DANISH MINISTRY
OF THE ENVIRONMENT
Environmental
Protection Agency

Survey and health assessment of chemical substances in essential oils and fragrance oils

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Survey of Chemical Substances in Consumer Products, **No. 92** 2008

The Danish Environmental Protection Agency will, when opportunity offers, publish reports and contributions relating to environmental research and development projects financed via the Danish EPA.

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Preface

The Danish Environmental Protection Agency has initiated a special effort to survey chemical substances in consumer products. The survey is accomplished by a series of projects with the purpose of illuminating the population's exposure to chemical substances and the possible risks related to this.

Essential oils, fragrance oils and air refreshers all contain fragrances in varying quantities. When using the products, fragrances and auxiliary substances are spread in the rooms where they are used and persons being present in the rooms are exposure to the substances.

The Danish Environmental Protection Agency has thus initiated a survey of the use of aromatherapy oils and fragrance oils with the aim of investigating the possible health effects caused by inhalation of chemical substances in the oils.

The successful implementation of the project has depended on information from a number of suppliers, importers, producers and users of products for aromatherapy and therefore we especially thanks all those who has contributed by answering questions and submitting product information.

The project's primary target group is the Danish Environmental Protection Agency, market actors as well as professional and private users of the products.

Steering group
The project has been followed by a steering group consisting of:

Anette Ejersted, Danish Environmental Protection Agency (Chairman)

Bettina Andersen, Danish Environmental Protection Agency

Shima Dobel, Danish Environmental Protection Agency

Carsten Lassen, COWI A/S

Inge Bondgaard, Eurofins Danmark A/S

Martin Silberschmidt, ms consult - International Public Health

Working group
The project was carried out by a multidisciplinary team consisting of: Carsten Lassen (project manager), Sven Havelund og Sonja Mikkelsen, COWI, Inge Bondgaard, Eurofins and Martin Silberschmidt, ms consult.

Summary and conclusions

As part of the Danish Environmental Protection Agency's programme for surveying chemical substances in consumer products, a survey of the use of essential oils and fragrance oils in Denmark was undertaken in order to examine possible health effects by inhalation of the chemical substances released from the oils.

The extension of the use of essential oils and fragrance oils

A large number of essential oils and fragrance oils are marketed for use in different kinds of aromatherapy. The focus of this investigation has been on the use of essential oils and fragrance oils for dispersion of fragrances in the home by use of candle diffusers and electrical fan diffusers. The use of candle diffusers is the most widely applied method for dispersion of these types of fragrances in the home and these diffusers are sold by many health food shops, materialists, hardware dealers, stores for life style and on the Internet.

Data on chemical substances were received from producers who submitted Material Safety Data Sheets and supplementary data sheets with information on the content of 26 substances on EU's list of fragrance allergens.

The survey identified more that 50 essential oils and 40 fragrance oils specifically stated as useful for this application, but several hundred different essential oils are marketed, which in principle may be used by the non-professional user. The total sale in Denmark in 2006 is estimated to be in the order of 300,000-700,000 flasks of essential oils and 100,000-300,000 flasks of fragrance oils. The flask size can be 1½, 5, 10 and 100 ml, respectively, with 10 ml as the most common. The total consumption is increasing.

By proper aromatherapy the oils are used specifically to obtain a particular therapeutic effect, but many users primarily use the oils to disperse a pleasant fragrance in the room in order to obtain a particular atmosphere. The possible beneficial effects of aromatherapy have not been in investigated.

Content of fragrance allergens

Data on the content of the 26 fragrance allergens on EU's list in 90 products were collected. Practically all of the essential oils and all fragrance oils contain one or several of the substances on the list, and in many products substances from the list constitute more than half of the product. Skin sensitizing is not covered by this investigation, but it is worth mentioning that the oils in some types of aromatherapy are in contact with the skin also; however, always heavily diluted.

Constituents of essential oils

Essential oils are natural oils extracted from plants, and each oil typically contains more than 100 different chemical substances. On the basis of Material Safety Data Sheets (MSDS) for the essential oils identified, a list of 52 constituents was compiled. These are either included in the list of dangerous substances (6 substances) or classified as dangerous by the producers' self classification.

By the producers' self classification none of the oils have been assigned the sentences R23 (Toxic by inhalation) or R42 (May cause sensitization by inhalation). The most frequent R-phrases for the oils are R38 (Irritating to skin), R43 (May cause sensitization by skin contact) and R65 (Harmful: may cause lung damage if swallowed). Tea tree oil and wintergreen oil have been assigned the sentence R22 (Harmful if swallowed). One oil (nutmeg oil) has been assigned the sentence R45 (May cause cancer) due to the presence of 5-allyl-1,3-benzodioxol, whereas. Products labeled R45 are forbidden to sell to the general public in Denmark. The Chemical Inspection Service has dealt with the infringement of the regulation and the product is no longer at the Danish Market.

Constituents of fragrance oils

Fragrance oils typically consist of a mixture of essential oils and so-called "nature-identical" constituents (i.e. synthetic substances with a chemical structure similar to the structure of constituents of natural oils). Some of the fragrance oils, however, consisted solely of synthetic substances, of which some cannot be designated "nature-identical". On the basis of MSDSs a list of 92 constituents, which are either included in the list of dangerous substances (6 substances) or classified as dangerous by the producers' self classification, was compiled. None of the substances were assigned the sentences R23 (Toxic by inhalation) or R42 (May cause sensitization by inhalation).

Labelling of the products

For the applications concerned, the products must be considered chemical products regulated by the Statutory Order on the classification, packaging, labelling, sale and storage of chemical substances and products. According to the statutory order at least eight of the ten purchased products should have been assigned the sentence R43 (May cause sensitization by skin contact), as they contain more that 1% d-limonene or citral, which are both classified with R43. It should appear from the label that the products are classified with R 43, and which constituent gives rise to the classification. None of the products were labelled correctly. The statutory order includes an exemption where the package contains no more than 125 ml, but this exemption does not apply to products classified with R43. However, most of the products were provided with instructions for avoiding contact with eyes, mucous membranes and skin because of the risk of irritation/allergy. The Chemical Inspection Service is dealing with the infringement of the regulation according to the labelling..

Analysis of constituents of selected products

Based on the lists of constituents of the oils, 15 constituents were selected for analysis. Already at this stage of the investigation it became clear that only limited information on the effects caused by inhalation of the substances would be available, and the list of selected substances consequently had a predominance of substances, which are also released from building materials, as there has been some attention to the effect of these substances in the indoor environment. A number of substances released from wood - including a range of terpenes - also constitute a significant part of many of the essential oils.

The results of the quantitative analysis of constituents of the oils were in accordance with the information on constituents from the MSDSs considering some natural variation in the composition of the oils. For some of the oils the analyses confirmed that classified substances constituted more than half of the products, e.g. more than 70% d-limonene in lemon oil and more than 70% citral in lemongrass oil were discovered.

Climate chamber tests
Five climate chamber tests were set up in order to investigate to what extent the substances are released to the room where the user stays. In three of the tests a candle diffuser, in which the oil is released from a little bowl with water heated by a tea light, was used. In two tests an electrical fan diffuser of the brand name Aroma Stream was used. In all tests 10 drops of oils were added. This corresponds to the upper limit for the recommended quantities; many suppliers recommend 1-5 drops only.

Results of the measurements
The results of the tests are difficult to interpret as the measured emission rates calculated on the basis of the measurements of the substances in the air evacuated from the chamber apparently were much lower than the rates, which could be expected from the quantities of the substances that disappeared from the diffusers. The explanation can be that the substances are decomposed or oxidized from when they were added until they were measured, but a contributing factor could also be that lower numbers are measured because of high atmospheric humidity in the chambers. It is a well-known fact that e.g. terpenes relatively rapidly oxidize in the air, and that the oxidation products contribute to the respiratory effects observed by exposure to the substances. Irrespective of the explanation and to be on the safe side it was decided to undertake two exposure assessments: One assessment based on the actually measured emission rates and a "worst case scenario" assessment, in which it is assumed that half of the added quantity of each substances is released to the room in a chemical state in which it may have an effect similar to the pure substance.

As the investigated oils are not necessarily the oils with the highest content of the substances, the "worst case scenario" was extended with a scenario in which it was assumed that the applied oils are those having the highest content of each substance. For d-limonene "worst case" would e.g. be to apply lemon oil with 72.5% d-limonene, for alpha-pinene it would be pine needle oil in which the substance constitutes 50%, and for diethyl phthalate it would be one of the fragrance oils in which diethyl phthalate constitutes 50%.

Exposure scenario
In the applied exposure scenario it is assumed that the fragrances are released at a constant emission rate for two hours to a standard room of 17.4 m^3 with an air exchange rate of 0.5 times per hour. The person stays in the room for 4 hours, and based on the emission rates, the average concentration to which the person is exposed during the 4 hours is calculated. This average concentration is compared to the concentration levels of possible effects.

Toxicity of the substances
Health data were collected for six of the substances with particular focus on information on health effects by inhalation. The six substances are d-limonene, alpha-pinene, benzyl alcohol, p-cymene, citral and camphor. For two of the substances, d-limonene and alpha-pinene, systematic reviews of human inhalation experiments are available. For the other four substances the information on health effects on humans by inhalation is very scarce or lacking. While a large number of investigations of the effects of the substances by dermal contact exist, in relation to the use of the substances in cosmetics, investigations of the effects of fragrances by inhalation in general are very rare.

For more of the substances irritating effects on humans and animals are described, but only at relatively high concentrations. D-limonene and alpha-

pinene are known as potent airway irritants after oxidation e.g. by ozone. By this process ultrafine particles are formed.

Health assessment

The health assessment applies to a large extent of so-called LCI values and limit values of the Danish Working Environment Authority. The LCI value is defined as the lowest concentration of a certain substance (Lowest Concentration of Interest), which according to our present knowledge at permanent exposure to the indoor air would not imply a risk of hazardous effects to humans. LCI values are used in Denmark and Germany for studies of effects in relation to releases of volatile chemical substances from wood and wood-based materials. For most of the applied LCI values irritation was the decisive effect**.** As the typical user of aromatic oils does not use them constantly, one should be on the safe side, if the calculated room concentrations during use of the aromatic oils are below the estimated LCI values. Limit values of the Danish Working Environment Authority are generally much higher than the LCI values, as they are applied in relation to shorter time of exposure. LCI values have been identified for four of the six substances closely assessed and for nine of the other substances. In addition to the six investigated substances, comparisons between exposure levels and LCI values or limit values were made for 10 additional substances. It should be noted that several of the LCI values are based on relatively limited data; by way of example the same value has been established for a number of terpenes by analogous considerations.

Health assessment on the basis of emission measurements

For the scenario where the concentration in the model room is estimated on the basis of the actual measurements, the calculated exposure levels, for all substances are below the LCI values and far below the limit values of the Danish Working Environment Authority. It is consequently estimated that the use of the oils in the way assumed in the exposure scenario does not result in any health risk from the evaluated substances.

Health assessment on the basis of worst case scenarios

By the worst case scenario based on the oils with the highest concentration of the substances, the exposure level is estimated to be substantially above the LCI values for many of the substances. This concerns e.g. d-limonene, alpha pinene, camphene, p-mentha-1.4-diene, p-mentha-1.3-diene, beta-Pinene and 3-carene. For diethyl phthalate in one of the fragrance oils the exposure level is close to the limit values of the Danish Working Environment Authority which is not appropriate by uses at home.

The results of this scenario indicate that it may not be appropriate to use the oils in these quantities (10 drops in a small room) frequently. The possibility of long term health effects, like chronic bronchitis or pneumonia, caused by repeated, short-term inhalations over longer periods, cannot with any certainty be excluded. At present, however, this assumption rests on no safe foundation according to the literature and experts consulted.

On the basis of the existing data it is not possible to estimate to what extent this worst case scenario is realistic, but the results indicate that there may be a need for further investigations of the problem; if necessary in a more scientific context also examining in which chemical form the substances are present in the air.

Particularly sensitive persons

The health assessment does not concern particularly sensitive persons. The

literature describes a particular group of people experiencing symptoms in their upper and lower airways when they breathe perfumes and fragrance containing products. These persons react with airway contraction when tested with a standard substance. This airway reaction is not associated with an allergic reaction, such as asthma. It is not known to what extent essential oils and fragrance oils contain substances that may elicit such reactions in sensitive persons.

Conclusion

The results of the investigation do not indicate any health risks by occational use of aromatic oils, subject to the fact that only a limited number of substances have been assessed. On the other hand, based of the results of the investigation it cannot be rejected that daily use of 5-10 drops of oils in smaller rooms for a prolonged period in the long term may result in airway irritation.

Recommendations

It is recommended, until more certain findings are available, to use small quantities only, to ventilate to room carefully when the fragrance effect is no longer desired, and not to make the use of fragrance diffusers an everyday phenomenon.

It is recommended to carry out further research on the possible effects of long term effects of inhalation of fragrances at concentrations relevant for the indoor environment and on the effects of simultaneous exposure to a number of chemical substances.

It is recommended that the consumers only use oils recommended by the producers specifically for this purpose and follow the instructions on the packaging. It is further recommended, before beginning to use candle diffusers or other ways to disperse the fragrances, to read the safety instructions provided by producers and suppliers on their web-sites or provided in books about the subject.

1 Introduction

1.1 Objective

The objective of this project is to

- survey which types of fragrance oils and aromatherapy oils are available on the Danish market;
- survey usage patterns for the different types;
- investigate whether there is a health risk for the consumers when they use these products, with a focus on inhalation.

1.2 Description of methodology

The progress of the project is illustrated in Figure 1.1 on the following page, showing the interrelated connection between the completed activities and the information flow throughout the project.

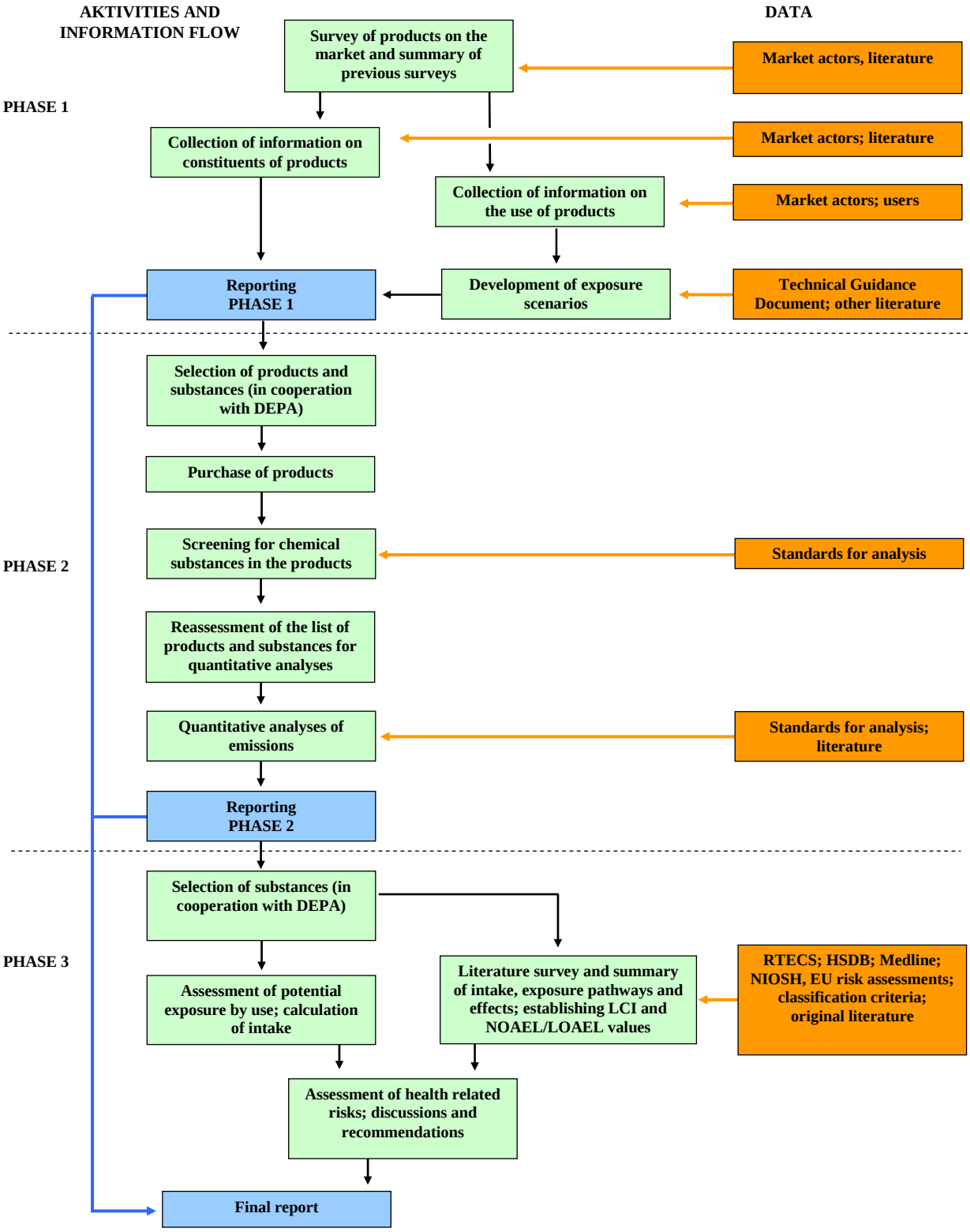


Figure 1.1
Overview of activities and information flow throughout the project

2 Survey

2.1 Delimitation of the survey

A long series of products are used for spreading fragrances at home and in the car. The products may be divided roughly in three groups:

- Traditional aroma fresheners: aroma balls, "Wunderbaums", electric air fresheners, etc.
- Joss sticks and scented incense tops;
- Essential oils and aroma oils used for aromatherapy.

This survey covers the third of the groups as the two other groups have been included in previous investigations.

Traditional air fresheners
A number of air fresheners have previously been examined for several known sensitizing fragrances in the project "Mapping of chemical substances in air fresheners and other fragrance liberating products", carried out by Eurofins for the Danish Environmental Protection Agency (DEPA) (Survey of chemical substances in consumer products no. 30, 2003, Danish only). In this project was included a survey of the market for air fresheners and 19 products were tested for the content of 24 specific fragrances, known for having a sensitizing effect when contact with the skin. In the project it was not investigated to which extent the substances are emitted to the room and whether the substances could have any impact by exposure to humans by inhalation.

Joss sticks and tops
The emission of chemical substances from burning incense was investigated in the project "Survey and emission of chemical substances from incense " (Survey of chemical substances in consumer products no. 39, 2003). In this project a screening of 12 types of incense products was made and afterwards a quantitative analysis of the emission of chemical substances from 6 selected incense sticks. The survey showed that it cannot be excluded that there can be health problems connected with use of scented incense products and especially the burn off products could cause health risks.

What is aromatherapy?
Aromatherapy is use of therapeutic oils. Primarily oils extracted from natural plant material are used, but on the market are also so-called "nature-identical" synthetic oils.

Where the traditional air fresheners primarily should add a scent of clean and freshness to the air, the use of aromatherapy oils has - as the name suggests - a broader perspective as it is assumed that exposure to the oils have a positive health effect on the user.

The oils are particularly said to have an influence on the mental condition of the user and different oils may for example be marketed as giving a sense of calm, a soporific effect, be relaxing, enforcing, refreshing, exhilarating or sexually stimulating. Where the oils are used directly on the skin (e.g. in baths

or by massage) the different essential oils are marketed as being stimulating for the skin, with a cleansing effect, stimulating for the blood circulation or as relaxation for the muscles.

Aromatherapy includes different uses of essential and other low-viscosity oils. At most uses the primary exposure to chemical substances in the oils is via inhalation and this project is directed specifically to these uses.

Essential oils are also used for dilution in massage oils and by this use the primary exposure will probably be through the skin. This usage of essential oil has been covered by a previous survey. In the project "Survey and health assessment of chemical substances in massage oils" (Survey of chemical substances in consumer products, no. 78, 2006) there was included an identification of essential oils being part of the massage oils.

This project is mainly directed towards the use of oils at home and the exposure of professional aroma therapists is not covered by the elaborated exposure assessments.

The term aromatherapy will be used widely and partly covers use of fragrances where the use is described as being part of an actual therapeutic process where, through a more systematic use of fragrances, the aim is a specific effect, partly "self-therapy" where the person uses the fragrance from a knowledge of their effect, for example from books - or just uses the oils because he/she finds it comfortable and pleasant.

2.2 The market for essential oils and fragrance oils

2.2.1 Product types

Oils that are used for aromatherapy can be divided into two groups:

- Pure essential oils extracted from natural plant material;
- Fragrance oils that are either a mixture of essential oils and synthetic "nature-identical" fragrances or pure mixtures of synthetic fragrances.

2.2.2 Actors on the market and turnover

Sale from shops
Store visits in the second largest town in Denmark (Aarhus) showed that essential oils were sold in the visited department stores (2), materialists (3 shops) and health food shops (2). All the stores also sold fragrance lamps, but not other aggregates for diffusion of the fragrances. The shops have from 5 to 50 fragrance variants on the shelf, but could typically obtain more. Two hardware dealers also sold fragrance lamps, but not the oils. One visited hobby shop sold essential oils, but the intended use was for making soaps and candies. One visited super market and one alternative life style shop sold neither oil nor lamps. If it is roughly assumed that all department stores, warehouses, materialists and health food shops sell essential oils, the total number of suppliers in these sectors are approximately 1400 (search on companies with this sector a primary category in Krak Markedsdata). To this should be added that the products will probably be distributed from some pharmacies and lifestyle shops.

The Internet

There are several internet shops selling products for aromatherapy. The shops typically sell products for the alternative therapy market and apart from essential oils and fragrance mixtures they also sell for example other types of oils, stones and crystals, tea and aromatic plants, pendulums and books on alternative therapy and life style.

Producers and importers
Based on store checks, internet search and other contact with actors on the market, the following companies have been identified marketing a wide range of oils:

- Natur-drogeriet A/S, Denmark
- Urtegaarden aps, Denmark
- RO-CO, Denmark
- Weibel Naturprodukter, Denmark
- The Body Shop, UK (Danish distributor: The Body Shop)
- Primavera Life GmbH, Germany (Danish supplier: Ulla Kvintel)
- Jurlique, Australia (Danish agent: Anne Frølund).

The Greek producer Apivita that has a broad range of essential oils has a Danish agent saying that essential oils or fragrance oils are not imported from Apivita.

Turnover
Production and import of essential oils and fragrance oils are not part of the statistic from Danish Statistics where these oils are listed with a number of other vegetable oils.

According to information from an important supplier there has been a considerable increase in the use of essential oils and fragrance oils with a 100% increase of sales during the last 2 years, but the consumption is still far below what is seen in e.g. Great Britain.

The total sale in Denmark has been estimated based on figures for one of the largest suppliers to the market. Based on this information it is estimated that total sales in 2006 seems to be approx. 300,000 to 700,000 bottles of essential oils and 100,000-300,000 bottles of fragrance oils. The bottles may be 1½, 5, 10 and 100 ml with 10 ml being the most frequent.

2.2.3 Consumer groups

There seem to be a tendency that more women than men are interested in aromatherapy and the use of essential oils. There also seems to be a tendency that more persons above 40 years of age than below use aroma oils. Many users of the products get to know these products through an aroma therapeutic session, but there are probably also many users of the lamps using the oils to spread a good atmosphere without being familiar with the effect of each of the oils. In aroma therapeutic sessions the use of fragrance oils are often combined with massage and healing. At some sessions the client must - after advise from the therapist - over a period use certain essential oils daily, but in view of achieving a desired effect.

There was found no information showing that children to a larger extent use aromatic oils at home, but children can also participate in aroma therapeutic sessions.

2.2.4 Found products

Essential oils
A long series of essential oils are marketed in Denmark. In table 2.1 is a list of oils found on the market, but the list probably does not include all essential oils marketed in Denmark. Apart from aromatherapy the oils are used as fragrances for other purposes, for example massage oils and production of candles, softeners, candies and perfumes. On the shop shelves and at homepages on the Intranet it is often not specifically mentioned whether the oils should be used for aromatherapy only and in principle all the oils could be used by the ordinary consumer in e.g. fragrance lamps. In the table there are oils specifically recommended (in books or at Danish internet pages) for use in aroma lamps or other uses where inhalation is the most important way of exposure. This applies for approximately 50 products.

