this specification.

All numeric values are herein assumed to be preceded by the term "about", whether or not explicitly indicated. The term "about" generally refers
10 to a range of numbers that one of skill in the art would consider equivalent to the recited value (i.e. having the same function or result). In many instances, the term "about" may be indicative as including numbers that are rounded to the nearest significant figure.

Although some suitable dimension ranges and/or values pertaining to
15 various components, features and/or specifications are disclosed, one of skill in the art, incited by the present disclosure, would understand desired dimensions, ranges and/or values may deviate from those expressly disclosed.

As used in this specification and the appended claims, the singular forms
20 "a", "an", and "the" include plural referents unless the content clearly dictates otherwise. As used in this specification and the appended claims, the term "or" is generally employed in its sense including "and/or" unless the content clearly dictates otherwise.

25 The following detailed description should be read with reference to the drawings in which similar elements in different drawings are numbered the same. The detailed description and the drawings, which are not necessarily to scale, depict illustrative embodiments and are not intended to limit the scope of the invention. The illustrative embodiments depicted are intended only as
30 exemplary. Selected features of any illustrative embodiment may be incorporated into an additional embodiment unless clearly stated to the contrary.

As illustrated in FIG. 1, a motor vehicle 1 may comprise a combustion
35 engine 2 with an exhaust system 3 including an exhaust pipe 4 and one or more catalytic converters 10 for decreasing pollutant emissions from the engine

exhaust. The combustion engine 2 may be, as illustrated, an internal combustion engine, and more particularly a reciprocating internal combustion engine with one or more cylinders. It may comprise an inlet manifold 5 and a fuel system, with e.g. fuel injectors 6, for feeding, respectively, air and fuel into the individual cylinders, and an exhaust manifold 7 for collecting the exhaust gases from the individual cylinders. It may also comprise a forced induction device, such as a turbocharger 8 with a turbine 8a, which may be located directly downstream from the exhaust manifold 7, so as to be driven by the exhaust gases, and a compressor 8b, which may be located directly upstream of the inlet manifold 5 and operatively coupled to the turbine 8a, so as to be driven by the latter to feed air under pressure into the engine. However, other forced induction devices, such as a supercharger, may be used instead, and the combustion engine 2 may even be naturally aspirated, that is, devoid of any forced induction device.

As shown in Fig. 1, the one or more catalytic converters 10 may be situated at a distance d downstream from the outlet of turbine 8a. Although in the illustrated example the exhaust system 3 comprises a single catalytic converter 10, the exhaust system 3 may instead comprise a plurality of catalytic converters, for instance a first catalytic converter, or pre-cat, located upstream in the exhaust system 3 so as to heat up faster on vehicle start up, so as to decrease cold start emissions, and a main catalytic converter located further downstream in the exhaust system 3, in a more convenient location, for instance under the motor vehicle's floorpan. The exhaust system 3 may further comprise exhaust content, flowrate and temperature sensors 12 located e.g. upstream of, between and/or downstream of the one or more catalytic converters 10. These sensors 12 may be connected to an engine control unit 13, which may in turn be connected to i.a. the fuel system to control the combustion engine 2.

The one or more catalytic converters 10 may in particular be three-way catalytic converters configured to catalyze the reduction of nitrogen oxides (NO_x) and the oxidation of carbon monoxide (CO) and unburnt hydrocarbons (HC) to decrease emissions of all these three pollutants. As seen in FIG. 2, such a catalytic converter 10 may comprise a housing 100 and a block of substrate 101 therein, with channels 102 extending in the direction of flow of the exhaust

gasses from an inlet 103 to an outlet 104. As seen in FIGS. 3A and 3B, on the walls of these channels 102, the substrate 101, which may in particular be a ceramic material, such as e.g. cordierite ceramic, for its thermal properties, may receive a coating 105 or "washcoat" containing one or more catalysts, which
5 may be selected among platinum-group metals (PGM), in particular rhodium, palladium and platinum. This coating 105 may also comprise an oxygen storage material such as cerium. Moreover, this coating 105 may change in composition over the length of the channels 102.

10 FIG. 3A illustrates a first-generation catalytic converter 10 wherein the coating 105 is divided in three distinct zones: an upstream coating zone 105a with a palladium concentration by weight Pd1a, a downstream coating zone 105b with a rhodium concentration by weight Rh1a, and an intermediate coating zone 105c, located between the upstream and downstream coating
15 zones 105a, 105b, as rich in rhodium as the downstream coating zone 105b and with a palladium concentration Pd2a of e.g. 5% of the palladium concentration Pd1a of the upstream coating zone 105a.

FIG. 3B illustrates a second-generation catalytic converter 10, using a
20 smaller amount of costly platinum-group metals, wherein the coating 105 is divided in two distinct zones: an upstream coating zone 105a with a palladium concentration Pd1b of e.g. 46% of the palladium concentration Pd1a of the upstream coating zone 105a of the first-generation catalytic converter and a rhodium concentration Rh1b of e.g. 57% of the rhodium concentration Rh1a of
25 the downstream coating zone 105b of the first-generation catalytic converter, and a downstream coating zone 105b with a palladium concentration Pd2b of e.g. 3% of the palladium concentration Pd1a of the upstream coating zone 105a of the first-generation catalytic converter 10 and the same rhodium concentration Rh1b as the upstream coating zone 105a of this second-
30 generation catalytic converter 10.

In use, after the combustion engine 2 is started, the exhaust gases may flow through the exhaust manifold 7 and the exhaust pipe 4 into the one or more catalytic converters 10. After a short light-off period, during which the
35 one or more catalytic converters 10 are heated up by the hot exhaust gases, their temperature may stabilize. Within the one or more catalytic converters 10,

the various chemical substances contained in the exhaust gases may react with each other, at reaction sites on the coating 105, where these chemical reactions may be catalyzed by the platinum-group metals contained therein and progress at reaction rates each according to a corresponding Arrhenius equation.

5

A fresh-state catalytic converter 10 may be modelled using a detailed chemistry approach, taking into account the composition of the various coating zones 105a,105b,105c. A plurality of chemical reactions, e.g. up to 35 different chemical reactions, may be modelled in order to consider reactions of pollutants
10 such as NO_x, CO and HC with e.g. oxygen (O₂), ammonia (NH₃) and water (H₂O) on reaction sites on the coating 105 which contain a catalyst, as well as oxygen storage reactions which are modeled using 2 different storage sites. Each one of these chemical reactions may be modelled, for each catalyst, using a corresponding Arrhenius equation, for multiple positions within a grid
15 representing the catalytic converter, and a flowrate of one or more reagents and/or reaction products of these chemical reactions, flowing out of the catalytic converter may be calculated by applying these reaction rates to an exhaust stream flowing through the catalytic converter. Calculating these flowrates at multiple time steps over a period of time and integrating them, it is
20 also possible to calculate corresponding cumulated outflows over that period of time.

FIGS. 4A, 4B and 4C illustrate an example of cumulated in- and outflows of, respectively CO, HC, and NO_x, into and out of a catalytic converter 10, in a
25 fresh state, in a set-up corresponding to that of FIG. 1, applying a WLTC test cycle from a cold engine start at t=0 s.

In FIG. 4A, curve 401 corresponds to a cumulated mass inflow of CO and curve 402 to a corresponding cumulated mass outflow of CO, according to
30 experimental data from a test bench with the same combustion engine 2 and exhaust system 3, with a distance d of 70 cm between the outlet of turbine 8a and the catalytic converter 10 to obtain a relatively long light-off period of about 70 to 90 s. Curve 403 corresponds to the corresponding cumulated mass outflow according to a simulation using the abovementioned detailed reaction
35 model. As can be seen, the simulation result may remain within a narrow $\pm 10\%$

band, limited by curves 402a and 402b, around the experimental result of curve 402.

In FIG. 4B, curve 411 corresponds to a cumulated inflow of HC and curve
5 412 to a corresponding cumulated mass outflow of HC, according to the
experimental data, and curve 413 corresponds to the corresponding cumulated
mass outflow according to a simulation using the abovementioned detailed
reaction model. As can be seen, the simulation result may remain within a
 $\pm 15\%$ band from the experimental result of curve 412. Curves 412a, 412b
10 represent, respectively, the lower and upper limits of a narrower, $\pm 10\%$ band
around curve 412.

In FIG. 4C, curve 421 corresponds to a cumulated inflow of NO_x and curve
422 to a corresponding cumulated mass outflow of NO_x , according to the
15 experimental data, and curve 423 to the corresponding cumulated mass outflow
according to a simulation using the abovementioned detailed reaction model. As
can be seen, the simulation result may mostly remain within a narrow $\pm 10\%$
band, limited by curves 422a, 422b around the experimental result of curve 422.

20 However, the reaction sites within the catalytic converter may be
progressively poisoned by substances (both reagents and reaction products)
contained in the exhaust gases, so that the reaction rates may progressively
decrease as the catalytic converter ages. Moreover, the effect of this aging may
not be the same on the rates of all chemical reactions within the catalytic
25 converter. Consequently, the results from testing fresh-state catalytic
converters cannot be easily extrapolated to aged-state catalytic converters.

In each Arrhenius equation, the activation energy may depend on the
active reaction site type, i.e. palladium, rhodium..., while the pre-exponential
30 factor may depend according to the amount of active reaction sites, their
quality, accessibility, and so on... Aging of the catalytic converter may mainly
impact the quality and accessibility of the active sites. Therefore, aging of the
catalytic converter may only affect the pre-exponential factor of the Arrhenius
equations, leaving the activation energies substantially unaffected. A detailed
35 reaction model of the catalytic converter in an aged state may thus be
developed from the model of the same catalytic converter in the fresh state by

individually adjusting just the pre-exponential factor of each Arrhenius equation so as to match experimental results from testing the catalytic converter in the aged state.

5 FIGS. 5A, 5B and 5C illustrate an example of cumulated in- and outflows of, respectively CO, HC, and NO_x, into and out of a first-generation catalytic converter such as that of FIG. 3A, in an intermediate aged state, in a set-up corresponding to that of FIG. 1, applying the WLTC test cycle from a cold engine start at t=0 s.

10

 In FIG. 5A, curve 501 corresponds to a cumulated mass inflow of CO, curve 502 to a corresponding cumulated mass outflow of CO, according to experimental data from the same test bench, wherein the first-generation catalytic converter has been previously aged to the intermediate aged state by
15 running the combustion engine 2 for a corresponding time period, whereas curve 503 represents the corresponding cumulated mass outflow according to a simulation using the abovementioned detailed reaction model, wherein the pre-exponential factor has been individually adjusted for the Arrhenius equation corresponding to each chemical reaction, to take the aging into account.
20 Parallel curves 502a and 502b represent, respectively, the lower and upper limits of a $\pm 10\%$ band around curve 502.

