

CLAIMS

1. A volatile liquid chemical compound physical parameter database construction method (100), characterized in that it comprises:
- 5 - a step (105) of controlled deposition of a chemical compound in an inert container,
 - a step (110) of airflow generation, the airflow being directed in the direction of the deposited chemical compound,
 - a step (115) of measurement of a quantity of evaporated chemical compound
 - 10 at different measurement times,
 - a step (120) of evaporation rate calculation depending on the measured evaporated chemical compound quantities measured,
 - a step (125) of volatility calculation depending on the evaporation rate calculated and
 - 15 - a step (130) of storing, in a database, the calculated evaporation rate and the volatility calculated.
2. A construction method (100) according to claim 1, which further comprises:
- a step (135) of computing at least one gas phase concentration of a chemical
 - 20 compound for a given volatility of chemical compound,
 - a step (140) of measurement of the psychophysical intensity of a chemical compound for at least one said gas phase concentration,
 - a step (145) of modeling of a mathematical formula of psychophysical intensity as a function of gas phase concentration based on at least two of the measured
 - 25 gas phase concentration values and
 - a step (150) of recording, in a database, the psychophysical intensity formula modeled parameters.
3. A construction method (100) according to claim 1 or 2, which comprises a plurality
- 30 of steps (105) of controlled deposition of a chemical compound at different temperature, the evaporation rate being calculated for each said temperature and stored during the step of storing.

4. A fragrance physical composition evolution prediction method (200) to provide predictive, real-time, fragrance performance metrics, characterized in that it comprises:
- a step (205) of selecting at least one chemical compound identifier in a computerized interface,
 - 5 - a step (210) of inputting, for each selected chemical compound, a quantity of said chemical compound,
 - a step (215) of modeling a deposition of the quantity of each selected chemical compound on a virtual surface,
 - a step (220) of simulating, by a computing system, for at least one (modeled)
10 deposited chemical compound, the stripped quantity of said chemical compound in an airflow for at least two different times as a function of:
 - the quantity of each said chemical compound,
 - a first value representative of a virtual surface size of the deposited chemical compound,
 - 15 - a second value representative of a virtual airflow directed at the deposited chemical compound configured to virtually strip the chemical compound from the surface,
 - a third value representative of an activity coefficient of each said chemical compound and
 - 20 - an evaporation rate or volatility associated to said chemical compound stored in a database constructed according to the database construction method of any one of claims 1 to 3 and
 - a step (225) of displaying, for each chemical compound, of an indicator representative of the computed evaporated mass of said compound over time.
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5. A prediction method (200) according to claim 4, further comprising a step (230) of computing a gas phase concentration of the virtually stripped chemical compound as a function of the stripped quantity computed, the step (225) of displaying being configured to display the gas phase concentration computed.
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6. A prediction method (200) according to claim 5 when claim 4 depends on claim 2, further comprising a step (235) of computing a psychophysical intensity of each selected chemical compound as a function of the gas phase concentration computed,

the step (225) of displaying being configured to display the psychophysical intensity computed over time.

7. A prediction method (200) according to claim 6, in which at least two chemical compounds are selected, the method further comprising a step (240) of computing a global psychophysical intensity comprising:

- a first step (241) of matching a value for concentration for each compound against the corresponding dose-response curve to provide a perceived intensity value for that compound,
- 10 - a second step (242) of matching each said perceived intensity value against a dummy dose-response curve to provide an artificial compound concentration value,
- a step (243) of addition of each artificial compound concentration value to form a virtual concentration value and
- 15 - a third step (244) of matching the virtual concentration value against the dummy dose-response curve to provide a total perceived intensity value for the composition.

the step of displaying being configured to display the global psychophysical intensity computed over time.

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8. A prediction method (200) according to either claim 6 or 7, in which at least two chemical compounds are selected, the method further comprising a step (245) of computing a psychophysical intensity linearity of the composition of said at least two compounds based on the computed psychophysical intensity of each selected chemical compound over time, the step (225) of displaying being configured to display the psychophysical intensity linearity of the composition of said at least two compounds.

30 9. A prediction method (200) according to any one of claims 6 to 8, which further comprises a step (250) of chemical compound identifier selection, said chemical compound identifier being selected if the psychophysical intensity at a given time is below a determined value and a step (255) of display of said chemical compound identifier.

10. A prediction method (200) according to any one of claims 4 to 9, in which at least two chemical compounds are selected to form a composition, the method further comprising a step (260) of computing of the composition evolution over time as a
5 function of the stripped quantity calculated over time.

11. A prediction method (200) according to any one of claims 4 to 9, which further comprises a liquid chemical compound physical parameter database construction step (100) comprising:

- 10 - a step (105) of controlled deposition of a chemical compound in an inert container,
- a step (110) of airflow generation, the airflow being directed in the direction of the deposited chemical compound,
- a step (115) of measurement of a quantity of evaporated chemical compound
15 at different measurement times,
- a step (120) of evaporation rate calculation depending on the measured evaporated chemical compound quantities measured,
- a step (125) of volatility calculation depending on the evaporation rate calculated and
- 20 - a step (130) of storing, in a database, the calculated evaporation rate and the volatility calculated.

12. A liquid chemical compound physical parameter database construction system (300), characterized in that it comprises:

- 25 - a means (305) of controlled deposition of a chemical compound in an inert container (306),
- a means (310) of airflow generation, the airflow being directed in the direction of the deposited chemical compound,
- a means (315) of measurement of a quantity of evaporated chemical compound
30 at different measurement times,
- a means (320) of evaporation rate calculation depending on the measured evaporated chemical compound quantities measured,
- a means (325) of volatility calculation depending on the evaporation rate calculated and

- a means (330) of storing, in a database, the calculated evaporation rate and the volatility calculated.

13. A fragrance physical parameter evolution prediction system (400) to provide
5 predictive, real-time, fragrance performance metrics, characterized in that it comprises:

- a means (405) of selecting at least one chemical compound identifier in a computerized interface,
- a means (410) of inputting, for each selected chemical compound, a quantity of said chemical compound,
- 10 - a means (415) of modeling a deposition of the quantity of each selected chemical compound on a virtual surface,
- a means (420) of simulating, by a computing system, for at least one (modeled) deposited chemical compound, the stripped quantity of said chemical compound in an airflow for at least two different times as a function of:
 - 15 - the quantity of each said chemical compound,
 - a first value representative of a virtual surface size of the deposited chemical compound,
 - a second value representative of a virtual airflow directed at the deposited chemical compound configured to virtually strip the chemical
 - 20 compound from the surface,
 - a third value representative of an activity coefficient of each said chemical compound and
 - an evaporation rate or volatility associated to said chemical compound stored in a database constructed according to the database construction
 - 25 method of any one of claims 1 to 3 and
- a means (425) of displaying, for each chemical compound, of an indicator representative of the computed evaporated mass of said compound over time.