Table 2.1
Essential oils on the Danish marked - either pure or in mixtures

Trade name	Oils specifically indicated as used for relevant applications	INCI Name *1	CAS No
Amyris oil	x	Amyris balsifera oil	8015-65-4
Orange oil	x	Pimpinella anisum extract	84775-42-8
Arnica oil	x	Citrus aurantium dulcis oil	8008-57-9
Valerian oil		Arnica montana extract	68990-11-4
Basil oil	x	Valeriana officinalis extract	8057-49-6
Benzoin oil	x	Ocimum basilicum	8015-73-4
Birch leave oil		Styrax benzoin extract	84929-79-3
Bergamot oil		Betula alba leaf extract	84012-15-7
Cajuput oil	x	Citrus aurantium bergamia oil	8007-75-8
Cinnamon leave oil	x	Melaleuca leucadendron extract	85480-37-1
Cedarwood oil		Cinnamomum zeylanicum	84649-98-9
Citronnella oil	x	Cedrus atlantica oil	8000-27-9
Lemon tree oil	x	Cymbopogon nardus oil	8000-29-1
Lemon oil	x	Citrus medica limonum extract	84929-31-7
Lemongrass oil	x	Cymbopogon citratus extract	89998-14-1
Cypress oil	x	Cupressus sempervirens extract	84696-07-1
Juniper oil	x	Juniperus communis extract	84603-69-0
Tarragon oil		Artemisia dracunculus Extract	90131-45-6
Eucalyptus oil	x	Eucalyptus citriodora oil	223748-96-7
Fennel oil	x	Foeniculum vulgare oil	8006-84-6
Frankincense oil	x	Boswellia carteri extract	89957-98-2
Pine needle oil	x	Abies sibirica oil	91697-89-1
Geranium oil	x	Pelargonium odoratissimum (bot)	-
Burdock extract		Arctium lappa extract	84012-13-5
Spruce oil (douglas)	x	Pseudotsuga menziesii resin	97926-19-7
Grapefruit oil	x	Citrus paradisi (bot)	-
Ginger oil		Zingiber officinale extract	84696-15-1
Hyssop oil		Hyssopus officinalis extract	84603-66-7
Jasmine oil		Jasminum officinale	90045-94-6
Vervain oil		Lippia citriodora extract	85116-63-8
Camphor oil	x	Cinnamomum camphora (bot)	-
Camomile oil	x	Chamomilla recutita oil	8002-66-2
Cardamom oil		Elettaria cardamomum oil	8000-66-6
Caraway seed oil	x	Carum carvi oil	8000-42-8
Coriander leave oil		Coriandrum sativum extract	84775-50-8
Coriander seed oil		Coriandrum sativum seed oil	246865-89-4
Curled mint oil	x	Eugenia caryophyllus extract	84961-50-2
Cove bud oil		Lavandula hybrida extract	91722-69-9
Lavandine oil	x	Lavandula angustifolia oil	90063-37-9
Lavender oil		Laurus nobilis extract	84603-73-6
Bay tree oil	x	Citrus medica extract	84929-31-7
Lime oil	x	Litsea Cubeba Oil	68855-99-2 / 90063-59-5
Lime tree oil		Tilia cordata oil	68916-81-4
Mandarin oil	x	Citrus nobilis oil	8008-31-9

Trade name	Oils specifically indicated as used for relevant applications	INCI Name *1	CAS No
Marjoram oil	x	Origanum majorana extract	84082-58-6
Mimosa absolu oil		Acacia dealbata extract	165800-52-2
Muskateller oil		Salvia sclarea extract	84775-83-7
Nutmeg oil		Myristica fragrans extract	84082-68-8
Myrrh oil	x	Commiphora myrrha extract	84929-26-0
Cloves leave oil	x	Eugenia caryophyllus leaf oil	8015-97-2
Neroli oil		Citrus aurantium extract	72968-50-4
Niaouli oil	x	Melaleuca viridiflora (bot)	-
Olibanum oil		Citrus sinensis (bot)	-
Sweet orange oil	x	Citrus aurantium amara extract	72968-50-4
Bitter orange flower oil		Urtica urens extract	90131-83-2
Small nettle oil		Origanum vulgare extract	84012-24-8
Palmrosa oil		Cymbopogon martini oil	84649-81-0
Patchouli oil	x	Pogostemon cablin oil	03-09-8014
Peppermint oil	x	Mentha piperita extract	84082-70-2
Peru balsam	x	Myroxylon pereirae extract	8007-00-9
Petitgrain oil	x	Citrus deliciosa (bot)	-
Seville orange oil		Citrus bigaradia (bot)	-
Damask rose oil	x	Rosa damascena oil	90106-38-0
Rose geranium oil	x	-Pelargonium graveolens	8000-64-2
Rose tree oil	x	Aniba rosaeodora extract	83863-32-5
Rosemary oil	x	Rosmarinus officinalis extract	84604-14-8
Sage oil	x	Salvia officialis extract	84082-79-1
Sandalwood oil	x	Amyris balsamifera oil	8015-65-4
Sandalwood oil, Mysore		Santalum album	84787-70-2
Sassafras oil		Sassafras officinale extract	84787-72-4
Anise seed star oil		Illicium verum oil	84650-59-9
Blackthorn oil		Prunus spinosa extract	90105-94-5
Tea tree oil	x	Melaleuca alternifolia oil	85085-48-9
Turpentine tree		Pistacia terebinthus (bot)	-
Thyme oil	x	Thymus Vulgaris Extract	84929-51-1
Vanilla oil		Vanilla planifolia extract	84650-63-5
Vetiver oil		Vetiveria zizanioides (bot)	-
Violet leave oil		Viola odorata extract	90147-36-7
Wintergreen oil		Gaultheria procumbens extract	90045-28-6
Ylang ylang oil	x	Cananga odorata extract	83863-30-3

*1 (bot) The botanical name is listed because the product is not on the INCI list.

The essential oils are often used in mixtures that is said to have various effects on the user. You can either buy ready-to-use oils or mix them yourself from recipes that can be found in books on aromatherapy. Examples of recipes for mixture of essential oils for fragrance lamps can be seen in table 2.2.

Table 2.2
Examples of mixtures of essential oils and their stated effect (Source: Unique Products 2007)

Soporific:	1 juniper, 2 lavender, 1 sandalwood, 1 ylang-ylang (candle diffuser and bath)
Relaxation after a hard day:	1 lavender, 1 geranium, 1 juniper, 1 sandalwood, 1 ylang-ylang (candle diffuser and bath)
New energy:	1 rosemary, 1 juniper, 1 eucalyptus, 1 geranium (candle diffuser and bath)
Winter blend:	1 eucalyptus, 1 lemon, 1 pine needle, 1 lavender (candle diffuser)
Tired/sore head:	1 lavender, 1 camomile, 1 peppermint or eucalyptus, 1 rosemary. (candle diffuser)

There is no statistic information on sales of each oil.

According to one supplier the most popular oils for candle diffusers are lavender, eucalyptus, bergamot and orange, whereas another suppler says that the most used are lavender, eucalyptus, peppermint, citronella, lemon grass, citrus oils (lemon, orange, bergamot, grape, etc.) rosemary, ylang ylang, patchouli and litsea.

Fragrance oils
A number of fragrance oils are marketed mainly consisting of mixtures of synthetic aroma substances and essential oils. Some, however, only consist of synthetic parts. The fragrance oils are often labelled "nature-identical", meaning that they consist of synthetic substances, identical with substances to be found in natural oils. In many cases there can be minor differences in for example the steric structure between the synthetic and natural substances. The reason for using the fragrance oils is partly that they elicit flower scents better than essential oils, partly that the oils are cheaper.

The composition of fragrance oils are generally considered to be confidential. Information on classified ingredients for a number of oils is based on information from safety data sheets listed in Appendix 3. The names of the fragrance oils are removed as the products can be linked to specific producers.

The oils are treated especially for use in aroma lamps and other uses related to aromatherapy. Examples of 40 fragrance oils sold in Denmark are shown in table 2.4 with information on the content of 26 potentially sensitizing substances (will be discussed later).

2.3 Use pattern for the products

Uses of essential oils and fragrance oils, where the primary way of exposure is inhalation cover (Lotus 1985, Mojay 1996, Web Which 2006 and consulted aroma therapists):

- **Diffusion of the substances to the air** in the room by use of candle diffusers, scented stones, electrical fragrance diffusers, etc.

- **Aroma cushions.** At certain cushions, drops are placed on a heated cushion which is then placed on for example your shoulders. The heat

and the effect of the essential oils last, according to the supplier, approx. 45 minutes. At other cushions a few drops are dripped on a cushion used as a sleeping pillow in bed.

- Aroma baths. Some drops of oil are added to the bath water.

- Inhalation: A small bowl is filled with boiling water. A few drops of essential oils are added. The user takes a towel over the head and inhales the vapour.

- Water basin method: A few drops of essential oils are added every morning to a water basin filled with hot water. The user moistens a washing cloth in the scented water, presses it against the face and breathes deeply. This is done a couple of times.

- Aroma sauna: 3-5 drops of oil in sufficient hot water are poured on the hot stones in the sauna.

- Aroma jewellery: The jewellery is filled with a few drops of essential oils with a pipette. The scent is emitted slowly over 2-3 weeks.

Aggregates to diffuse the fragrances

There is a long series of aggregates for diffusing the fragrances to the room. In all cases 2 to 10 drops are used and diffused to the room over a period of up to some hours. By contact to suppliers and searching the Danish homepages the following aggregates have been found, illustrated in the following:

- Candle diffusers: A few drops of essential oils are added to a small bowl with little water. Under the bowl is a tea light heating up the bowl, the water evaporates and diffuses the fragrances in the room. One or several oils can be used in combination depending on which scent or effect is desired. Lamps seem to be the most extended use and candle diffusers are sold from many stores and from several internet shops. There are a large number of different designs, all functioning according to the same principles. Some suppliers suggest adding 2-5 drops, others 5-10.

- Aroma figures and stones: Drops of oil are added which slowly evaporates. Works without heating.

- Ceramic lamp ring. A few drops of oil are added to the ring placed on an electric bulb. When the bulb is lit, the heat will diffuse the scent of the oil out in the room.

- Fragrance spray. Works by vaporizing the oil and thus diffusing it out in the room.

- Electric fragrance diffusers (Aroma Stream or aroma mouse): Consists of a cotton-wool-like material and a fan. 1-10 drops of essential oil are dripped on the material and the air flow from the fan diffuses the fragrance in the room. The oil is not heated. On the Internet a lot of American web sites have these products, but there is only found one Danish web site selling these products.

Apart from the above a Danish supplier has given information about the following aggregates that are not possible to find by contacting suppliers of oil for aromatherapy or on the Internet.

- Electric bowl: a few drops of essential oils are dripped into a small bowl that is heated electrically and thus diffusing the scent to the room. It is a bit the same principle as with candle diffusers, but no water is used. There is no use of a fan.

- Wool-cotton roundel: A few drops of essential oil are dripped on the wool-cotton roundel (a porous slice that is placed on a warm radiator.

Examples of products for diffusing the scents are shown below.

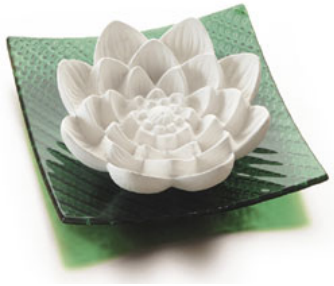
Candle diffusers

Source: Urtegården at http://www.urtegaarden.dk/Default.aspx?ID=42

"***Candle diffusers are used to spread the scent from the fragrance oils and the essential oils slowly and agreably. Fill the bowl of the lamp with water, add 5-10 drops of oil and lit the candle***"

Aroma figure, Angel

Source: Urtegården at http://www.urtegaarden.dk/Default.aspx?ID=527



Aroma stone - lotus

Source: Den Naturlige Butik

http://www.dennaturligebutik.dk/product.asp?product=4683&sub=0&page=1

"***Add a few drops of your favorite oil to create exactly the atmosphere you want***"

Ceramic lamp ring

Source: No. 29atrade

http://www.No. 29trade.dk/

*"**Add oil and place on an electric bulb - normal large size. When the bulb is lit, the heat diffuses the scent of the oil into the room**".*

Fragrance spray

Source: PrimaVera
http://www.primavera-life.de/de/produkte/sairsprays.php

Aroma pillow

Source: Duft og Natur

http://shop.duftnatur.dk/aroma_terapi/aroma_puder_og_kirsebaerpuder/aroma_hvedepude_roed_cirkulationsfremmende.html

*"**With each pillow comes 5 ml of essential oils that you can drop on the inner pillow after heating (in micro oven or ordinary oven). The heat and the effect of the essential oil last approx. 45 minutes**".*

Aroma diffuser

Source: BodyMind Company

http://bodymindcompany.zafi.netimage.dk/index.php?pid=3&item_id=274

"***Aroma Stream offers a clean, safe and efficient method to spread an aroma in a room without use of fire. A stream of air simply evaporates the essential oil and keeps its scent in its pure form. In this way heating of the oil is avoided, which can burn it, change its scent and qualities.***"

"***With most essential oils one drop is enough on a part of the filter insertion. When you want a new fragrance Aroma Stream should just be on until the scent of the existing oil is evaporated where after a new oil can be added to the same filter insertion***"

Aroma mouse

Source: BodyMind Company

http://bodymindcompany.zafi.netimage.dk/index.php?pid=3&item_id=273

"***The Aroma mouse is a portable fragrance diffuser. You can use it everywhere in your home and clinic as it uses batteries and has an ordinary plug outlet***"

"***There are 5 refill pads in the package and you can easily order more pads for the Aroma mouse. The pads can be used over a longer period with one aroma per pad. Drip approx. 10 drops per pad depending on the sixe of the room and how strong you would like the aroma to be***"

Aroma jewellery

"***In the jewellery is added scent after your own choice - we recommend 2 drops of essential oil - a pipette is enclosed for filling the oil. The fragrance lasts 2-3 weeks where after you must fill up again***"

Source: Description in a shop selling the jewellery. Own photo.

Apart from these usages, we searched on electrical fragrance diffusers and air fresheners and found 2 product groups beyond the limits of this project.

- Electric fragrance diffusers, sold to dog and cat owners to diffuse calming pheromones (behavioural fragrances);
- Electric air fresheners for the professional market (ex. Pure for Sure and Dan Dryer Fresh-air).

2.4 Constituents

2.4.1 Essential oils

The essential oils typically contain more than 100 different chemical substances. As it is a question of natural oils there can be differences between extracts from the same plant depending on which sort, growth place, weather conditions when growing and the method of how to extract the oils. The main parts are however often the same, but in different concentrations.

Examples of chemical content of selected essential oils are shown in Appendix 2. The statements are based on scientific investigations of the content of each oil and there will be deviations between the mixture of the analysed oils and the concrete oils on the Danish market.

The most important classes of substances found in essential oils are listed below (Tisserand and Balacs 1995) with examples of substances mentioned in this report:

- Hydrocarbons:
  - Terpenes (camphene, pinene, limonene, Myrcene, Caryophyllene);

- Oxidized compounds:
  - Alcohols (citronellol, geraniol, farnesol, linalool, nerolidol, menthol, terpineol);
  - Aldehydes (cinnamal);
  - Ketones (pulegone);
  - Esters (benzylbenzoate, methylsalicylate, methylbenzoate, methoxyphenylacetate);
  - Phenols (eugenol, iso-eugenil, cresol);
  - Ethers and oxides;
  - Peroxides;
  - Furanes (dimethylbenzofurane);
  - Lactones (coumarin);
  - Acids;

- Other compounds:
  - Sulphur compounds;
  - Nitrogen compounds.

Information about the constituents of essential oils has been collected from companies marketing the products in Denmark.

The essential oils typically have their own CAS number and in many cases the only information on the products' safety data sheets is that the product

contains this CAS number in a 100% concentration. The datasheet may be supplemented by a datasheet showing the content of 26 sensitizing substances. In other cases the companies list which chemical substances classified dangerous are contained in the oils. The classification is primarily based on the companies' self-classification of dangerous substances.

26 fragrances allergens

Many of the 26 fragrance allergens that must be declared according to Appendix 3 in the Statutory Order on Cosmetics (BEK no. 422) are found in essential oils and fragrance oils. As the essential oils in many cases are used in cosmetics, the suppliers have elaborated datasheets showing the oils' content of the 26 substances. The presence of the substance in cosmetic products must be stated when the concentration exceeds 0.001% in products that are not cleansed off and 0.01% in products that are cleansed off.

The list with all 26 substances can be seen in Appendix 1. The fragrance allergens are assessed as such based on their effect at skin contact.

26 fragrance allergens in essential oils

Table 2.3 shows the content of 26 substances in a number of essential oils listed to be used for aroma therapy. For some of the essential oils constituents are listed in oils from two different suppliers. Out of 26 substances, 14 of the substances are present in one or several of the essential soils. The substances d-limonene and linalool are the most frequent and are present in the major part of the products.

In some of the oils the fragrance allergens constitute more than 50% of the products. D-limonene constitute thus more than 50% of orange oil, lemon oil, mandarin oil and grapefruit oil (max. in orange oil 94%), linalool constitute more than 50% of coriander oil and rose tree oil (max. in rose tree oil of 94%) whereas citral, cinnamal and eugenol constitute more than 50% of lemongrass oil, cassia tree oil and cove bud oil (max. 75% in lemongrass oil).

From one of the producers it has been stated that the products contain limonene (CAS no. 138-86-3) whereas for similar products from other producers it has been listed as d-limonene (CAS no. 5989-27-5). Limonene (CAS no. 138-86-3) is a mixture of (R) and (S) enantiomeren of limonene. In literature it is mentioned that for example oils from citrus fruits contain limonene in the form of (R) antimeren d-limonene which has a characteristic citrus scent, whereas S (enantiomeren l-limonene has a terpentine smell. Limonene and d-limonene have the same classification according to the list of dangerous substances, but limonene (CAS no. 138-86-3) is not on the list of the 26 substances.

Citral and d-limonene that are both on the list of dangerous substances are classified with R38 and R43 and present with more than 1% in most of the oils.

26 fragrance allergens in fragrance oils

In table 2.4 information is given on the constituents of the 26 substances in a number of fragrance oils stated to be used for aromatherapy. 18 of the 26 substances are part of the fragrance oils. For confidentiality reasons the fragrance oils are listed with a number. In appendix 3 is information about some of the oils and their constituents based on safety data sheets. The

numbers refer to, for products listed in appendix 2, the sequential numbering in this appendix. The fragrance oils are typically named after aromatic flowers or fruits or have exotic names as Satsuma, Erotica, Africa Spa and Flower Meadow.

Apart from the mentioned fragrance oils there are also fragrance oils on the market being a mixture of some of these fragrance oils and some of the mentioned essential oils. Apart from this there is to a certain extent also pure mixtures of essential oils called "aroma oils".

As for the essential oils d-limonene and linalool are part of most of the oils, but also citronellol is a constituent in the main part of the fragrance oils. In a very large part of the products, substances from the 26-list constitutes more than half of the product. In one of the products none of the substances are present.

Table 2.3
Content of fragrances from EU's 26-substances-list in essential oils from Danish suppliers. The concentration is shown in %. Only substances that constitutes more than 0.1% are listed. If the substance constitutes more than 10%, it has been marked in bold.

	Benzyl alcohol	Benzyl benzoate	Benzyl salicylate	Cinnamal	Cinnamyl alcohol	Citral	Citro-nellol	Coumarin	Eugenol	Farnesol	Geraniol	Iso-eugenol	d-Limonene	Linalool
Orange oil						0.2	0.1						**94.25**	0.4
Basil oil									1.2				0.5	1.5
Bergamot oil						<1	<0.5				<8		**<34**	**<16**
Bergamot oil													**24-55**	1.5-2
Cajeput oil	ca. 3													
Cedar wood oil										<2.3				
lemon oil						4	0.1						**67**	0.75
lemon oil						<6					<0.1		**<65**	<0.3
Citronelle oil						<4	**<13**		<2.4		**<25**		<2.6	<1.1
Citronelle oil						1.7	1				24		3	1
Lemongrass oil						**75.5**	1		0.05		3.25		8	2.5
Cypress oil													**16.5**	0.4
Cypress oil													2.55	0.81
Juniper oil													4-8	
Eucalyptus oil													8	
Fennel oil													4	
Pine needle oil													**11.75**	
Pine needle oil													4-9	
Geranium oil						0.7	**32.8**				**14**		0.5	2.5
Grapefruit oil						1							**93**	0.2
Ginger oil						0.7							2	0.6
Camphor oil													7	
Cassia tree oil		1		**90**	1			4	0.5				0.1	
Coriander oil											3		5	**78**
Cove bud oil									**50-100**					
Cove bud oil									**<80**					
Lavender oil														**29.8**
Litsea cubeba oil						**<75**	<0.5			<0.8	<2.6		**<19**	<6

	Benzyl alcohol	Benzyl benzoate	Benzyl salicylate	Cinnamal	Cinnamyl alcohol	Citral	Citro-nellol	Coumarin	Eugenol	Farnesol	Geraniol	Iso-eugenol	d-Limonene	Linalool
Mandarin oil													**79.5**	0.3
Mandarin oil							<0.5						**<96**	<1.5
Marjoram oil													0.25	5.4
Muskateller oil											1.4		0.6	**24**
Nutmeg oil							0.16		0.6		0.3	0.6	8	0.4
Patchouli oil														
Peppermint oil													1.2	0.1
Petitgrain oli						<0.7				<0.2	<4.6		<2.8	**<24**
Rosegeranium oil						<4	<33				**<35**		<0.2	<8
Rose tree oil		0.4					0.55				1.9		0.25	**94**
Rose tree oil		<2.2									<3.3		<1.2	**<92**
Rosemary oil													5	0.75
Rosemary oil													<6	<1.5
Sage oil											0.1		**12.5**	2.25
Sage oil													0.5-3	0.2-0.8
Sandalwood oil (West Indian)										<0.3				
Anise seed star oil													3	1.5
Tea tree oil													1.15	0.15
Wintergreen oil													0.5	
Ylang Ylang oil	0.4	8.4	3.8						0.5	2.8	2.4	0.4		**15.8**
Ylang Ylang oil		<15	<8						<1.3	<12	<2.5		<0.1	**<11**

* Substances below the detection limit in all products is not included in the table

Table 2.4
Content of fragrances from EU's 26-substances-list in fragrance oils from Danish suppliers. The concentration is shown in %. Only substances that constitute more than 0.1% is listed. If the substance constitutes more than 10%, it has been marked in bold.

*1	Amyl-cinna-mal	Benzyl alcohol	Benzyl benzo-ate	Benzyl salicy-late	Benzyl cinna-mate	Cinna-mal	Cinna-myl alcohol	Citral	Citro-nellol	Cou-marin	Eugenol	Farnesol	Geraniol	Hexyl cinna-malde-hyde	Hy-droxycit-ronellal	Iso-eugenol	d-Limo-nene	Linalool
Nr 1			0.49						1.24	3.4			0.1				5.3	8.1
No. 2		0.68						0.54	1.49	5.02	2.81		1.31				**17.83**	6.21
No. 3			**17.62**						0.94				0.11				0.94	0.63
No. 4			5.00					0.29	**16.44**				0.46				**17.74**	2.02
No. 5			**13.34**				3.50	0.14	4.07		2.05		**10.59**				8.29	**12.28**
No. 6			**12.01**				3.15	0.13	3.66		1.85		9.53	**10.00**			7.46	**11.05**
No. 7							**10.50**		3.50						**18.00**	3.00	0.53	1.12
No. 8		0.60	0.49						7.00		0.25		0.13				0.42	**21.05**
No. 9								0.22	**13.50**		2.87						**12.42**	9.28
No. 10					1.43				**18.81**								4.06	**16.12**
No. 11	**15.00**						6.00		**15.00**				**10.00**					**10.00**
No. 12		1.36	0.13		0.45				**18.23**		0.59		0.12				7.06	**16.89**
No. 15		7.00							1.81	6.01							**11.04**	**15.66**
No. 16																		**10-20**
No. 17		0.85	8.94		0.11				8.47	1.00	0.65		2.43				**10.23**	**18.44**
No. 18		0.64	6.54					0.11	**10.30**	1.00	0.28		1.62				4.70	**12.68**
No. 19									**64.44**				4.60					0.20
No. 20			10.02		0.22				**38.36**		0.83		4.63					3.75
No. 21																		5-10
No. 22							**10.20**		3.36							5.50		**13.02**
No. 23		0.30	**24.85**						2.24	**16.00**	0.14		0.48				5.62	3.96
No. 24			0.18		0.58				0.18									0.20
No. 25																		
No. 26		0.94	0.80						**14.25**		0.39		0.75				**14.98**	**18.00**
No. 27		**24.9**																
No. 28																		
No. 29																		

*1	Amyl-cinna-mal	Benzyl alcohol	Benzyl benzo-ate	Benzyl salicy-late	Benzyl cinna-mate	Cinna-mal	Cinna-myl alcohol	Citral	Citro-nellol	Cou-marin	Eugenol	Farnesol	Geraniol	Hexyl cinna-malde-hyde	Hy-droxycit-ronellal	Iso-eugenol	d-Limo-nene	Linalool
No. 30									1.7									
No. 31								0.2		0.3			0.3					
No. 32			1-5															**1-5**
No. 33													0.1-1					
No. 34								2									0.9	
No. 35																	3	
No. 36																		
No. 37									1-5									
No. 38						2.5-5				2.5-5								
No. 40			6.7					9.70					0.18				**26.26**	8.33
No. 41			2.79		0.55				**10.49**				1.67				5.53	6.60
No. 42							**12.50**		6.44		4.00		0.46				0.39	0.16
No. 43		3.92	9.00					0.32	1.35		0.29						**34.94**	2.92
No. 44		3.50	**22.00**		0.55					0.60							5.55	4.68
No. 45								0.14	**28.6**		0.14		**28.6**					7;0
No. 46	**60.00**								**10.00**				5.00				5.50	**11.50**
No. 47		8.50	7.06	0.11	0.75				**11.40**		3.69	0.10						**27.94**

*1 Numbers refer to numbering in Appendix 3.

Constituents classified hazardous

As previously mentioned the safety datasheets from some suppliers contain information about constituents included in the list of dangerous substances, the 26-substances-list or which are classified dangerous by the company's self-classification.

Table 2.5 below shows a list of all the substances on the safety datasheets with the classification according to the list of dangerous substances.

In view of selecting substances for laboratory analysis and health assessments it is listed in the table whether the substances previously have been examined in the consumer projects by the Danish Environmental Protection Agency, the AT limit values (set by the Danish Working Environment Authority), LCI values and German NIK values.

The limit values of the Danish Working Authority have been made for content in the air in the working climate (AT 2007) whereas the LCI values (Lowest Concentration of interest) have been made especially for indoor climate.

The LCI values have been defined as the lowest concentration of a given substance, which, based on present knowledge, don't cause any risk for hazardous effects on humans by exposure in indoor climate. LCI values were introduced in Denmark in a survey on degassing of wood and wooden materials (Larsen et al. 1999). LCI is not considered an actual limit value for indoor climate, but an estimate for when there can be expected to be irritations, typically of mucous membranes and skin irritations in a particular indoor climate. The listed LCI values mainly derive from Jensen et al. (2001) which is a scientific article based on the above investigation. For substances not being part of Jensen et al. (2001), but part of a previous report from European Collaborative Action on Indoor Air Quality and its Impact on Man (ECA-IAQ 1999), values from this report is stated. The listed LCI values in the ECA-IAQ (1999) derive from a Finnish study referred to in the report.

The German NIK values (AgBB 2005) equal the LCI values and have been calculated according to the same principles. The values are used in Germany for assessment of degassing from building materials to the indoor climate.

The same data set is shown in table 2.6 where the concentration of the substances in each of the essential oils is listed. There is information on the substances from two producers and one of them generally classifies more of the constituents so that it is not possible to make an unambiguous comparison between the products.

In the table the producers' own classification of the products with R-phrases is listed related to health effects. The most frequent R-phrases are R38 (Irritating to skin), R43 (May cause sensitization by skin contact) and R65 (Harmful: may cause lung damage if swallowed). As it can be seen the own classification is not identical where there is information from several producers.

Tea tree oil and wintergreen oil have been assigned the sentence R22 (Harmful if swallowed). One oil (nutmeg oil) has been assigned the sentence R45 (May cause cancer) due to the presence of 5-allyl-1,3-benzodioxol, whereas. Products labeled R45 are forbidden to sell to the general public in Denmark. The Chemical Inspection Service has dealt with the infringement of the regulation and the product is no longer at the Danish Market

It is worth mentioning that none of the oils are classified with the sentences R23 (Toxic by inhalation) or R42 (May cause sensitization by inhalation).

Apart from this, several of the oils are classified as being hazardous (to a varying extent) for organisms living in water and may cause undesired long term effects in the water environment.

