

## Supporting Information

Environmental profile of the production of fragrance ingredients used in cosmetic products: comparative analysis of results obtained by Life Cycle Assessment and the Green Chemistry-based eco-design tool GREEN MOTION™

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## 1 Data sources for ingredients modelling

Sources of data to model raw material and production process for all the fragrance ingredients studied are summarized in Table 1.

Table 1: Description of data sources for fragrance ingredients modeling

Category	Ingredients	Produced inhouse or bought	Starting raw material	Raw material data source	Manufacturing process data (Mane production unit or supplier data)
<b>Essentials oils (EO) and Jungle Essences™</b>	Lavender EO	Bought	Flower	Specific	Supplier data
	Elemi EO	Produced	Resin	Adapted from WFLDB	MANE – Natural extracts
	Iris EO	Produced	Rhizome	Bibliography	
	Vetiver EO	Bought	Root	Specific	MANE's supplier
	Pure vanilla Jungle Essence™	Produced	Beans	WFLDB	MANE – Natural extracts
	Pure pink berry Jungle Essence™	Produced	Pink berry	Specific	
<b>Essences by expression</b>	Orange flower absolute	Bought	Fruit	Ecoinvent	Supplier data
<b>Natural extracts with volatile solvent - Absolutes</b>	Orange absolute	Produced	Flower	Specific	MANE – Natural extracts
	Jasmine absolute	Produced			
	Narcissus absolute	Produced			
	Rose absolute	Produced			
<b>Natural extracts with volatile solvent - Resinoids</b>	Benzoin resin	Produced	Resin	Specific	MANE – Natural extracts
	Labdanum resinoid	Produced	Leafy branches	Specific	
	Labdanum absolute	Produced		Specific	
	Vanilla absolute	Produced	Beans	WFLDB	
<b>Isolated natural ingredients</b>	cis-3-Hexenol (natural)	Bought	Mint leaves	Adapted from WFLDB	MANE – Fractionation
<b>Bio-based ingredients with a fossil-based moiety</b>	Iso E super	Bought	Myrcene <sup>e</sup>	Ecoinvent (CST) Specific (pine)	Supplier data
	Vetiveryl acetate	Produced	Vetiver essence	Specific	MANE – Synthesis
	Myrcene (from crude sulfate turpentine)	Bought	Wood chips	Ecoinvent	MANE's supplier / MANE – Fractionation
	Myrcene (from pine)	Bought	Pine resin	Specific	
<b>Fossil-based ingredients</b>	Hexyl salicylate	Bought	Synthesized from petrochemical materials	Ecoinvent	Supplier data
	Ethyl 2-methyl butyrate	Produced			MANE – Synthesis
	Hedione	Bought			Supplier data
	cis-3-Hexenol (fossil)	Bought			
<b>Biotechnology ingredients</b>	Antillone	Produced	Natural ingredient	Specific	MANE – at plant level
	gamma-Octalactone	Produced		Specific	
	Tropicalone	Produced		Specific	

## 2 Production process: modelling of energy and water requirements

Each ingredient is associated to a specific production unit (see Table 1 above). Global energy and water requirements in MANE's plant are known for 3 types of production units: natural extracts, synthesis, and fractionation; and are estimated based on energy and water uses at the global plant level for the biotechnology production unit.

Energy and water requirements are linked to the process duration and to the process type. The latter is mainly defined by the heating type. Process type and process duration are specifically monitored by MANE for each ingredient. These two parameters have thus been used to estimate the specific energy and water requirements for each ingredient.

Based on Mane's knowledge of their processes, each type of process is ranked depending on its energy and water requirements per hour, and an "Energy and water equivalence coefficient (EC)" has been estimated to compare each process to a reference (Expanded steam process). Values are summarized in Table 2.

Table 2: Equivalence coefficients to estimate the needs of a specific process

Type of process	Energy and water equivalence coefficient (EC)
Expanded steam (reference)	1
Steam with a pressure of 3 bars	2
Steam with a pressure of 6 bars	3
Steam with a pressure of 15 bars	4
Heating with oil	4
Pyrolysis using gas	6

The global energy and water requirements of a production unit correspond to the energy and water necessary for an average ingredient produced in this unit. This average ingredient corresponds to an average process duration and process type.

To calculate this average, it was assumed that each ingredient is produced in the same proportion as the other ingredients of the same production unit (they were selected to be representative).

