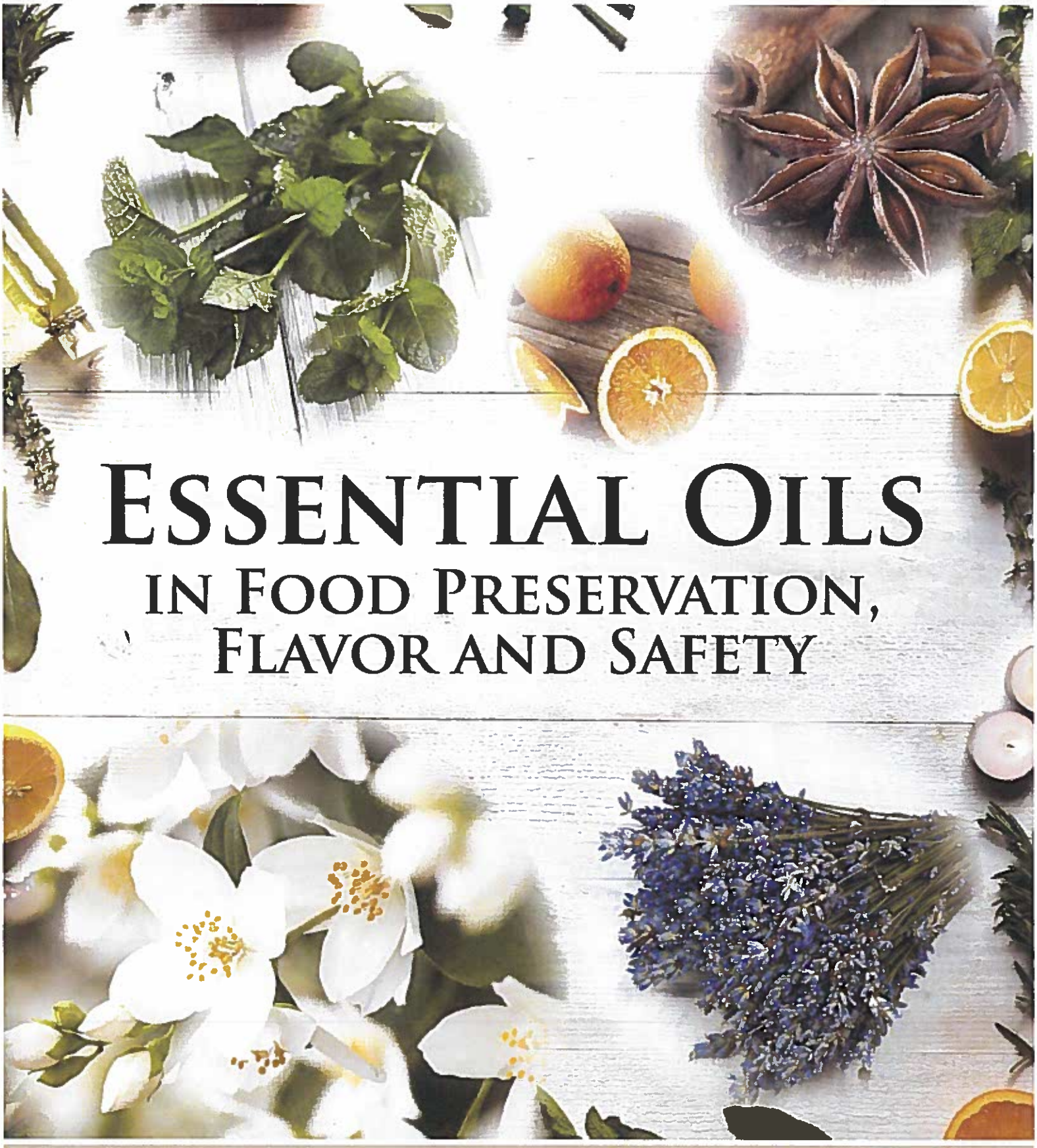

Essential Oils
in Food Preservation, Flavor and Safety

Edited by
Victor R. Preedy

Chapter 11

Essential Oils as Flavors in Carbonated Cola and Citrus Soft Drinks

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List of Abbreviations

AEDA Aroma extract dilution analysis
GC-MS Gas chromatograph-mass spectroscope
GCO Gas chromatography-olfactometry
GMP Good manufacturing practice
GRAS Generally regarded as safe
HPLC High-performance liquid chromatograph
ISO International Organization for Standardization
LLCE/SAFE Liquid–liquid continuous extraction/solvent-assisted flavor evaporation
SDLC Soft drink licensing company
SPME Solid phase microextraction
TCCC The Coca-Cola Company
TNI Transnational Institute

INTRODUCTION

Essential Oils, Spices, and Aromatic Plants

Essential oils (EOs) are pure or partly purified mixtures of lipophilic substances, usually obtained as a liquid from a named plant part. EOs have taste and odor because they contain volatile aroma-active compounds (i.e., molecules that elicit a distinctive taste and smell). An EO may be called the "oil of" the plant from which it was obtained—usually by distillation, expression, or solvent extraction. An EO is termed "essential" in the sense that it has a distinctive/characteristic aroma, scent, or essence of the plant from which it came. The term *aromatic plant* describes a plant known for one or more EOs.