In table 25 it can also be seen which of the substances that has been health assessed in previous consumer project. Apart from these substances, the following, only being part of fragrance oils, have been subject to a health assessment (see table 2.7):

101-86-0	Hexylcinnamalaldehyde	Consumer project no. 69
122-40-7	Amylcinnamal	Consumer project no. 69
31906-04-4	Lyral	Consumer project no. 69

Table 2.5
Detected substances in essential oils that are on the list of dangerous substances, either being danger classified by the producers own classification. AT limit values and whether the substances have previously been assessed in a consumer project by DEPA.

CAS No	Chemical name (as stated on the safety data sheet)	Synonym	Classification according to list of dangerous substances	AT limit values (AT 2007)	Previously assessed in consumer projects	LCI / NIK value µg/m³
60-12-8	2-Phenylethanol		-	-		
76-22-2	Bornan-2 one	Camphor	-	2 ppm 12 mg/m³ (synthetic)	Proj. no. 79	
78-70-6	Linalool		-	-	Proj. no. 55; 69	
79-92-5	Camphene		-	-	Proj. no. 36	LCI: 250
87-44-5	beta-Caryophyllene		-	-		LCI: 1000 *3
89-82-7	Pulegone		-	-		
91-64-5	Coumarin		-	-	Proj. no. 69	
93-15-2	1,2 Dimethoxy-4(2-propenyl)-benzol	Methyleugenol	-	-	Proj. no. 55	
93-28-7	4-Allyl-2-methoxyphenylacetate	Eugenyl acetate	-	-		
93-58-3	Methylbenzoate		-	-		
94-59-7	5-allyl-1,3-benzodioxol	Safrole	CARC2;R45 Xn;R22 MUT3;R68	-		
97-53-0	Eugenol		-	-	Proj. no. 55	
97-54-1	Isoeugenol		-	-		
98-55-5	p-Ment-1-en-8-ol		-	-		
99-85-4	p-Mentha-1,4-diene	Gamma-Terpinene	-	-		LCI: 250
99-86-5	p-Mentha-1,3-diene	Alpha-Terpinene	-	-		LCI: 250
99-87-6	p-Cymene	Methylisopropylbenzene	-	25 ppm 135 mg/m³		
100-51-6	Benzylalcohol		Xn;R20/22	-	Proj. no. 43	NIK: 440 LCI: 100
103-41-3	Benzyl cinnamat		-	-	Proj. no. 78	

CAS No	Chemical name (as stated on the safety data sheet)	Synonym	Classification according to list of dangerous substances	AT limit values (AT 2007)	Previously assessed in consumer projects	LCI / NIK value µg/m³
104-54-1	Cinnamyl alcohol		-	-		
104-55-2	Cinnamal		-	-	Proj. no. 78	
104-93-8	4-Methylanisole		-	-		
105-87-3	2,6-Octadien-1-ol-3,7-dimethylacetate	Geranyl acetate	-	-		
106-22-9	Citronellol		-	-	Proj. no. 78	
106-24-1	Geraniol		-	-	Proj. no. 55	
106-25-2	Nerol		-	-		
118-58-1	Benzylsalicylate		-	-		
119-36-8	Methylsalicylate		-	-	Proj. no. 79	
120-51-4	Benzylbenzoate		Xn;R22	-	Proj. no. 43;55	
123-35-3	Myrcene		-	-		LCI: 1700 *1
138-86-3	Limonene	Dipenten	R10 XI;R38 R43 N;R50/53	75 ppm (tentative)		NIK: 1400 LCI: 300
140-67-0	Estragole		-	-		
150-84-5	3,7-Dimethyl-6-octen-1-yl-acetate	Citronellyl acetate	-	-		
464-49-3	Camphor		-	-		
491-07-6	cis-5-Methyl-2-(1-methylethyl)-1-cyclohexanone	Isomentone	-	-		
494-90-6	4,5,6,7-tetrahydro-3,6-dimethylbenzofuran	Menthofuran	-	-		
562-74-3	p-Menth-1-en-4-ol		-	-		
586-62-9	p-Mentha-1,4(8)-dien		-	-		LCI: 1000 *1
2216-51-5	L-Menthol		-	-		
4180-23-8	trans-Anethole		-	-		
4221-98-1	(R)-5-isopropyl-2-methylcyclohexa-1,3-dien		-	-		
4602-84-0	Farnesol		-	-		
5392-40-5	Citral		XI;R38 R43	-	Proj. no. 78	
5989-27-5	d-Limonene		R10 XI;R38 R43 N;R50/53	-	Proj. no. 36; 43	LCI: 300
7212-44-4	No. 50dol		-	-		
7785-26-4	(1S)-(-)-alpha-Pinene		-	-		
7785-70-8	(1R)-(+)-alpha-Pinene		-	-		
80-56-8 *"	alpha-Pinene				Proj. no. 36	NIK: 1400 LCI: 250
8000-41-7	Terpinol		-	-		
18172-67-3	beta-Pinene		-	-		NIK: 1400 LCI: 250
13466-78-9	3,7,7-Trimethylbicoclo[4.1.0]hept-3-ene	3-carene;	-	-		NIK: 1400 LCI: 250

LCI = "lowest concentration of interest" (Jensen *et al.* 2001). For substances marked with *1 LCI value is from ECA-IAQ (1999).

NIK = "Niedrigst interessierende Konzentrationen", equivalent to LCI (AgBB 2005).

*2: CAS No is not stated on the safety data sheets. Same designation as for the two CAS No. above.

Table 2.6
Content of dangerous substances in essential oils from two suppliers and R-phrases* related to health. Classification of product as stated on safety data sheets.

Product	Concentration in percentage of the oil								Indicated classification of the product							
	50-100	25-49.99	20-24.99	10-19.99	5-9.99	2.5-4.99	1-2.49	<1	R 21	R 22	R 36	R 38	R 43	R 45	R 65	R 68
Orange oil	d-Limonene						Myrcene	alpha-Pinene				x	x		x	
Basil oil	Estragole						Linalool; p-mentha-1,4-dien	d-limonene; 1,2-Dimethoxy-4-(2-propenyl)-benzol; beta-Pinene; alpha-Pinene								
Bergamot oil		d-Limonene				Linalool beta-Pinene					x	x	x		x	
Cedar wood oil							Farnesol						x			
Lemon oil	d-Limonene			beta-Pinene	p-Mentha-1,4-diene	Citral	alpha-Pinene; Myrcene; p-Cymene; Terpinol					x	x		x	
Lemon oil	d-Limonene										x	x	x		x	
Citronelle oil			Geraniol	Citronellol		Limonen						x	x			
Lemongrass oil	Citral					Geraniol	d-Limonene					x	x			
Cypress oil		alpha-Pinene		3,7,7-Trimethyl-bicoclo[4.1.0]hept-3-en; d-Limonene			p-Mentha-1,4(8)-dien; Myrcene	beta-Pinene; p-Mentha-1,3-dien	x							
Juniper oil	**not complete**				d-Limonene										x	
Eucalyptus oil	**not complete**															
Fennel oil	trans-Anethole					alpha-Pinene; estragol	alpha-Pinene ; (R)-5-Isopropyl-2-methylcyclohexa-1,3-dien	2-Limonen								
Pine needle oil		alpha-Pinene		beta-Pinene; 3,7,7-Trimethylbico-clo[4.1.0]hept-3-en; d-Limonene	d-Limonene	beta-Caryophyllene; p-Mentha-1,4(8)-dien	Myrcene; Camphene						x		x	
Geranium oil		Citronellol		Geraniol	2-Phenylethanol	cis-5-Methyl-2-(1-methylethyl)-1-cyclohexanone	2,6-Octadien-1-ol-3,7-dimethylacetate; d- Linalool; 3,7-Dimethyl-6-octen-1-yl acetate					x	x			

Product	Concentration in percentage of the oil								Indicated classification of the product							
	50-100	25-49.99	20-24.99	10-19.99	5-9.99	2.5-4.99	1-2.49	<1	R 21	R 22	R 36	R 38	R 43	R 45	R 65	R 68
Grapefruit oil	d- Limonene						Citral; Myrcene	alpha-Pinene				x	x		x	
Ginger oil					Camphene; (R)-5-Isopropyl-2-methylcycloheca-1,3-diene		alpha-Pinene; d-Limonene	Nerolidol					x		x	
Camphor oil				beta-Pinene; p-Mentha-1,4-dien; alpha-Pinene	p-mentha-1,3-diene	d-Limonene; p-Cymene	p-Mentha-1,4-(8)dien						x		x	
Cassia tree oil	Cinnamal						Coumarin		x			x	x			
Coriander oil	Linalool				alpha-Pinene, p-Mentha-1,4- diene	Camphor; d-Limonene	Geraniol; Camphene, p-Cymene; Myrcene	p-mentha-1,4(8)-diene; beta-Pinene				x	x		x	
Cove bud oil	Eugenol			4-Allyl-2-methoxypnenyl acetate								x	x			
Lavender oil		Linalool						Camphene							x	
Litsea oil		Citral			D-limonene						x	x	x		x	
Mandarin oil	d-Limonene			p-Mentha-1,4-dien			Myrcene; alpha-Pinene	beta-Pinene; p-Mentha-1,4-(8)diene; p-Cymene				x	x		x	
Muskatel Sage oil			Linalool				Geraniol	d-Limonene				x	x			
Nutmeg oil				beta-Pinene; alpha-Pinene	d-Limonene	p-Mentha-1,4(8)-diene; beta-Caryophyllene	p-Mentha-1,4-dien; p-Menth-1-en4-ol; camphene; 5-allyl-1,3-benzodioxol; (R)-5-isopropyl-2-methylcyclohexa-1,3-diene; p-mentha-1,3-dien; Myrcene	p-Cymene					x	x	x	x
Patchouli oil											x	x				
Peppermint oil		L-Menthol				cis-5-Methyl-2-(1-methylethyl)-1-cyclohexanone	d-Limonene; 4,5,6,7-tetrahydro-3,6-dimethylbenzofuran; Pulegone	alpha-Pinene; beta-Pinene				x	x			
Peru balsam		Benzylbenzoate		Benzyl cinnamat			Farnesol; Coumarin						x			
Petitgrain oil				Linalool												
Rosegeranium oil		Geraniol	Citronellol		Linalool						x	x	x		x	

Product	Concentration in percentage of the oil								Indicated classification of the product							
	50-100	25-49.99	20-24.99	10-19.99	5-9.99	2.5-4.99	1-2.49	<1	R 21	R 22	R 36	R 38	R 43	R 45	R 65	R 68
Rose tree oil	Linalool					Geraniol	d-Limonene					x	x			
Rosemary oil					Camphor; alpha-Pinene	beta-Pinene; Camphene; Camphor; d-Limonene	p-Mentha-1,4-diene	p-Cymene					x		x	
Rosemary oil	Not- complete			Camphene							x	x	x			
Sage oil	Not- complete														x	
Sandal wood oil	Not- complete							Farnesol								
Anise seed star oil	trans-Anethole						Estragole; d-Limonene	alpha-Pinene					x			
Tea tree oil		p-Menth-1-en-4-ol		p-Mentha-1,4-diene	p-Mentha-1,3-diene; p-Ment-1-en-8-ol	p-Mentha-1,4(8)-dien; d-Limonene;	Myrcene; beta-Caryophyllene; alpha-Pinene; p-Cymene			x		x	x		x	
Wintergreen oil	Menthyl salicy-late							d-Limonene		x	x					
Ylang ylang oil				Linalool	Benzyl benzoate; 4- Methyl anizole	Methyl benzoate	Benzyl salicylate; Farnesol; geraniol						x			
Ylang ylang oil				Benzyl benzoate; Linalool	Benzyl salicylate; Linalool		Geranil; Eugenol	d-Limonene				x			x	

* The used R-phrases:

R 21 harmful by skin contact
R 22 Harmful if swallowed
R 36 Irritating to eyes
R 38 Irritating to the skin
R 43 May cause sensitization by skin contact
R 45 May cause cancer
R 65 Harmful: may cause lung damage if swallowed
R 68 May cause permanent damage to health

The R-phrases are for the entire product. Each substance in the products may have other R-phrases. R-phrases for environmental impacts are not listed in the table..

2.4.2 Fragrance oils

All constituents listed on the safety data sheet, that have been supplied by producers of fragrance oils, are listed in table 2.7.

For each of the 80 substances their classification is given according to the List of Dangerous Substances and material safety data sheet, which fragrance oils they are part of and the content in weight percentage in each fragrance oil.

As it can be seen for some of the essential oils being part of the fragrance oils, only the oil's CAS number is listed and not the constituents of the oil. As a consequence there might be a large number of classified constituents that are not on the list.

It is again worth mentioning that none of the constituents are classified with R42 (May cause sensitization by inhalation).

None of the substances are on the Danish Working Environment Authority's list of limit values (AT 2007).

Table 2.7
Constituents of fragrance oils, their classification according to list of dangerous substances and safety data sheet, and which products they are part of with which percentage.

CAS No	Chemical name (English translation of name indicated in the MSDS)	Classification according to the List of Dangerous Substances	Classification according to the MSDS	Products	Weight percentage
60-12-8	Phenethyl alcohol	-	Xi;R36	No. 19	20-40
				No. 4, No. 7, No. 11, No. 20, No. 22	10-20
				No. 9, No. 14, No. 15, No. 24	5-10
				No. 8, No. 10, No. 38, No. 26, No. 32, No. 37	1-5
64-17-4	Ethanol	-	F; R11	No. 48	2.5-5
64-19-7	Acetic acid	R10 C;R35	C; R 10-35	No. 49	1-2.5
77-83-8	Ethyl methylphenylglycidate	-	-; R 52/53	No. 49	1-5
78-70-6	Linalool	-	Xi;R38	No. 8, No. 10, No. 50, No. 38, No. 22, No. 26	10-20
				No. 9, No. 11, No. 12, No. 15, No. 51, No. 21	5-10
				Nr 1, No. 2, No. 14, No. 20, No. 23, No. 32	1-5
79-77-6	3-buten-2-one,4-(2,6,6,-trimethyl-1-cyclohexen-1-yl)-,(E)-	-	N;R51/53;	No. 7	10-20
				No. 23, No. 52	1-5
80-54-6	p-t-Butyl-alpha-methylhydrocinnamaldehyde	-	Xn; R22-43	No. 22	5-10
				No. 52, No. 11	1-2.5
84-66-2	Diphenyl phthalate	-	-	No. 53, No. 49, No. 11, No. 54	50-100
				No. 55	25-50
				No. 52, No. 38	5-10
				No. 22	1-2.5
88-41-5	2-tert-butylcyclohexyl acetate	-	Xi; R38-52/53	No. 53	10-20

CAS No	Chemical name (English translation of name indicated in the MSDS)	Classification according to the List of Danger-ous Substances	Classification according to the MSDS	Products	Weight percent age
91-64-5	Coumarin	-	Xn;R22;R43	No. 23	10-20
				Nr 1, No. 15	5-10
				No. 2, No. 38, No. 21, No. 51, No. 38, No. 56, No. 55	1-5
				No. 31	0.3
93-18-5	2-ethoxy naphthalene	-	Xi-N; R 38-51/53	No. 34	0.2
97-54-1	Phenol, 2-methoxy-4-(1-propenyl)-	-	Xn;R22 Xi;R43	No. 22	5-10
				No. 7	1-5
98-55-5	Alpha-Terpineol		Xi; R38	No. 27	1.5
100-51-6	Benzylalcohol	XN;R20/22	Xn;R20/22 Xi;R43	No. 15	5-10
				No. 12, No. 57, No. 14	1-5
101-84-8	Phenyl ether	-	N; R 51/53	No. 38	1-2.5
101-86-0	2-(phenylmethylene)-Octanal	-	Xi;R43	No. 6	5-10
				No. 37, No. 11, No. 58	1-5
102-20-5	Benzylcarbinyl alpha-toluate	-	N; R 51/53	No. 32	0.1-1
103-05-9	alpha,alpha-dimethyl-Benzenepropanol	-	Xi; R 38	No. 37	1-5
103-82-2	phenyl acetic acid	-	Xi;R36/37/38	No. 20	1-5
103-95-7	Alpha-methyl-p-isopropylphenylpropanalde-hyde	-	Xi;R38 N;R51/53	No. 15	5-10
				No. 32	5-25
				No. 30, No. 36	1.0
				No. 28, No. 22	0.1-1
104-54-1	Cinnamyl alcohol	-	Xi;R43	No. 7, No. 22	10-20
				No. 5, No. 6, No. 22, No. 19, No. 55	1-5
				No. 11	5-10
104-55-2	Cinnamal	-	Xn; R21-38-43	No. 38	2.5-5
104-67-6	gamma-Undecalactone	-	N; R 51/53	No. 32, No. 35	0.1-1
105-21-5	4-Heptanolide		Xi; R 36/37/38	No. 28	1-5
105-53-3	Diethyl malonate	-	Xi; R 36	No. 33	1-5
105-87-3	Geranyl acetate	-	Xi; R 36/38	No. 32	1-5
105-95-3	Ethylene brassolate	-	N;R 51/53	No. 27, No. 35	1.7
106-22-9	Citronellol	-	Xi;R38 N;R51/53	No. 19	60-80
				No. 20	20-40
				No. 4, No. 8, No. 9, No. 10, No. 11, No. 12, No. 26	10-20
				No. 38, No. 51, No. 21, No. 11	5-10
				No. 2, No. 7, No. 57, No. 15, No. 22, No. 23, No. 30, No. 37, No. 22, No. 52, No. 38, No. 19	1-5
				Nr 1, No. 3, No. 24	0.1-1
106-24-1	Geraniol	-	Xi;R38 R43	No. 5, No. 6, No. 11, No. 19	5-10
				No. 2, No. 38, No. 20, No. 21, No. 38, No. 55	1-5
				No. 33. No. 31	0.1-1

CAS No	Chemical name (English translation of name indicated in the MSDS)	Classification according to the List of Danger-ous Substances	Classification according to the MSDS	Products	Weight percent age
107-75-5	Hydroxycitronellal	-	Xi;R36-R43	No. 7	10-20
				No. 36, No. 22, No. 8	1-10
				No. 30	1-2.5
112-30-1	1-Decanol	-	Xi;R36/38 N;R51/53	No. 50	1-5
				No. 38	0.1-1
112-31-2	n-Decylaldehyde	-	Xi;R38;	No. 5, No. 6, No. 57, No. 34	1-5
112-53-8	1-Dodecanol	-	Xi;R38 N;R50/53	No. 5, No. 6	1-5
112-54-9	Duodecylaldehyd C.12	-	Xi;R38;N;R51/53	No. 9	1-5
				Nr 1, No. 8, No. 11, No. 57, No. 14, No. 15, No. 38	0.1-1
115-95-7	Linalylacetate	-	Xi;R38	No. 57	20-40
				No. 2, No. 5, No. 8	10-20
				No. 6, No. 7, No. 15, No. 26	5-10
				No. 10, No. 12, No. 50, No. 22, No. 23	1-5
				No. 26	5-10
118-58-1	Benzyl salicylate	-	Xi,N; R 43-51/53	No. 8	<1
120-51-4	Benzylbenzoate	XN;R22	Xn;R22 Xi;R43	No. 14, No. 23, No. 27	20-40
				No. 3, No. 5, No. 6, No. 20	10-20
				No. 57, No. 38, No. 7, No. 51	5-10
				No. 4, No. 12, No. 51, No. 24, No. 32, No. 36	1-5
121-33-5	Vanillin	-	Xi;R43	No. 3	20-40
				No. 15	5-10
				No. 4, No. 8, No. 10, No. 38, No. 23, No. 26	1-5
122-00-9	Para-metylacetophenone	-	Xn;R22	No. 14	1-5
122-40-7	Amylcinnamaldehyde	-	Xi;R38 R43	No. 21	40-60
				No. 11	10-20
				No. 8, No. 38, No. 22, No. 52	1-5
122-78-1	Fenylacetaldehyde	-	Xi;R43;	No. 38	1-5
123-68-2	Allyl hexanoate	-	N; Xn; R 21/22-51/53	No. 33	0.1-1
124-13-0	n-Octyl Aldehyde	-	Xi;R 10-36/38	No. 34	1.5
127-91-3	beta-Pinene	-	Xn-N; R 10-50/53-65	No. 37	0.1-1
128-51-8	6,6-Dimethyl-2-norpinen-2-ethanyl acetate	-	R 52/53	No. 38	2.5-5
				No. 55	1-2.5
142-19-8	Allyl heptylate	-	Xn,N; R21/22-38-50/53	No. 53	5-10
150-84-5	Citronellyl acetate	-	Xi-N; R 38-51/53	No. 32	0.1-1
1205-17-0	2-Methyl-3-(3,4-methylenedioxy-phenyl)propanal	-	N;R 51/53	No. 27	0.6
1222-05-5	1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethyl cyclopenta[g][2]benzopyran	-	N; R 50/53	No. 53	<1
1335-46-2	Methyl ionone	-	N; R 51/53	No. 37, No. 52	1-5

CAS No	Chemical name (English translation of name indicated in the MSDS)	Classification according to the List of Danger-ous Substances	Classification according to the MSDS	Products	Weight percent age
1506-02-1	AHTN	-	Xn, N; R 22-50/53	No. 58	<1
2050-08-0	Amyl salicylate	-	N, R51/53	No. 38, No. 55	<1
4180-23-8	trans-Anethole	-	N; R51/53	No. 34	0.3
4949-11-8	2-Ethyl-3-hydroxy-4-pyrone	-	Xn; R 22	No. 35	1-5
5392-40-5	Citral	XI;R38 R43	Xi;R38 R43	No. 12, No. 34	1-5
				No. 31	0.1-1
5989-27-5	D-limonene	R10 XI;R38 R43 N;R50/53	R10 Xi;R38 R43 N;R50/53	No. 26	10-20
				No. 2	5-10
				Nr 1, No. 10, No. 35	1-5
				No. 34	0.9
6259-76-3	Hexyl salicylate	-	Xi-N; R 38-50/53	No. 32	1-5
				No. 36	0.1-1
6658-48-6	3 - (p - cumenyl) - 2 - methylpropionaldehyde	-	Xi; R43	No. 37	5-10
8000-41-7	Terpen alcohol	-	Xi; R38	No. 22	25-50
8021-36-1	Opoponax resinoid	-	Xi;R43	No. 38	1-5
8028-48-6	Orange oil	-	Xn;R10;R43;R65	No. 57	20-40
				No. 4, No. 9, No. 50, No. 38	5-10
				Nr 1, No. 5, No. 6, No. 51	1-5
27939-60-2	Dimethyl cyclohexene carboxaldehyde	-	Xi; R 36/38-43-52/53	No. 33	0.1-1
28219-61-6	2-Ethyl-4-(2,2,3-trimethylcyclopent-3-en-yl)-but-2-en-1-ol	-	Xi-N; R 38-50/53	No. 37	1-5
				No. 28, No. 32	0.1-1
31906-04-4	4-(4-Hydroxy-4-methyl pentyl)-3-cyclohexene-1-carboxaldehyde	-	Xi; R43	No. 11	5-10
				No. 30	2.0
32388-55-9	Acetyl cedrene	-	N; R 50/53	No. 32	1-5
37677-14-8	Isohexenyl cyclohexenyl carboxaldehyde	-	N; R51/53	No. 34	0.3
54464-57-2	1-(Octahydrotetramethyl-2-naphthyl)ethanone	-	N; R 51/53	No. 37, No. 30	1-5
				No. 32	0.1-1
63500-71-0	Tetrahydro-4-methyl-2-(2-methylpropyl)-2H-pyram-4-ol	XI;R36	Xi; R36	No. 27, No. 30	1-5
68039-49-6	2,4-DIMETHYL-3-CYCLOHEXENE CARBOX-ALD	-	Xi; R 36/38-43-52/53	No. 29, No. 53	0.2-2.5
68155-67-9	1 - (1,2,3,4,6,7,8,8a - octahydro - 2,3,8,8 - tetramethyl - 2 - naphthyl)ethan - 1 - one	-	N; R 51/53	No. 36	10-25
68647-72-3	Orange oil terpenes sweet	-	Xn-N; R 10-38-50/53-65	No. 37	0.1-1
80623-07-0	Ethyltricyclo (5,2,10,2,2) decane-2-carboxylate	-	Xi-N; R 38-51/53	No. 34	0.2
83863-30-3	Ylang-ylang oil III	-	Xn;R65 Xi;R38	No. 25	100

CAS No	Chemical name (English translation of name indicated in the MSDS)	Classification according to the List of Danger-ous Substances	Classification according to the MSDS	Products	Weight percent age
84238-29-9	Vetivert resinoid	-	Xi;R43	No. 2	1-5
84238-39-1	Patchouli oil	-	Xn;R65;	No. 4	5-10
				No. 2, No. 3, No. 5, No. 6, No. 23, No. 15	1-5
84650-11-3	Geranium oil	-	Xi;R38 R43 Xn;R65	No. 20	5-10
84776-65-8	Lavender oil	-	Xi;R43 Xn;R65	No. 2	5-10
				No. 9, No. 15, No. 38	1-5
84929-31-7	Lemon oil	-	R10 Xi;R43	No. 2	10-20
				No. 4, No. 9	5-10
				No. 5, No. 6, No. 51, No. 26	1-5
84929-38-4	Madarin orange oil	-	Xn; R 65	No. 36	1-10
84929-61-3	Carrot oil	-	R10 Xn;R65	Nr 1	1-5
84929-79-3	Styrax resinoid	-	Xi;R43	No. 10	5-10
				No. 12, No. 14, No. 20, No. 22, No. 24	1-5
84961-50-2	Cove bud oil	-	Xi;R38 Xn;R21/22 R65	No. 5, No. 6, No. 9, No. 20	1-5
85085-61-6	Bay oil	-	Xn;R22 R65	No. 2	1-5
89957-91-5	Bergamot oil	-	Xn;R65 Xi;R43	No. 12, No. 15	10-20
				No. 4, No. 57, No. 14, No. 38, No. 21, No. 23	5-10
				No. 5, No. 6, No. 9,No. 50	1-5
89957-98-2	Olibanum oil	-	R10 Xn;R65	No. 3, No. 23	1-5
89998-15-2	Citronelle oil	-	Xi;R43	No. 5, No. 6	1-5
90045-28-6	Gaultheria oil (Wintergreen)	-	Xn;R22 Xi;R36 R43	Nr 1	5-10
90063-59-5	Litsea-cubeba oil	-	Xi;R38	No. 5, No. 6, No. 9	1-5
90082-51-2	Geranium oil	-	Xi;R43 Xn;R65	No. 19	10-20
				No. 5, No. 6	5-10
				No. 4, No. 38, No. 51, No. 26	1-5
91722-69-9	Lavendin oil	-	Xi;R38 R43 Xn;R65	No. 26	1-5
99811-75-3	Cedar wood oil		Xi;R43;Xn;R65;	No. 5, No. 6, No. 24	5-10
				No. 2, No. 3, No. 15, No. 38, No. 23	1-5
100081-14-1	Musk ketone	-	N; R50/53	No. 22	1-2.5
				No. 53, No. 8, No. 55	<1

*1 See explanation in table notes for table 2.5 re NIK and LCI.