Knowing the duration and the process type of each ingredient, an average of all durations and process types has been calculated, according to the below equation:

$$Average\ Process_{prod\ unit} = \frac{1}{n} * \sum_{i=1}^n (Process\ duration_{ing\ i} * EC_{ing\ i})$$

With:

$\sum_{i=1}^n (Process\ duration_{ing\ i} * EC_{ing\ i})$ : the arithmetic mean of process duration and process type of all ingredients of a given production unit.

n: total number of ingredients in the same production unit

The estimation of the energy and water requirements for a specific ingredient is then calculated with a rule of three, thanks to the specific data of the ingredient and to the average process of the production unit, with the following equation:

$$Energy\ and\ Water\ Requirements_{ing\ x} = \frac{Process\ duration_{ing\ x} * EC_{ing\ x}}{Average\ Process_{prod\ unit}} * Energy\ and\ Water\ requirements_{prod\ unit}$$

with  $Process\ duration_{ing}$ : the duration of the process of the ingredient,  
 $EC_{ing}$ : the equivalence coefficient for the ingredient,  
 $Ing_i$ : all the ingredients produced in the same production unit as ingredient x,  
 $Energy\ and\ Water\ Requirements_{prod\ unit}$ : electricity, gaz and water needs of the production unit  
per kg of produced ingredient or per kg of starting raw material.

As for ingredients not manufactured by MANE but by suppliers, they were calculated by extrapolation with the corresponding MANE production unit and adapted, when possible, to the country of production.

### 3 Environmental results of fragrance ingredients

List of abbreviation:

- Climate change (CC)
- Water consumption (WC)
- Ecotoxicity, freshwater (EC)
- Eutrophication, freshwater (EF)
- Eutrophication, marine (EM)
- Acidification (A)
- Land use (LU)
- Eutrophication, terrestrial (ET)
- Mineral, fossil & ren resource depletion (RD)
- Particulate matter (PM)
- Ionising radiation (IR)
- Photochemical ozone formation (POF)
- Ozone depletion (OD)
- Human toxicity, cancer & non-cancer (HT)

Single scores (in mPt):

	Lavender EO	Elemi EO	Iris EO	Vetiver EO	Pure Vanilla Jungle Essence™	Pure Pink berry Jungle Essence™	Orange essence	Orange flower absolute	Jasmine absolute
Total	2,03E+01	1,48E+00	4,55E+01	3,75E+00	1,43E+01	6,76E+00	6,04E-01	2,08E+02	2,71E+02
CC	1,68E+00	2,40E-01	8,47E+00	5,45E-02	1,63E+00	2,41E+00	1,03E-01	6,89E+01	5,49E+01
WC	3,01E-03	6,89E-04	1,88E-02	3,95E-04	5,52E-04	9,44E-03	1,20E-02	1,20E+00	4,51E-01
EC	2,10E+00	8,44E-01	2,72E+00	2,50E-02	1,19E-01	1,84E+00	2,61E-01	2,47E+01	3,13E+01
EF	5,95E-01	3,09E-02	6,50E-01	5,80E-03	1,96E+00	6,31E-01	5,48E-02	8,30E+00	1,01E+01
EM	1,75E-01	8,30E-03	1,90E-01	2,65E-03	1,71E+00	5,53E-02	2,70E-02	1,43E+00	2,21E+00
A	2,99E-01	9,07E-03	1,77E-01	2,98E-03	9,26E-03	8,06E-02	2,04E-02	2,00E+00	4,04E+00
LU	5,20E+00	3,22E-02	2,98E+01	3,60E+00	6,83E+00	4,89E-02	1,07E-01	3,22E+01	2,49E+01
ET	2,32E-01	4,98E-03	1,10E-01	1,80E-03	5,57E-03	4,52E-02	1,54E-02	1,34E+00	2,95E+00
RD	6,41E-01	4,37E-02	1,28E+00	9,55E-03	1,95E+00	7,67E-01	4,77E-02	1,13E+01	1,24E+01
PM	1,15E-07	1,86E-09	6,78E-08	1,10E-08	3,34E-09	2,18E-08	8,05E-09	6,59E-07	1,49E-06
IR	2,91E-04	1,42E-04	7,68E-03	9,97E-06	1,38E-04	1,62E-03	1,22E-05	6,49E-02	4,40E-02
POF	1,54E-01	1,02E-02	2,90E-01	3,88E-03	1,41E-02	6,97E-02	5,78E-03	2,77E+01	5,09E+01
OZ	1,01E-03	1,41E-04	6,66E-03	4,63E-05	1,40E-04	1,28E-03	3,47E-05	5,81E-02	4,96E-02
HT	9,24E+00	2,58E-01	1,80E+00	4,33E-02	7,53E-02	8,05E-01	-5,10E-02	2,85E+01	7,66E+01