Most EOs contain hydrocarbons and oxygenated compounds, mainly as terpenes and terpenoids, with molecular weights no larger than 300Da. EOs are well known for their uses in food and beverages and in medicine and cosmetics (Sellar, 2001; Baser and Buchbauer, 2010). The plant parts (usually dry) bearing EOs are often called spices; these have been widely used since the middle ages, in the days of the alchemists. Spices are generally regarded as safe flavorings in foods and beverages. However, EOs used in nutrition and medicine need to be handled professionally in accordance with strict good manufacturing practices.

The International Organization for Standardization (ISO) has established over 100 standards for EOs. Examples include ISO 3217:1974, which addresses oil of lemongrass; ISO/TR210:1999, on the general rules for packaging, conditioning, and storage of EOs; ISO 7359:1985, which discusses the analysis of EOs by gas chromatography on packed columns; ISO 4720:2009 on nomenclature; and ISO 25157:2013 on the EO of Chinese Kushui-type roses. These ISO standards are listed in the ISO catalog (2013) and are widely used to guide the production, quality control, marketing, and use of EOs worldwide.

Carbonated Soft Drinks

Carbonated soft drinks ("sodas") are cold, nonalcoholic beverages. This chapter focuses on cola and citrus sodas that contain EOs from the following aromatic plants: coca—*Erythroxylum coca* (Erythroxylaceae); cinnamon—*Cinnamomum*

† Deceased

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(Lauraceae); nutmeg—*Myristica fragrans* (Myristicaceae); coriander—*Coriandrum sativum* (Apiaceae); neroli—*Citrus aurantium* (Rutaceae); lemon—*Citrus limon* (Rutaceae); lime—*Citrus limetta* (Rutaceae); orange—*Citrus sinensis* (Rutaceae); and vanilla—*Vanilla planifolia* (Orchidaceae). A soda may contain the synthetic equivalent of any of the foregoing flavorings and may contain no more than 0.5% v/v of ethanol (Alcoholfree.co.uk., 2012). Other names by which sodas are called include "fizzy drink" and "mineral," among others (D'Amato et al., 2011; Vaux, 2011).

The first popular soda, Coca-Cola or Coke, produced by The Coca-Cola Company (TCCC), at a stage in its history contained oils from all the plants enumerated above (TCCC, 2013). The self-styled lemon-lime sodas contain lemon and lime oils as the main flavorings, with or without orange oil as a minor component. Orange sodas contain orange oil as the main flavoring, with or without lemon and lime oils as minor components. Lemon, lime, neroli, and orange oils are collectively called citrus oils.

Sodas are prepared from purified water, sugar (or other sweetener), EOs, colors and preservatives, and carbon dioxide (CO_2). Some quantities of natural fruit juice are sometimes incorporated in sodas. In the soda industry, EOs and other strategic ingredients, including colors, are supplied by big soft-drink licensing companies (SDLCs) as concentrates to smaller, licensed bottling companies ("bottlers") (May, 1998; Benson, 2004; TNI Conflict & Debate Paper 13, 2006; TCCC, 2013). This somewhat feudal arrangement has existed since the late nineteenth century and operates worldwide, except in Cuba and North Korea (TCCC, 2013). During the 1970s and 1980s, some emerging economies attempted to change the order of things, but they were unsuccessful.

Some instructive and informative developments in the history of the soda industry include the following:

1. Fanta, a popular orange soda, was invented in Germany in 1940 during World War II, when there was no communication between the US-based SDLC (the Coke Company and eventual owner of Fanta trademark) and the German bottler licensed to it (Mikkelson, 2011).
2. Campa-Cola was invented in India in the 1970s, following the expulsion of the Coke Company from that country (Coca-Cola India, 2013; Campa-Cola Website, 2013). However, following the liberalization policy of Narasimha Rao's premiership, the Coke Company returned to India in 1993 and Campa-Cola ceased to exist.
3. There were several scores of independent bottlers (i.e., bottlers not licensed to any of the US-based SDLCs) that operated in Nigeria in the 1980s. However, by the early 1990s, they had all become defunct or affiliated with a US-based SDLC operating in Nigeria.
4. In Nigeria, the many scores of independent bottlers during the 1980s obtained their concentrates from independent suppliers of concentrates based in Asia, such as Campa Beverages Limited in India (Campa-Cola Website, 2013), and Europe, such as Britvic Soft Drinks in the United Kingdom (Britvic Website, 2013).

Most of the history and dynamics of the soda industry are fairly well documented. Some of the industry's activities, such as SDLC–bottler arrangements, have been around for a long time. The 1980s was quite important in the history of the soda industry worldwide; the author's activities in the beverage industry as a scientific officer during at this time partly informs the writing of this book chapter.