 In FIG. 5B, curve 511 corresponds to a cumulated mass inflow of HC, curve 512 to a corresponding cumulated mass outflow of HC, according to
25 experimental data, and curve 513 to the corresponding cumulated mass outflow according to the simulation using the abovementioned detailed reaction model with individually adjusted Arrhenius equations. Parallel curves 512a and 512b represent, respectively, the lower and upper limits of a $\pm 10\%$ band around curve 512.

30

 In FIG. 5C, curve 521 corresponds to a cumulated mass inflow of NO_x, curve 522 to a corresponding cumulated outflow of NO_x, according to experimental data, and curve 523 to the corresponding cumulated outflow
35 according to a simulation using the abovementioned detailed reaction model using the abovementioned detailed reaction model with individually adjusted

Arrhenius equations. Parallel curves 522a and 522b represent, respectively, the lower and upper limits of a $\pm 10\%$ band around curve 522.

As can be seen from FIGS. 5A to 5C with individually-adjusted Arrhenius equations, the accuracy of the simulation results for this aged-state first-generation catalytic converter may remain close to that of the simulation results for the fresh-state first-generation catalytic converter. This is further confirmed by the comparative graphs of FIGS. 6A to 6H, comparing experimental and simulated results for CO, HC and NO_x cumulated emissions (by mass), at two different points in time, with the first-generation catalytic converter in a fresh state and three different aged states.

More precisely, FIGS. 6A and 6B show the experimental and simulated cumulated emissions of CO, HC and NO_x (by mass) at, respectively, a cold start timing t_{cs} , defined as the moment when the substrate 101 reaches a temperature of 400°C, and a final time step t_{end} , which for the WLTC test cycle may be 1800 s after engine start, for the fresh-state first-generation catalytic converter. FIGS. 6C and 6D show the same for the first-generation catalytic converter at a first aged state, FIGS. 6E and 6F for the first-generation catalytic converter at a second aged state and FIGS. 6G and 6H for the first-generation catalytic converter at a third aged state.

While the simulation results for the aged-state catalytic converter may remain thus close to the experimental results, individually adjusting the Arrhenius equation for each chemical reaction can be extremely laborious, potentially requiring synthetic gas bench tests of each coating zone of the catalytic converters, as well as validation experiments in engine test benches and/or chassis dynamometer test benches, and this for each configuration and aged state of the catalytic converter.

30

It has been our surprising insight that it may be possible to group the various chemical reactions for each catalyst in a smaller number of groups of chemical reactions, wherein the aging of the catalytic converter has a similar impact on all the chemical reactions of one group, so that the all the Arrhenius equations for that group of chemical reactions may be simultaneously adjusted to the aged state of the catalytic converter using a common aging coefficient

35

for all reactions of that group of chemical reactions with that catalyst, and this independently of the composition of each coating zone within the catalytic converter.

- 5 For example, the chemical reactions may be grouped according to reagents and/or reaction products to form six groups according to Table 1 for each of the catalysts:

Groups	Type of reactions
Group 1	Reactions with O ₂
Group 2	Reactions with NO
Group 3	Reactions with NH ₃ and N ₂ O
Group 4	Reactions with slow Ce
Group 5	Reactions with fast Ce
Group 6	Reactions with H ₂ O

Table 1: Groups of chemical reactions

10

If three catalysts, e.g. platinum, palladium and rhodium, are taken into consideration, 18 common aging coefficients will correspond to each aged state.

- 15 To calculate each common aging coefficient for an aged state, a first step may be that of dividing the pre-exponential factor A_{aged} of each individually adjusted Arrhenius equation of the detailed reaction model of the catalytic converter in that aged state by the pre-exponential factor A_{fresh} of the Arrhenius equation for the same chemical reaction and catalyst in the detailed reaction
- 20 model in the fresh state, to obtain individual aging coefficients X for each chemical reaction and catalyst, according to the following equation:

$$X = \frac{A_{aged}}{A_{fresh}}$$

- 25 The common aging coefficient X_{Group} for a group of N chemical reactions with a catalyst for that aged state may then be calculated as an average of the individual aging coefficients X_i for the chemical reactions within that group of chemical reactions, with that catalyst, at that aged state:

$$X_{Group} = \frac{\sum_1^N X_i}{N}$$

For instance, if the group of chemical reactions with O₂ having rhodium as a catalyst comprises the chemical reactions of O₂ with CO, O₂ with HC and O₂ with H₂, the common aging coefficient X_{O₂,Rh} for this group of chemical reactions with rhodium as a catalyst may be calculated as:

$$X_{O_2,Rh} = \frac{X_{O_2+CO,Rh} + X_{O_2+HC,Rh} + X_{O_2+H_2,Rh}}{3}$$

wherein X_{O₂+CO,Rh}, X_{O₂+HC,Rh} and X_{O₂+H₂,Rh} are the individual aging coefficients calculated for the chemical reactions of O₂ with, respectively, CO, HC and H₂, at the same aging state, with rhodium as a catalyst.

The individual aging coefficients may be calculated for multiple aging states, possibly from experimental data at each of these multiple aging states. Common aging coefficients for each of these aging states may then be calculated by averaging the individual aging coefficients for each aging state, group of chemical reactions and catalyst, and further common aging coefficients may still be interpolated, from these common aging coefficients, for intermediate aging states.

In FIG. 7, for an exemplary catalytic converter 10, circles plot the individual aging coefficients for the chemical reaction of O₂ with CO, crosses plot the individual aging coefficients for the chemical reaction of O₂ with HC and triangles plot the individual aging coefficients for the chemical reaction of O₂ with H₂, with rhodium as a catalyst, in a fresh state and various aged states. Squares plot the common aging coefficients resulting from averaging, for each aged state, the corresponding individual aging coefficients, and a line links these squares to illustrate an aging law resulting from linear interpolation between these common aging coefficients.

Because the aged state may affect all the chemical reactions within one reaction group similarly, and individual divergences from the corresponding common aging coefficient may balance each other out if they involve a common reagent and/or reaction product, the individual pre-exponential factors of the

Arrhenius equations for each group of chemical reactions in the reaction model for the aged state may be replaced by the pre-exponential factors for the fresh state, multiplied by the corresponding common aging coefficient for each chemical reaction group, without significantly affecting the accuracy of this reaction model.

FIGS. 8A, 8B and 8C further illustrate the example from FIGS. 5A, 5B and 5C of cumulated in- and outflows of, respectively CO, HC, and NO_x, into and out of the first-generation catalytic converter 10.

As in FIG. 5A, in FIG. 8A curve 501 corresponds to the cumulated mass inflow of CO, curve 502 to the corresponding cumulated mass outflow of CO, according to experimental data from the same test bench, wherein the first-generation catalytic converter 10 has been previously aged to the intermediate aged state by running the combustion engine 2 for a corresponding time period, and curve 503 represents the corresponding cumulated mass outflow according to the simulation using the abovementioned detailed reaction model, wherein the pre-exponential factor has been individually adjusted for the Arrhenius equation corresponding to each chemical reaction, to take the aging into account. In addition to these previous curves, parallel curves 503a and 503b represent, respectively, lower and upper limits of a $\pm 15\%$ band around curve 503, and curve 801 represents the corresponding cumulated mass outflow according to a simulation using a reaction model wherein the pre-exponential factor for the Arrhenius equations has been adjusted by groups of chemical reactions, with a single corresponding common aging coefficient for each group of chemical reactions and catalyst, to take into account the aged state of the first-generation catalytic converter.

As in FIG. 5B, in FIG. 8B curve 511 corresponds to the cumulated mass inflow of HC, curve 512 to a corresponding cumulated mass outflow of HC, according to experimental data, and curve 513 to the corresponding cumulated mass outflow according to the simulation using the abovementioned detailed reaction model with individually adjusted Arrhenius equations. In addition to these previous curves, parallel curves 513a and 513b represent, respectively, lower and upper limits of a $\pm 15\%$ band around curve 513, and curve 811 represents the corresponding cumulated mass outflow according to a simulation

using the reaction model wherein the pre-exponential factor for the Arrhenius equations has been adjusted by groups of chemical reactions, with a single corresponding common aging coefficient for each group of chemical reactions and catalyst, to take into account the aged state of the first-generation catalytic converter.

As in FIG. 5C, in FIG. 8C curve 521 corresponds to a cumulated mass inflow of NO_x, curve 522 to a corresponding cumulated mass outflow of NO_x, according to experimental data, and curve 523 to the corresponding cumulated mass outflow according to a simulation using the abovementioned detailed reaction model using the abovementioned detailed reaction model with individually adjusted Arrhenius equations. In addition to these previous curves, parallel curves 523a and 523b represent, respectively, lower and upper limits of a $\pm 15\%$ band around curve 523, and curve 821 represents the corresponding cumulated mass outflow according to a simulation using the reaction model wherein the pre-exponential factor for the Arrhenius equations has been adjusted by groups of chemical reactions, with a single corresponding common aging coefficient for each group of chemical reactions and catalyst, to take into account the aged state of the first-generation catalytic converter.

As can be seen from FIGS. 8A to 8C with individually-adjusted Arrhenius equations, adjusting the Arrhenius equations by catalysts and groups of chemical reactions rather than individually, to take the aged state of the first-generation catalytic converter into account, still does not significantly affect the accuracy of the outcome of the corresponding simulation. This is further confirmed by the comparative graphs of FIGS. 9A to 9D, comparing experimental results for CO, HC and NO_x cumulated emissions, at two different points in time, with catalytic converters in two aged states, with corresponding results from simulations using individually adjusted Arrhenius equations and simulations using groups of Arrhenius equations adjusted with common aging converters. These bar plots show the deviation of the cold start emissions and the final cumulative emissions. The end of the cold start is defined as the time to reach 400°C for the catalyst bed temperature. It can be seen that the maximum deviation of the group-adjusted reaction model with respect to the individually-adjusted model is just 11%.

Another surprising insight is that the common aging coefficients and aging laws thus derived for one or more groups of chemical reactions, with one or more catalysts, from experimental results using a catalytic converter may be applied to extrapolate emissions from another, differently-configured catalytic converter. For example, common aging coefficients derived from experimental results from testing a first-generation catalytic converter as illustrated in FIG. 3A can be applied in the simulation of the same chemical reactions in a second-generation catalytic converter, as illustrated in FIG. 3B, with the same aged state.