2.5 Labelling, legislation and recommendations

Definition

Essential oils and fragrance oils are in a grey area concerning which legislation applies to the products. Some use of the oils will be under the cosmetics legislation whereas products for other usage will fall under the chemical legislation. In order to decide which legislation the products are covered by it is necessary to make an assessment of where the products are sold, at what purpose, appraisals and labelling.

Cosmetic products are denotes in the Statutory Order on Cosmetic Products as "***any substance or preparation intended to come into contact with various parts of the surface of the human body (skin, hair of the head and other hair, nails, lips and external genital organs) or with the teeth and the mucous membranes in the oral cavity, with the exclusive of main purpose of cleaning and perfuming them, changing their appearance and/or correcting body odours and/or protecting or keeping them in good condition***". When essential oils are used for example as additives to the bath tub they will be in contact with the human body and can be regarded as "bath and shower preparations" which are on the recommended list of products that can be considered to be cosmetic products.

The question is, however, whether the products are designated for this purpose or whether it is just a use of the product. The products are generally marketed as used for aromatherapy where the major part of the usages are beyond the limits of the cosmetic legislation as they are not intended to be in contact with the listed parts of the surface of the human body. It also seems to be the general opinion among companies marketing the products that the products are covered by the legislation for chemical substances and products.

2.5.1 Classification and labelling according to chemical legislation

According to Act on Chemical Substances and Products (LBK nr 1755 of 22/12/2006) any producer or importer of a chemical substance or product before sale or import hereof get information on the qualities and effects of the substance or product in order that he/she can classify, pack and label it according to the law.

Classification of constituents and products and the subsequent labelling for chemical products must be made according to the Statutory Order on classification, packing, labelling, sale and storage of chemical substances and products (BEK nr. 329 of 16/05/2002).

For a long series of chemical substances, the classification can be seen in Statutory Order on the list of dangerous substances (BEK no. 923 of 28/09/2005), but for substances not on the list, producers and importers must make their own self-classification based on the principles in the legislative order.

As is can be seen from table 2.5 and 2.7 a long series of essential oils and fragrance oils contain substances that are either on the list of dangerous substances or are classified as harmful to your health by one or several producers.

The rules for classification and labelling of the products based on classification of constituents can be seen in Statutory Order on classification, packing, labelling, sale and storage of chemical substances and products and depend on classification and concentration of each of the substances. Chemical products must be classified for fire and explosion hazards according to the same criteria as single substances only with specific rules for gas mixtures. As a main rule, the classification of products is based on the classification of each substance and their concentration. Test data on product level may, if they are available, be used for classification for most health and environmental impacts with the exception of CMR (carcinogenic, mutagenic or toxic for reproduction) effects, aspiration hazard, bioaccumulation and biodegradation and danger for the ozone layer.

For the examined substances and products it is especially the content of substances with local irritating effects and/or sensitizing impacts that has a consequence for labelling of the products. For each of the substances there may be other effects that have not been considered here.

Irritant effects
For products containing one substance classified as irritant(Xi) with R36, R37 and/or R38 the product must also be classified as irritant with R36, R37 and/or R38 if the substance is present in concentrations above 20% unless any individual limits are given in the list of dangerous substances. This for example applies for products containing more than 20% d-limonene and citral.

For products containing several substances with this classification, a summation formula with a concentration limit for the products' classification in the actual danger category for each substance in the product is used. This means that the product, where the total concentration of substances classified with R38 (e.g. d-limonene and citral) is above 20%, should be classified as irritant with R38.

Sensitizing effects
Products containing a substance classified as sensitized must be classified as sensitizing with R43 and assigned the danger symbol and designation Xi, if the concentration of the substance with R43 is higher or equals 1%. This for example applies to products containing more than 1% d-limonene or citral.

For products containing several substances with this classification, the classification is determined based on each of the constituents whose concentration equals or exceeds the general concentration limits listed in the Statutory Order or any individual limits given in the list of dangerous substances.

Labelling
Products containing hazardous chemical substances must be marked with a label showing:

a) danger category and danger symbols,

b) R-phrases and

c) S-phrases.

This means that packing for essential oils or fragrance oils, classified according to above-mentioned rules must be labelled with danger category and danger symbols, R-phrases and S-phrases.

However, if the content of the pack is 125 ml or less (which is typical for essential oils and fragrance oils) labelling with R-phrases and S-phrases is not required:

- In the case of highly flammable, flammable, oxidizing and irritant substances or products. This also applies in the case of the same volume of harmful substances not retailed to the general public;

- In the case of a chemical product classified as dangerous for the environment with the danger symbol N, highly flammable, oxidising or irritant with R36, R37 and/or R38.

In a similar way, labelling with S-phrases is not required if the content of the package/bottle is 125 ml or less:

- In the case of a chemical product classified as flammable or dangerous for the environment without the danger symbol N.

Constituents should be listed in accordance with current rules.

On the label of chemical products, classified as sensitising, it should for example be listed which substances cause the classification of the product. For products containing more than 1% d-limonene there should be danger symbol, danger designation Xi and R-phrases for the product and it should be stated that it contains d-limonene.

Chemical products not classified sensitizing but containing at least one substance classified sensitizing in a concentration of more than 0.1%, unless a lower limit is specified in the list of dangerous substances , must bear the inscription on the label:"Indeholder (navnet på det sensibiliserende stof). Kan udløse allergisk reaktion" [Contains (name of sensitizing substance). May produce an allergic reaction].

Based on the gathered information on the content of sensitizing substances in the products it may be concluded that on the packaging of the main part of the products, classification and names of the sensitizing substances they contain must be stated.

2.5.2 Labelled in accordance with the cosmetics legislation

If the products are mainly marketed for uses covered by the cosmetics legislation products should be labelled with an INCI declaration. One of the things to be stated is the presence of 26 fragrances with particularly labelling requirements when the concentration is above 0.001% in products that are not cleansed off and 0.01% in products that are cleansed off.

If the essential oils are marketed as cosmetic products, what they normally are not, a very large part of the products should be marked with one or several of the 26 sensitizing substances.

2.5.3 Labelling of products and recommendations

Recommendations on the packaging of 10 purchased products are shown in table 2.8.

Table 2.8
Recommendations on the packaging of purchased products.

Product name	No	Type	Recommendation on packaging	Attached recommendation
Rosemary oil	1	Essential oil	Plant part: Twigs Avoid contact with eyes, mucous membranes and skin due to risk for irritation/hypersensitivity. To be used in drops/diluted in a recommended dose. To be kept closed and away from children.	None
Lemon oil	2	Essential oil	Plant part: Ecological fruit peel Avoid contact with eyes, mucous membranes and skin due to risk for irritation/hypersensitivity. To be used in drops/diluted in a recommended dose. To be kept closed and away from children.	None
Tea tree oil	3	Essential oil	Plant part: Leaves Avoid contact with eyes, mucous membranes and skin due to risk for irritation/hypersensitivity. To be used in drops/diluted in a recommended dose. To be kept closed and away from children.	None
Lemongrass oil	4	Essential oil	Plant part: Grass Avoid contact with eyes, mucous membranes and skin due to risk for irritation/hypersensitivity. To be used in drops/diluted in a recommended dose. To be kept closed and away from children.	None
No. 5	5	Fragrance oil	Contain natural or nature-identical fragrances. Avoid contact with eyes, mucous membranes and skin due to risk for irritation/hypersensitivity. To be diluted and used externally only Should be kept closed and away from children.	None
No. 2	6	Fragrance oil	Contain natural or nature-identical fragrances. Avoid contact with eyes, mucous membranes and skin due to risk for irritation/hypersensitivity. To be diluted and used externally only Should be kept closed and away from children.	None
No. 6	7	Fragrance oil	Avoid contact with eyes, mucous membranes and skin due to risk for irritation/hypersensitivity. To be diluted and used externally only Should be kept closed and away from children.	None
No. 38 *1	8	Fragrance oil	Aromatic oil. Must be kept away from children. Avoid mucous membranes and eye contact. Only essential oils are for internal use.	None
No. 27	9	Fragrance oil	Read folder on safety before use. May cause an allergic reaction. Keep away from children. If swallowed contact doctor and present this bottle or label	None
No. 34 *1	10	Fragrance oil	Read the ..... before use	None

*1 Text - including missing words- is identical with the text on the packaging

Based on analyses of constituents of the products, all the products except no. 27 and no. 38 should be classified with R43 as they contain either d-limonene or citral, both classified R43 in concentrations above 1%. They should also be marked with danger symbol and danger designation Xi and with R43 on the packaging and it must be stated which ingredients have caused the classification. As no. 38 contains >>0.1% d-limonene this oil it should also be labelled "Contains (name of the sensitizing substance). May cause an allergic reaction."

None of the purchased products was labelled with information that they contained sensitizing substances and they were not labelled correctly. Most distributors' catalogues and homepages have general recommendations with precautionary rules.

An example is on the homepage for Unique Products where the Danish agent has the following rules of precaution [translated into English]: (http://www.danishbusiness.com/tekst/foraroma.htm):

"***Rules of precaution*":**

The oils are very concentrated and should only be used in small quantities.

If you suffer from too high blood pressure, epilepsy of progressive nerve diseases, you should not use essential oils as they in some cases may worsen the situation. If you're pregnant it is also recommended that you do not use essential oils.

The oils are for external use only. They should not be in contact with eyes or mucous membranes.

They should be stored out of children's reach. Do not use undiluted essential oils directly on the skin.

If you have a tendency to allergy you should make an allergy test before using the oil for the first time.

Orange oil, bergamot oil, lemon oil, grapefruit, mandarin oil should not be used 12 hours before sunbathing and for perfuming of clothes."

2.6 Summary of previous investigations on chemical substances in traditional air fresheners

The Danish Environmental Protection Agency has previously carried out a survey of chemical substances air fresheners and other fragrance liberating products (Pors & Fuhlendorff 2003). The survey did not include products for aromatherapy.

Through contact to suppliers of these products a number of different types of air fresheners were found. The results of the survey could be concluded as follows:

- Suspending – few manufactures (3-4), several fragrances (10-15);
- Electrical – several manufactures (5-8), several fragrances (5-10);
- Spray – few manufactures (2-3), several fragrances (5-10);
- Balls – few manufactures (2-3), several fragrances (10-15);
- Gel plates/pressure cans - several producers (5-8), several fragrances (10-15).

From the manufacturers it was informed that 5% of the population in Denmark uses air fresheners in their cars or home and out of the total sale of air fresheners it was assumed that the households using air fresheners approximately uses 26 air fresheners on average a year.

In the investigation 19 air fresheners and fragrance balls, covering the market in various groups, were analyzed. The products were selected to represent the various areas of application and origin, and a certain sales volume..

The tests were analyzed for the presence of 24 ingredients that EU's scientific committee has identified as allergens (same list as the 26 ingredients mentioned in the present study exclusive of oak moss extract and three moss extract).

At least one of the 24 constituents were detected in all samples. Single ingredients were detected from 3.5 mg/kg to 62,000 mg/kg (6.2 weight %). For the total content of the constituents the concentrations varied from 10 mg/kg to 162,000 mg/kg (16%weight %). Five of the products had a total content of the 24 constituents $\geq$ 10%.

There were also made qualitative analyses for a number of solvents: ethylacetate, isopropanol, ethanol, isoamylacetate, isoamylbutyrate and hexane acid ethylester.

Solvents were present in six of the products. Two of these products were fragrance products from vacuum cleaners and the other products were all liquids for various purposes.

The survey did not include measurement of the release of fragrances from the products or a health assessment of the possible exposure of the users.

3 Exposure scenarios

Based on the description of use patterns, an exposure scenario has been chosen; diffusion of fragrances in a room by use of aroma lamps, fragrance streamer, and aroma pillows, etc.

At some occasions 2-10 drops are used which, over a short period, is diffused to a room where the user is present. The most used method is use of candle diffuser, but aroma figures and stones, ceramic lamp ring or electrical air fresheners in principle work the same way. There may be a difference in which substances are emitted and which quantities depending on whether the oils are heated, but the scenario to which degree the user will be exposed to the different substances will mainly be the same. By use of fragrance spray the diffusion will take place over a very short period, but it will still be a variant of the same basic scenario.

Description of use pattern
The typical use of a candle diffuser is to fill a bowl with 20 ml of water and add 2-10 drops of oil into the water. In some cases the oil may be seen as a separate phase, but some of the substances will be dissolved in the water. It can either be a fragrance oil, a single essential oil or a mixture of essential oils. The lamp is placed in the room where you are, typically the living room or another room. A candle is lit under the bowl and the water is heated gradually to approx. 50° C and the aroma substances will evaporate and be emitted to the air. The candle typically puts out after a period of ½ to 2 hours and the lamp is cooling off. The remaining water is either poured out or additional water is added.

The typical user uses the lamp occasionally, but some users use the candle diffusers on a daily basis.

Exposure happens when the user inhales the air in the room where the aroma lamp is used.

Exposure model
The used exposure model is described in the following. For each parameter included in the calculations, abbreviations will be used in accordance with the descriptions used for similar scenarios in EU's Technical Guidance Document (TGD 2003). However, some of the parameters that are part of the present model are not covered by examples in TGD 2003.

When calculating the possible exposure by use of aroma lamps the following worst case parameters are used:

- Quantity of oil to be used, Q_{prod}: 10 drops ~ 0.4 g .
- Volume of the room, V_{room}: 17.4 m^3 (equals a small room, is used as a standard room for exposure calculations in relation to exposure calculations for emission of substances from building materials).
- Time the lamp is used, T_{use}: 2 hours

- Time of exposure at use cycle, $T_{contact}$: 4 hours (the person has left the room or a thorough air circulation has been made before then)

- Air exchange rate, R_{room}: 50% per hour

- No of use cycles per day, n: = 1

- Body weight, BW = 60 kg for women and 70 kg for men (standard i TGD 2003)

- Respiration rate, IH_{air}: 20 m^3/day for adults equals 0.83 m^3/hour or 0.014 m^3/min (standard i TGD 2003)

Exposure of a person in the room will be a function of the actual persons' respiration rate and the concentration of the substance in the room.

The concentration in the room will however vary during a use cycle and it is thus necessary to calculate the exposure by integrating the varied exposure in a use cycle.

Concentration in the room
The concentration in the room depends on the rate of which the substances are emitted to the room, the size of the room and the rate the substances are removed from the room by exchanging with the surroundings.

Changes in the concentration in the room within a time period can be expressed by the formula:

$$\frac{dC}{dt} = \frac{R}{V_{room}} - \frac{Q}{V_{room}} * C_{air}$$

as

C_{air} is the concentration of the substance in the room at the time t

R is quantities of what is added by emission in the time period dt

V_{room} is the volume of the room

Q is the quantity removed from the room by ventilation in the time period dt

As there is a gradually heating of the water, the emission rate (and thus the quantity added to the room) will gradually increase in the beginning of the period and it will later decrease when the concentration of the actual substance in the candle diffuser falls. To simplify, we calculate that the total quantity of substances emitted to the room is emitted with the same average rate as within a two hours period.

In figure 3.1 the concentration sequence at a total emission of 60 mg of the substance has been shown, equivalent to the emission of d-limonene from 10 drops no. 34 oil used in the climate chamber test no. 3. On the figure is shown the concentration sequence in the room, when the 60 mg are assumed to be emitted during 0.5 and 2 hours, respectively.

We have here chosen a numeric solution of the calculations where all calculations are made stepwise in intervals of 1 minute.

It is assumed that the person stays in the room for 4 hours, so that the average concentration in these 4 hours is calculated. The average concentration in these 4 hours is 1,450 µg/m^3 when the oil is emitted for 30 minutes and 1,320 µg/m^3, if the emission takes place for 2 hours. The average concentration the person is exposed to is thus not very depending on how quick the oil evaporates, whereas the maximum concentration the person is exposed to is higher when the evaporation takes place within a shorter period.

For the exposure assessment a scenario is used where it is estimated that the oil is emitted equally over a period of 2 hours.

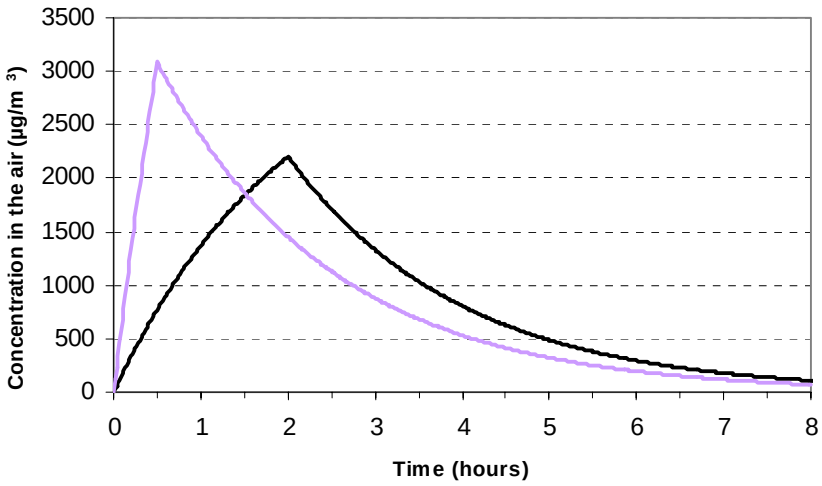


Figure 3.1
Concentration in the air in a 17.4 m^3 room with an air circulation rate of 50% per hour. It is assumed that 60 mg in total of the substance is emitted at a constant rate for ½ time (gray curve) and 2 hours (black curve). The 60 mg equals the content of the d-limonene in 10 drops of oil no. 34 used in climate chamber tests.

Total quantity of substance emitted to the room in a user cycle can be calculated as:

$$M_{subst,emiss} = Q_{prod} * FC_{prod} * E_{stof}$$

where

$M_{subst,emiss}$ is the total amount of substance emitted during a user cycle (in mg)

Q_{prod} is the quantity of oil added to the candle diffuser (in kg)

FC_{prod} is the concentration of the actual substance in the oil (in mg/kg)

E_{stof} is the emission factors for the substance, i.e. the part of the substance in the added oil liberated to the air during a user cycle (out of scale)

Q_{prod} is determined by weighing the 10 drops of oil added to the lamp,

FC_{prod} is determined by use quantitative analyses of content, whereas

E_{stof} is determined by use of climate chamber tests.

Inhalatory intake

A person staying in the room will inhale a part of the substance, depending on the persons' respiration rate and the concentration of the substance in the air in the room.

A part of the inhaled substance will be absorbed via the respiratory tract. The quantity that is inhaled, the inhalatory intake, depends on to which degree the substance appears as a gas or is linked to aerosols of different size.

Calculations show that in cases where the total quantity in 0.5 hour, the person will, during a 4 hour user cycle, inhale 8.1% of the emitted quantity, i.e. mainly the same quantity as when the total quantity is emitted over 2 hours. It is thus of less importance how fast the substances are emitted within a 4 hours user period.

4 Results of analysis program

4.1 Selection of products for analysis

The preliminary contact to Danish knowledge centres indicated that there is not much knowledge about these products and the possible impact from their constituents via exposure to the respiratory tract. There is considerable material on the substances impact to the skin by exposure, but this knowledge is not immediate useful to assess exposure via the respiratory tract.

At least 17 of the substances have previously been assessed in connection with other consumer product projects. Only one of the reviews of health impacts of the substances contained information about possible effects at exposure via the respiratory tract.

Tisserand & Balacs (1995) give in the book "Essential oil safety. A guide for health care professionals" a thorough review of health aspects related to essential oils. There is a number of essential oils that may contain various dangerous substances, but these oils are not among the oils identified in this project and marketed for aromatherapy.

The book also concludes about exposure via the respiratory tract that: "***Inhalation is an important route of exposure because the role of odour in aromatherapy, but from a safety standpoint it presents a very low level of risk to most people…..The only risk would be from prolonged exposures(perhaps 1 hour or more) to relatively high levels of essential oil vapour, such as could occur when directly sniffing from a bottle of undiluted oil. This could lead to headaches, vertigo, nausea and lethargy***".

In the book a number of substances are pointed out having a possible health effect, however not particularly by exposure via the respiratory tract. The following has a critical effect:

- safrole (CAS No 94-59-79) - carcinogenic;
- estragole (CAS No 140-67-0) - carcinogenic;
- trans-anethole (CAS No 4180-23-8) - weak oestrogenic activity;
- thujone (CAS No 546-80-5) - acute poisonous;
- methyleugenol (CAS No 93-15-2) - genotoxic.

It should be noticed that none of the 5 substances is included in the list of dangerous substances. Out of the 5 substances, thujone is not listed as a constituent of the oils used for aromatherapy.

Four of the oils have previously been examined for presence of the 26 sensitizing substances. The results are in accordance with the results presented here based on information from producers considering the variations to be expected.

Some of the constituents of the oils are also part of wooden building materials and are in this connection assessed to be released to the indoor climate. LCI

values have been found for 11 substances as listed in table 4.1. It has been found relevant to include substances with LCI values, as it will be possible to relate the LCI values to the calculated room concentrations when using candle diffusers.

According to one of the suppliers, the most popular essential oils for candle diffusers are lavender, eucalyptus, bergamot and orange, whereas another supplier lists eucalyptus, peppermint, citronella, lemongrass, citrus oils (lemon, orange, bergamot, grape, and other), rosemary, ylang ylang, patchouli and litsea.

An initial literature search showed that reviews have been made on impacts from exposure via the respiratory tract for d-limonene and alpha-pinene.

The table below shows the substances that at first were selected for quantitative analysis of constituents. The list was subsequently reduced to 15 substances by taking out substances that are only present in smaller quantities in few oils and omit substances that structurally are similar to other substances on the list and that have the same LCI value.

A number of products have then been selected based on 3 criteria: 1) all substances should be covered; 2) products should specifically be used for candle diffusers; 3) relatively many fragrance oils are selected because their constituents are less known. A number of the fragrance oils contain essential oils whose constituents are not shown, and it should thus be expected that many of the fragrance oils contain more of the selected substances than listed in table below. These fragrance oils will contain a large part of the selected substances and are thus appropriate for climate chamber tests.

The selected products are:

- Essential oils: Rosemary oil, citrus oil, tea tree oil, lemon grass oil;
- Fragrance oils: No. 38, No. 5, No. 2, No. 6, No. 27, No. 34.

The following oils were selected for climate chamber tests based on the criteria that they in total cover the main part of the 15 constituents: Rosemary oil, tea tree oil, No. 38, No. 5, and No. 34.

The following climate chamber tests are made:

- Candle diffuser with rosemary oil, No. 34 and No. 5;
- Aroma Stream with tea tree oil and No. 38.

Table 4.1
Background data for selection of substances and products.

CAS No	Chemical name (English translation of name indicated in the MSDS)	Synonymous	Classification according to the List of Dangerous Substances	AT limit value (AT 2007)	Products (concentration of the substances in percentage	LCI / NIK value µg/m³
Substances selected for laboratory analysis						
76-22-2	Camphor		-	2 ppm 12 mg/m³ (synthetic)	Coriander oil (2.5-5) Rosemary oil (5-10)	
79-92-5	Camphene		-	-	Rosemary oil (2.5-10) Ginger oil (5-10) Nutmeg oil, coriander oil, pine needle oil (1-2,5) Lavender oil (<1)	LCI: 250
84-66-2	Diethyl phthalate		-	3 mg/m³	No. 55, No. 49, No. 11 (25-50) No. 38 (5-10); No. 22 (1-2.5)	
87-44-5	beta-Caryophyllene		-	-	Pine needle oil (1-2.5) Nutmeg oil (2.5-5) Tea tree oil (1-2.5)	LCI: 1000 *1
99-87-6	p-Cymene	Methylisopropylbenzen	-	25 ppm 135 mg/m³	Camphor oil (2.5-5) Lemon oil, coriander oil, tea tree oil (1-2,5) Mandarin oil, nutmeg oil, rosemary oil (<1)	
100-51-6	Benzylalcohol		Xn;R20/22	-	Cajeput oil (ca. 3) Ylang ylang oil (ca. 0.4) No. 15, No. 47 (5-10) No. 12, No. 57, No. 14 (1-5)	NIK: 440 LCI: 100
112-31-2	n-Decylaldehyde		-		No. 5, No. 6, No. 57, No. 34 (1-5)	NIK: 1400 LCI: 3,100 *1
120-51-4	Benzylbenzoate		XN;R22		Ylang ylang oil No. 14, No. 23, No. 27 (20-40) No. 3, No. 5, No. 6, No. 20 (10-20) No. 4, No. 12, No. 51, No. 24, No. 32, No. 36 (5-10)	
123-35-3	Myrcene		-	-	Orange oil, lemon oil, Cypress oil, pine needle oil, Grapefruit oil, Coriander oil, mandarin oil, nutmeg oil, Tea tree oil(1-2.5)	LCI: 1700
140-67-0	Estragole		-	-	Basil oil (50-100) Fennel oil (2.5-5) Anise seed star oil (1-2.5)	-

CAS No	Chemical name (English translation of name indicated in the MSDS)	Synonymous	Classification according to the List of Dangerous Substances	AT limit value (AT 2007)	Products (concentration of the substances in percentage	LCI / NIK value µg/m³
586-62-9	p-Mentha-1,4(8)-diene		-	-	Cypress oil (1-2.5) Pine needle oil, camphor oil, nutmeg oil, tea tree oil (2.5-5) Coriander oil, mandarin oil (<1)	LCI: 1000 *1
4180-23-8	trans-Anethole		-	-	Anise oil, fennel oil (50-100) No. 34 (0.3)	-
5392-40-5	Citral		XI;R38 R43	-	Lemongrass oil, litsea cubeba oil (75) No. 12, No. 34 (1-5); No. 31 (0.1-1)	
5989-27-5	d-Limonene		R10 XI;R38 R43 N;R50/53	-	A range of essential oils. Typically present in concentrations above 50% in oils of citrus fruits. No. 26 (10-20); No. 2 (5-10) Nr 1, No. 10,No. 35 (1-5); No. 34 (0,9)	NIK og LCI værdier for limonen
7785-26-4; 7785-70-8; 80-56-8	alpha-Pinene		-	-	Cypress oil, pine needle oil (25-50) Camphor oil, nutmeg oil, (10-20) Fennel oil (2.5-5); coriander oil (5-10) lemon oil, mandarin oil, tea tree oil (1-2,5) Orange oil, basilica oil, grapefruit oil, peppermint oil, anise seed star oil (<1)	NIK: 1400 LCI:250 (CAS 80-56-8)
Substances not selected for analysis						
93-15-2	Methyleugenol		-	-	Basil oil (<1)	-
94-59-7	5-allyl-1,3-benzodioxol	Safrole	CARC2;R45 Xn;R22 MUT3;R68	-	Nutmeg oil (1-2.5) [usually not applied in candle diffusers]	
138-86-3	Limonene	Dipentene	R10 XI;R38 R43 N;R50/53	75 ppm (tentative)	Mentioned for many products, but it is assumed, that the substance predominantly is present as d-limonene	NIK: 1400 LCI: 300
13466-78-9	3,7,7-Trimethylbicoclo[4.1.0]hept-3-ene	3-carene	-	-	Pine needle oil (10-20)	NIK: 1400 LCI: 250
18172-67-3	beta-Pinene		-	-	Lemon oil, pine needle oil, camphor oil (10-20) Bergamot oil, rosemary oil (2.5-5) Basil oil, cypress oil, coriander oil, mandarin oil, peppermint oil(<1), cassis oil, No. 19 (0.1-1)	NIK: 1400 LCI 250

*1 LCI = "lowest concentration of interest" (Jensen *et al.* 2001). For substances marked with *1 LCI value is taken from ECA-IAQ (1999).