HISTORY OF SPICES AND THE POLITICAL ECONOMY OF THE SODA INDUSTRY WORLDWIDE

A spice is defined as an aromatic plant substance used as flavoring. Spices have been very important in human history, culture, and civilization. Wars have been fought and deals have been made over spices. Europe's desire for "spices of the East" fueled Vasco da Gama's discovery of the sea route to India.

The primary driving force of the industry worldwide is none other than EOs. John Pembroke's famous cola formula (Jackson, 1978) became popular more from the seven spices it contained than from the psychoactive alkaloids in coca leaf. Ever since that formula in 1885—and the later inventions of Pepsi in 1893, 7Up in 1929, Fanta in 1940, Tango in 1950, Mirinda in 1960, and Sprite in 1961—sodas have been a major contributor to the global economy in form of a multibillion dollar industry. In 2012 for example, the Coca Cola Company of USA planned to spend $30 billion to bring about global growth in the company in year 2013. It produces and markets over 500 brands, with a portfolio of $16 billion, consumers in over 200 countries with an average drinking rate of 1.8 billion servings daily. Also in India, Coca-Cola was the leading soft drink till 1977 and after its return in 1993, it has made significant investments to ensure that the beverage is available to more and more people in a country of over a billion persons, reaching even the remote and inaccessible parts of that country. The politico-economic importance and effect of the soda industry cannot be over-emphasized because of the capital and labor intensive nature which has potent multiplier effect both up and down

streams. The Coca-Cola Company for example is one of the world's top 10 private employers having more than 700,000 employees (Melnick and Jackson, 2002).

INDUSTRIAL PRODUCTION OF SODAS

A schematic representation of the processes and the materials required in soda production is shown in Figure 1. Major requirements are water and water treatment chemicals, sugar, CO_2, chemicals used in preservation (e.g., benzoates) and in