	Narcissus absolute	Rose absolute	Benzoin resinoid	Labdanum resinoid	Labdanum absolute	Vanilla absolute	cis-3-Hexenol (natural)	Iso E super	Vetiveryle acetate
Total	2,09E+02	1,84E+02	3,18E-01	1,07E+01	2,27E+01	1,13E+02	5,30E+01	1,91E+00	9,14E+00
CC	8,72E+01	3,32E+01	6,80E-02	7,57E-01	3,17E+00	1,23E+01	8,04E+00	3,48E-01	4,54E-01
WC	2,98E-01	3,88E-01	3,79E-04	1,75E-02	4,17E-02	3,18E-03	3,51E-01	1,09E-02	1,06E-02
EC	2,61E+01	1,93E+01	8,74E-02	6,42E-01	2,31E+00	4,35E-01	5,19E+00	7,48E-01	7,61E-01
EF	6,20E+00	7,75E+00	1,65E-02	3,45E-01	1,80E+00	1,56E+01	5,31E+00	1,06E-01	1,39E-01
EM	1,36E+00	1,51E+00	2,81E-03	1,64E-01	2,09E-01	1,36E+01	3,32E+00	9,27E-03	1,33E-02
A	2,03E+00	3,37E+00	2,84E-03	8,80E-02	1,91E-01	4,93E-02	2,18E+00	1,26E-02	1,83E-02
LU	1,41E+00	2,39E+01	4,58E-03	5,98E-01	6,37E-01	5,47E+01	1,14E+01	2,02E-01	7,22E+00
ET	1,32E+00	2,47E+00	1,45E-03	5,70E-02	9,20E-02	2,95E-02	1,71E+00	5,45E-03	8,51E-03
RD	1,28E+01	8,09E+00	2,34E-02	2,33E-01	7,15E-01	1,54E+01	1,81E+00	1,24E-01	1,48E-01
PM	6,45E-07	1,31E-06	9,16E-10	3,84E-08	1,16E-07	2,28E-08	1,14E-06	1,54E-08	2,82E-08
IR	8,69E-02	2,69E-02	4,16E-05	1,81E-04	3,27E-04	4,20E-04	7,34E-04	5,34E-05	3,60E-04
POF	5,34E+01	5,28E+01	8,73E-02	8,99E+00	1,37E+01	4,81E-01	4,44E-01	2,64E-02	3,43E-02
OZ	7,80E-02	3,41E-02	4,06E-05	2,67E-04	8,20E-04	5,11E-04	2,59E-03	1,41E-04	2,84E-04
HT	1,67E+01	3,08E+01	2,33E-02	-1,19E+00	-1,08E-01	3,59E-01	1,33E+01	3,17E-01	3,30E-01

	Myrcene (from crude sulfate turpentine)	Myrcene (from pine)	Hexyl salicylate	Ethyl 2-methyl butyrate	Hedione	cis-3-Hexenol (fossil-based)	Antillone	γ-Octalactone	Tropicalone
Total	5,94E-01	2,92E-01	1,15E+00	5,01E-01	9,17E+00	6,36E-01	4,72E+01	3,58E+00	7,27E+01
CC	5,69E-02	3,94E-02	2,93E-01	1,17E-01	3,30E+00	2,67E-01	3,32E+00	5,11E-01	4,92E+00
WC	2,79E-03	1,40E-04	3,53E-03	1,50E-03	1,66E-02	7,20E-04	2,12E-02	2,14E-02	2,88E-02
EC	1,21E-01	1,45E-01	3,62E-01	1,99E-01	2,77E+00	1,47E-01	7,07E+00	1,60E+00	1,02E+01
EF	2,61E-02	1,46E-02	1,44E-01	4,23E-02	8,02E-01	6,20E-02	1,21E+00	1,73E-01	1,84E+00
EM	3,07E-03	8,26E-04	6,76E-03	3,66E-03	3,11E-01	5,56E-03	8,11E-01	7,05E-02	1,21E+00
A	3,08E-03	9,79E-04	1,36E-02	4,83E-03	7,25E-02	8,03E-03	4,28E-01	2,57E-02	6,69E-01
LU	2,78E-01	1,68E-03	5,94E-03	6,06E-03	5,66E-02	4,06E-03	3,71E+00	2,68E-01	5,54E+00
ET	1,94E-03	4,94E-04	4,21E-03	2,52E-03	2,72E-02	3,58E-03	3,30E-01	1,76E-02	5,16E-01
RD	4,09E-02	4,28E-02	1,31E-01	4,44E-02	6,63E-01	5,46E-02	2,55E+00	3,04E-01	3,93E+00
PM	4,95E-09	4,48E-10	6,49E-09	2,35E-09	4,65E-08	4,49E-09	1,65E-07	1,49E-08	2,59E-07
IR	2,18E-05	2,25E-05	5,20E-05	8,54E-05	2,36E-04	1,44E-05	4,87E-04	2,01E-04	7,19E-04
POF	4,10E-03	1,06E-03	1,14E-02	6,27E-03	8,79E-02	1,16E-02	2,21E-01	3,29E-02	3,60E-01
OZ	3,84E-05	2,34E-05	1,13E-04	5,33E-05	1,06E-03	7,28E-05	1,12E-03	1,64E-04	1,67E-03
HT	5,65E-02	4,45E-02	1,74E-01	7,26E-02	1,07E+00	7,22E-02	2,75E+01	5,61E-01	4,35E+01