NIK = "Niedrigst interessierende Konzentrationen", equals LCI (AgBB 2005).

*2: CAS No is not specifically shown on the substances safety data sheets. Overall designation for the two CAS No. as above.

4.2 Methods of analysis

4.2.1 Quantitative description of constituents

A partial test of the product is extracted with dichloromethane for one hour on a shaking table and is left over night. A partial test of the extract is taken out and analyzed directly by a combined gas chromatography and mass spectrometry (GC/MS). The content is calculated quantitatively. Analyses are carried out as duplicate determination, i.e. two determinations on the same product. Standards are made for all 15 specific components.

The uncertainty of the analyses is 10-15% RSD. The detection limit is 10-100 mg/kg.

4.2.2 Climate chamber test

The products are tested in two relevant user situations. 10 drops of the products (weighed) for each climate chamber test. The arrangements were placed in climate chambers with a known air circulation and humidity and temperature of the intake air.

Candle diffuser: 20 ml water was filled in the bowl. 10 drops of oil was added to the water. A tea light was lit under the bowl just before test start.

Aroma Stream: The device has a filter in the bottom that can be taken out and oils are added. 10 drops of oil were added to the filter and the device was assembled. The fan was started just before test start.

The used candle diffuser

Aroma Stream. Source: BodyMind Company http://bodymindcompany.zafi.netimage.dk/index.php?pid=3&item_id=274

The emissions from the products is collected on ATD-tubes with the absorption material Tenax starting after 15 minutes, 2 hours and 4 hours respectively. With this absorption material, substances can be collected which are in a gas phase.

After 15 minutes, collection is made for 10 minutes and for the two subsequent tests for 20 minutes. The short test period after 15 minutes is due to the

fact that otherwise the amount of emitted substance would exceed the capacity of the tubes.

The ATD-tubes are desorbed thermally and the content is analyzed for 15 specific components and TVOC (Total Volatile Organic Compounds) by combined gas chromatography and mass spectrometry (GC/MS). Reference method for ATD: ISO 16000-6.

The reporting limit is 1 µg/hour. Total uncertainty for test and analysis: 20-30% RSD.

The climate chamber tests were made using a method identical to the method used for emission test of VOC (Volatile Organic Compounds) from building materials after ISO 16000-9, 2006. These tests are reported as a steady state room concentrations in µg/m³ air in a standard room (accordingly) with a volume of 17.4 m³, air circulation of 0.5 times/hour, temperature of 23° C and relatively humidity of 50% RH. As this calculation method assume a constant emission at the measured rate of approx. 8 hours before, a steady state situation is achieved which is not fulfilled in these tests and instead it has been chosen to calculate room concentrations subsequently based on the exposure model with the same room size and air circulation, but with the emission over a shorter period.

Chamber conditions

Material: Plexiglas. Volume: 28 litre. Multistage air clean-up. A blind test was made in the empty room with or without light before each test. The added air had a temperature of 23° C and a relatively humidity of 50% RH. The relative humidity increased during the tests in the tests where the oil was added to 20 ml of water. The air circulation was 4.3 times per hour.

It will take some time before a steady state has been achieved where the quantity of the emitted substance sucked out of the climate chamber equals the quantity emitted from a source within the chamber. As it can be seen from the below figure, a steady state situation is not established in the climate chamber after approx. one hour if a source is placed in the room with a constant source strength. This means that after 15 minutes considerably lower concentrations are measured than the actual, but it has been chosen to make the test at this early point in time to ensure that not all the fragrances were emitted before the start of the collection.

At constant source strength, after 15 and 25 minutes, there will be measured 67% and 85% respectively of the actual emission rates and totally seen a measurement from 15 to 25 minutes will be 76% of the actual emission rate. As the results, at least for Aroma Stream, shows falling source strength, this underestimation will partly be outweighed by the fact that the source strength is falling. As there are no grounds for a correct correction of this uncertainty in measuring, no adjustments have been made, but this uncertainty is considered by the assessment of the results.

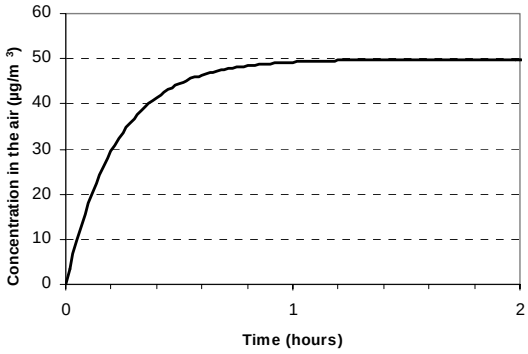


Figure 4.1
Course of concentration in a climate chamber with air circulation of 4.3 times per hour in which a source with constant source strength is placed.

4.3 Quantitative determination of constituents

Results of the quantitative determination of constituents of 15 oils are shown in table 4.2. Results of two parallel determinations are given on the same oil.

The measured concentrations in the four essential oils correspond to the information on the safety data sheet considering that a certain variation must be expected in the content of the natural oils. The very high concentrations of more than 70% d-limonene in citrus oil and above 70% citral in lemongrass oil have thus been confirmed by these analyses.

For the six fragrance oils it is for most of the substances not possible to compare the measured concentration with the concentrations stated in the safety datasheets as the safety data sheets typically only give information on a substance level for the synthetic substances, whereas for the essential oils being part of the fragrance oils, only information on the quantities is given. The measured content benzyl benzoate and diethyl phthalate is in accordance with the information on the safety data sheets. It can be seen that d-limonene is present in most of the oils in high concentrations, but by comparing to the safety data sheets it is seen that d-limonene primarily will be part of the fragrance oils as constituents of citrus oil and other essential oils.

Table 4.2
Results from the analysis of 15 specific substances in essential oils and fragrance oils. The unit is mg/kg. A and B show the result of two parallel analysis of the same oil.

	D.l.	Rosemary oil		Lemon oil		Tea tree oil		Lemongrass oil	
		A	B	A	B	A	B	A	B
alpha-Pinene	100	110,000	120,000	21,000	21,000	23,000	23,000	1,200	1,100
Camphene	100	52,000	53,000	860	870	-	-	5,300	5,000
Myrcene	100	11,000	11,000	23,000	22,000	11,000	10,000	15,000	13,000
Benzylalcohol	100	<1,000*	<1,000*	-	-	-	-	-	-
para-Cymene	100	22,000	22,000	8,800	9,600	31,000	18,000	560	490
d-Limonene	100	41,000	42,000	730,000	720,000	11,000	11,000	2,900	2,400
Terpinolene	100	480	490	2,900	2300	38,000	38,000	220	168
Camphor	100	110,000	110,000	-	-	-	-	2,500	2,300
Estragole	100	-	-	-	-	-	-	-	-
n-Decylaldehyde	100	-	-	820	880	-	-	3,800	3,500
Citral **	100	-	-	22,000	22,000	470	470	780,000	730,000
trans-Anethole	100	-	-	-	-	-	-	-	-
beta-Caryophyllene	100	33,000	33,000	2,400	2,300	4,900	4,800	18,000	16,000
Diethyl phthalate	100	-	-	-	-	-	-	-	-
Benzylbenzoate	100	-	-	-	-	-	-	-	-

D.l.: detection limit
-: not detected above the detection limit
*: Increased detection limit due to interference
** Sum of cis and trans-citral.

Table 4.2 continued

	D.l.	No. 5		No. 2		No. 6		No. 38	
		A	B	A	B	A	B	A	B
alpha-Pinene	100	1,800	1,800	4,900	5,200	1,700	1,700	-	-
Camphene	100	290	300	380	410	220	210	-	-
Myrcene	100	50,000	49,000	50,000	52,000	45,000	45,000	660	620
Benzyl alcohol	100	-	-	<1,000*	<1,000*	-	-	5,800	5,800
para-Cymene	100	1,600	1,600	4,100	4,300	870	850	-	-
d-Limonene	100	83,000	82,000	250,000	240,000	74,000	72,000	1,100	1,000
Terpinolene	100	1,200	1,200	8,600	9,200	1,200	1,200	-	-
Camphor	100	<1,000*	<1,000*	5,700	6,000	<2,000*	<2,000*	-	-
Estragole	100	-	-	-	-	-	-	-	-
n-Decylaldehyde	100	6,100	6,200	-	-	6,500	6,500	-	-
Citral **	100	13,000	13,000	9800	10,000	16,000	16,000	160	160
trans-Anethole	100	-	-	-	-	-	-	-	-
beta-Caryophyllene	100	4,300	4,700	<5,000*	<5,000*	4,600	4,400	<10,000*	<10,000*
Diethyl phthalate	100	-	-	-	-	-	-	96,000	95,000
Benzyl benzoate	100	110,000	140,000	100	-	140,000	120,000	5,500	5,400

Table 4.2 continued

	D.l.	No. 27		No. 34	
		A	B	A	B
alpha-Pinene	100	-	-	960	930
Camphene	100	-	-	-	-
Myrcene	100	-	-	3,700	3,400
Benzyl alcohol	100	<500*	<500*	-	-
para-Cymene	100	-	-	240	230
d-Limonene	100	260	220	210,000	200,000
Terpinolene	100	-	-	-	-
Camphor	100	-	-	-	
Estragole	100	-	-	-	-
n-Decylaldehyde	100	-	-	58,000	55,000
Citral **	100	-	-	19,000	18,000
trans-Anethole	100	-	-	2,300	2,200
beta-Caryophyllene	100	-	-	-	100
Diethyl phthalate	100	-	-	-	-
Benzyl benzoate	100	240,000	240,000	-	-

D.l.: detection limit
-: not detected above the detection limit
*: Increased detection limit due to interference
** Sum of cis and trans-citral.

4.4 Climate chamber test

4.4.1 Candle diffuser

The measurement results of the emission of 16 substances from rosemary oil and the two fragrance oils No. 5 and No. 34 from the candle diffuser can be seen in table 4.3.

Table 4.3
Emissions of 15 specific substances from rosemary oil and the two fragrance oils no. 5 and no. 34. The unit is µg/time (emission rate). A and B show the results of two parallel climate chamber tests on the same oil.

Substance	R.g.	Rosemary oil		No. 5		No. 34	
		A	B	A	B	A	B
Gram sample (10 drops)		0.45	0.47*	0.39	0.41	0.29	0.30
15-25 min. after start							
alpha-Pinene	1	6,000	2,400*	390	410	140	110
Camphene	1	3,900	1,400*	120	100	-	-
Myrcene	1	360	88*	190	310	140	110
Benzyl alcohol	1	5.7	1.2*	-	-	-	1.3
para-Cymene	1	420	260*	480	270	84	95
d-Limonene	1	340	340*	2,500	4,600	>5,300	>4,900
Terpinolene	1	18	5.8*	29	28	-	-
Camphor	1	840	480*	370	270	-	-
Estragole	1	-	-	-	-	-	-
n-Decylaldehyde	1	-	-	-	-	55	36
Citral **	1	-	-	13	16	13	11
trans-Anethole	1	-	-	-	-	-	-
beta-Caryophyllene	1	12	2.8*	2	8.0	-	1.2
Diethyl phthalate	1	-	-	-	-	-	-
Benzyl benzoate	1	-	-	20	42	-	-

Substance	R.g.	Rosemary oil		No. 5		No. 34	
		A	B	A	B	A	B
TVOC		43,000	18,000*	10,000	14,000	>11,000	>10,000
120-140 min. after start							
alpha-Pinene	1	18	45	-	1	-	-
Camphene	1	14	29	-	-	-	-
Myrcene	1	-	-	8	22	-	-
Benzylalcohol	1	-	-	1	3	-	-
para-Cymene	1	13	28	3	5	-	-
d-Limonene	1	10	28	28	58	14	15
Terpinolene	1	-	-	1	2	-	-
Camphor	1	93	330	1	-	-	-
Estragole	1	-	-	-	-	-	-
n-Decylaldehyde	1	-	-	-	-	-	-
Citral **	1	-	-	33	22	-	-
trans-Anethole	1	-	-	-	-	-	-
beta-Caryophyllene	1	28	73	3	2	-	-
Diethyl phthalate	1	-	-	-	3	-	-
Benzylbenzoate	1	-	-	1,300	350	1.8	-
TVOC		730	1,800	2,700	1,800	96	84
240-260 min. after start							
alpha-Pinene	1	11	13	-	-	-	-
Camphene	1	9.5	9.8	-	-	-	-
Myrcene	1	-	-	2	11	-	-
Benzyl alcohol	1	-	1.7	-	-	-	-
para-Cymene	1	7.6	9.7	2	3	-	-
d-Limonene	1	6.4	11	12	26	11	13
Terpinolene	1	-	-	-	1	-	-
Camphor	1	19	24	1	-	-	-
Estragole	1	-	-	-	-	-	-
n-Decylaldehyde	1	-	-	-	-	-	-
Citral **	1	-	-	7	24	-	-
trans-Anethole	1	-	-	-	-	-	-
beta-Caryophyllene	1	10	2.7	-	1	-	-
Diethyl phthalate	1	-	-	-	-	-	-
Benzyl benzoate	1	-	-	23	17	-	-
TVOC		270	720	180	840	6.0	6.0

R.g: Reporting limit

- : Not detected above reporting limit

* At the test 15-25 min only 0,329 gram was added at chamber B.

** Sum of *cis*- and *trans*-citral.

TVOC The sum of Volatile Organic Components calculated as toluene.

4.4.2 Aroma Stream

Measurement results of emission of 15 substances from tea tree oil and fragrance oil No. 38 evaporated with Aroma Stream are shown in table 4.4.

Table 4.4
Emissions of 15 specific substances from tea tree oil and fragrance oil no. 38. The unit is µg/time (emission rate). The two results show double indications on the same oil.

	R.g.	Tea tree oil		No. 38	
		A	B	A	B
Gram sample (10 drops)		0.46	0.48	0.34	0.39
15-25 min. after start					
alpha-Pinene	1	4,300	4,000	84	47
Camphene	1	-	-	29	6
Myrcene	1	840	770	140	92
Benzyl alcohol		14	6	4	-
para-Cymene	1	1,100	1,200	880	370
d-Limonene	1	920	550	360	140
Terpinolene	1	1,300	1,600	-	-
Camphor	1	-	-	-	-
Estragole	1	-	-	-	-
n-Decylaldehyde	1	-	-	-	-
Citral **	1	-	-	-	-
trans-Anethole	1	-	-	-	-
beta-Caryophyllene	1	1.3	2.8	1.8	1.2
Diethyl phthalate	1	-	-	-	-
Benzyl benzoate	1	-	-	-	-
TVOC, 2 timer		36,000	36,000	8,500	5,200
120-140 min. after start					
alpha-Pinene	1	39	140	-	-
Camphene	1	0.4	-	-	-
Myrcene	1	-	120	3.6	18
Benzyl alcohol	1	-	-	4.6	16
para-Cymene	1	390	820	1.6	5.3
d-Limonene	1	140	240	11	17
Terpinolene	1	670	1,700	-	1.7
Camphor	1	-	-	-	-
Estragole	1	-	-	-	-
n-Decylaldehyde	1	-	-	-	-
Citral **	1	-	-	-	-
trans-Anethole	1	-	-	-	-
beta-Caryophyllene	1	110	220	1.4	3.5
Diethyl phthalate	1	-	-	-	-
Benzyl benzoate	1	-	-	-	-
TVOC, 2 timer		22,000	45,000	960	2,200
240-260 min. after start					
alpha-Pinene	1	14	24	-	-
Camphene	1	-	-	-	-
Myrcene	1	-	6.0	3.6	4.0
Benzyl alcohol	1	-	-	4.0	7.6
para-Cymene	1	58	130	1.2	-
d-Limonene	1	18	40	4.6	4.3
Terpinolene	1	96	240	-	-
Camphor	1	-	-	-	-

	R.g.	Tea tree oil		No. 38	
		A	B	A	B
Estragole	1	-	-	-	-
n-Decylaldehyde	1	2.3	-	-	-
Citral **	1	-	-	-	-
trans-Anethole	1	-	-	-	-
beta-Caryophyllene	1	5.2	17	1.6	3.0
Diethyl phthalate	1	-	-	-	-
Benzyl benzoate	1	-	-	-	-
TVOC, 4 timer		2,300	5,700	580	980

R.g: Reporting limit

- : Not detected above reporting limit

* At the test 15-25 min only 0,329 gram was added at chamber B.

** Sum of *cis*- and *trans*-citral.

TVOC The sum of Volatile Organic Components calculated as toluene.

4.5 Interpretation of analysis results

At all the climate chamber tests it can be seen that the emission rates are relatively low considering the quantities of each substance being part of the 10 drops of oil added to the candle diffuser or Aroma Stream. In the following the results will be elaborated further.

4.5.1 Aroma Stream

Tea tree oil

The measured emission rates with results for tea tree oil in Aroma Stream can be seen in figure 4.2. For each measuring period, a measuring point is given in the middle of the interval at 20, 130 and 250 minutes respectively.

There is a regular fall in the emissions rates for four of the substances whereas for alpha-pinene the rates are significantly higher in the beginning and at the same time a relatively low rate after 130 minutes.

The emission rate for beta-caryophyllene was unexpectedly low for the period 15-25 minutes. The same is the case for the emission measurement of beta-caryophyllene from rosemary oil, No. 38 and No. 5 from this testing period, but there is no explanation to this.

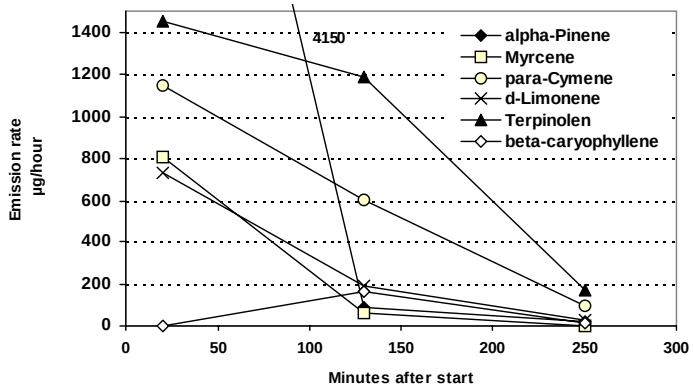


Figure 4.2
Measured emission rates from tea tree oil in Aroma Stream. Value of 4,150 for alpha-Pinene is out of scale. The unit is µg/time. The average of two tests.

In order to normalize the rates to the content of the substances in tea tree oil the same results is shown in figure 4.3, where emission factors indicating the emission in % of the quantity of the substances added to Aroma Stream.

It can be seen that substances with a relatively high emission factor after 20 minutes have an equivalently low emission factor after 130 minutes which indicates that the relatively low rate after 130 minutes is due to the fact that a large part of the substances have already disappeared. Alpha-pinene and myrcene with high rates in the beginning thus have low rates after 130 minutes where the rates are less than 1/10 of the rates in the beginning. It should be noted that the emission factor has been calculated in relation to the starting quantity of the substance and not the remaining quantity at different points in time. Held together with the very low rates after 250 minutes, the results indicate that the main part of the oils have disappeared after four hours.

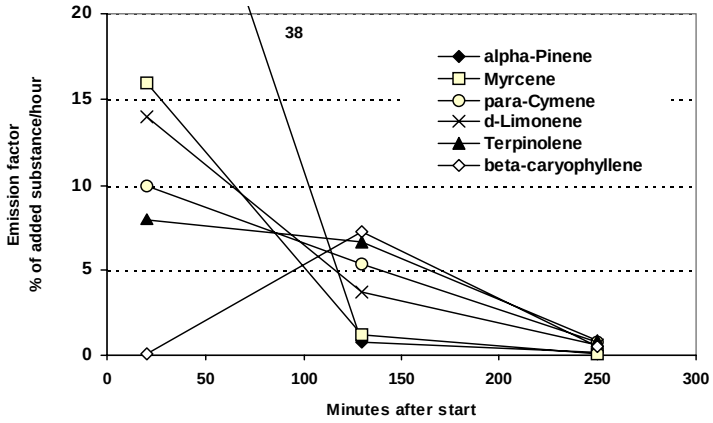


Figure 4.3
Measured emission factors from tea tree oil in Aroma Stream. Value at 38% for alpha-Pinene is out of scale. The emission factor in percentage shows how large a part of the added substance will be emitted during an hour with the measured emission rates. The average of two measurements.

A calculation based on the measured emission rates indicates however that for most of the substances less than 25% has been collected on the ATD-tubes, whereas for alpha-pinene there has been collected 51% of the added quantity (table 4.5). The total quantity emitted has been calculated for each time interval based on a line drawn through the two nearest measuring points. The emission in the period 0-2 hours has thus been calculated as 2 hours emission with the emission rate at 60 minutes (stated in µg/hour) based on the line through the measuring points for 20 and 130 minutes. For some of the substances an exponential fall probably better describes the actual development in the emission rates, but there are too few measuring points to make somewhat certain fits for an exponential tendency line. Control measurements show that the calculated emissions, if exponential functions are used, are close to the emissions stated in table 4.5 calculated on the basis of linear functions.

A simple test where the weight loss was measured after Aroma Stream had functioned for 2 hours showed for the fragrance oil No. 38 that approx 40% of the oil had disappeared after 2 hours. Similar tests were not made for the other oils. The tests indicate that the low rates are probably not due to the fact that the substances generally are absorbed strongly to the filter or diffuse into the plastic material.

Table 4.5
Tea tree oil in Aroma Stream. Total emission in respectively first 2 hours and first 4 hours in µg and in percentage of the content of the substances in the added oil. Average of two measurements.

	Content of 0.46 g oil added		Estimated total emission First 2 hours		Estimated total emission First 4 hours	
	%	µg	µg	% of addef	µg	% of added
alpha-Pinene	2.30	10,810	5,347	49	5,462	51
Myrcene	1.05	4,935	1,068	22	1,137	23
para-Cymene	2.45	11,515	1,904	17	2,649	23
d-Limonene	1.10	5,170	1,074	21	1,307	25
Terpinolene	3.80	17,860	2,707	15	4,153	23
beta-Caryophyllene *	0.49	2,280	123 *	5	313	14

* The measurements of beta-caryophyllene in the time period 15-25 minutes are unexpectedly low for all oils. There has been found no explanation of this.

Creation of decomposition and oxidation products

A possible explanation of the relatively low emission factors at the same time as the substances seems to disappear may be that the substances are either broken down or react with other substances after they have been transmitted to the air where substances are formed that are not part of the measuring program. The reactions will partly happen as gas phase reactions in the room, on surface particles or in the actual ATD-tubes before measuring.

The fact that e.g. terpenes oxidize in the air is a well known case, but the question is whether it happens to an extent so that 50-70% of the substances have reacted before measured. The substances are in relatively high concentrations in the chamber and it should be expected that the half life period depend on the relationship between the substances and the other reactants.

In an assessment on d-limonene from the International Programme for Chemical Safety (IPCS 1999) it is indicated that d-limonene emitted to the atmosphere is expected to quickly become part of a gas phase reaction with

photo chemically made radicals, ozone and nitrate radicals. It has further been mentioned that it is important when analyzing limonene in the air also to analyze the oxidation products as limonene is quickly oxidized in the air. Based on the experimentally determined rate constants, a lifetime has been calculated for d-limonene at the reaction with photo chemically made hydroxyl radicals in 0.3-2 hours. The equivalent life times at reaction with ozone is 2-2.6 hours, whereas the life time at night hour reactions with nitrate radicals has been calculated to 0.9-9 minutes. Further circumstances and concentrations of reaction substances are not listed in the statements, but it is said that the atmospheric lifetime for d-limonene during daytime is estimated at 12-48 minutes. It is not perfectly clear whether life time actually means average lifetime.

Another reference shows a half-life time for d-limonene at 46 minutes at an ozone concentration of 50 ppb (Wainman ***et al*** 2000). Indoor ozone concentrations are in Denmark from approx. 10 up to approx. 70 ppb (Wolkorff 2004).

There is a long series of studies describing how the oxidation of d-limonene has an effect on the creation of fine particles in the air of the indoor climate (Vartiainena ***et al***. 2006; Weinman ***et al***. 2000).

It should be expected that the other substances in a similar way are part of the reactions even though the rates would be different. It is difficult to say whether the reactions could take place in such high rates in the climate chamber with high concentrations of a number of VOCs at the same time, but the stated reaction times for limonene indicated that such reactions may have a significant influence on the quantity of pure substances in the atmosphere in the climate chamber.

A completely different question is whether the reaction products will have any of the effects seen for the pure substances, so that by a health assessment it is necessary also to include the reaction products. This is further discussed in chapter 5 under health assessment.

Fragrance oil No. 38

Calculated emission factors for 5 substances from fragrance oil No. 38 can be seen in table 4.6. Emissions of alpha-pinene, camphene and para-Cymene were also measured above the reporting limit, but the measured concentrations in the oil were below the detection limit and it was thus not possible to calculate emission rates for these substances. The results show emission rates for Myrcene and d-limonene that are relatively high compared to the emission rates measured for tea tree oil (figure 4.3). The calculated emission factors for benzyl alcohol, Diethyl phthalate and benzyl benzoate in the period 15-25 minutes is 0.08%/hour for Benzyl alcohol and 0 for the two other substances. There has been found no explanation why no emission has been measured from the three substances.