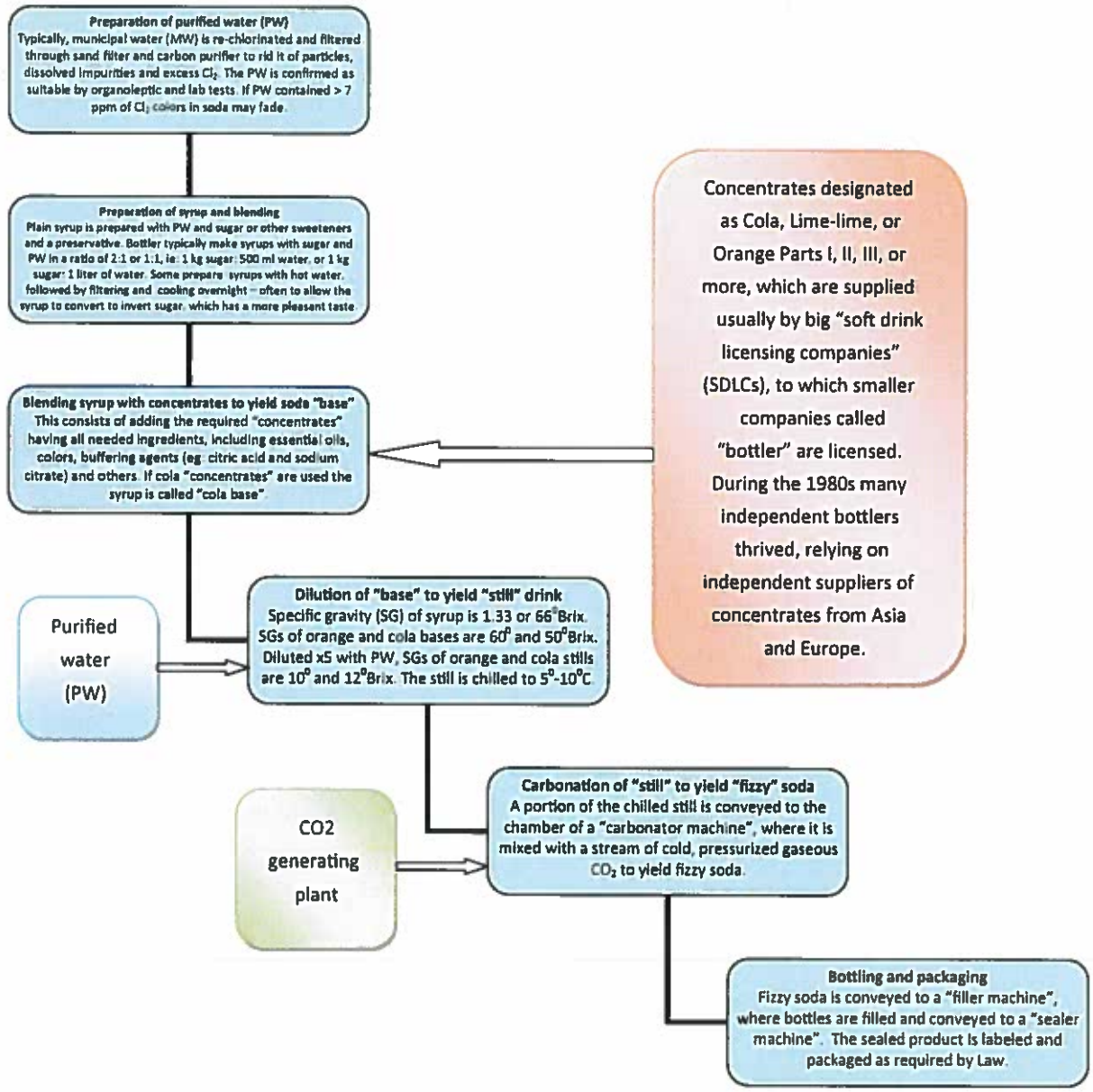


FIGURE 1 Schematic representation of soda production. The sweetener and the syrup produced from it must meet quality control specifications. The specific gravity (SG) of syrup or soda is measured in degrees Brix (°Brix) using a Brix hydrometer. Syrup prepared with refined sugar and water in a ratio of 1 kg–500 ml is given a value of 66 °Brix. Blended orange syrup normally has SG of 60 °Brix, while that of cola or lemon-lime syrup is 50 °Brix. Syrups are diluted 5× with carbonated water. Thus the SG of orange soda is 12 °Brix, while that of soda and lemon-lime is 10 °Brix. Usually orange sodas are given less carbonation than cola and lemon-lime sodas.

sanitation (e.g., sodium bicarbonate), and concentrates. The most strategic inputs of the industry—the EOs—are incorporated in the concentrates.

ESSENTIAL OILS IN COLA AND CITRUS SODA CONCENTRATES

Essential Oils as Flavorings in Sodas

Soda concentrates come as cola, lemon-lime, or orange. They are typically supplied by SDLCs to licensed bottlers. Bottlers not licensed to an SDLC buy their concentrates from independent producers or suppliers. A given soda can have one or more EOs combined into one or more concentrate formulas (containing Parts I, II, III, and more), along with colors and other ingredients, depending upon the brand and supplier. The other ingredients are usually granular substances, such as buffering agents (e.g., citric acid, sodium citrate, phosphoric acid, potassium phosphates) and additional preservatives. During the blending of syrup (Figure 1), the various parts are incorporated in a particular order and method, as described on labels affixed to the said parts. The ingredients contained in cola and citrus parts, including Eos, are given in Tables 1–3.

It is the EOs in concentrates that interact with other flavorings, such as sweeteners, acids, and CO_2, to give a soda its distinctive taste and aroma. The alleged secrets of SDLCs regarding a particular soda lie in the choice and combination of a wide range of EOs (which can have synthetic equivalents).

Essential Oils Used in Cola and Citrus Concentrates

Cola concentrate contains EOs from coca leaf, cinnamon bark, nutmeg seed, coriander seed, neroli flower, lemon peel, lime peel, orange peel, and vanilla seed (Table 1). Lemon-lime and orange soda concentrates contain EOs from all the citrus fruits, including neroli in the case of lemon-lime soda (Table 2). While the dominant oil in orange soda is orange oil (Table 3), those of lemon-lime soda are lemon, lime, and neroli oils. Each of these oils contains scores of different molecular components; some of the leading molecular entities are shown in Table 4 (cola soda concentrate) and Table 5 (citrus soda concentrates). Table 5 further compares and contrasts citrus oils in terms of molecular constituents to explain organoleptic similarities and contrasts between the different citrus oils.

TABLE 1 Ingredients of Cola Concentrate

Ingredient	Remark
Essential oils: • Coca • Cinnamon • Orange • Lemon • Lime • Neroli • Nutmeg • Vanilla Other ingredient: • Kola nut extract (or other sources of caffeine) • Benzoic acid (or other preservatives) • Buffer (e.g., citric acid/Na citrate) • Caramel color • Chelating agent • Emulsifying agent (e.g., gum Arabic) • Glycerin • Natural juice concentrate (in some brands) These ingredients are contained in parts designated as Cola Parts I, II, III, or more depending on brand or region.	Coke originally contained caffeine from the kola nut and cocaine from coca leaf and was flavored with vanilla and other ingredients. Today, however, most colas use other flavorings and other sources of caffeine. The original Coca-cola or coke was invented in 1886 in the US by a Pharmacist, Pemberton, whose coke formula was inspired by Mariani's 1863 recipe for Cocawine (Hamblin, 2013). In most countries worldwide colas usually contain most or all the ingredients listed in the left column. Most use sugar or HFCS. Low or zero sugar colas contain little or no syrups or may use sweeteners such as aspartame, sucralose, or others (Poundstone, 1983; D'Amato et al., 2011).

Though called cola, a cola soda may not contain cola extract, or even caffeine. The primary flavorings of colas today are sugar, citrus oils, cinnamon, vanilla, and phosphoric or citric acid. SDLCs or manufacturers of cola concentrates invent distinctively different tastes for each brand by adding trace ingredients like nutmeg. However, the flavorings most associated with colas are vanilla and cinnamon.