For this, a reaction model of the second-generation catalytic converter in a fresh state may be developed, comprising another set of Arrhenius equations for the chemical reactions within this second-generation catalytic converter, taking into account the different concentration and distribution of catalysts along its channels, and eventually matching experimental results from testing the second-generation catalytic converter in the fresh state. In this reaction model, additional chemical reactions and species may be considered. For instance, even if only C_3H_6 was considered among hydrocarbons (HC) in the detailed reaction model for the first-generation catalytic converter, chemical reactions involving CH_4 may be considered in the detailed reaction model for the second-generation catalytic converter.

To adapt this reaction model of the second-generation catalytic converter to an aged state, the pre-exponential factors of its Arrhenius equations may be multiplied by the corresponding common aging coefficients for their corresponding chemical reaction groups, catalysts and aged state. The additional chemical reactions considered in this reaction model may be associated to one or more existing reaction groups, so that the corresponding common aging coefficients may also be applied to their Arrhenius equations. A flowrate of one or more reagents and/or reaction products of all the chemical reactions considered in the thusly adapted reaction model, flowing out of the second-generation reaction catalytic converter may be calculated by applying these reaction rates to an exhaust stream flowing through the catalytic converter. Calculating these flowrates at multiple time steps over a period of time and integrating them, it is also possible to calculate corresponding cumulated outflows over that period of time.

FIGS. 10A, 10B and 10C illustrate an example of cumulated in- and outflows of, respectively CO, HC, and NO_x, into and out of a second-generation catalytic converter such as that of FIG. 3, in a first aged state, in a set-up corresponding to that of FIG. 1, applying the WLTC test cycle from a cold engine start at t=0 s.

In FIG. 10A, curve 1001 corresponds to a cumulated mass inflow of CO, curve 1002 to a corresponding cumulated mass outflow of CO, according to experimental data from the same test bench, wherein the second-generation catalytic converter 10 has been previously aged to the first aged state by running the combustion engine 2 for a corresponding time period. Parallel curves 1002a and 1002b represent, respectively, lower and upper limits of a $\pm 15\%$ band around these experimental data, whereas curve 1003 represents the corresponding cumulated mass outflow according to a simulation using a reaction model of the second-generation catalytic converter in a fresh state, and curve 1004 represents the corresponding cumulated mass outflow according to a simulation using a reaction model of the second-generation catalytic converter in the first aged state, wherein the pre-exponential coefficients of the Arrhenius equations of the reaction model of the second-generation catalytic converter in the fresh state have been adjusted by applying the corresponding common aging coefficients obtained for the first-generation catalytic converter in the same first aged state.

In FIG. 10B, curve 1011 corresponds to a cumulated mass inflow of HC, curve 1012 to a corresponding cumulated mass outflow of HC, according to experimental data. Parallel curves 1012a and 1012b represent, respectively, lower and upper limits of a $\pm 15\%$ band around these experimental data, whereas curve 1013 represents the corresponding cumulated mass outflow according to the simulation of the second-generation catalytic converter in a fresh state, and curve 1014 represents the corresponding cumulated outflow according to the simulation adjusted by applying the corresponding common aging coefficients obtained for the first-generation catalytic converter in the same first aged state.

In FIG. 10C, curve 1021 corresponds to a cumulated mass inflow of NO_x, curve 1022 to a corresponding cumulated mass outflow of NO_x, according to

experimental data. Parallel curves 1022a and 1022b represent, respectively, lower and upper limits of a $\pm 15\%$ band around these experimental data, whereas curve 1023 represents the corresponding cumulated mass outflow according to the simulation of the second-generation catalytic converter in a fresh state, and curve 1024 represents the corresponding cumulated mass outflow according to the simulation adjusted by applying the corresponding common aging coefficients obtained for the first-generation catalytic converter in the same first aged state.

As can be seen from FIGS. 10A to 10C the accuracy of the simulation results using those common aging coefficients remains high, the adjusted reaction model adequately taking into consideration the aged state of the second-generation catalytic converter.

These reaction models and simulation methods may be implemented in a computer, which may comprise a processing unit and a memory. They may be embodied in a computer program, which may be stored in a computer-readable data storage medium, and comprise a set of instructions which, when the program is carried out by a computer, cause the computer to carry out the computer-implemented simulation method.

Such a computer-implemented simulation method may be used, for example, to evaluate the impact of aging on the emissions from an exhaust system incorporating a novel catalytic converter without having to carry out additional tests of actual examples of the novel catalytic converter. For instance, an instantaneous flowrate of the one or more reagents and/or reaction products out of the catalytic converter 10, calculated using this computer-implemented simulation method, may be compared with a predetermined flowrate threshold, to verify performance of the novel catalytic converter. Alternatively or in combination with this, a cumulated outflow of the one or more reagents and/or reaction products of the group of chemical reactions out of the catalytic converter 10 over a period of time, calculated using this computer-implemented simulation method, may also be compared with a predetermined cumulated outflow threshold to verify performance of the catalytic converter 10.

Such computer-implemented simulation methods, coupled with engine models, can support real driving emissions evaluation for motor vehicle manufacturers who want to prevent exceeding mandatory emission thresholds along the entire life of the motor vehicle 1. Numerous routes and driving profiles may be simulated, with variously-aged exhaust systems 3 and catalytic converters 10 in order to reduce the number of prototype exhaust systems as well as the number of real tests on the road or on chassis dynamometer test benches. This may be integrated in a production process, wherein the mass-fabrication of the novel catalytic converter 10 is launched after verification of its performance using the computer-implemented simulation method. This can also support a better design of the catalytic converter 10 with a broader range of evaluation (dimensioning, catalyst loading) without a need for specific prototypes. Moreover, such computer-implemented simulation can help reduce prototyping and testing costs.

Furthermore, the computer-implemented simulation method may also be integrated in an engine control process, wherein engine control parameters are adjusted so that the flowrate of the one or more reagents and/or reaction products out of the catalytic converter 10, calculated using the computer-implemented simulation method, does not exceed a predetermined threshold, and the thusly adjusted engine control parameters are applied to control the combustion engine 2. For example, in the set-up of FIG. 1, the engine control unit 13 may be a computer programmed to carry out this engine control process.

Those skilled in the art will recognize that the present invention may be manifested in a variety of forms other than the specific embodiments described and contemplated herein. Accordingly, departure in form and detail may be made without departing from the scope of the present invention as described in the appended claims.

CLAIMS

1. A computer-implemented method for simulating chemical reactions in a catalytic converter (10) in an aged state, comprising the steps of:

5 applying, to a group of Arrhenius equations, a single corresponding common aging coefficient according to the aged state of the catalytic converter (10), by multiplying a pre-exponential factor of each Arrhenius equation of the group of Arrhenius equations by the corresponding common aging coefficient, wherein each Arrhenius equation from among the group of Arrhenius equations
10 corresponds to a chemical reaction from among a group of chemical reactions with a catalyst in the catalytic converter (10);

 calculating reaction rates for the group of chemical reactions using the group of Arrhenius equations with the corresponding common aging coefficient; and

15 calculating a flowrate of one or more reagents and/or reaction products of the group of chemical reactions, out of the catalytic converter (10), by applying the reaction rates for the group of chemical reactions to an exhaust stream flowing through the catalytic converter (10).

20 2. The computer-implemented method of claim 1, wherein all chemical reactions within the group of chemical reactions involve a common chemical substance as reagent and/or reaction product.

3. The computer-implemented method of claim 2, wherein the step of
25 calculating a flowrate of one or more reagents and/or reaction products out of the catalytic converter (10) includes calculating a flowrate of the common chemical substance out of the catalytic converter (10).

4. The computer-implemented method according to any one of claims 1
30 to 3, wherein the corresponding common aging coefficient is an average of individual aging coefficients, each corresponding to an individual chemical reaction from among the group of chemical reactions with the catalyst.

5. The computer-implemented method of claim 4, wherein each
35 individual aging coefficient is a quotient of a pre-exponential factor of an Arrhenius equation determined for the corresponding individual chemical

reaction in a reference catalytic converter (10) in said aged state, divided by a pre-exponential factor of an Arrhenius equation determined for the corresponding individual chemical reaction in the reference catalytic converter (10) in a fresh state.

5

6. The computer-implemented method of claim 5, wherein the Arrhenius equations determined for each individual chemical reaction in the reference catalytic converter (10) in the aged and fresh states are determined from experimental data.

10

7. The computer-implemented method according to any one of claims 1 to 6, wherein the corresponding common aging coefficient for the aged state is interpolated from common aging coefficients for different aged states.

15

8. The computer-implemented method according to any one of claims 1 to 7, further comprising the steps of:

applying, to one or more other groups of Arrhenius equations, one or more other corresponding common aging coefficients, all also according to the aged state of the catalytic converter (10), by multiplying a pre-exponential factor of each Arrhenius equation of the one or more other groups of Arrhenius equations by another corresponding aging coefficient from among the one or more other corresponding common aging coefficients, wherein each Arrhenius equation from each one or more other group of Arrhenius equations corresponds to a chemical reaction from among one or more other groups of chemical reactions with a catalyst in the catalytic converter (20);

25

calculating reaction rates for the one or more other groups of chemical reactions using the one or more other group of Arrhenius equations with the one or more other common aging coefficients; and

calculating a flowrate of one or more reagents and/or reaction products of the one or more other groups of chemical reactions, out of the catalytic converter, by applying the reaction rates for the one or more other groups of chemical reactions to an exhaust stream flowing through the catalytic converter (10).

30

9. The computer-implemented method according to any one of the previous claims, wherein the reaction rates are calculated for multiple positions within a grid representing the catalytic converter (10).

5 10. The computer-implemented method according to any one of the previous claims, further comprising a step of comparing, with a predetermined flowrate threshold, the flowrate of the one or more reagents and/or reaction products out of the catalytic converter (10), to verify performance of the catalytic converter (10).

10 11. The computer-implemented method according to any one of the previous claims, wherein the flowrate of one or more reagents and/or reaction products of the group of chemical reactions, out of the catalytic converter (10), is calculated for multiple time steps within a period of time.

15 12. The computer-implemented method of claim 11, wherein the exhaust stream flowing through the catalytic converter varies in flowrate, composition and/or temperature during the period of time.

20 13. The computer-implemented method according to any one of claims 11 or 12, further comprising a step of calculating a cumulated outflow of the one or more reagents and/or reaction products of the group of chemical reactions out of the catalytic converter (10) over the period of time.

25 14. The computer-implemented method according to claim 13, further comprising a step of comparing the cumulated outflow with a predetermined cumulated outflow threshold to verify performance of the catalytic converter (10).

30 15. A process for producing catalytic converters (10), comprising the steps of:

simulating, in a computer system, chemical reactions within a catalytic converter (10) according to a predefined set of specifications by using the computer-implemented method according to any one of claims 1 to 14; and

35 fabricating catalytic converters (10) according to the predefined set of specifications.