### Characterisation:

Climate change (CC)	kg CO2 eq	Eutrophication, terrestrial (WTE)	mol N eq
Water consumption (WC)	m3	Mineral, fossil & ren resource depletion (RD)	kg Sb eq
Ecotoxicity, freshwater (EC)	CTUe	Particulate matter (PM)	disease inc.
Eutrophication, freshwater (EF)	kg P eq	Ionising radiation (IR)	kBq U-235 eq
Eutrophication, marine (EM)	kg N eq	Photochemical ozone formation (POF)	kg NMVOC eq
Acidification (A)	mol H+ eq	Ozone depletion (OD)	kg CFC11 eq
Land use (LU)	Pt	Human toxicity, cancer & non-cancer (HT)	CTUh

	Lavender EO	Elemi EO	Iris EO	Vetiver EO	Pure Vanilla Jungle Essence™	Pure Pink berry Jungle Essence™	Orange essence	Orange flower absolute	Jasmine absolute
CC	5,35E+01	7,63E+00	2,69E+02	1,73E+00	5,19E+01	7,64E+01	6,04E-01	2,19E+03	1,74E+03
WC	1,22E-01	2,79E-02	7,59E-01	1,60E-02	2,23E-02	3,82E-01	1,03E-01	4,86E+01	1,83E+01
EC	8,15E+02	3,29E+02	1,06E+03	9,72E+00	4,64E+01	7,15E+02	1,20E-02	9,63E+03	1,22E+04
EF	1,09E-02	5,65E-04	1,19E-02	1,06E-04	3,58E-02	1,16E-02	2,61E-01	1,52E-01	1,84E-01
EM	2,28E-01	1,08E-02	2,48E-01	3,45E-03	2,23E+00	7,20E-02	5,48E-02	1,87E+00	2,88E+00
A	1,15E+00	3,48E-02	6,79E-01	1,14E-02	3,55E-02	3,09E-01	2,70E-02	7,66E+00	1,55E+01
LU	1,68E+04	1,04E+02	9,61E+04	1,16E+04	2,20E+04	1,58E+02	2,04E-02	1,04E+05	8,01E+04
ET	4,95E+00	1,06E-01	2,34E+00	3,83E-02	1,19E-01	9,63E-01	1,07E-01	2,86E+01	6,29E+01
RD	1,11E-03	7,59E-05	2,22E-03	1,66E-05	3,39E-03	1,33E-03	1,54E-02	1,96E-02	2,15E-02
PM	7,41E-06	1,20E-07	4,37E-06	7,12E-07	2,15E-07	1,41E-06	4,77E-02	4,25E-05	9,57E-05
IR	3,05E+00	1,49E+00	8,04E+01	1,04E-01	1,44E+00	1,70E+01	8,05E-09	6,79E+02	4,60E+02
POF	4,27E-01	2,83E-02	8,03E-01	1,07E-02	3,89E-02	1,93E-01	1,22E-05	7,65E+01	1,41E+02
OZ	7,20E-06	1,00E-06	4,73E-05	3,29E-07	9,92E-07	9,07E-06	5,78E-03	4,12E-04	3,52E-04
HT	1,71E-04	4,78E-06	3,33E-05	8,01E-07	1,39E-06	1,49E-05	3,47E-05	5,29E-04	1,42E-03