TABLE 2 Ingredients of Lemon-Lime Concentrates

Ingredient	Remark
Essential oils from parts of the following fruit: • Lemon • Lime • Neroli • Orange (minor in some brands) Other ingredient: • Benzoic acid (or other preservatives) • Buffer (e.g., citric acid/sodium citrate) • Caffeine (only in some brands) • Calcium disodium EDTA (a chelating agent) • Conc. Natural flavors or juices (in some brands) • Emulsifier (e.g., gum Arabic) • Erythorbic acid (to preserve freshness) • Brominated vegetable oil (in some brands) • Phenylalanine (in some brands as a sweetener) • Yellow 5 (only in some colored brands) • Red 40 (in some colored brands) These ingredients are contained in concentrate parts designated lemon-lime Parts I, II, or III, depending upon brand, country or region.	Lemon-lime sodas are of two kinds—the clear variety and the cloudy. The clear include: 7Up, Sprite, and Sierra Mist. Among the cloudy are: Schweppes bitter lemon and Krest bitter lemon, which contain quinine as additional flavoring. Tripp, a lemon-lime soda of Indian origin was popular in Nigeria during the 1980s, but has since disappeared. Limca, also of Indian origin, is similar to Tripp, and is popular in Nigeria, India and the US. The cloudy appearance of lemon-lime sodas makes them look like real lemon or lime juice. This, in combination with their reputation or status as being free from artificial colors, account for their immense popularity. Although the clear and colorless appearances of Sprite and 7Up do not make them look like lemon or lime juice, their colorlessness bespeaks their non-content of artificial colors. Cloudy lemon-lime sodas are called "lemonade" or "cloudy lemonade" in the UK and most Commonwealth Nations, including Nigeria, where a lemonade brand "Rainbow" was very popular but during the Nigeria Civil War (1967–1970). Because some lemon-lime sodas like Sprite and 7Up are clear and can be mistaken for soda water (i.e., carbonated water), it has become a tradition in the soda industry to present lemon-lime sodas in clear green bottles while soda waters are presented in clear and colorless bottles. Taking a cue from the fact that lemon-lime drinks were popular even before the era of carbonation, some producers currently offer noncarbonated version of their lemon-lime sodas. These include 7Up (Nimbooz) and Minute Maid (Nimbu pani), which are popular in India.

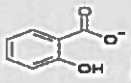
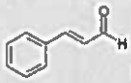
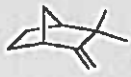
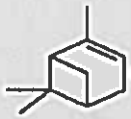
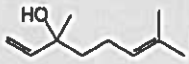
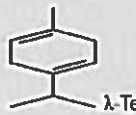
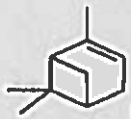
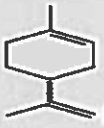
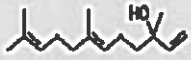
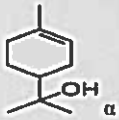
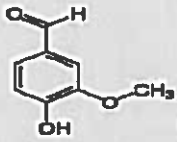
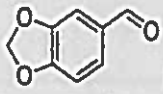
7Up, the oldest of the clear and colorless version of lemon-lime sodas, was invented in 1920 by Charles Grigg, and launched in 1929. It then contained lithium citrate—a mode stabilizing drug, until 1950, when it was discontinued. Attempts to re-formulate 7Up so it can be marketed as "100% natural" climaxed in 2006, with removal EDTA, and replacement of Na-citrate with K-citrate. But the claim was challenged, since the drink had high fructose corn syrup (HFCS). In 2011 however, HFCS was replaced with sugar in the formulation called 7Up Retro (Cadbury-Schweppes, 2008).