A subsequent test, where the filter was measured at start and after 2 hours, it showed that 39% of the oil had evaporated after 2 hours. The emission of TVOC the first two hours may, based on a regression line between the measurements of the emission of TVOC in the periods 15-25 minutes and 220-240 minutes, be calculated to 9,990 µg equivalent to 2.7% of the weight of the added oil.

The composition of the oil is not known, but the figures indicate that together with data for rosemary oil, the measured emissions of the VOCs are considerably lower than the evaporated quantity.

Table 4.6
Fragrance oil no. 38 in Aroma Stream. Emission factors for constituents of the three measuring periods and content in added oil. Average of two measurements.

	Content of added oil (0.365 g)		Emission factor (% of content of oil per hour)		
	%	µg	15- 25 min	120-140 min	220-240 min
Myrcene	0.06	234	50	4.6	1.6
Benzyl alcohol	0.58	2,117	0.08	0.5	0.3
d-Limonene	0.11	383	65	3.7	1.2
Diethyl phthalate	9.6	34,858	0	0.001	0
Benzyl benzoate	0.55	1,989	0	0.001	0

4.5.2 Candle diffuser

The candle diffuser generally shows a more pronounced decrease in the emission between the first and the second measurement than in the tests with Aroma Stream. The measured emission rates for rosemary oil shown in figure 4.4 indicate that the main part of the substances evaporates within the first two hours.

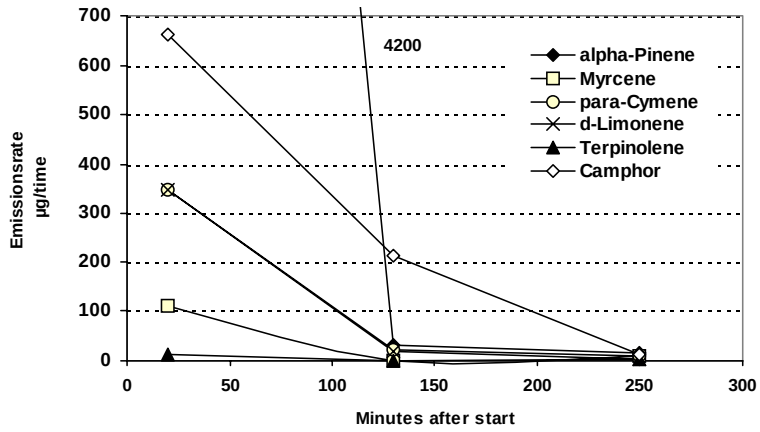


Figure 4.4
Measured emission rates from rosemary oil in candle diffuser. Value of 4,200 for alpha-pinene is out of scale.

But as for the measurements of Aroma Stream, the measured rates are considerably below the quantities that seem to disappear.

In table 4.7 is shown the calculated rates in percentage of the substance quantities added to the lamp in form of rosemary oil. The total emission has been calculated by assuming that the measured rate at 15-25 minutes represents an average rate for the first 2 hours. On the contrary to what is the case with Aroma Stream, it cannot - in this set up - be assumed that the emission gradually is reduced as it is a fact that the oil is dissolved in water and that the temperature increases. However, the uncertainty of this calculation can hardly explain the low rates that more likely are due to some of the same mechanisms resulting in low rates in the tests with Aroma Stream.

Apart from the creation of reaction products it may in this test also have an effect that part of the substances adsorb to or are dissolved in water drops created in the chamber due to the high humidity. With the used ATD-tube, substances adsorbed to water particles will not be collected and measured.

In order to illustrate the results of the climate chamber test, a simple test has been made with the evaporation of rosemary oil from the candle diffuser (same model as used in the chamber). After 15 minutes the water was well heated and there was still a visible layer of oil on the surface. All the water had evaporated after 1 hour and 40 minutes. No oil, after the last bit of water had evaporated, could be observed in the bowl and in the following 15 minutes there were no significant odour from the lamp (subjectively determined by the author) which is accordance with the fact that the test after 130 minutes showed very limited emission of fragrances.

There was not observed any change in the odour either after the water had evaporated. Addition of one drop of oil to the hot diffuser immediately gave a very strong odour and the oil disappeared within a few minutes. It seems as if the substances in the oil evaporates with the water, but it is not possible to say whether the rates measured in the period 15-25 minutes is representative for the rates through the whole period. It seems to be pretty certain that approx. 99% of the substances are emitted to the air shortly after the water has evaporated.

It should be noticed that some aroma therapists recommend to turn off the diffuser before all the water has evaporated, but it is not indicated on any recommendations for the used diffuser. If the diffuser is blown out after an hour where half of the water has evaporated and then left in the room there will of course evaporate a smaller quantity than if you let all the water evaporate, but it is reasonable to assume that at least half of the substances in the added oil will still evaporate.

Table 4.7
Rosemary oil in candle diffuser. Calculated emission in the first 2 hours in µg and in percentage of the substances in the added oil (emission factor).

	Content of added oil (0.46 g)		Estimated total emission First 2 hours	
	%	µg	µg	Emission factor % of added
alpha-Pinene	11.50	54,050	9,429	17
Camphene	5.25	24,675	5,900	24
Myrcene	1.10	5,170	486	9
para-Cymene	2.20	10,340	791	8
d-Limonene	4.15	19,505	826	4
Terpinolene	0.05	228	26	12
Camphor	11.0	51,700	1,526	3
beta-Caryophyllene	3.3	15,51o	16	0.1

4.6 Selection of substances for health assessment

Out of the 15 substances examined, six substances have been selected for a closer health assessment.

The substances have been selected based on the following criteria:

- The substances are part of a number of the oils in significant quantities;
- It has been shown that the substances are emitted in such large quantities from the oils examined in the climate chamber that it is possible to calculate a concentration in the air;
- There are AT limit values and/or LCI/NIK values (can both be used directly for comparison, but also indicates that data is available);
- The substances are on the list of dangerous substances;
- The substances are mentioned in literature on aroma therapy as having a possible health effect;
- It is realistic to find information on the substances' possible effect by exposure via the respiratory tract;
- The selected substances should represent several substance groups (e.g. not all should be terpenes).
- Four of the substances were not chosen because the emissions were below the detection limit so that concentration could not be calculated in the test room: estragole, n-decylaldehyde, trans-anethole and Diethyl phthalate.

Based on these criteria the following substances have been selected for health assessment:

d-Limonene CAS No. 5989-27-5	Part of all tested oils (up to 73%) and in most other oils. AT limit value and LCI/NIK values On the list of dangerous substances. Knowledge of literature on exposure via the respiratory tract
alpha-Pinene CAS No. 7785-26-4 and 7785-70-8	Part of 9 of the examined oils (op to 11%) and concentrations of up to 50% other oils NIK value Knowledge of literature on exposure via the respiratory tract
p-Cymene CAS No. 99-87-6	Part of 9 of the examined oils (up to 2%) and in concentrations of up to 5% in other oils AT limit value
Benzyl alcohol CAS No.100-51-6	Part of 4 of the examined oils (up to 0.5%) and in concentrations up to 10% in other oils. On the list of dangerous substances NIK value
Camphor	Part of the 5 examined oils (up to 11%) and in concentrations of up to 10% in other oils
Citral	Part of 8 of the examined oils (up to 75%) and in a number of other oils On the list of dangerous substances

5 Health assessment

The aim of aromatherapy is to achieve a certain psychical and physical state of the treated person. The result is achieved by the scent from the oil influencing the smell receptors in the mucous membranes in the nose, which then sends impulses via the olfactory nerve to different brain centres.

This report is about the possible health damaging effects caused by inhalation of certain chemical substances being part of aromatherapy oils. The survey concentrates on effects that can be achieved in the respiratory tract (nose, trachea, bronchi) or in the lower part of the lungs (alveolus) or in the remaining part of the body after the substances have gone through the bloodstream via the lungs.

The effect of the fragrances on the olfactory nerve is not included in the assessment. Effects by exposure to the skin or by swallowing are also not included in this assessment.

Actual health damaging inhalation effects may occur as irritation of the respiratory tract or by toxic impact on the respiratory tract and the lower pulmonary segments. When a substance has reached the bloodstream via the lungs it is transported round in the body to all organs and by this way the substance may have a hazardous effect (systemic effect). Apart from this, certain substances may have negative health effects such as being carcinogenic, genotoxic or influencing the immune system.

An additional health damaging effect of the examined substances is the possibility for sensitizing the respiratory tract i.e. an effect that may cause asthma. This is reasonable as several of the substances in focus have a sensitizing effect on the skin (so-called delayed type 4 allergy) and is called for allergens. Sensitizing in the nose or the respiratory tract follows another immunological mechanism than the skin. It is a so-called type-1 immediate allergy causing hay fever (rhinitis allergica) and asthma (asthma bronchiale). There is however no direct relation between the two allergy mechanisms. A substance that is skin allergen does not necessarily also cause allergy in the respiratory tract.

By reviewing the literature for the 6 selected substances the above considerations have been used for guidance. Comments on the substances' health damaging effects by inhalation are limited to the described area and there has not been searched for information on the substances' allergenic effect by exposure via the skin and the substances' effect on the skin have not been assessed (most of them have been assessed earlier) whereas certain systemic effects to a certain extent will be described.

5.1 Search of data

Background data for toxic effects by inhalation have been found in:

- DTV-online search in HSDB and RTECS;
- The European Chemicals Bureau (ECB);
- ChemID light with relevant underlying databases;

- IARC Website;
- NIOSH Website.

Apart from the above, original literature has been searched for using the search parameters: substance name and "inhalation" and substance name and "exposure" in the following databases:

- PubMed;
- Medline;
- Scopus.

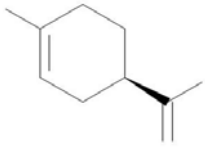
Furthermore there has been searched for original literature by a DTV-online search for CAS no. and "inhalation" in Chemical Abstracts.

Information has also been collected from Danish experts from the National Research Centre for the Working Environment, The Danish Research Centre for Chemical Sensitivities, and Department for Environmental and Occupational Medicine, Institute of Public Health, University of Aarhus and from international experts from ***Research Institute for Fragrance Materials*** in USA and from the ***Tisserand Institute*** in Great Britain.

A review of several survey reports from the Danish Environmental Protection Agency has given useful information about some of the substances and the procedures, for example survey report no. 36 on chemical substances in printed matter (Hansen & Eggert 2003), no. 49 on emission of chemical substances from exotic wood (Witterseh 2004) and no. 82 on selected respiratory tract sensitizing substances in consumer products (Boyd & Mogensen 2007), as they threat several of the substances investigated in this report (e.g. d-limonene, alpha-pinene, citral).

5.2 Toxicity in selected substances by inhalation

5.2.1 D-limonene

Chemical name	(R)-p-mentha-1,8-diene
Synonym	+Dipentene (R)-p-mentha-1,8-diene (S)-p-mentha-1,8-diene trans-1-methyl-4-(1-methylvinyl)cyclohexene (±)-1-methyl-4-(1-methylvinyl)cyclohexene Limonene D-limonene L-limonene
CAS-No.	5989-27-5
EINECS No.	227-813-5
Molecular formula	$C_{10}H_{16}$
Molecular structure	
Legislation:	
Classification as per list of dangerous substances	R10 XI;R38 R43 N;R50/53
List of undesirable substances.	On the list as the substance has been assessed as allergenic by skin contact and is one the 26 allergenic fragrances assessed by SCCNFP.
IUCLID-dataset	Yes
Cosmetics	The fragrance is declared in cosmetics if used in quantities above o.01% in products that are cleaned and o.001% in products that are not cleaned.
Physical chemical substances:	
Melting point, °C	-89 - -96.9
Boiling point, °C	170-180
Vapour pressure (Pa)	2.66644 hPa at 25° C
Physical state	Liquid
Octanol-water partition coefficient, (log Pow)	4,.57
Water solubility (mg/L)	very low (<0.1 g/100 mL at 19.5 C)

Available information on toxicity related to inhalation

D-limonene has very low acute toxicity in humans and test animals. There is no genotoxic, teratogenic or embryo-toxic effect described in the found literature. Its effect on the respiratory tract is controversial. By inhalation the substance is readily absorbed into the blood wherefrom it is absorbed by fatty tissues and eliminated through the kidneys. D-limonene is a strong immunological active substance at a relatively low concentration (Josefson 1993).

Human exposure by inhalation of 450 mg/m^3 d-limonene gives significant reduction of lung capacity, but not of the other respiratory functions. No irritating effect on eyes, nose, throat or the upper and lower respiratory tract and no

influence of the central nervous system has been reported. Tests have shown a ready uptake of 70% of the dose during two hours exposure (Falk-Filipson ***et al***. 1993, Beije and Lundberg 1993).

Inhalation tests with mice show a decrease in respiratory rate at 1076 ppm as a result of sensory irritation. This reaction seems to resemble the human response, as NOEL for sensory irritation is 80 ppm in humans whereas it is 100 ppm in mice. A mild bronchoconstrictive effect at mice is seen at 1000 ppm (Larsen ***et al***. 2000).

Inhalation of d-limonene prevents bronchial obstruction in sensitized rats by reaction with ozone. Histologically there is an inflammatory inhibitory effect. (Keinan ***et al***. 2005).

Airways irritants in the form of ultrafine particles can be formed by reaction between ozone and unsaturated volatile organic compounds - especially limonene and alpha-pinene. (Wolkoff ***et al***. 2000; Rohr ***et al***. 2003). Nøjgaard ***et al***. (2005) report that oxidation products of terpenes (e.g. limonene) contain unidentified irritants that may be responsible for a part of the reported eye and airway complaints in indoor environments.

Exposure of rats to 6 ppm d-limonene and 0.8 ppm ozone for three hours causes inflammatory changes in the lungs (Sunil ***et al***. 2007).

D-limonene is not in itself an allergen, but allergens are created by auto-oxidation (Karlberg ***et al***. 1992).

According to IARC (1999) it is estimated that the substance d-limonene cannot be classified in relation to its carcinogenic effect on humans (Group 3).

When humans inhale d-limonene a stimulation of the autonomic nervous system is observed with increased b blood pressure, subjective alertness and restlessness as well as subjective mental and emotional reactions (Heuberger ***et al***. 2001).

Limit values for d-limonene:

AT limit value (AT 2007): 75 ppm (tentative)
NIK (AgBB 2005): 1400 µg/m^3
LCI (Jensen ***et al***. 2001): 300 µg/m^3

5.2.2 Alpha-Pinene

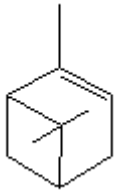
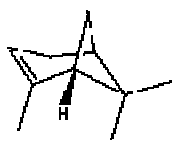
The substance is linked to several CAS numbers. In the following data have been collected for three:

1) 80-56-8: alpha-Pinene (non-specified mixture of below substances)

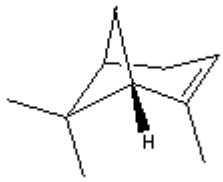
2) 7785-26-4: (-)-alpha-Pinene

3) 7785-70-8: (+)-alpha-Pinene

Both enantiomers, (-)-alpha-pinene and (+)-alpha-pinene, are present in natural oils.

Chemical name	alpha-Pinene
Synonym [1)]	2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene 2-Pinene Acitene A alpha-Pinene Cyclic dexadiene pin-2(3)-ene
CAS-No.	80-56-8
EINECS No.	201-291-9
Molecular formula	$C_{10}H_{16}$
Molecular structure	
Legislation:	
Classification according to list of dangerous substances	Not on the list
Lists of undesirable substances……	No
IUCLID-dataset	Yes
Cosmetics	
Physical chemical properties:	
Melting point, °C	-64
Boiling point, °C	155
Vapour pressure (Pa)	Not identified
Physical state	Liquid
Octanol-water partition coefficient, (log Pow)	4.83
Water solubility (mg/L)	Not identified
Chemical name [19]	(1S)-(-)-alpha-Pinene
Synonym [1)]	(1S)-(1)-alpha-Pinene (1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene (1S)-(-)-alpha-Pinene (-)-alpha-Pinene Dipentene Pinen
CAS-No.	7785-26-4
EINECS No.	232-077-3
Molecular formula	$C_{10}H_{16}$
Molecular structure	

[1] www.chemfinder.com

Legislation:	
Classification as per list of dangerous substances	Not on the list
List of undesirable substances.	No
IUCLID-dataset	No
Cosmetics	
Physical chemical properties	
Melting point, °C	-64
Boiling point, °C	155 - 156
Vapour pressure (Pa)	NA
State	Liquid
Octanol-water partition coefficient, (log Pow)	4.4 8)
Water solubility (mg/L)	NA
Chemical name [29]	(1R)-2,6,6-trimethylbicyclo[3.1.1]hept-2-ene
Synonym [1)]	(+)-alpha-Pinene (1R)-(+)-alpha-Pinene (1R)-2,6,6-trimethylbicyclo[3.1.1]hept-2-ene
CAS-No.	7785-70-8
EINECS No.	232-087-8
Molecular formula	$C_{10}H_{16}$
Molecular structure	
Legislation:	
Classification as per list of dangerous substances	Not on the list
List of undesirable substances	No
IUCLID-dataset	No
Cosmetics	
Physical/chemical properties	
Melting point, °C	-62
Boiling point, °C	155
Vapour pressure (Pa)	Not identified
Physical state	Not identified
Octanol-water partition coefficient, (log Pow)	Not identified
Water solubility (mg/L)	Not identified

Available information on toxicity related to inhalation:

The substance may cause the same effects as turpentine. The substance may, if inhaled in high concentrations cause heart beat, dizziness, disturbance of the nervous system, chest pain, bronchitis and inflammation of the kidneys (Gosselin ***et al.*** 1984).

Alpha-Pinene is toxic to rats and mice when inhaled (Lewis 1999).

[2] www.chemfinder.com

For humans there are no subjective inconveniences or influence of the lung function by inhalation of alpha-pinene at concentrations of 450 mg/m^3. The main relative blood uptake of the substance was 62% of the amount supplied (Edman ***et al***. 2003; Filipson 1996).

The substance may cause irritation in the lungs (Rohr ***et al***. 2002).

An inhalation study with mice shows that the substance causes irritation in the upper respiratory tract (reduced respiration rate) at doses between 100 and 3691 ppm (Nielsen ***et al***. 2005). Limit value for effect from (+)-alpha-pinene is 70 ppm, equivalent to GV dose of 40 ppm for humans. At concentrations above 200 ppm, contraction of the respiratory tract is seen. NOEL for sensory irritation is 72 ppm.

At concentrations of (+/-)-alpha-pinene below 81 ppm there was no contraction of the respiratory tract in humans. Neither (+) or (–)-alpha-pinene below 82 ppm has shown any effect on the central nervous system in humans (Falk ***et al***. 1990).

Animal inhalation studies show that at 6-12 g/m^3 there is irritating effect of the respiratory tract for (+)- alpha-pinene, but not for (–)-alpha-pinene. No risk for harmful health effects on humans (Mersch-Sundermann 2007).

Inhalation of alpha-pinene has a moderate effect on the autonomic nervous system resulted in increased blood pressure and increased concentration of stress hormones in the blood (catecholamine) (Haze ***et al***. 2002).

The following animal toxicological data have been identified in IUCLID:

- LC_{LO} (inhalation, rat) = 625 µg/m^3
- LC_{LO} (inhalation, porpoise) = 572 µg/m^3
- LC_{LO} (inhalation, mouse) = 364 µg/m^3.
- (LC_{LO} = lowest concentration at which death occurred)

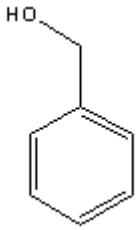
Limit values for alpha-pinene
AT limit value (AT 2007): None

NIK (AgBB 2005): 1400 µg/m^3

LCI (Jensen ***et al***. 2001): 250 µg/m^3 (CAS No.: 80-56-8)

NOEL for lung symptoms: 25 mg/m³ (Larsen ***et al***. 1999).

5.2.3 Benzyl alcohol

Chemical name	Benzyl alcohol
Synonym	alpha-Hydroxytoluene alpha-toluenol Benzyl alcohol Benzenecarbinol Benzenemethanol Benzoyl alcohol (hydroxymethyl)benzene Hydroxytoluene Phenylcarbinol Phenylmethanol Phenylmethyl alcohol
CAS-No.	100-51-6
EINECS No.	202-859-9
Molecular formula	C_7H_8O
Molecular structure	
Legislation: Classification as per list of dangerous substances List of undesirable substances. IUCLID-dataset Cosmetics	 Xn;R20/22 (at conc.>=25%) No Yes The fragrance is declared in cosmetics if used in quantities above 0.01% in products that are cleaned and 0.001% in products that are not cleaned.
Physical/chemical properties: Melting point, °C Boiling point, °C Vapour pressure (Pa) Physical state Octanol-water partition coefficient, (log Pow) Water solubility (mg/L)	 -15.3 205 not identified oily liquid 1.10 4.29 g/100 mL

Available information on toxicity related to inhalation

Vapours may cause irritation of eyes, nose and throat (US Coast Guard referred in HSDB and RTECS). Vapours cause irritation in eyes, nose and throat with cough and bad throat, but there is no quantitative data and benzyl alcohol is not classified as irritant. (Koniezko and Czerczak 2003).

According to Cosmetic Ingredient Review the substance is not carcinogenic or genotoxic (CIR 2001).

There is uncertainty as regards the human toxicological data. The following has been identified in RTECS (2007 data without reference) regarding inhalation:

- LC_{50} (mouse, inhalation): > 500 mg/m^3.

- LC_{100} (rat, inhalation, 8 hours): 200 - 300 ppm - a value that must be seen in relation to the following value which is also referred to in (RTECS, data without reference. 2007):

- LC_{50} (rat, inhalation, 8 hours): 1000 ppm, also referred to as LC_{Lo}(RTECS, data without reference. 2007).

According to IUCLID there is the following data for inhalation:

- LC_{50} (rat, inhalation, 4 hours): results range from >4,178 to >9 mg/l.

Vapour from the substance is assessed to be able to penetrate intact skin (Opdyke 1979).

Inhalation of the substance may cause cough, dizziness and headache (IPCS, 2000).

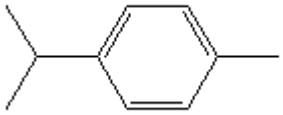
The substance has only caused negative results in Ames Tests (CCRIS database, 2007).

Limit values for benzyl alcohol
AT Limit values (AT 2007): None

NIK (AgBB 2005): 440 µg/m^3

LCI (Jensen ***et al***. 2001): 100 µg/m^3.

5.2.4 p-Cymene

Chemical name	p-Cymene
Synonym	1-Methyl-4-isopropylbenzene 1-Methyl-4-isopropylbenzene para-Cymene 4-isopropyltoluene p-methyl cumene 4-methyl isopropylbenzene Cymol Dolcymene Methyl-4-(1-methylethyl)benzene
CAS-No.	99-87-6
EINECS No.	202-796-7 [3)]
Molecyle formula	$C_{10}H_{14}$ [1)]
Molecyle structure	 1)
Legislation: Classification as per list of dangerous sub-stances List of undesirable substances. IUCLID-dataset Cosmetics	 Not on the list No Yes
Physical/chemical properties: Melting point, °C Boiling point, °C Vapour pressure (Pa) Physical state Octanol-water partition coefficient, (log Pow) Water solubility (mg/L)	 -67 176 - 178 Not identified Flammable liquid 4.10 Unsolvable

Available information on toxicity related to inhalation
Vapours have been assessed not to cause irritation in the throat (IPCS 2000).

Inhalation is mentioned to cause dizziness, drowsiness and vomiting, but there is no information about concentration (NIOSH 1997).

Inhalation tests with humans show a significant increase in amylase content in sputum, which seems to be provoked by stimulation of the olfactory nerve rather than nerves in the respiratory tract (Hanawa 2007).

Rat inhalation tests with 0.50 and 250 ppm for 4 weeks show changes in the brain that resemble the toxicity of solvents (Lam 1996).

Rats and porpoise inhalation, 100 mg/kg. During 48 hours 60-80% of the dose had been eliminated through urine in form of 18 metabolites (Walde 1983).

[3] http://ecb.jrc.it/esis/index.php?PGM=ein

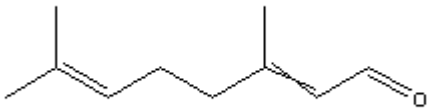
The following human toxicological data for inhalation has been identified for the substance:

LC_{50} (mouse, inhalation) = 19,500 mg/m^3 (RTECS, data without reference. 2007).

Limit values

AT Limit values (AT 2007): 25 ppm, 135 mg/m^3
NIK (AgBB 2005): None
LCI: None

5.2.5 Citral

Chemical name	Citral
Synonym	3,7-Dimethyl-2,6-octadienal cis-3,7-Dimethyl-2,6-octadienal cis-Citral' cis/trans-3,7-Dimethyl-2,6-octadienal Citral A Citral B Citral, mixture of cis and trans CITRAL NATURAL CITRAL SINTETICO Geranal Geranial Geranialdehyde Lemarome n Neral trans-3,7-Dimethyl-2,6-octadienal
CAS-No.	5392-40-5
EINECS No.	226-394-6 [4)]
Molecular formula	$C_{10}H_{16}O$
Molecular structure	
Legislation: Classification as per list of dangerous substances List of undesirable substances. IUCLID-dataset Cosmetics	 Xi; R38 - R43 Yes Yes The fragrance is declared in cosmetics if used in quantities above 0.01% in products that are cleansed off and 0.001% in products that are not cleansed off.
Physical/chemical properties: Melting point, °C Boiling point, °C Vapour pressure (Pa) Physical state Octanol-water partition coefficient, (log Pow) Water solubility (mg/L)	 < 20 [5)] 225 5) < 100 at 50 degrees C Liquid Not identified 0.01 - 0.1 g/100 ml at 18 degrees

Available information on toxicity in relation to inhalation

Inhalation tests with pregnant rats during 6-15 days with 10, 35 and 68 ppm. The pregnant animals show toxic effects at 68 ppm, but no effect on foetus has been observed at this concentration. The substance is not teratogenic (Gaworksi ***et al***. 1992).

[4] http://ecb.jrc.it/esis/index.php?PGM=ein
[5] IUCLID dataset on http://ecb.jrc.it

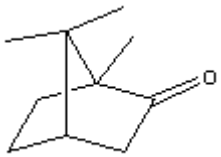
Rat/mouse inhalation tests give LC_{50} of 12,500 ppm. The substance is moderately toxic (Luo ***et al***. 2005).