	Narcissus absolute	Rose absolute	Benzoin resinoid	Labdanum resinoid	Labdanum absolute	Vanilla absolute	cis-3-Hexenol (natural)	Iso E super	Vetiveryle acetate
CC	2,77E+03	1,05E+03	2,16E+00	2,40E+01	1,01E+02	3,92E+02	5,30E+01	1,11E+01	1,44E+01
WC	1,21E+01	1,57E+01	1,53E-02	7,07E-01	1,69E+00	1,28E-01	8,04E+00	4,41E-01	4,28E-01
EC	1,01E+04	7,52E+03	3,40E+01	2,50E+02	8,97E+02	1,69E+02	3,51E-01	2,91E+02	2,96E+02
EF	1,14E-01	1,42E-01	3,02E-04	6,31E-03	3,29E-02	2,86E-01	5,19E+00	1,94E-03	2,54E-03
EM	1,77E+00	1,96E+00	3,66E-03	2,13E-01	2,72E-01	1,78E+01	5,31E+00	1,21E-02	1,73E-02
A	7,79E+00	1,29E+01	1,09E-02	3,37E-01	7,33E-01	1,89E-01	3,32E+00	4,84E-02	7,02E-02
LU	4,53E+03	7,69E+04	1,48E+01	1,93E+03	2,05E+03	1,76E+05	2,18E+00	6,52E+02	2,33E+04
ET	2,82E+01	5,26E+01	3,09E-02	1,22E+00	1,96E+00	6,29E-01	1,14E+01	1,16E-01	1,81E-01
RD	2,22E-02	1,40E-02	4,07E-05	4,03E-04	1,24E-03	2,67E-02	1,71E+00	2,15E-04	2,57E-04
PM	4,15E-05	8,43E-05	5,90E-08	2,47E-06	7,46E-06	1,47E-06	1,81E+00	9,90E-07	1,82E-06
IR	9,09E+02	2,81E+02	4,35E-01	1,89E+00	3,42E+00	4,39E+00	1,14E-06	5,59E-01	3,76E+00
POF	1,48E+02	1,46E+02	2,41E-01	2,49E+01	3,78E+01	1,33E+00	7,34E-04	7,30E-02	9,50E-02
OZ	5,54E-04	2,42E-04	2,88E-07	1,90E-06	5,82E-06	3,63E-06	4,44E-01	1,00E-06	2,02E-06
HT	3,09E-04	5,71E-04	4,31E-07	-2,21E-05	-1,99E-06	6,66E-06	2,59E-03	5,87E-06	6,11E-06

	Myrcene (from crude sulfate turpentine)	Myrcene (from pine)	Hexyl salicylate	Ethyl 2- methyl butyrate	Hedione	cis-3- Hexenol (fossil- based)	Antillone	$\gamma$ - Octalactone	Tropicalone
CC	1,81E+00	1,25E+00	9,29E+00	3,73E+00	1,05E+02	8,48E+00	1,05E+02	1,62E+01	1,56E+02
WC	1,13E-01	5,68E-03	1,43E-01	6,06E-02	6,71E-01	2,91E-02	8,56E-01	8,66E-01	1,17E+00
EC	4,70E+01	5,65E+01	1,41E+02	7,75E+01	1,08E+03	5,71E+01	2,75E+03	6,23E+02	3,95E+03
EF	4,78E-04	2,68E-04	2,63E-03	7,75E-04	1,47E-02	1,14E-03	2,21E-02	3,16E-03	3,36E-02
EM	4,00E-03	1,08E-03	8,81E-03	4,77E-03	4,05E-01	7,25E-03	1,06E+00	9,19E-02	1,57E+00
A	1,18E-02	3,75E-03	5,21E-02	1,85E-02	2,78E-01	3,08E-02	1,64E+00	9,87E-02	2,56E+00
LU	8,97E+02	5,42E+00	1,91E+01	1,95E+01	1,82E+02	1,31E+01	1,20E+04	8,64E+02	1,78E+04
ET	4,14E-02	1,05E-02	8,99E-02	5,37E-02	5,80E-01	7,64E-02	7,04E+00	3,75E-01	1,10E+01
RD	7,10E-05	7,43E-05	2,26E-04	7,70E-05	1,15E-03	9,47E-05	4,42E-03	5,27E-04	6,82E-03
PM	3,19E-07	2,88E-08	4,18E-07	1,51E-07	3,00E-06	2,89E-07	1,07E-05	9,62E-07	1,67E-05
IR	2,28E-01	2,36E-01	5,44E-01	8,94E-01	2,47E+00	1,50E-01	5,10E+00	2,11E+00	7,52E+00
POF	1,13E-02	2,92E-03	3,15E-02	1,73E-02	2,43E-01	3,22E-02	6,11E-01	9,11E-02	9,97E-01
OZ	2,73E-07	1,66E-07	8,04E-07	3,79E-07	7,49E-06	5,17E-07	7,97E-06	1,17E-06	1,19E-05
HT	1,05E-06	8,25E-07	3,21E-06	1,34E-06	1,97E-05	1,34E-06	5,09E-04	1,04E-05	8,06E-04