TABLE 3 Ingredients of Orange Concentrates

Ingredient	Remark
Essential oils from the following fruit parts: • Orange (as the major citrus oil) (Vora et al., 1983) • Lemon (as the minor citrus oil) • Lime (as the minor citrus oil) • Others (from, e.g., mango, raspberry, apple, pineapple, blackcurrant, and so on) Other ingredient: • Benzoic acid (or other preservatives) • Brominated vegetable oil (in some brands) • Buffer (e.g., citric acid/Na citrate) • Calcium disodium EDTA (to protect flavor) • Carotene (or artificial colors) • Conc. orange juice/other natural flavors • Caffeine (only in some brands) • Emulsifier (e.g., gum Arabic) • Erythorbic acid (for freshness in some brands) • Rosin or gum Arabic • Yellow 5 These ingredients are contained in parts designated as Orange Parts I, II, or more depending upon brand **Flavor variety**: Orange sodas vary with country, brand, and date. About 100 varieties are currently marketed worldwide. In the UK, for example, orange sodas contain orange essence in addition to other essences—lemon, lime, mango, passion fruit, peach, and apricot. **Color**: Artificial colors are allowed in many countries, but in some only natural colors from carrot, pumpkin, or other food plants are used. **Natural fruit juice**: Some brands of orange soda contain small amounts of natural fruit juice.	Fanta, invented in Germany in 1940 is the most popular orange soda worldwide, but the version sold in the US (Fanta Orange) differs from those sold elsewhere (Orange Fanta). The original Fanta had orange juice and a color like orange juice, while Fanta Orange is red-orange and has a candy-like flavor. Fanta Orange was the second drink to be produced by the Coke Company. Some orange sodas contain sodium hexametaphosphate—a sequestrant or chelating agent that complexes with Cu^{2+}, Fe^{2+}, Fe^{3+} and Ni^{2+} that would otherwise be available to catalyst fat peroxidation, an undesirable. Some orange sodas also contain BVO—a densifying/emulsifying agent added to prevent ringing, but causes colors to stick to the tongue. Other popular orange sodas include: Tango, Mirinda, Slice, Sumol, Crush, and Tropicana Twist. **Tango** is an orange soda sold in the UK, Ireland, Sweden, Norway and Hungary, and used to be sold in Nigeria during the 1960s. It was first launched in 1950 by Corona, which was bought over by Beecham in 1958, and later by Britvic in 1987 (Britvic Brand Website, 2013). Like other orange sodas, Tango may contain other flavors—apple, lemon, cherry, and blackcurrant.

Brominated vegetable oils (BVOs) are vegetable oil in which some atoms of hydrogen have been replaced by bromine. The resulting product may have a specific gravity (SG) of up to 1.33. Thus, when a BVO is mixed with a lighter oil like a citrus oil, a mixture with an SG closer to that of water (SG≈1) is produced. Oil-in-water droplets (emulsions) containing BVOs tend to remain suspended in water rather than "ring out"—i.e., separate and float (Bendig et al., 2012). Similar effects can be produced by food additives like sucrose acetate isobutyrate (E444) or glycerol ester of wood rosin (E445). "E" stands for food additive permitted in the European Union.

TABLE 4 Molecular Components of Essential Oils Used in Producing Cola Soda Concentrate

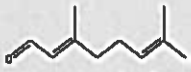
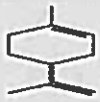
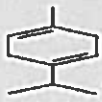
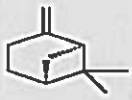
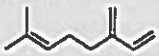
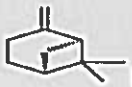
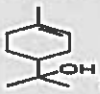
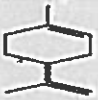
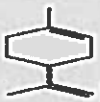
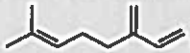
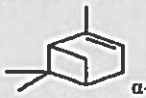
Name of Essential Oil	Key Components	Structures of Key or Other Top Components in Terms of Quantity Present (% w/w)
Coca leaf oil (0.06–0.13% w/w)	The key component is methyl salicylate.	 Methyl salicylate
Cinnamon bark oil	The key component is cinnamaldehyde (65–80% w/w). Others are ethyl eugenol, β-caryophyllene, linalool, and methyl chavicol, limonene, α-terpineol, and so on.	 Cinnamaldehyde
Nutmeg seed oil (5–15% w/w)	The compositions (w/w) are: camphene or sabinene (50%); α-pinene (20%); dipentene, or racemic mixture of limonene (8%); linalool (6%); borneol (6%); λ-terpineol (6%); geraniol (6%); myristcin (4%); eugenol (4%); and safrole (0.6%).	 Camphene  α-Pinene
Coriander seed oil	The main components (w/w) are linalool (77.5%), λ-terpinene (4.6%), α-pinene (4.0%), limonene (1.3%), geraniol (0.6%), and 2-decenal (0.2%).  Linalool	 λ-Terpinene  α-Pinene
Neroli flower oil (0.8–1% w/w) Other citrus oils as in a citrus soda concentrate	The components of Tunisian neroli oil are: limonene (27.5%); nerolidol (17.5%); α-terpineol (14.0%); α-terpinyl acetate (11.7%); farnesol (8.0%); β-ocimene (4.3%); γ-elemene (3.4%); δ-3-carene (2.4%); β-terpinyl acetate (1.7%).  Limonene	 Nerolidol  α-Terpineol
Vanilla seed extract	The volatiles of fermented vanilla seed comprise 85% w/w vanillin, piperonal (heliotropin) and over 100 other aroma compounds.	 Vanillin  Piperonal

Cola concentrates contain lemon, lime, neroli, and orange oils just like some citrus concentrates. Neroli oil has nerolidol as a key component, but other citrus oils contain little or none.

Formulation of Essential Oils into Soda Concentrates

A soda typically consists of over 99% w/w water, sugar, and other ingredients, and less than 0.5% w/w EOs. Because these oils are hydrophobic, a soda is really a very dilute oil-in-water suspension. Therefore, the concentrate must be presented as a concentrated oil-in-water emulsion.