The substance is in the Chemical Carcinogenesis Research Information System (CCRIS) referred with negative Ames Tests and has not been assessed by IARC.

According to York ***et al***. (1989) the substance is not teratogenic.

Limit values
Limit value (AT 2007): None
NIK (AgBB 2005): None
LCI: None.

5.2.6 Camphor

Chemical name	Camphor
Synonym [1)]	(±)-Camphor 1,7,7-Trimethylbicyclo[2.2.1]-2-heptanone 1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one 1,7,7-Trimethylnorcamphor 2-Camphanone 2-camphonone Camphore Caladryl Camphor Oil Gum camphor Radian B
CAS-No.	76-22-2
EINECS No.	200-945-0
Molecular formula	$C_{10}H_{16}O$
Molecular structure	
Legislation: Classification as per list of dangerous substances List of undesirable substances. IUCLID-dataset Cosmetics	 Not on the list No No
Physical chemical properties: Melting point, °C Boiling point, °C Vapour pressure (Pa) Physical state Octanol-water partition coefficient, (log Pow) Water solubility (mg/L)	 177 207 Liquid 2.38 0.12 g/100 mL

Short summary on available information on toxicity in relation to inhalation
Nose in and expiratory resistance was not changed by inhalation of the substance by humans (Eccles ***et al***. 1987).

Five minutes inhalation provokes a subjective sense of chill and improved air flow through the nose. The substance stimulates chill receptors in the mucous membrane in the nose (Burrow ***et al***. 1983).

Inhalation of concentration above 2 ppm may cause irritation in nose and throat (IPCS 1989).

At concentrations above 6 mg/m^3 the substance may cause serious health effects on animals (OHSA, 1989).

Porpoise inhalation tests at 500 µg/l reduce chemically provoked cough reflex. At lower concentrations no effect was observed (Laude ***et al***. 1994).

According to HSDB web the substance is not carcinogenic and IARC has not evaluated the substance.

The following human toxicological data have been identified:

- LC_{50} (rat, inhalation) = 500 mg/m^3 (RTECS data without reference, 2007)

- LC_{50} (mouse, inhalation) = 450 mg/m^3 (RTECS data without reference, 2007).

Limit values

Limit value (AT 2007): 2 ppm, 12 mg/m^3
NIK (AgBB 2005): None
LCI (Jensen ***et al***. 2001): 250 µg/m^3

5.3 Exposure to selected substances by inhalation

Concentrations of the selected substances in the model room calculated based on tests in the climate chamber can be seen in table 5.1. What is indicated is an average concentration for four hours after start. For calculation of the average concentration during the four hours the exposure model, presented in chapter 3, has been used. It is assumed that the substances are emitted with a constant rate for 2 hours and that the concentration in the room, subsequently, will gradually decrease due to air circulation.

As background for the calculations, data for those of the tested oils - in each of the experimental setups - where the substances have the highest concentration has been used. have been used in each arrangement

In order to take the uncertainty on the interpretation of the measuring results into account, the calculated values are both based on actual emission tests and worst case scenarios.

Concentrations in model rooms based on actual tests
The emission rate during the first two hours is calculated differently for the two setups.

For the tests with the candle diffuser it has been assumed that the emission during the 2 hours is at the same level as measured in the period 15-25 minutes. From the measurements it is obvious that this is not the case - after 2 hours the emission is considerably lower. By the calculation it is considered that there will be an inherent tendency that the measured rates are lower than the actual rates as a steady state has not yet been established in the climate chamber.

For the tests with Aroma Stream a regression line has been used as described in chapter 4.5.1.

"Worst case" scenario based on examined oils

It seems to be quite certain that the emission of substances is considerably larger than the quantities collected and measured but it is not obvious why. The differences may be due to a combination of many factors: the substances are broken down or creating reaction products before the measurement; the collection is not efficient because some of the substances are absorbed by water particles; the measuring uncertainty is biased, or a steady state in the test chamber has not yet been established before the first measurement and the emission is consequently underestimated. For Aroma Stream an alternative explanation could be that the substances are absorbed to the filter, but this has not been confirmed by a simple weight loss test. It can thus not be rejected that the actual emissions would be higher, and as the oxidation products for several of the substances have been demonstrated to also have sensitizing effects on the respiratory tract, there is, to be on the safe side in the assessments, used a worst case where 50% is emitted during the first hours.

As a result of the measuring results for tea tree oil in Aroma Stream shown in figure 4.2, there will be a difference depending on how large a part is actually emitted, but the data material is too vague to make precise calculations for each substance.

In the table is also given AT limit values and LCI and NIK values used for assessment of exposure level in the indoor climate.

Table 5.1
Concentration of selected substances calculated based on measurement in climate chambers.

Substance	Product	Concentration in product %	Concentration in model room based on measurements (average first 4 hours), µg/m³ *1	Worst case concentration in model room (average first 4 hours), µg/m³ *2	AT limit value µg/m³	LCI µg/m³	NIK µg/m³
Experiments with candle diffuser:							
d-Limonene	No. 34	20.5	> 190	665	75 ppm (tentative)	300	1,400 *3
alpha-Pinene	Rosemary oil	11.5	175	580		250	
Camphor	Rosemary oil	11	25	560	2 ppm 12,000 (synthetic)	250	
Citral	No. 34	1.9	0.2	60			
p-Cymene	Rosemary oil	2.2	12.7	110	25 ppm 135,000		
Benzyl alcohol	Rosemary oil	0.1	<0.1 *4	10		100	440
Experiments with Aroma Stream: *2							
d-Limonene	Tea tree oil	1.1	20	60	75 ppm (tentative)	300	1,400 *3
alpha-Pinene	Tea tree oil	2.3	100	120		250	
Camphor	-	-	-	-			
Citral	Tea tree oil	0.5	0	30			
p-Cymene	Tea tree oil	2.5	35	130	25 ppm 135,000		
Benzyl alcohol	No. 38	0.6	0.2 *4	25		100	440

*1 The concentrations for fragrance oils have been calculated based on the assumption that the emission continues for two hours with the same rate as measures in the period 15-25 minutes. The emission for Aroma Stream has been calculated based on the regression line between the two measuring points in 20 min and 130 minutes, respectively.

*2 Worst case concentration is for both scenarios calculated by roughly estimating that 50% of the substances in the added oil has been emitted and are in the room either in form of pure substances or reaction products.

*3 NIK values for limonene (CAS No. 138-86-3).

*4 There is no explanation to the measured low values for benzyl alcohol, but the result should be interpreted with caution.

"Worst case" scenario based on oils with the highest concentration

The oils that have been included in the climate chamber tests are not necessarily the oils with the highest concentration. For example is the highest concentration of d-limonene in the examined oils 20.5% in no. 34, but the concentration of the d-limonene in citrus oil was measured to 72.5%. It must thus be expected that there could be a considerably higher concentration in the model room if citrus oil was used in the setups.

In view of describing a "worst case scenario", a calculation has been made using the exposure model using the highest registered concentration of the substance in any product. For products where the concentration in safety data sheets has been indicated with an range the highest value in the range has been used. It has been assumed that for the setups 0.4 g product is added

equivalent to 10 drops (based on the measured average of the 10 climate chamber tests).

It has furthermore been assumed that 50% of the quantity of each substance added evaporates to the room during a 2 hour period. There are several circumstances indicating that the actual emission rates could be of that size even though it would vary from substance to substance depending on the substances' physical/chemical properties. Alternatively you could argue for a worst case scenario where 100% is emitted, but this does not seem to be the case in the actual use situations.

The average concentration of a number of terpenes (d-limonene, alpha-pinene, camphene, p-mentha-1.4-diene, p-mentha-1.3-diene, beta-pinene and 3-carene) during the first four hours is considerably above the LCI values. The highest concentration is for d-limonene in citrus oil, where the concentration in the room is more than 10 times higher than the LCI value.

For diethyl phthalate the average concentration is 2,400 µg/m^3 close to the Danish Working Environment Agency's limit value of 3,000 µg/m^3.

Table 5.2
Worst case scenario where it is assumed that half of the added quantity of substance is emitted during the first two hours.

Substance	Example of product *1	Maximum concentration in product % *2	Concentration in model room (average first 4 hours) µg/m³ *3	AT limit value µg/m³ or ppm	LCI µg/m³ *4	NIK µg/m3 *4
d-Limonene	lemon oil	72.5	3,490	75 ppm (tentative)	300	1,400*1
alpha-Pinene	Pine needle oil	50	2,400		250	1400
p-Cymene	Tea tree oil	2.5	120	25 ppm 135,000		
Benzyl alcohol	No. 15	10	480		100	440
Camphor	Rosemary oil	11	530	2 ppm 12,000 synthetic	250	
Citral	Lemongrass oil	75.5	3,630			
Dietylphthalat	No. 39	50	2,400	3,000		
Myrcene	Orange oil	2.5	120		1000 *4	
n-Decalaldehyd	No. 34	5	240		400	1400
Camphene	Rosemary oil	10	480		250	
beta-Caryophyllene	Nutmeg oil	5	240		1000 *4	
p-Mentha-1,4-diene	Camphor oil	20	960		250	
p-Mentha-1,3-diene	Camphor oil	10	480		250	
p-Mentha-1,4(8)-diene	Tea tree oil	5	240		1000 *4	
beta-Pinene	Lemon oil	20	960		250	1400
3-Carene	Pine needle oil	20	960		250	1400

*1 Examples of products where the substance has the highest concentration; the substance may be present in similar concentrations in other products.

*2 Represents highest reported concentration in safety data sheets or actual measurements. In cases where the safety data sheet indicated ranges the highest value of the range is listed.

*3 It has been estimated that 0.4 g product is used, equivalent of 10 drops (average of measurements at climate chamber tests). It is assumed that 50% of the added quantity of the substance is emitted to the air during 2 hours. The concentration shows a total concentration of the substance and possible reaction products.

*4 Based on Jensen *et al.* 2001. For substances marked with *4 there is no values in Jensen *et al.* 2001, and instead the LCI values from ECA-IAQ (1999) have been listed.

5.4 Risk assessment of health aspects

The risk assessment of health aspects for the six examined substances is very difficult to carry out. Partly there is not sufficient data from human inhalation tests; partly the measured concentrations and the calculated ***worst case scenario*** values are very uncertain. The risk assessment has consequently been made on an uncertain basis and must be taken with many different reservations for the results and conclusions of the assessment.

Lacking and defective data in literature

By going through the literature and by personal inquiries to Danish and foreign experts, not much useful and valid information about the six examined substances have come forward on the health effects by inhalation.

For two substances, d-limonene and alpha-pinene there are systematic reviews of inhalation tests in humans. For the other four substances, the information is very scarce and defective. One substance, benzyl alcohol, has been classified as hazardous by inhalation in concentrations above 25%. For several of the substances there are experimental tests of inhalation by rats and mice. Based on these animal tests, the LCI values have been calculated by using correction factors 100 and 1000. It is problematic to use these surveys as a scientific basis for a risk assessment of health impacts.

The Danish experts with expertise in climate chambers and indoor climate problems have no supplementary information about health effects caused by inhalation of the six selected substances. Dr. Elberling from the Danish Research Centre for Chemical Sensitivities says that according to a Danish survey there are people who get nuisance in the upper and/or lower respiratory tract by inhalation of fragrance and these persons have a so-called "bronchial hyper-reaction" meaning that they - as a contracts to none-hypersensitive persons - react with contractions in the respiratory tract when tested with specific substances. This hyper activity is not related to an allergic reaction such as asthma. It is uncertain whether the mentioned fragrances contain any of the six tested substances.

Missing data for standards
There is insufficient information for the current standards for the six substances. There are AT limit values for three of the substances valid for the working environment i.e. 8 hours exposure per day. Otherwise there are LCI/NIK values for respectively five and three of the substances used for indoor climate assessments. These values relate to exposure in the indoor climate 24 hours a day, 7 days a week.

There is a considerable difference between the Danish LCI-values and the German NIK-values with a factor 5 difference for d-limonene and alpha-pinene, and a factor 4 for benzyl alcohol. It is not obvious what the differences are due to, but it illustrates that caution should be taken when health assessments are based on these values.

There is a considerable quantitative difference of up to 300 times between the AT limit values and the LCI values which is linked to the different exposure situations the values are used for.

Uncertainty in own test results
The quantitative climate chamber tests of concentration of the six substances during evaporation from Aroma Stream and candle diffusers have an uncertainty that makes it difficult to determine a concentration as basis for the risk assessment of health impacts as it is not obvious in which form the substances are.

Selection of LCI-value as a basis for health related risk assessment
The risk assessment is based on LCI values for the five substances whereas there is no immediately accessible values for citral. It is estimated that concentrations listed as LCI values are so low that they should be considered as safe for a health assessment at a maximum 4 hours exposure by inhalation.

The definition of LCI is described in chapter **Fejl! Henvisningskilde ikke fundet.**. For several of the substances the LCI value is determined based on the very poor knowledge on effects. There are considerable safety margins used by the determination of the LCI. Irritation was the most decisive health effect

of the substances for the determination of the LCI value. More serious health effects were found at a much higher concentrations.

We have found one single (human) NOEL value for lung symptoms for alpha-pinene at 25,000 µg/m³. This value equals the set LCI value for the substance with a safety factor of 100. This example again shows that the LCI-values are considered to be very certain for this risk assessment.

Health related risk assessment has been made for:

- (A) calculated concentrations in model rooms based on actual measurements in climate chamber tests for the six examined products;
- (B) calculated "worst case" concentrations in model room based on climate chamber test for the six examined products;
- (C) calculated "worst case" concentrations in model rooms for products with highest content of the six substances based on information of concentrations on safety data sheets.

A. The calculated concentrations above 4 hours in model rooms (table 5.1) are all below the listed LCI values, for d-limonene and alpha-pinene, however the concentrations are of the same size. For p-cymene, benzyl alcohol and camphor one to two times lower. There is consequently not expected to be any health risk related to the intended use.

B. The calculated "worst case" concentrations in model rooms (table 5.1) are approximately twice as high as the LCI values for d-limonene, alpha-pinene and camphor, whereas they are about the LCI value for p-cymene and benzyl alcohol. Under these circumstances a health risk for the first mentioned three substances cannot be ignored completely - it is however very limited - but it is assessed that there will be no risk for the remaining three.

C. Here the listed concentrations for d-limonene and alpha-pinene exceed the LCA value with at factor 10, for benzyl alcohol with a factor 5 and camphor a factor 2 (table 5.2). Similar exceeding is seen for at number of other substances that are not further assessed here. The exceeding indicates a possible; however low health risk at constant exposure in the indoor climate. Bearing in mind that the NOEL value for lung effects in humans is approx. 25,000 µg/m3 there is a good safety margin, at least for alpha-pinene/terpenes.

Assessment of toxicity

For none of the substances a significant toxicity has been observed, neither in human inhalation tests nor in animal inhalation tests.

Assessment of irritating effects on the respiratory tract

For several of the substances there have been described irritating effects on humans and animals but only at high concentrations.

D-limonene in a (high) concentration of 450,000 µg/m^3 causes a reduction of the lungs vital capacity for humans. At high concentration it causes a fall in the respiration rate in rats. These effects have been observed at extremely high concentrations.

D-limonene and alpha-pinene are known as potential irritant for the respiratory tract after oxidation, e.g. with ozone. In this process ultrafine particles are created.

By inhalation of camphor, test persons experience a sensation of chill in the nose with a better air passage. Objective measurements have not been able to confirm an improvement of the nose's air flow. The sensation of chill is due to influence of the nervous receptors in the mucous membranes in the nose

Assessment of sensitizing
None of the examined substances has a respiratory sensitizing effect. In 2008 on Institute for Research on Fragrance Materials (IRFM) a study is planned of benzyl alcohol's possible sensitizing/allergic effect on the respiratory tract.

Assessment of systemic and other biological effects
When inhaled, all substances are quickly absorbed in the blood. Adult test persons who inhaled d-limonene while they were doing a light manual labour of 50 W (expression of working intensity), 70% of the given dose was found in the blood after 2 hours. A large part of the substances are subsequently absorbed into the fatty tissue. They are transformed to other chemical substances (metabolites) and the major part is excreted through the kidneys. A small part of the inhaled dose is found in the expired air.

Inhalation of camphor by humans showed sign of stimulation of the autonomic nervous system in form of increased blood pressure immediately after inhalation whereas other fragrances have the opposite effect. Inhalation of d-limonene and alpha-pinene causes increased blood pressure and a stress-like condition in rats.

There have not been described any biological effects on other organs.

For none of the examined substances any carcinogen, genotoxic or foetus damaging effects have been observed.

Discussion
This risk assessment focuses primarily on health effects as a consequence of a short (2-4 hours) inhalation of one single substance. It is not likely that health effects arise long time after a short-period inhalation. But the possibility for a long-term health effect, such as chronic bronchitis or pneumonia, emerging after repeated short-period inhalations over a longer time period cannot with certainty be precluded. According to literature and contacted experts there is however no basis for this assumption.

Most aromatherapy oils contain several active substances that are inhaled during the treatment. The risk assessment only concentrates on one of the active substances. This makes a health assessment further complicated and uncertain because several substances in one and same aroma oil product may have different, partly additive or reverse health effects by inhalation.

This risk assessment, comparing the measured concentrations in a climate chamber with a fixed LCI value, does not consider a group of people reacting with respiratory symptoms by exposure to fragrances in a very low concentration as e.g. persons with multiple chemical sensitivity.

Conclusions
The results of the survey do not indicate that, apart from people being sensitive to fragrances, there are considerable health problems by inhalation of a-

romatherapy oils occasionally with the reservation that only a limited number of constituents have been examined. On the contrary, based on the results of the examination it cannot be rejected that daily use of 5-10 drops of oil in a small room for a prolonged period in the long term may result in airway irritation.

Recommendations

It is thus recommended, until more certain results are available, that small quantities are used, to ventilate the room carefully air when the fragrance effect is no longer wanted and that use of fragrance oil is not a daily occurrence.

It is recommended that the consumers only use oil specifically recommended by the producers for this purpose and follow the recommendations given on the packaging. It is also recommended that before using a diffuser candle or diffuses the fragrances in another way to read the safety recommendations given by the producers and suppliers at their web-sites or given in books on the subject.

It is recommended that more and better climate chamber and inhalation tests on humans are made if there is a suspicion of health effects on humans. Targeted provocation tests can also be made as the expertise and interest for the problem is present among Danish experts. It is recommended that further research is made on the possible effects of long term impact of inhalation of aroma substances in concentrations relevant in the indoor climate and on the effects of simultaneously exposure to a long series of chemical substances.

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Appendix 1: 26 fragrances covered by Directive 2003/15/EC

Name according to Directive 2003/15/EC	CAS No.
Amyl cinnamal	122-40-7
Amylcin namyl alcohol	101-85-9
Anisyl alcohol	105-13-5
Benzyl alcohol	100-51-6
Benzyl benzoate	120-51-4
Benzyl cinnamate	103-41-3
Benzyl salicylate	118-58-1
2-(4-tert-Butylbenzyl)propionaldehyde	80-54-6
Cinnamal	104-55-2
Cinnamyl alcohol	104-54-1
Citral	5392-40-5
Citronellol	106-22-9
Coumarin	91-64-5
d-Limonene	5989-27-5
Eugenol	97-53-0
Farnesol	4602-84-0
Geraniol	106-24-1
Hexyl cinnam-aldehyde	101-86-0
Hydroxy-citronellal	107-75-5
Hydroxy-methylpentyl-cyclohexenecarboxaldehyde	31906-04-4
Isoeugenol	97-54-1
Linalool	78-70-6
Methyl heptin carbonate	111-12-6
3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	127-51-5
Oak moss extract	90028-68-5
Treemoss extract	90028-67-4

Appendix 2: Constituents of a number of essential oils

On a homepage for a British fragrance producer, The Good Scents Company (http://www.thegoodscentscompany.com/) there are detailed lists of the composure of constituents of more than 60 different essential oils.

The lists are taken from various scientific articles referred to in the American magazine Perfumes & Fragrances (P&F). As the content of chemical substances in essential oils will vary according to the specific sort of the plan, growth conditions, climate conditions, etc. there will be a variation in the composure, but the lists gives a good hint on what to expect.

Lemongrass oil

Lemongrass oil. Cas No 8007-02-1

Content i %	Substance
22,7	beta-caryophyllene
18,5	T-cadinol
10,3	(E)-alpha-bergamotene
10,1	alpha-humulene
8,3	eugenol
5,4	(E)-methyl cinnamate
3,4	cubenol
3,2	linalool
2,8	spathulenol
2,2	caryophyllene oxide
2,1	gamma-cadinene
0,8	(Z)-delta-bisabolene
0,6	alpha-copaene
0,4	beta-elemene
trace	methyl chavicol

References:

C-K. Shu and B. M. Lawrence, Reasons for the variation in composition of some commercial oils. In: Spices, Flavor chemistry and antioxidant Properties. Edits., S. J. Risch and C-T. Ho, pp. 183-195, Amer. Chem. Soc. Symposium Series 660, A.C.S., Washington (1997).

P&F 23, No. 4, 37, (1998) Allured Publishing Corporation, Carol Stream, IL.

Lemon oil

Lemon oil, California. CAS No. 8008-56-8

Content i %	Substance
65,65	limonene + 1,8-cineole + (E)-beta-ocimene
11,13	beta-Pinene
8,32	gamma-terpinene
1,85	sabinene
1,75	alpha-Pinene
1,58	Myrcene
1,18	geranial
0,74	neral
0,6	neryl acetate
0,55	beta-bisabolene
0,52	geranyl acetate
0,38	(E)-alpha-bergamotene + citronellyl propionate
0,38	alpha-thujene
0,34	Terpinolene
0,22	beta-caryophyllene

Content i %	Substance
0,16	alpha-terpinene
0,16	alpha-terpineol
0,14	para-Cymene
0,13	(Z)-sabinene hydrate + linalool
0,12	nonanal
0,11	terpinen-4-ol
0,09	(E)-beta-ocimene
0,08	citronellal
0,08	octanal
0,06	camphene
0,06	citronellol + nerol
0,05	decanal
0,04	alpha-bisabolol
0,04	alpha-phellandrene
0,03	(Z)-alpha-bergamotene
0,03	campherenol
0,03	citronellyl acetate
0,03	2,3-dimethyl-3-(4-methyl-3-pentenyl)-2-norbonanol
0,03	(E)-beta-farnesene
0,03	geraniol
0,03	perillaldehyde
0,03	undecanal
0,02	alpha-humulene
0,01	borneol
0,01	exo-(Z)-4,7-dimethyl bicyclo(3.2.1)oct-3-en-6-one
0,01	dodecanal + decyl acetate
0,01	geranyl propionate
0,01	(E)-sabinene hydrate + octanol
0,01	beta-santalene
0,009	undecyl acetate
0,008	camphor
0,007	(E)-limonene 1,2-oxide
0,007	methyl geranate
0,007	neryl propionate
0,006	(Z)-limonene 1,2-oxide
0,004	No. 50dol
0,004	piperitone

References:

T. S. Chamblee, B. C. Clark. G. B. Brewster, T. Radford and G. A. Iacobucci, Quantitative analysis of the volatile constituents of lemon peel oil. Effects of silica gel chromatography on the imposition of its hydrocarbon and oxygenated fractions. J. Agric, Food Chem., 39, 162-169 (1991).
P&F 17, No. 1, 45, (1992) Allured Publishing Corporation, Carol Stream, IL.

Rosemary oil

Rosemary oil, Morocco. CAS No: 8000-25-7

Content i %	Substance
9,56-12,72	alpha-Pinene
7,42-10,80	camphor
5,53-7,83	beta-Pinene
43,53-53,48	1,8-cineole
3,21-3,98	camphene
3,00-4,51	borneol
2,41-4,32	beta-caryophyllene
1,86-2,06	limonene
1,27-1,60	Myrcene
0,99-1,40	para-Cymene
0,93-1,19	gamma-terpinene
0,73-1,76	linalool
0,69-0,91	terpinen-4-ol
0,52-0,66	alpha-terpinene
0,37-0,51	beta-farnesene
0,29-0,36	Terpinolene
0,27-5,43	alpha-humulene
0,18-0,77	delta-cadinene
0,15-0,20	delta-3-carene
0,14-0,21	sabinene
0,12-0,86	bornyl acetate
0,10-0,23	tricyclene
0,08-0,98	alpha-cadinene
0,06-0,13	beta-bisabolene
0,04-0,19	(E)-sabinene hydrate
0,04-0,13	isopinocamphone
0,00-trace	6,6-dimethyl(3.1.1)bicyclohept-3-ene-2-butylene
0,00-trace	alpha-thujene
0,00-2,46	alpha-terpineol
0,00-0,80	alpha-santalene
0,00-0,46	verbenone
0,00-0,30	lavandulyl acetate
0,00-0,27	(Z)-beta-ocimene
0,00-0,23	lavandulol
0,00-0,13	germacrene D
0,00-0,13	gamma-muurolene
0,00-0,12	viridiflorene
0,00-0,11	T-cadinol
0,00-0,10	caryophyllene oxide
0,00-0,10	nerol
0,00-0,07	geranyl acetate
0,00-0,06	(E)-beta-ocimene
0,00-0,05	geraniol
0,00-0,02	linalyl acetate

References:

J. C. Chalchat, R. P. Garry, A. Michet, B. Benjilali and J. L. Chabart, Essential oils of rosemary (Rosmarinus officinalis L.). The chemical composition of the oils of various origins (Morocco, Spain, France). J. Essent. Oil Res., 5, 613-618 (1993).
P&F 20, No. 1, 47, (1995) Allured Publishing Corporation, Carol Stream, IL.

Rosemary oil, Spain. CAS No: 8000-25-7

Content i %	Substance
27,3	camphor
22,2	1,8-cineole
10,8	gamma-terpinene
9	borneol
6,3	verbenone
4,4	alpha-Pinene
3,8	alpha-terpineol
3,2	alpha-phellandrene
2,8	camphene
1,8	para-Cymene
1,7	beta-caryophyllene
1,6	terpinen-4-ol
1,4	bornyl acetate
1,3	linalool
1	sabinene
0,8	alpha-humulene
0,5	delta-3-carene
0,3	gamma-eudesmol
0,3	beta-Pinene
0,2	carvacrol
0,2	caryophyllene oxide

References:

C. Bourrel, G. Vilarem, G. Michel and A. Gase, Etude des proprietes bacteriostatiques et fongistatiques en milieu solide de 24 huiles essentielles preamblement analysees. Rivista Ital. EPPOS, (16), 3-12 (1995).
P&F 22, No. 5, 71, (1997) Allured Publishing Corporation, Carol Stream, IL.