16. A process for controlling a combustion engine (2), comprising the steps of:

simulating, in a computer system, using the computer-implemented method according to any one of claims 1 to 14, chemical reactions within a catalytic converter (10) incorporated in an exhaust system (3) of the combustion engine (2), with an exhaust stream corresponding to a given set of engine control parameters;

adjusting the engine control parameters so that the calculated flowrate of the one or more reagents and/or reaction products out of the catalytic converter (10) does not exceed a predetermined threshold; and

applying the adjusted control parameters to control the combustion engine (2).

17. A computer program product comprising a set of instructions that, when carried out by a computer, cause it to carry out the computer-implemented method of any one of claims 1 to 14.

18. A computer-readable data storage medium comprising a set of instructions that, when carried out by a computer, cause it to carry out the computer-implemented method of any one of claims 1 to 14.

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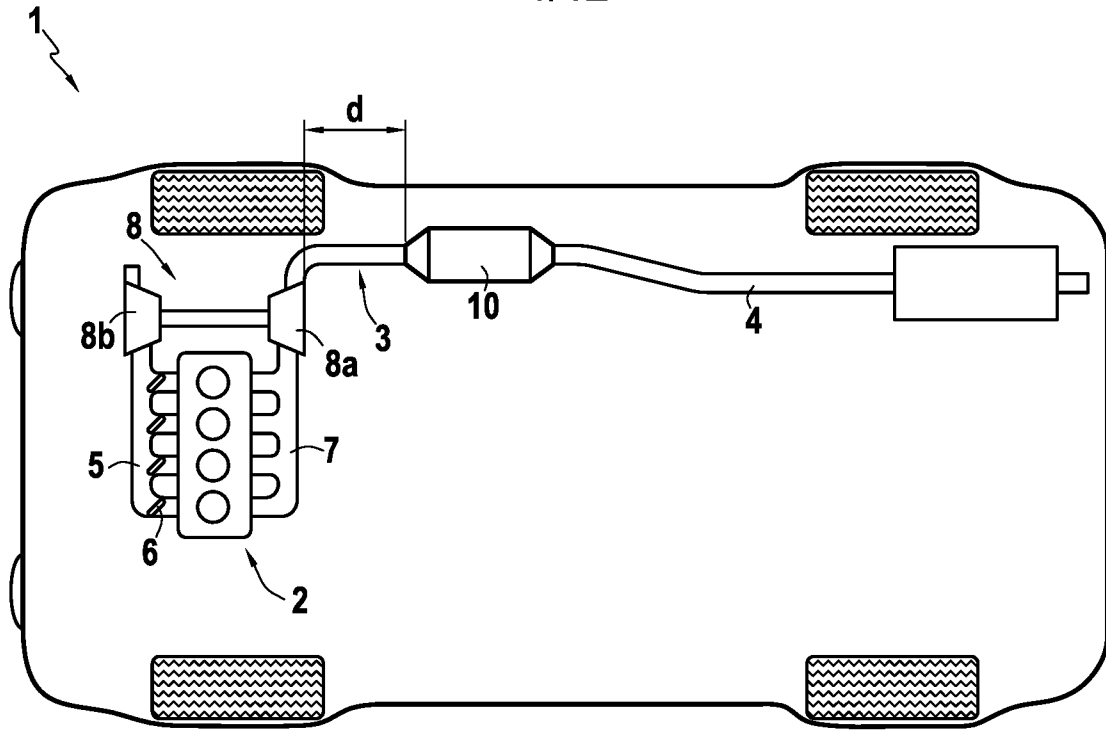


FIG.1

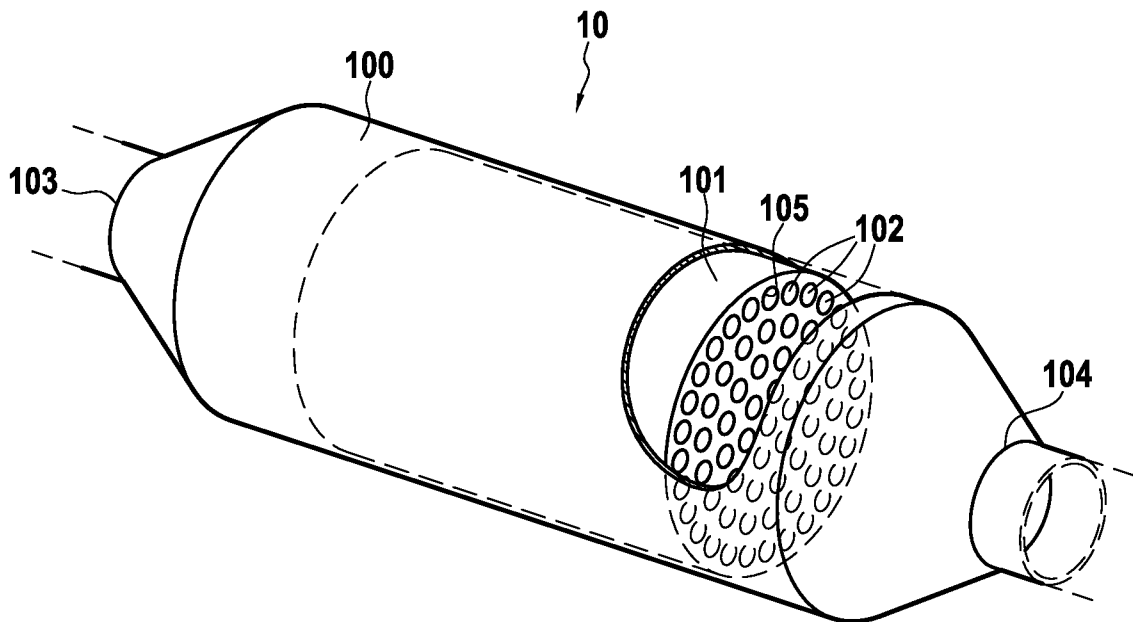


FIG.2

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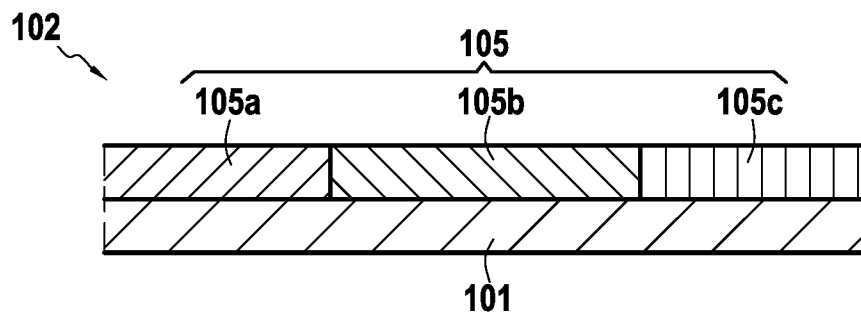