TABLE 5 Molecular Components of Essential Oils Used in Producing Citrus Soda Concentrates

Name of Essential Oil	Key Components (in % w/w)	Structures of Key or Other Top Components in Terms of Quantity Present (% w/w)
Lemon oil	Limonene (54.6); γ-Terpinene (19.1); β-Pinene (14.5); α-Pinene (3.9); Geranial (2.3) and Myrcene (1.5).  Geranial It is noteworthy that both γ-Terpinene (19.1) and geranial (2.3)—also called lemonal or citral, are conspicuous in lemon but below detection or much lower in both lime and orange.	 Limonene  λ-Terpinene  β-Pinene
Lime oil	Limonene (74.8); γ-Terpinene (0.1); β-Pinene (1.4); α-Pinene (0.3) and Myrcene (7.1) (Khan and Abourashed, 2010).  Myrcene It is noteworthy that myrcene is much higher in lime (7.1) than in lemon (1.5) and orange (2.1–4.3).	 Limonene  β-Pinene  Myrcene
Neroli flower oil (0.8–1% w/w)	Tunisian neroli oil has: limonene (27.5%); nerolidol (17.5%); α-terpineol (14.0%); α-terpinyl acetate (11.7%); farnesol (8.0%); β-ocimene (4.3%); γ-elemene (3.4%); δ-3-carene (2.4%); β-terpinyl acetate (1.7%).	 Nerolidol  α-Terpineol
Orange oil	Limonene (94.2); β-Pinene (0.2–1.0); α-Pinene (0.7–1.4); and Myrcene (2.1–4.3) (Coleman et al., 1969).  Limonene It is noteworthy that limonene is much higher in orange (94.2) than in lemon (54.6) and lime (74.8).	 Limonene  Myrcene  α-Pinene

All the citrus oils contain limonene and other components in common, (Wang et al., 2012), which partly accounts for their similar aromas. The differences in the concentrations of components partly account for the dissimilarities. Sprite, Sierra Mist and 7UP appear to contain neroli oil judging from their contents of nerol and neral according to the study by Hausch (2010).

The most notable natural emulsifying agent used in the soda industry is gum Arabic. Other natural gums, glycerin, and artificial carboxymethyl cellulose, can also be used. Brominated vegetable oils (BVOs), which have specific gravities (SGs) close to that of syrup (i.e., 1.33) can also be used to stabilize oil-in-water emulsions. As previously stated, concentrates come in parts; at least one of these parts containing one or more EOs will be presented as a syrup-like liquid. Such a liquid cola or orange part may contain, for example, lemon oil, caramel (in the case of cola) or other colors (in the case of orange), glycerin or other polyhydric alcohol, gum Arabic or other emulsifying agent, buffers, and preservatives, including chelating agents. The EO may be presented in a vehicle of vegetable oil or polyhydric alcohol. In countries where BVOs are allowed, orange or other concentrates may contain BVO.

A concentrate normally has an SG greater than 1 so that it can blend more readily with syrup. A typical concentrate can be produced by an SDLC or its proxy as follows:

1. A predetermined quantity of water or other solvent is placed in the tank of an emulsifying blender. This may be followed by the addition of another solvent, such as vegetable oil or glycerin. The resulting mixture is then blended for a specified length of time.
2. A predetermined quantity of an emulsifier (e.g., a 10% w/v solution of gum Arabic in water) is added and blended for a given duration. This may be followed by the addition of and blending with other ingredients, such as BVO, colors, buffers, and chelating agents, and other preservatives previously dissolved or suspended in suitable solvents. An ingredient like caffeine (previously dissolved in water or aqueous solvent) may be added at this point or in a later stage.
3. A predetermined quantity of EO (presented in a suitable vehicle, such as a vegetable oil or polyhydric alcohol) is added to the mixture and blended for a specified duration.
4. Samples of the resulting emulsion are subjected to a number of required tests (by the SDLC or its proxy), which the emulsion must pass before it is packaged and shipped to bottlers. Such tests include determining SG, stability, and other parameters that determine the usability and durability of the emulsion, as well as the suitability and drinkability of the soda produced therefrom by the bottler.

A typical preservative used in the industry to control microbial growth is benzoic acid or a suitable salt thereof. A typical chelating agent used to control peroxidation of oils is ethylenediaminetetraacetic acid or any of its suitable analogues thereof. The reason for using a chelating agent is that it can sequester from solution metallic ions that would otherwise catalyze oil peroxidation, making such oils rancid with offensive organoleptic features. Ingredients used in producing cola and citrus soda concentrates are given in Tables 1–3. The key molecular components of EOs used in colas and in citrus sodas are given in Tables 4 and 5.