Tea tree oil

Tea tree oil, Australia. CAS No: 68647-73-4

Content i %	Substance
41.1	1,8-cineole
8.7	alpha-terpineol
6.8	para-Cymene
5.9	Terpinolene
4.6	gamma-terpinene
4.1	limonene
3.6	linalool
3.2	alpha-Pinene
2.5	beta-caryophyllene
1.6	alpha-humulene
1.5	alpha-selinene
1.5	beta-selinene
1.5	terpinen-4-ol
1.2	guaiol
0.8	beta-Pinene
0.7	beta-eudesmol
0.6	gamma-eudesmol
0.6	alpha-terpinene
0.5	gamma-curcumene
0.5	alpha-phellandrene
0.4	cadina-1,4-diene
0.4	geraniol
0.3	caryophyllene oxide
0.3	beta-elemene
0.3	alpha-farnesene
0.3	beta-guaiene
0.3	alpha-ylangene
0.2	para-Cymenene
0.2	beta-phellandrene
0.1	Myrcene
trace	bulnesol
trace	delta-cadinene
trace	gamma-cadinene
trace	alpha-cadinol
trace	T-cadinol
trace	calamenene
trace	camphene
trace	delta-3-carene
trace	alpha-copaene
trace	delta-elemene
trace	gamma-elemene
trace	elemol
trace	alpha-maaliene
trace	alpha-muurolol

Content i %	Substance
trace	(E)-beta-ocimene
trace	(Z)-beta-ocimene
trace	beta-sesquiphellandrene
trace	sabinene
trace	thujopsene

References:

D. N. Leach, S. G. Wyllie, J. G. Hall and I. Kyratzis, Enantiomeric composition of the principal components of the oil of Melaleuca alternifolia. J. Agric. Food Sci., 41, 1627-1632 (1993).

P&F 22, No. 2, 59, (1997) Allured Publishing Corporation, Carol Stream, IL.

Appendix 3: Constituents of fragrance oils

The following lists of constituents of fragrance oils are based on safety data sheets from the producers of the oils. The data sheets only include constituents classified with one or several R-phrases.

CAS no	Chemical name (as indicated in MSDS)	Self classification	Weight-percent
No. 1			
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	0,1-1
112-54-9	duodecylaldehyde C.12	Xi;R38;N;R51/53	0,1-1
5989-27-5	(R)-p-mentha-1,8-diene	R10 Xi;R38 R43 N;R50/53	1-5
78-70-6	Linalool	Xi;R38	1-5
8028-48-6	Orange oil	Xn;R10;R43;R65	1-5
84929-61-3	carrotolie	R10 Xn;R65	1-5
90045-28-6	gaulterieolie (vintergrønt)	Xn;R22 Xi;R36 R43	5-10
91-64-5	2H-1-Benzopyran-2-On	Xn;R22;R43	5-10
No. 2			
106-24-1	2,6-Octadien-1-Ol, 3,7-dimethyl-	Xi;R38 R43	1-2
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	1-5
78-70-6	Linalool	Xi;R38	1-5
84238-39-1	patchouli oil	Xn;R65;	1-5
85085-61-6	bayolie	Xn;R22 R65	1-5
91-64-5	2H-1-Benzopyran-2-On	Xn;R22;R43	1-5
99811-75-3	Cedar wood oil	Xi;R43;Xn;R65;	1-5
84238-29-9	vetivert resinoid	Xi;R43	1-5
5989-27-5	(R)-p-mentha-1,8-dien	R10 Xi;R38 R43 N;R50/53	5-10
84776-65-8	Lavender oil	Xi;R43 Xn;R65	5-10
115-95-7	linalylacetat	Xi;R38	10-20
84929-31-7	citronolie	R10 Xi;R43	10-20
No. 3			
106-22-9	6-Octen-1-Ol, 3,7-dimethylpatchouli oil	Xi;R38 N;R51/53	0,1-1
84238-39-1	patchouli oil	Xn;R65;	1-5
89957-98-2	olibanum oil	R10 Xn;R65	1-5
99811-75-3	Cedar wood oil	Xi;R43;Xn;R65;	1-5
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	10-20
121-33-5	vanillin	Xi;R43	20-40
No. 4			
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	1-5
121-33-5	vanillin	Xi;R43	1-5
90082-51-2	Geranium oil	Xi;R43 Xn;R65	1-5
8028-48-6	Orange oil	Xn;R10;R43;R65	5-10
84238-39-1	patchouli oil	Xn;R65;	5-10
84929-31-7	citronolie	R10 Xi;R43	5-10
89957-91-5	bergamotolie	Xn;R65 Xi;R43	5-10
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	10-20
60-12-8	Benzenethanol	Xi;R36	10-20
No. 5			
104-54-1	Cinnamyl alcohol	Xi;R43	1-5

CAS no	Chemical name (as indicated in MSDS)	Self classification	Weight-percent
112-31-2	decylaldehyd C.10	Xi;R38;	1-5
112-53-8	1-Dodecanol	Xi;R38 N;R50/53	1-5
8028-48-6	Orange oil	Xn;R10;R43;R65	1-5
84238-39-1	patchouli oil	Xn;R65;	1-5
84929-31-7	citronolie	R10 Xi;R43	1-5
84961-50-2	Cove bud oil	Xi;R38 Xn;R21/22 R65	1-5
89957-91-5	bergamotolie	Xn;R65 Xi;R43	1-5
89998-15-2	citronelleolie	Xi;R43	1-5
90063-59-5	litsea-cubebaolie	Xi;R38	1-5
106-24-1	2,6-Octadien-1-Ol, 3,7-dimethylGeranium oil	Xi;R38 R43	5-10
90082-51-2	Geranium oil	Xi;R43 Xn;R65	5-10
99811-75-3	Cedar wood oil	Xi;R43;Xn;R65;	5-10
115-95-7	linalylacetat	Xi;R38	10-20
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	10-20
No. 6			
104-54-1	Cinnamyl alcohol	Xi;R43	1-5
112-31-2	decylaldehyd C.10	Xi;R38;	1-5
112-53-8	1-Dodecanol	Xi;R38 N;R50/53	1-5
8028-48-6	Orange oil	Xn;R10;R43;R65	1-5
84238-39-1	patchouli oil	Xn;R65;	1-5
84929-31-7	citronolie	R10 Xi;R43	1-5
84961-50-2	Cove bud oil	Xi;R38 Xn;R21/22 R65	1-5
89957-91-5	bergamotolie	Xn;R65 Xi;R43	1-5
89998-15-2	citronelleolie	Xi;R43	1-5
90063-59-5	litsea-cubebaolie	Xi;R38	1-5
106-24-1	2,6-Octadien-1-Ol, 3,7-dimethyllinalylacetat	Xi;R38 R43	5-10
115-95-7	linalylacetat	Xi;R38	5-10
90082-51-2	Geranium oil	Xi;R43 Xn;R65	5-10
99811-75-3	Cedar wood oil	Xi;R43;Xn;R65;	5-10
101-86-0	A-Hexylcinnamaldehyd	Xi;R43	5-10
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	10-20
No. 7			
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	1-5
97-54-1	Phenol, 2-methoxy-4-(1-propenyl)-	Xn;R21/22 Xi;R36/38 R43	1-5
115-95-7	linalylacetat	Xi;R38	5-10
120-57-0	heliotropin kryst.	Xi;R36/37/38	5-10
104-54-1	Cinnamyl alcohol	Xi;R43	10-20
107-75-5	Octanol, 7-hydroxy-3,7-dimethyl	Xi;R36-R43	10-20
60-12-8	Benzenethanol	Xi;R36	10-20
79-77-6	3-buten-2-one,4-(2,6,6,-trimethyl-1-cyclohexen-1-yl)-,(E)-	N;R51/53;	10-20
No. 8			
112-54-9	duodecylaldehyd C.12	Xi;R38;N;R51/53	0,1-1
121-33-5	vanillin	Xi;R43	1-5
122-78-1	fenylacetaldehyd	Xi;R43;	1-5
60-12-8	Benzenethanol	Xi;R36	1-5
106-22-9	6-Octen-1-Ol, 3,7-dimethyllinalylacetat	Xi;R38 N;R51/53	10-20
115-95-7	linalylacetat	Xi;R38	10-20
78-70-6	Linalool	Xi;R38	10-20
No. 9			
112-54-9	duodecylaldehyd C.12	Xi;R38;N;R51/53	1-5
84776-65-8	Lavender oil	Xi;R43 Xn;R65	1-5
84961-50-2	Cove bud oil	Xi;R38 Xn;R21/22 R65	1-5
89957-91-5	bergamotolie	Xn;R65 Xi;R43	1-5

CAS no	Chemical name (as indicated in MSDS)	Self classification	Weight-percent
90063-59-5	litsea-cubebaolie	Xi;R38	1-5
60-12-8	Benzenethanol	Xi;R36	5-10
78-70-6	Linalool	Xi;R38	5-10
8028-48-6	Orange oil	Xn;R10;R43;R65	5-10
84929-31-7	citronolie	R10 Xi;R43	5-10
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	10-20
No. 10			
115-95-7	linalylacetat	Xi;R38	1-5
121-33-5	vanillin	Xi;R43	1-5
5989-27-5	(R)-p-mentha-1,8-dien	R10 Xi;R38 R43 N;R50/53	1-5
60-12-8	Benzenethanol	Xi;R36	1-5
84929-79-3	styrax resinoid	Xi;R43	5-10
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	10-20
78-70-6	Linalool	Xi;R38	10-20
No. 11			
112-54-9	duodecylaldehyd C.12	Xi;R38;N;R51/53	0,1-1
104-54-1	Cinnamyl alcohol	Xi;R43	5-10
106-24-1	2,6-Octadien-1-Ol, 3,7-dimethyl-	Xi;R38 R43	5-10
78-70-6	Linalool	Xi;R38	5-10
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	10-20
122-40-7	Amylcinnamaldehyd	Xi;R38 R43	10-20
60-12-8	Benzenethanol	Xi;R36	10-20
No. 12			
100-51-6	benzylalcohol	Xn;R20/22 Xi;R43	1-5
115-95-7	linalylacetat	Xi;R38	1-5
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	1-5
120-57-0	heliotropin kryst	Xi;R36/37/38	1-5
5392-40-5	citral	Xi;R38 R43	1-5
84929-79-3	styrax resinoid	Xi;R43	1-5
78-70-6	Linalool	Xi;R38	5-10
106-22-9	6-Octen-1-Ol, 3,7-dimethylbergamotolie	Xi;R38 N;R51/53	10-20
89957-91-5	bergamotolie	Xn;R65 Xi;R43	10-20
No. 13			
112-54-9	duodecylaldehyd C.12	Xi;R38;N;R51/53	0,1-12
100-51-6	benzylalcohol	Xn;R20/22 Xi;R43	1-5
106-22-9	6-Octen-1-Ol, 3,7-dimethyldecylaldehyd	Xi;R38 N;R51/53	1-5
112-31-2	C.10	Xi;R38;	1-5
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	5-10
89957-91-5	bergamotolie	Xn;R65 Xi;R43	5-10
115-95-7	linalylacetat	Xi;R38	20-40
8028-48-6	Orange oil	Xn;R10;R43;R65	20-40
No. 14			
112-54-9	duodecylaldehyd C.12	Xi;R38;N;R51/53	0,1-1
100-51-6	benzylalcohol	Xn;R20/22 Xi;R43	1-5
122-00-9	para-metylacetofenon	Xn;R22	1-5
78-70-6	Linalool	Xi;R38	1-5
84929-79-3	styrax resinoid	Xi;R43	1-5
60-12-8	Benzenethanol	Xi;R36	5-10
89957-91-5	bergamotolie	Xn;R65 Xi;R43	5-10
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	20-40
No. 15			
112-54-9	duodecylaldehyd C.12	Xi;R38;N;R51/53	0,1-1
106-22-9	6-Octen-1-Ol, 3,7-dimethylpatchouli oil	Xi;R38 N;R51/53	1-5

CAS no	Chemical name (as indicated in MSDS)	Self classification	Weight-percent
84238-39-1	patchouli oil	Xn;R65;	1-5
84776-65-8	Lavender oil	Xi;R43 Xn;R65	1-5
99811-75-3	Cedar wood oil	Xi;R43;Xn;R65;	1-5
100-51-6	benzylalcohol	Xn;R20/22 Xi;R43	5-10
103-95-7	cyclamenaldehyd	Xi;R38 N;R51/53	5-10
115-95-7	linalylacetat	Xi;R38	5-10
121-33-5	vanillin	Xi;R43	5-10
60-12-8	Benzenethanol	Xi;R36	5-10
78-70-6	Linalool	Xi;R38	5-10
91-64-5	2H-1-Benzopyran-2-On	Xn;R22;R43	5-10
89957-91-5	bergamotolie	Xn;R65 Xi;R43	10-20
No. 16			
112-30-1	1-Decanol	Xi;R36/38 N;R51/53	1-5
115-95-7	linalylacetat	Xi;R38	1-5
89957-91-5	bergamotolie	Xn;R65 Xi;R43	1-5
8028-48-6	Orange oil	Xn;R10;R43;R65	5-10
78-70-6	Linalool	Xi;R38	10-20
No. 17			
112-30-1	1-Decanol	Xi;R36/38 N;R51/53	0,1-1
112-54-9	duodecylaldehyd C.12	Xi;R38;N;R51/53	0,1-1
106-24-1	2,6-Octadien-1-Ol, 3,7-dimethylvanillin	Xi;R38 R43	1-2
121-33-5	kryst.	Xi;R43	1-5
122-78-1	fenylacetaldehyd	Xi;R43;	1-5
60-12-8	Benzenethanol	Xi;R36	1-5
8021-36-1	opoponax resinoid	Xi;R43	1-5
84776-65-8	Lavender oil	Xi;R43 Xn;R65	1-5
90082-51-2	Geranium oil	Xi;R43 Xn;R65	1-5
91-64-5	2H-1-Benzopyran-2-On	Xn;R22;R43	1-5
99811-75-3	Cedar wood oil	Xi;R43;Xn;R65;	1-5
106-22-9	6-Octen-1-Ol, 3,7-dimethylbenzylbenzoate	Xi;R38 N;R51/53	5-10
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	5-10
8028-48-6	Orange oil	Xn;R10;R43;R65	5-10
89957-91-5	bergamotolie	Xn;R65 Xi;R43	5-10
78-70-6	Linalool	Xi;R38	10-20
No. 18			
120-57-0	heliotropin kryst.	Xi;R36/37/38	1-5
8028-48-6	Orange oil	Xn;R10;R43;R65	1-5
84929-31-7	citronolie	R10 Xi;R43	1-5
90082-51-2	Geranium oil	Xi;R43 Xn;R65	1-5
91-64-5	2H-1-Benzopyran-2-On	Xn;R22;R43	1-5
106-22-9	6-Octen-1-Ol, 3,7-dimethylbenzylbenzoate	Xi;R38 N;R51/53	5-10
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	5-10
78-70-6	Linalool	Xi;R38	5-10
Nr 19			
90082-51-2	Geranium oil	Xi;R43 Xn;R65	10-20
60-12-8	Benzenethanol	Xi;R36	20-40
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	60-80
No. 20			
106-24-1	2,6-Octadien-1-Ol, 3,7-dimethyl-	Xi;R38 R43	1-2
78-70-6	Linalool	Xi;R38	1-2
103-82-2	fenyleddikesyre	Xi;R36/37/38	1-5
84929-79-3	styrax resinoid	Xi;R43	1-5
84961-50-2	Cove bud oil	Xi;R38 Xn;R21/22 R65	1-5

CAS no	Chemical name (as indicated in MSDS)	Self classification	Weight-percent
84650-11-3	Geranium oil	Xi;R38 R43 Xn;R65	5-10
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	10-20
60-12-8	Benzenethanol	Xi;R36	10-20
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	20-40
No. 21			
106-24-1	2,6-Octadien-1-Ol, 3,7-dimethyl-	Xi;R38 R43	1-5
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	5-10
78-70-6	Linalool	Xi;R38	5-10
89957-91-5	bergamotolie	Xn;R65 Xi;R43	5-10
122-40-7	Amylcinnamaldehyd	Xi;R38 R43	40-60
No. 22			
106-22-9	6-Octen-1-Ol, 3,7-dimethyllinalylacetat	Xi;R38 N;R51/53	1-5
115-95-7	linalylacetat	Xi;R38	1-5
84929-79-3	styrax resinoid	Xi;R43	1-5
97-54-1	Phenol, 2-methoxy-4-(1-propenyl)-	Xn;R22 Xi;R43	5-10
104-54-1	Cinnamyl alcohol	Xi;R43	10-20
60-12-8	Benzenethanol	Xi;R36	10-20
78-70-6	Linalool	Xi;R38	10-20
No. 23			
106-22-9	6-Octen-1-Ol, 3,7-dimethyllinalylacetat	Xi;R38 N;R51/53	1-5
115-95-7	linalylacetat	Xi;R38	1-5
121-33-5	vanillin kryst.	Xi;R43	1-5
78-70-6	Linalool	Xi;R38	1-5
79-77-6	3-buten-2-one,4-(2,6,6,-trimethyl-1-cyclohexen-1-yl)-,(E)-	N;R51/53;	1-5
84238-39-1	patchouli oil	Xn;R65;	1-5
84929-38-4	mandarine oil	R10 Xn;R65	1-5
89957-98-2	olibanum oil	R10 Xn;R65	1-5
99811-75-3	Cedar wood oil	Xi;R43;Xn;R65;	1-5
89957-91-5	bergamotolie	Xn;R65 Xi;R43	5-10
91-64-5	2H-1-Benzopyran-2-On	Xn;R22;R43	10-20
120-51-4	benzylbenzoate	Xn;R22 Xi;R43	20-40
No. 24			
106-22-9	6-Octen-1-Ol, 3,7-dimethylheliotropin	Xi;R38 N;R51/53	0,1-1
120-57-0	kryst.	Xi;R36/37/38	1-5
84929-79-3	styrax resinoid	Xi;R43	1-5
60-12-8	Benzenethanol	Xi;R36	5-10
99811-75-3	Cedar wood oil	Xi;R43;Xn;R65;	5-10
No. 25			
83863-30-3b	ylang-ylang olie III	Xn;R65 Xi;R38	100
No. 26			
121-33-5	vanillin	Xi;R43	1-5
60-12-8	Benzenethanol	Xi;R36	1-5
84929-31-7	citronolie	R10 Xi;R43	1-5
90082-51-2	Geranium oil	Xi;R43 Xn;R65	1-5
91722-69-9	lavendinolie	Xi;R38 R43 Xn;R65	1-5
115-95-7	linalylacetat	Xi;R38	5-10
106-22-9	6-Octen-1-Ol, 3,7-dimethyl-	Xi;R38 N;R51/53	10-20
5989-27-5	(R)-p-mentha-1,8-dien	R10 Xi;R38 R43 N;R50/53	10-20
78-70-6	Linalool	Xi;R38	10-20

CAS no	Chemical name (as indicated in MSDS)	Self classification	Weight-percent
No. 27			
120-51-4	Benzyl benzoate	Xn;R 22	24,9
105-95-3	Ethylene brassolate	N;R 51/53	1,7
98-55-5	Alpha-Terpineol	Xi; R38	1,5
63500-71-0	Tetrahydro-4-methyl-2-(2-methylpropyl)-2H-pyram-4-ol	Xi; R36	1,5
1205-17-0	2-Methyl-3-(3,4-methylenedioxyphenyl)propanal	N;R 51/53	0,6
No. 28			
28219-61-6	2-Ethyl-4-(2,2,3-trimethylcyclopent-3-en-yl)-but-2-en-1-ol	Xi-N; R 38-50/53	0,1-1
103-95-7	Alpha-methyl-p-isopropylphenylpropanaldehyde	Xi-N; R 38-51/53	0,1-1
105-21-5	4-heptanolide	Xi; R 36/37/38	1-5
No. 29			
68039-49-6	2,4-DIMETHYL-3-CYCLOHEXENE CARBOX-ALD	Xi; R 36/38-43-52/53	0,2
No. 30			
54464-57-2	1-(1,2,3,4,5,6,7,8-octahydro-2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one	N;R 51/53	2,0
103-95-7	Alpha-methyl-p-isopropylphenylpropanaldehyde	Xi; R38	1,0
63500-71-0	2-(iso butyl)-4-hydroxy-4-methyl tetrahydro-pyran	Xi; R36	1,4
106-22-9	Citronellol	Xi-N; R 38-43-51/53	1,7
107-75-5	Hydroxycitronellal	Xi; R 36-43	1,6
31906-04-4	4-(4-Hydroxy-4-methyl pentyl)-3-cyclohexene-1-carboxaldehyde	Xi; R43	2,0
No. 31			
5392-40-5	Citral	Xi; R 38-43	0,2
91-64-5	Coumarin	Xn; R 22-43	0,3
106-24-1	Geraniol	Xi; R 38-43	0,3
No. 32			
32388-55-9	Acetyl cedrene	N; R 50/53	1-5
54464-57-2	1-(octahydrotetramethyl-2-naphthyl)ethanone	N; R 51/53	0,1-1
28219-61-6	2-Ethyl-4-(2,2,3-trimethylcyclopent-3-en-yl)-but-2-en-1-ol	Xi-N; R 38-50/53	0,1-1
60-12-8	Phenethyl alcohol	Xi, R 36	1-5
78-70-6	Linalool	Xi; R 38	1-5
103-95-7	Alpha-methyl-p-isopropylphenylpropanaldehyde	Xi-N; R 38-51/53	5-25
120-51-4	Benzyl benzoate	Xn; R 22	1-5
150-84-5	Citronellyl acetate	Xi-N; R 38-51/53	0,1-1
105-87-3	Geranyl acetate	Xi; R 36/38	1-5
6259-76-3	Hexyl salicylate	Xi-N; R 38-50/53	1-5
102-20-5	Benzylcarbinyl alpha-toluate	N; R 51/53	0,1-1
104-67-6	gamma-Undecalactone	N; R 51/53	0,1-1
No. 33			
27939-60-2	Dimethyl cyclohexene carboxaldehyde	Xi; R 36/38-43-52/53	0,1-1
105-53-3	Diethyl malonate	Xi; R 36	1-5
123-68-2	Allyl hexanoate	N; Xn; R 21/22-51/53	0,1-1
106-24-1	Geraniol	Xi; R 38-43	0,1-1
No. 34			
93-18-5	2-ethoxy naphthalene	Xi-N; R 38-51/53	0,2
37677-14-8	Isohexenyl cyclohexenyl carboxaldehyde	N; R51/53	0,3
5392-40-5	Citral	Xi; R38-43	2,0
80623-07-0	Ethyltricyclo (5,2,10,2,2) decane-2-carboxylate	Xi-N; R 38-51/53	0,2
5989-27-5	D-limonene	Xn-N; R 10-38-43-50/53	0,9
112-31-2	n-Decylaldehyde	Xi; R38	5,0

CAS no	Chemical name (as indicated in MSDS)	Self classification	Weight-percent
124-13-0	n-Octyl Aldehyde	Xi;R 10-36/38	1,5
4180-23-8	trans-Anethole	N; R51/53	0,3
No. 35			
105-95-3	Ethylene brassylate	N; R 51/53	1-5
4949-11-8	2-Ethyl-3-hydroxy-4-pyrone	Xn; R 22	1-5
5989-27-5	D-limonene	Xn-N; R 10-38-43-50/53	3,0
77-83-8	Ethyl methylphenylglycidate	-; R 52/53	1-5
104-67-6	gamma-Undecalactone	N; R 51/53	0,1-1
No. 36			
68155-67-9	1 - (1,2,3,4,6,7,8,8a - octahydro - 2,3,8,8 - tetra-methyl - 2 - naphthyl)ethan - 1 - one	N; R 51/53	10-25
120-51-4	Benzyl benzoate	Xn; R22	1-10
103-95-7	p - cumenyl - 2 - methylpropionaldehyde	Xi; R38	1-10
107-75-5	Hydroxycitronellal	Xi; R36-43	1-10
84929-38-4	Madarin orange oil	Xn; R 65	1-10
6259-76-3	Hexyl salicylate	Xi-N; R38-50/53	0,1-1
No. 37			
6658-48-6	3 - (p - cumenyl) - 2 - methylpropionaldehyde	Xi; R43	5-10
101-86-0	2-(phenylmethylene)-Octanal	Xi; R43	1-5
60-12-8	Phenethyl alcohol	Xi; R36	1-5
1335-46-2	Methyl ionone	N; R 51/53	1-5
54464-57-2	1 - (1,2,3,4,5,6,7,8 - octahydro - 2,3,8,8 - tetrame-thyl - 2 - naphthyl)ethan - 1 - one	N; R 51/53	1-5
28219-61-6	2-Ethyl-4-(2,2,3-trimethylcyclopent-3-en-yl)-but-2-en-1-ol	Xi-N; R 38-50/53	1-5
103-05-9	alpha,alpha-dimethyl-Benzenepropanol	Xi; R 38	1-5
106-22-9	Citronellol	Xi-N; R 38-43-51/53	1-5
127-91-3	beta-Pinene	Xn-N; R 10-50/53-65	0,1-1
68647-72-3	Orange oil terpenes sweet	Xn-N; R 10-38-50/53-65	0,1-1
No. 38			
84-66-2	Diethyl phthalate		5-9,9%
106-22-9	Citronellol	Xi;N; R38-43-51/53	2,5-5%
104-55-2	Cinnamal	Xn; R 21-38-43	2,5-5%
128-51-8	Nopylacetate	R 52/53	2,5-5%
106-24-1	3,7-Dimethylocta-2,6-dien-1-ol	Xi; R38-43	2,5-5%
91-64-5	2H-1-Benzopyran-2-on	Xn; R22-43	1-2,49%
101-84-8	Diphenylether	N; R 51/53	1-2,49%
100081-14-1	Moscusketon	N; R5o/52	<1%
2050-08-0	Pentyl-2-hydroxybenzoate	N; R 51/53	<1%
No. 39			
84-66-2	Diethyl phthalate		25-49,99%
91-64-5	2H-1-Benzopyran-2-on	Xn; R22-43	1-2,49%
106-24-1	3,7-Dimethylocta-2,6-dien-1-ol	Xi; R38-43	1-2,49%
104-54-1	trans-3-Phenyl-2-propen1-ol	Xi; R43	1-2,49%
128-51-8	Nopylacetate	R 52/53	1-2,49%
101-84-8	Diphenylether	N; R 51/53	<1%
100081-14-1	Moscusketon	N; R5o/52	<1%
2050-08-0	Pentyl-2-hydroxybenzoate	N; R 51/53	<1%