FIG.3A

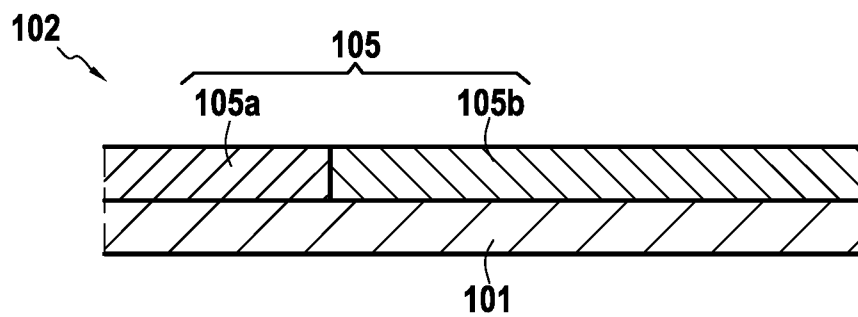


FIG.3B

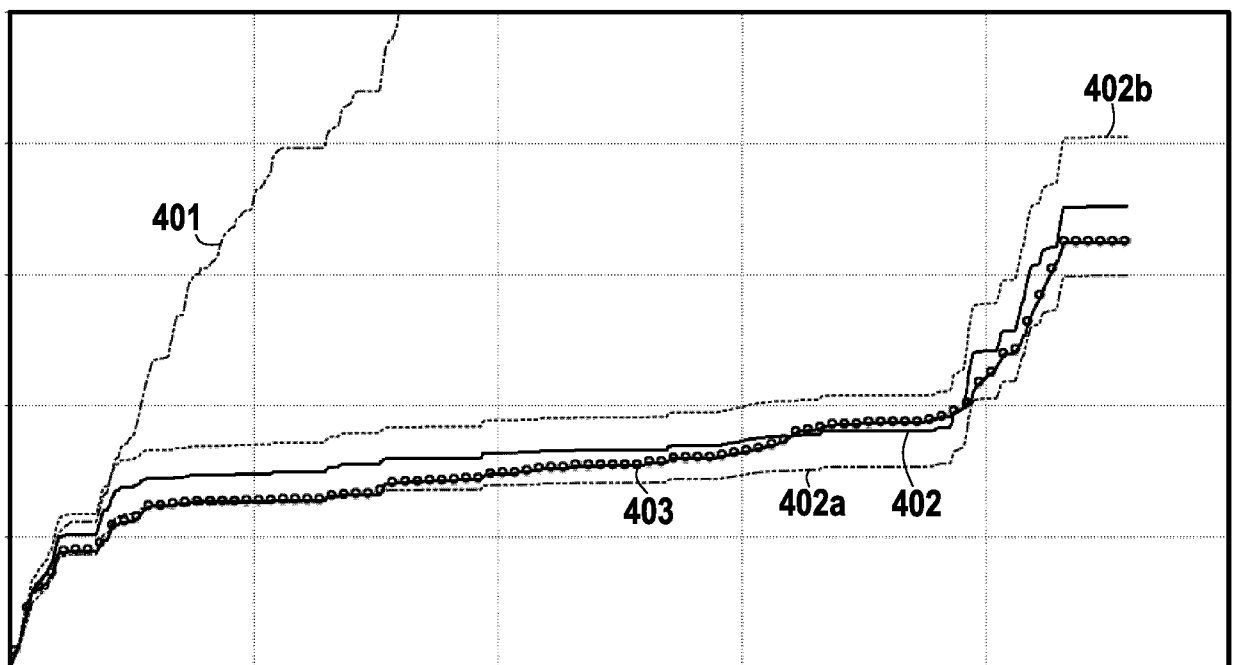


FIG.4A

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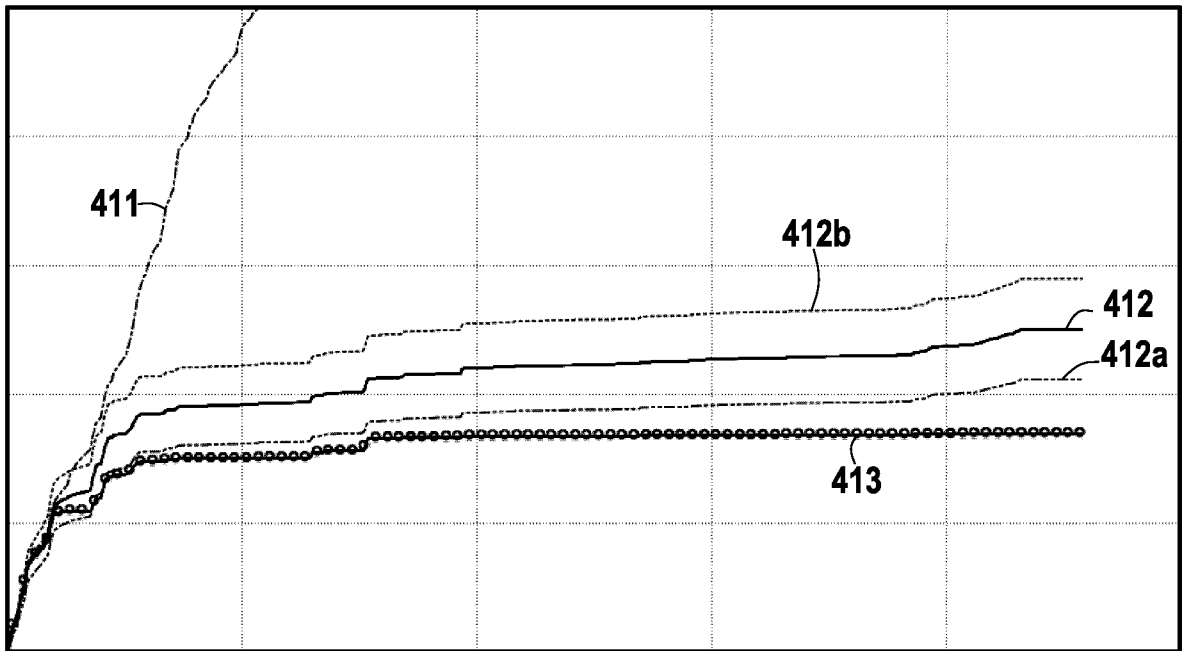


FIG. 4B

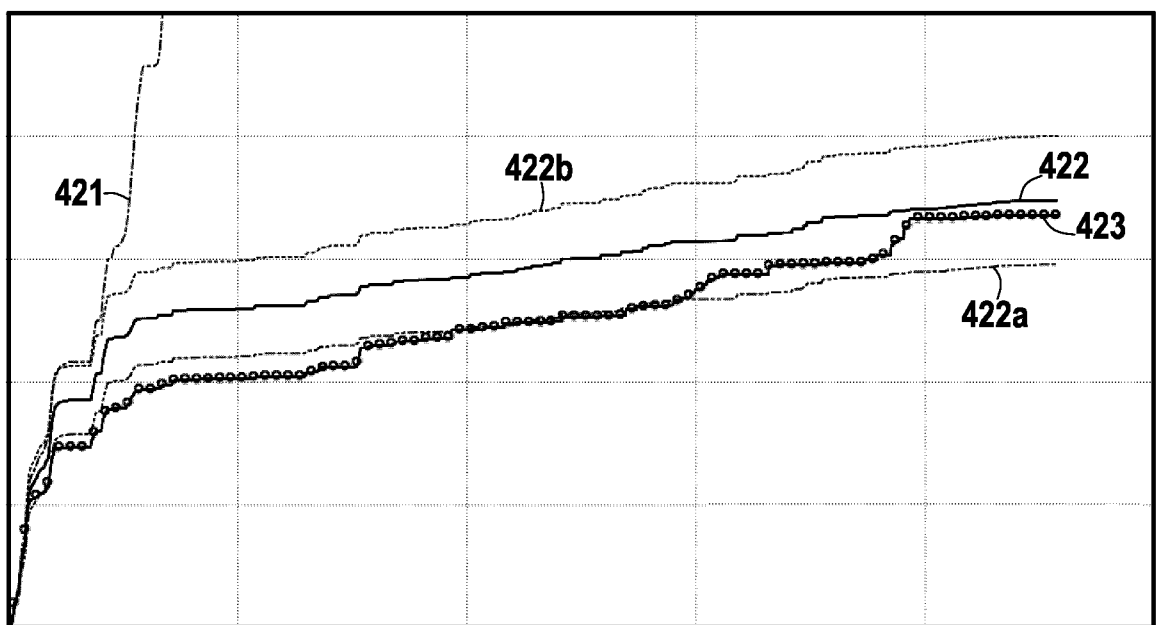


FIG. 4C

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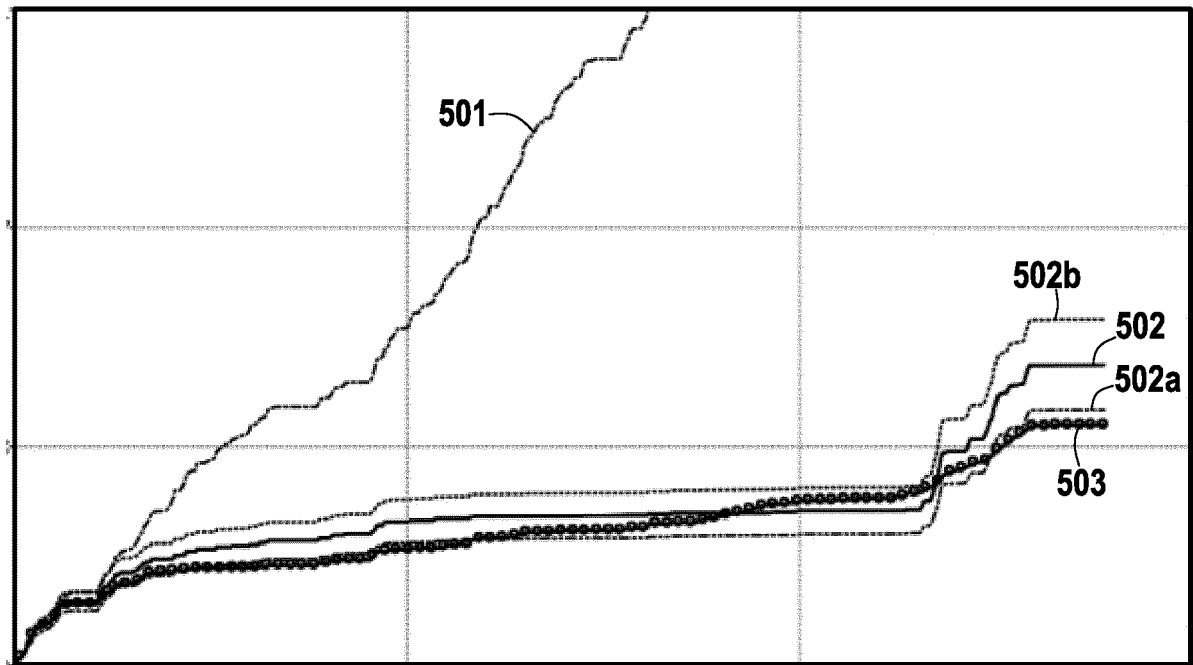


FIG.5A

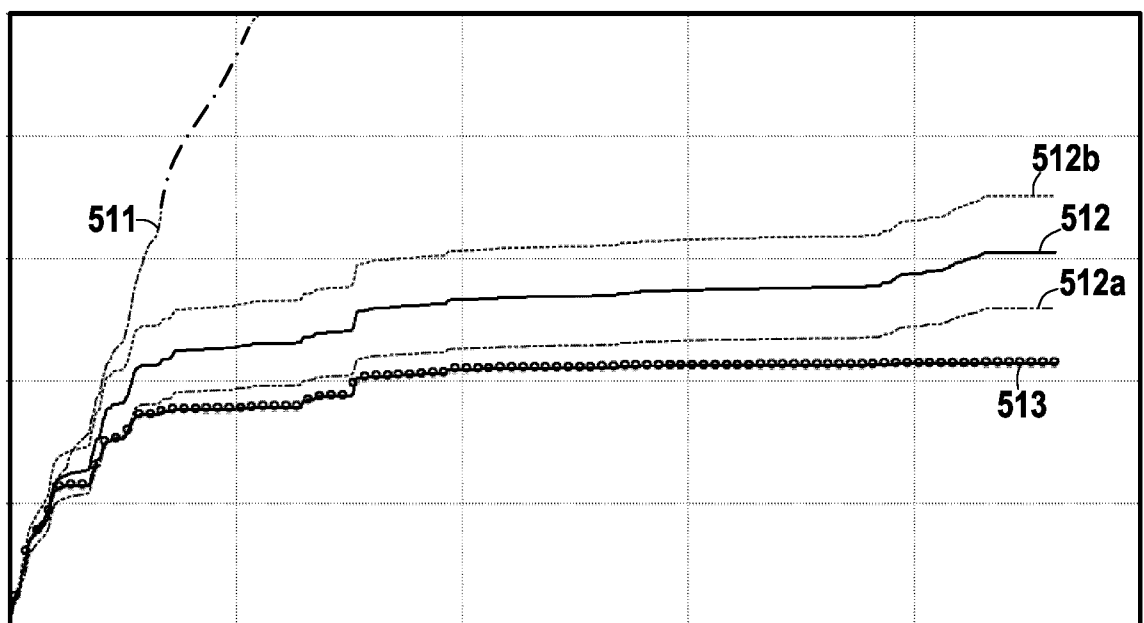


FIG.5B

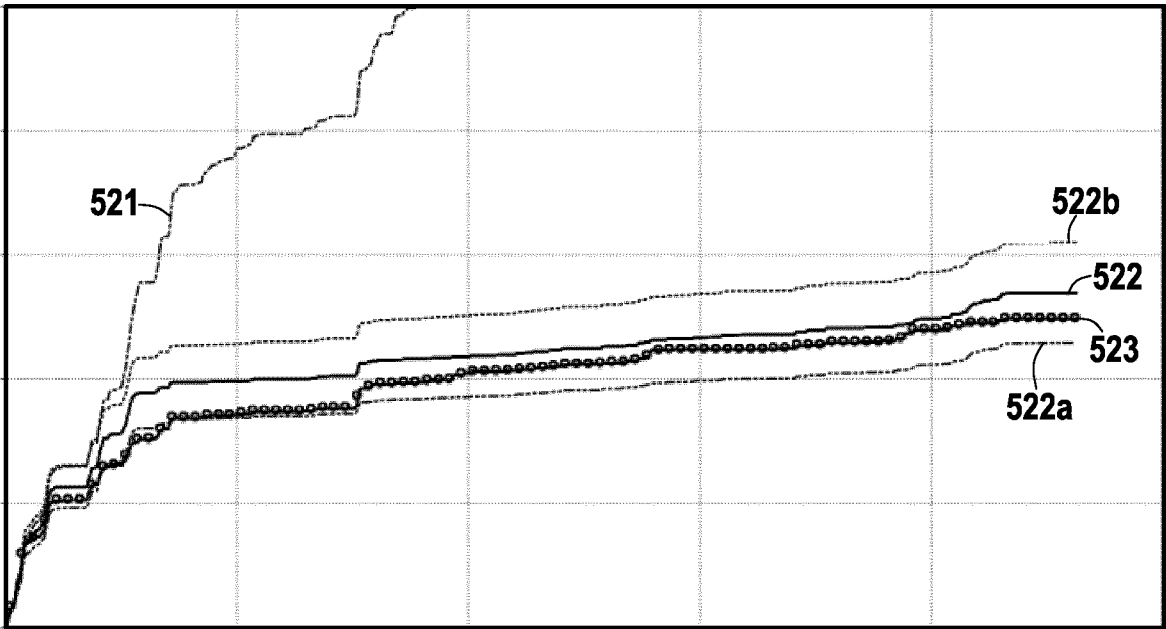


FIG.5C

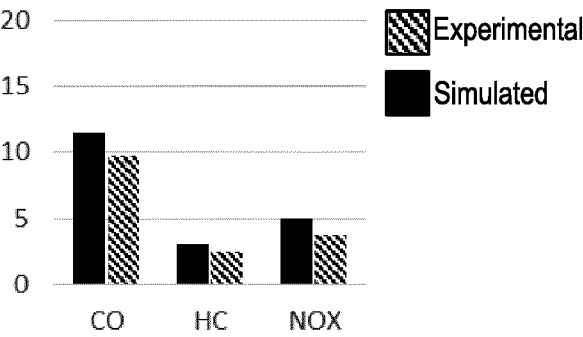


FIG.6A

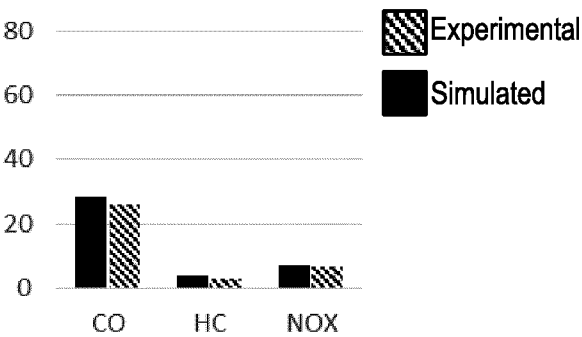


FIG.6B

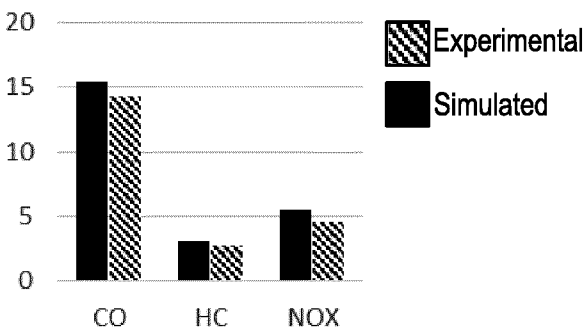


FIG.6C

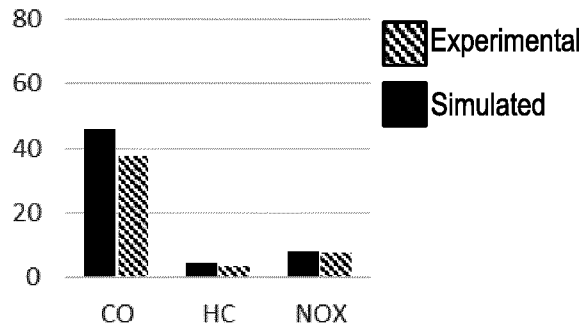


FIG.6D

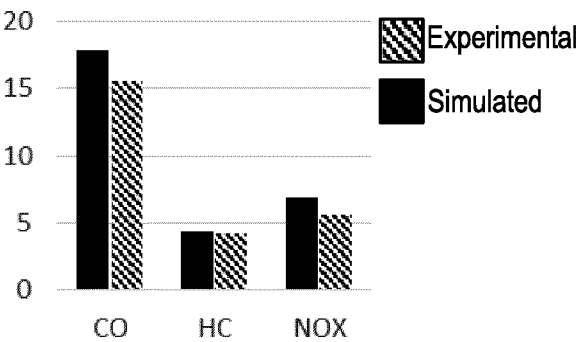


FIG.6E

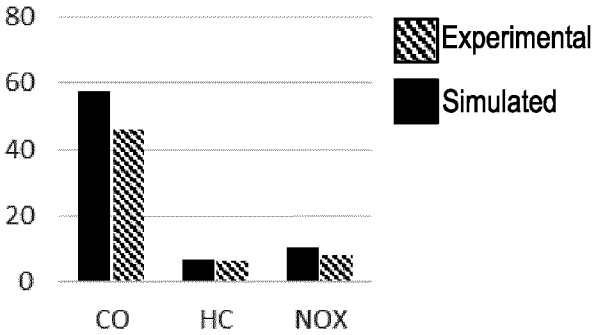


FIG.6F

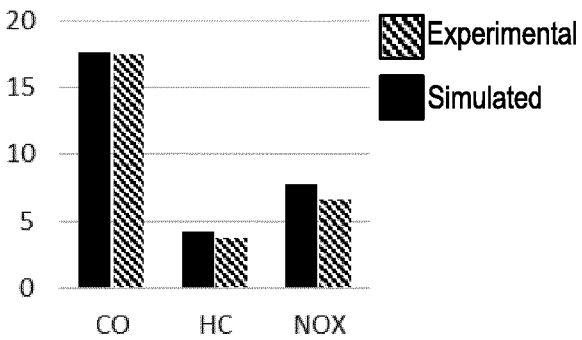


FIG.6G

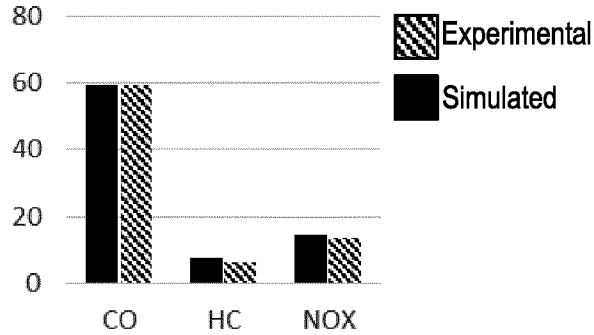


FIG.6H

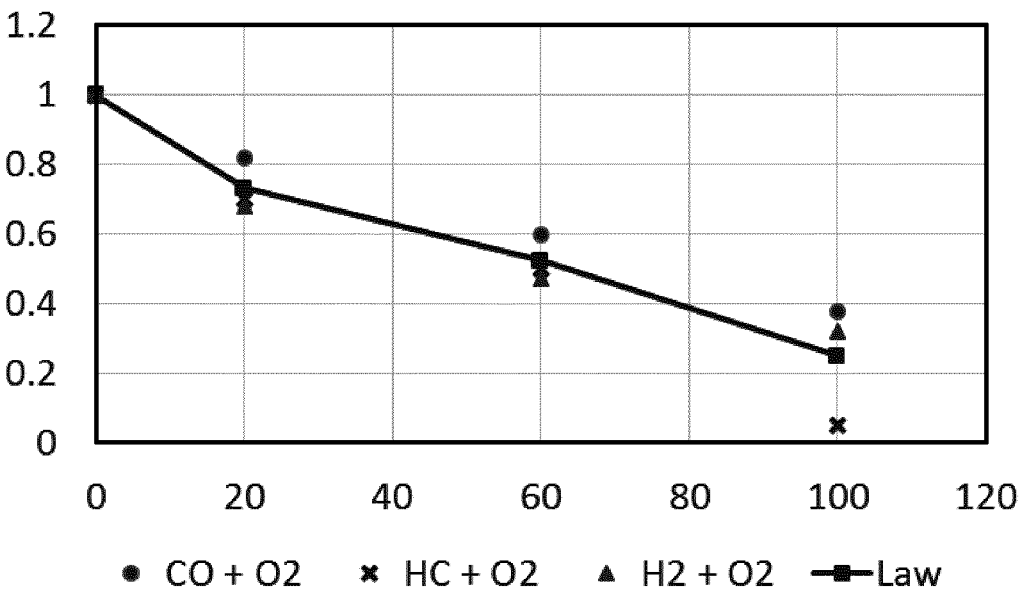


FIG.7

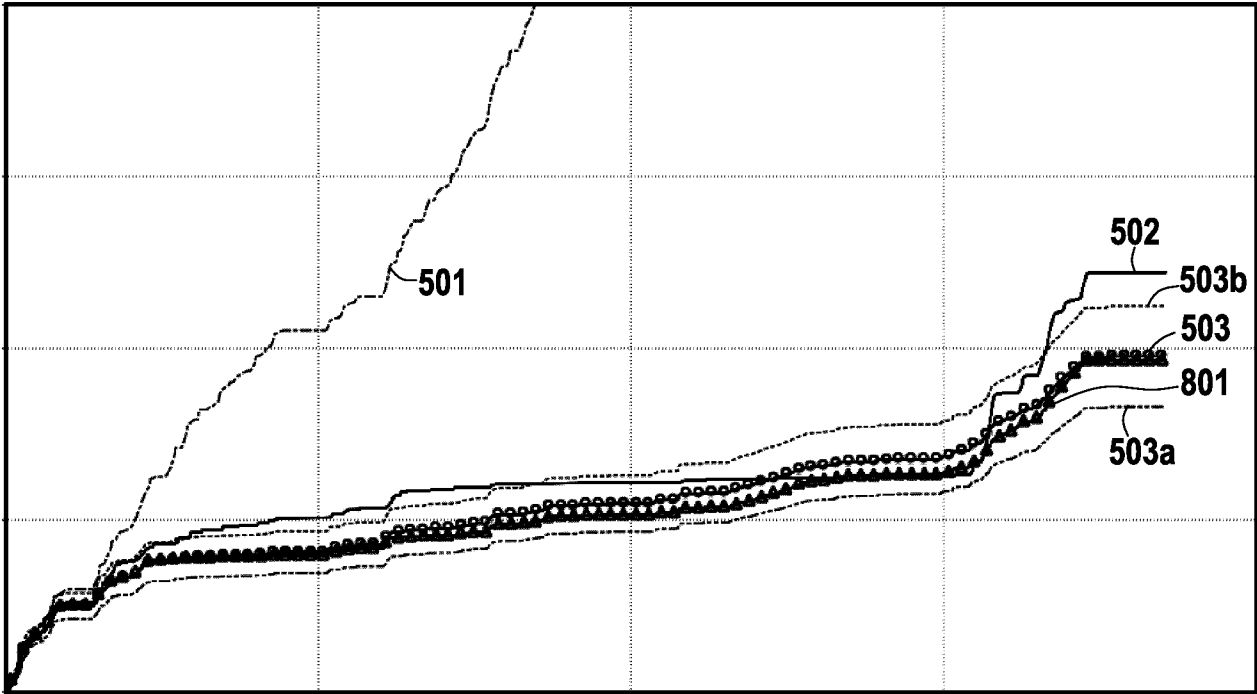


FIG. 8A

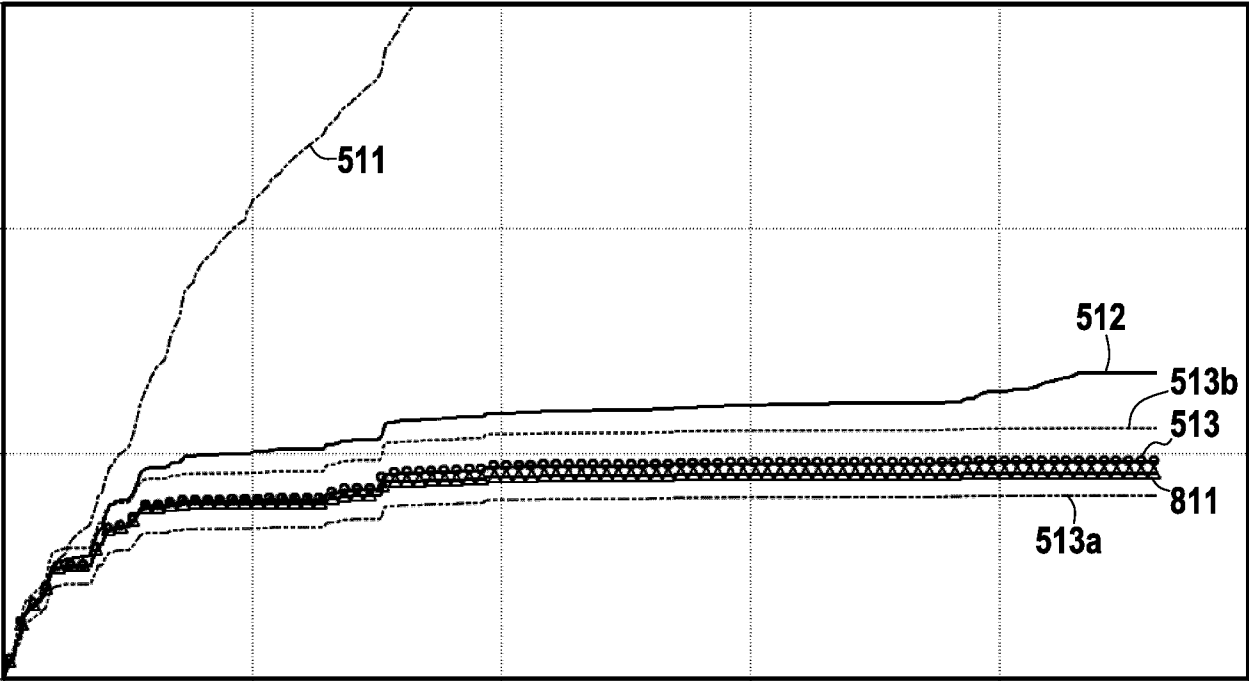


FIG. 8B

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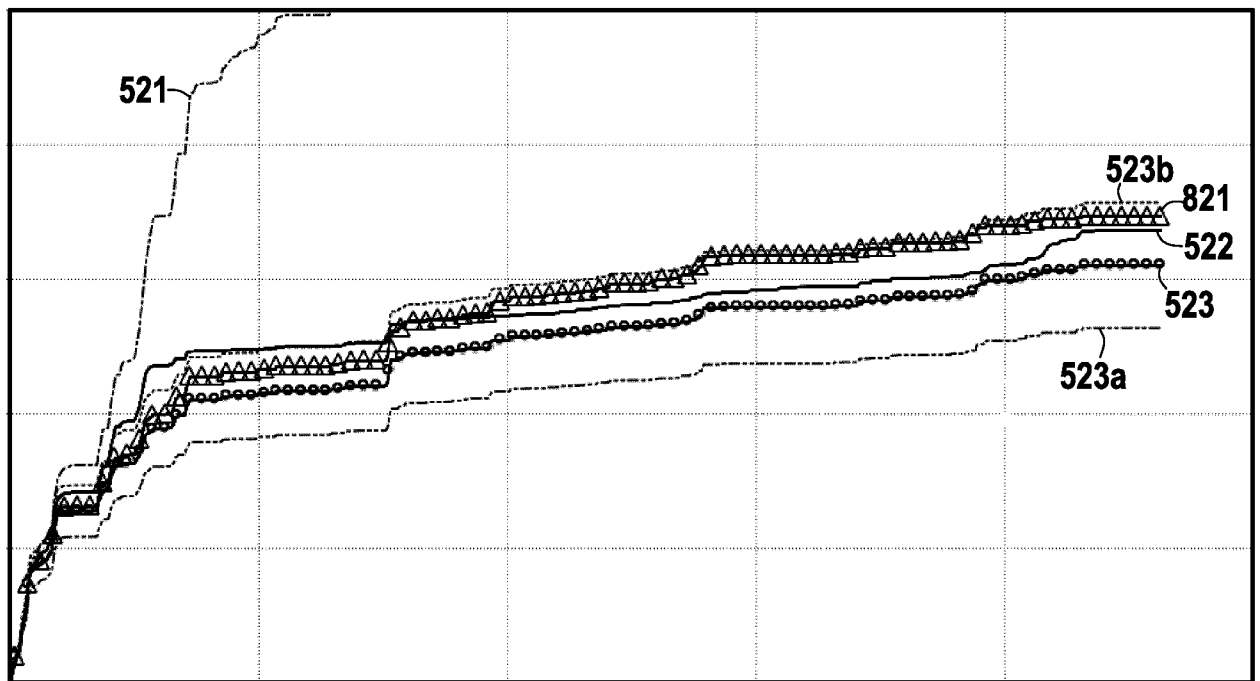


FIG.8C

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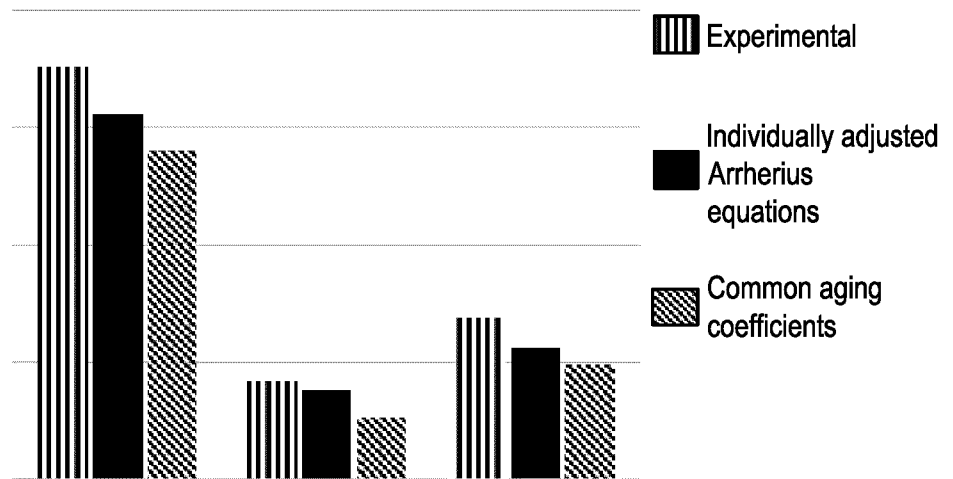


FIG.9A

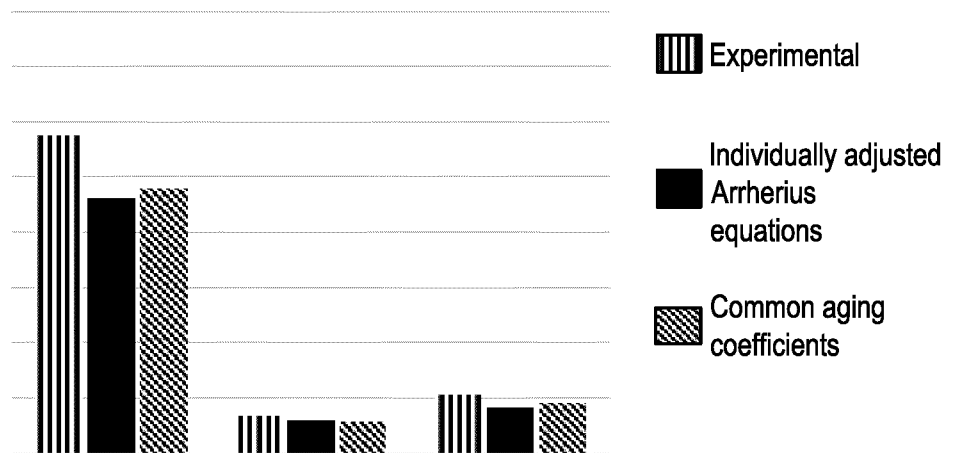


FIG.9B

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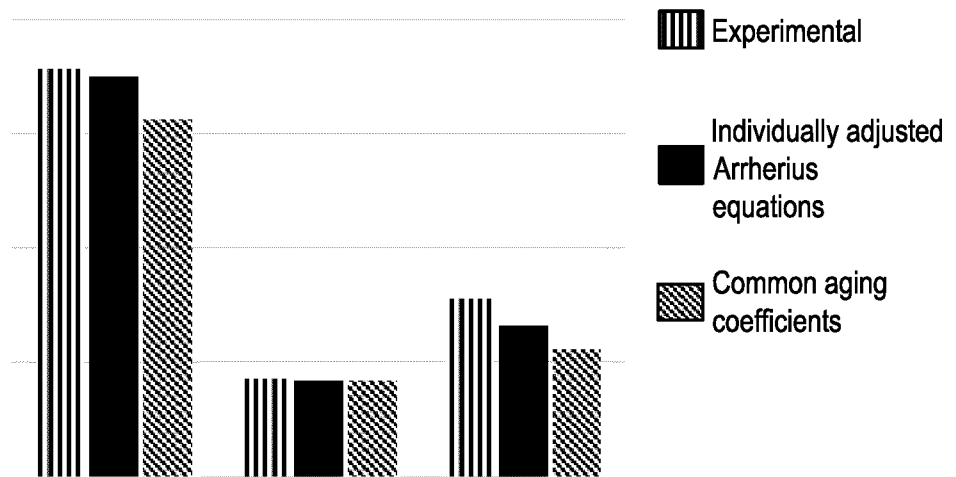


FIG.9C

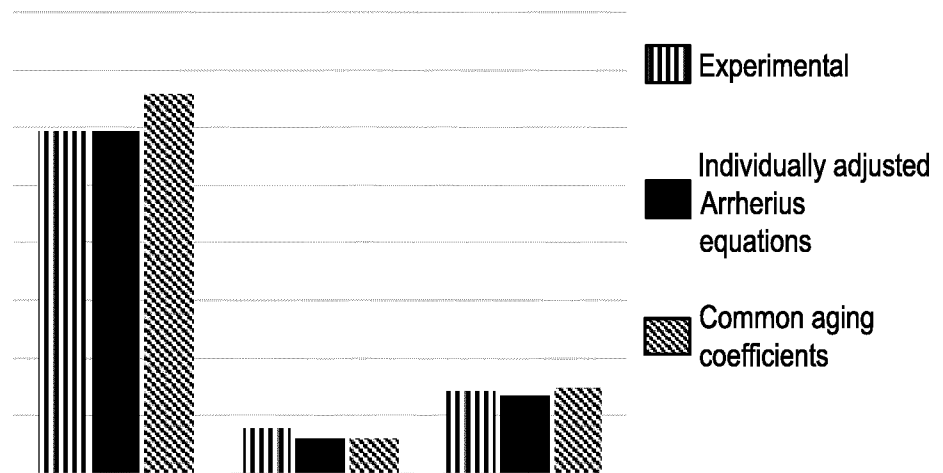


FIG.9D

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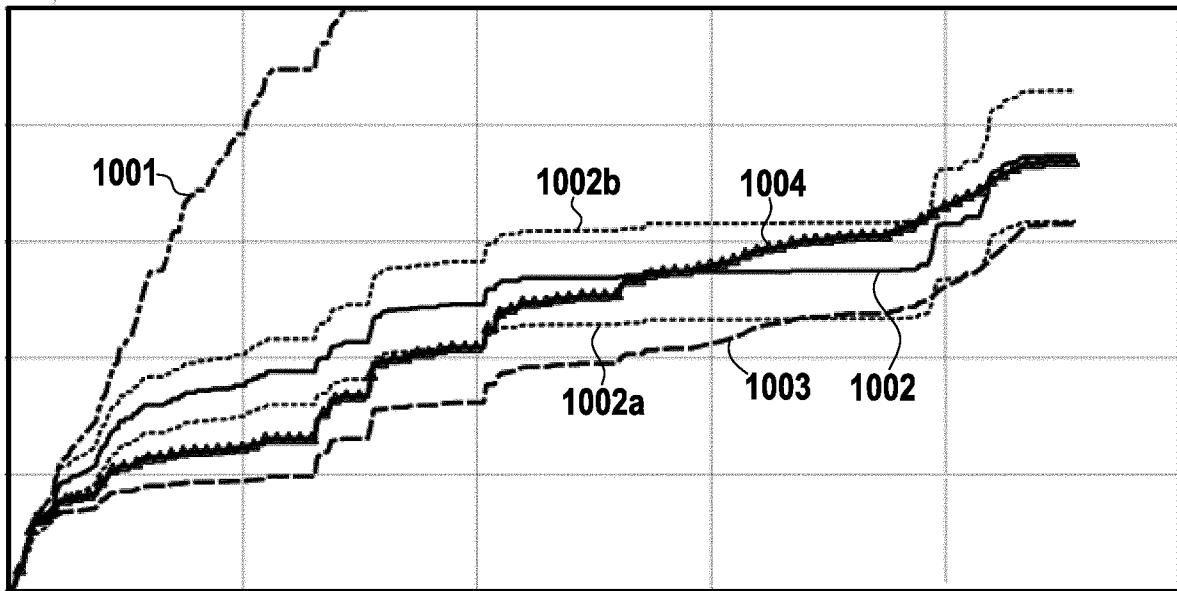


FIG.10A

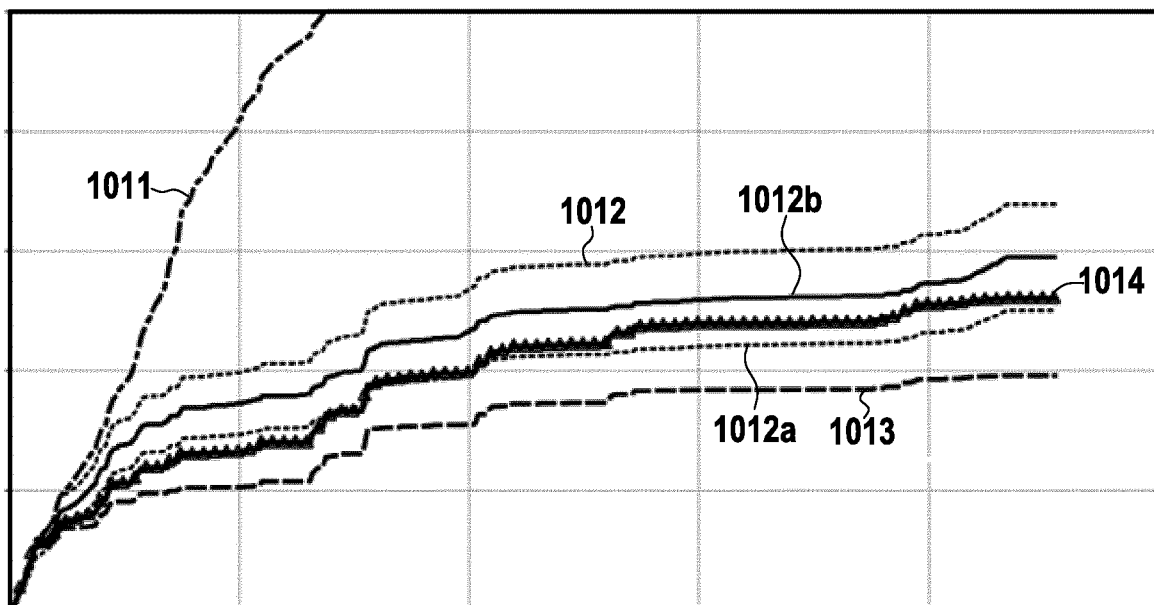


FIG.10B

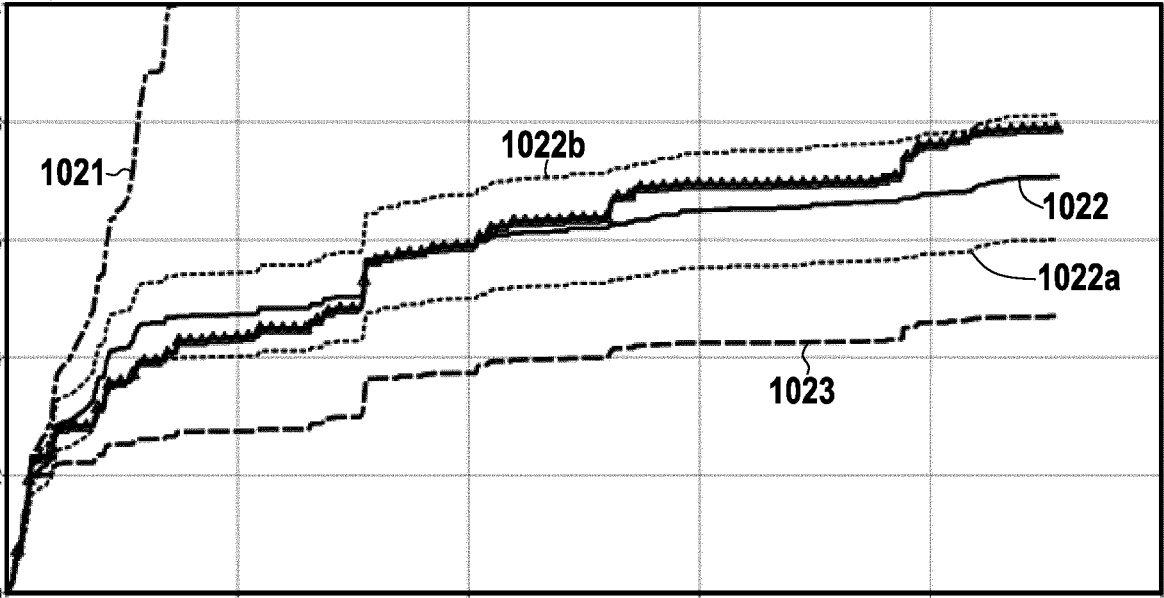


FIG.10C

INTERNATIONAL SEARCH REPORT

International application No
PCT/EP2019/066613

A. CLASSIFICATION OF SUBJECT MATTER
INV. F01N3/00 F01N11/00
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)
F01N

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, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	EP 1 544 431 A1 (FORD GLOBAL TECH LLC [US]) 22 June 2005 (2005-06-22) paragraph [0043]; claims 1, 4; figure 2 -----	1-18
X	WO 2011/093771 A1 (SCANIA CV AB [SE]; WESTERBERG BJOERN [SE]) 4 August 2011 (2011-08-04) claim 1; figures 1-2 -----	1-18
X	EP 2 543 840 A1 (FORD GLOBAL TECH LLC [US]) 9 January 2013 (2013-01-09) claims 1-5; figure 1 -----	1-18



Further documents are listed in the continuation of Box C.



See patent family annex.

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Date of the actual completion of the international search

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INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No

PCT/EP2019/066613

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
EP 1544431	A1	22-06-2005	DE 60311483 T2 31-10-2007 EP 1544431 A1 22-06-2005
WO 2011093771	A1	04-08-2011	EP 2529092 A1 05-12-2012 SE 1050084 A1 28-07-2011 WO 2011093771 A1 04-08-2011
EP 2543840	A1	09-01-2013	EP 2543840 A1 09-01-2013 US 2013008149 A1 10-01-2013