ADVANCED EQUIPMENT AND TECHNIQUES USED IN FLAVOR RESEARCH AND SODA TECHNOLOGY

Briefly, advanced equipment and techniques used in soda technology include the following:

1. Liquid–liquid continuous extraction/solvent-assisted flavor evaporation is a key technique used in extracting aroma-active compounds from sodas and similar media (Engel et al., 1999).
2. Gas chromatography-olfactometry is a technique used in detecting aroma-active compounds. It works in conjunction with another technique called aroma extract dilution analysis. This technique has been well described and applied by Hausch (2010).
3. Solid-phase microextraction combined with stable isotope dilution assays is used in quantifying aroma-active compounds (Hausch, 2010; Bertuzzi et al., 2013).
4. A gas chromatograph-mass spectroscope equipped with a comprehensive library is standard requirement for the identification and quantification of aromatic compounds in flavor chemistry (Verzera et al., 2004).
5. It is often essential and convenient to quantify benzoic acid in soda samples using high-performance liquid chromatography.
6. High sensitivity (0.01 mg) analytical balance in addition to other such related needs of an advanced analytical laboratory is necessary for the weighing of the small quantities of essential oils and aroma-active compounds found in sodas.

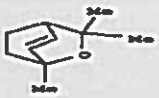
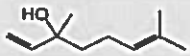
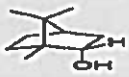
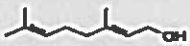
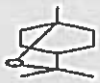
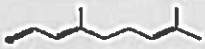
TYPICAL CONCENTRATIONS OF ESSENTIAL OIL MOLECULES IN SODAS

Table 6 shows the typical levels of EO molecules in three lemon-lime sodas: Sprite, Sierra Mist, and 7Up.

CONCLUSION

A search of the literature on sodas reveals that many previous trade secrets are now in the domain of public knowledge. Modern techniques allow scientists to discover the flavor secrets of sodas (i.e., the unique combinations of EOs as flavorings) and to invent new formulations, although questions remain. For example, when a soda contains more than one citrus oil (e.g., lemon, lime, orange, neroli), how much of each is present? This is a challenge because each oil contains scores of aroma-active terpenes and terpenoids (the main molecular entities of EOs that exist as a complex mixture of isomers) and thus are difficult to analyze. In addition, other EOs used in sodas contain similar terpenes and terpenoids as do the citrus oils. Finally, the nature of the techniques used in flavor analysis are such that the analyst

TABLE 6 Typical Concentrations of Essential Oil Molecules in Three Commercial Lemon-Lime Sodas

Molecule	Structure	Concentration of Component in ng/g of De-carbonated Soda as Mean or (Range at 95% Confidence Interval)		
		Sprite	Sierra Mist	7Up
Dehydrocineole		1550 (1360–1740)	2630 (2380–2890)	2750 (2490–3010)
Linalool		220 (202–239)	296 (277–314)	378 (353–403)
Borneol		201 (189–213)	53.8 (52.6–55.1)	58.6 (52.1–65.1)
Octanal		168 (155–181)	449 (411–487)	347 (332–362)
Decanal		61.3 (54.8–67.8)	191 (183–199)	133 (121–145)
Geraniol		47.5 (39.9–55.0)	67.5 (59.3–75.7)	119 (105–132)
Nonanal		33.5 (31.8–35.2)	54.3 (53.7–55.0)	42.1 (35.5–48.6)
Nerol		32.9 (29.5–36.4)	35.0 (29.8–40.2)	49.5 (43.2–55.9)
Isoborneol		32.5 (29.8–35.3)	16.0 (14.4–17.7)	12.2 (10.8–13.6)
Cineole (Eucalyptol)		29.7 (28.3–31.1)	17.4 (16.9–17.9)	15.5 (15.2–15.7)
Geranial (e-Citral)		5.64 (3.36–7.91)	6.58 (4.65–8.52)	10.0 (6.11–13.9)
Neral (z-Citral)		3.58 (2.46–4.70)	3.83 (2.65–5.01)	4.59 (3.56–5.63)

The data are after Hausch (2010), using liquid–liquid continuous extraction/solvent-assisted flavor evaporation (LLCE/SAFE), gas chromatography-olfactometry (GCO) and solid phase microextraction (SPME) combined with stable isotope dilution assays (SIDA). The masses of de-carbonated beverages were: Sprite—97.4 ± 1.55; Sierra Mist—97.8 ± 1.50; and 7Up—99.0 ± 0.18% w/w of their carbonated masses (Hausch, 2010).

or flavorist must continually contend with the possibility of artifacts in the matrix, which distort the true picture of desired components. A major implication of this situation is that the quality control of EOs in sodas is determined not by bottlers but at the level of concentrate formulation. Today's technology permits the production of tastier and safer sodas, using concentrates made with select synthetic flavorings that impart the desired taste and aroma.

SUMMARY POINTS

- Essential oils are obtained from plants containing aroma-active compounds. They are used in food and beverage, cosmetics, and pharmaceutical industries as flavoring agents, fragrance, and medicines.
- Chemically, these aroma-active compounds are terpenes and terpenoids. Each essential oil can characteristically be used to identify the plant source.
- Knowledge of these constituents has been used in the formulation of concentrates for soda flavoring.
- The soda industry has existed since the late nineteenth century and is currently a multibillion dollar industry, impacting global economy.

- Essential oils from various fruit-based spices are key components of the concentrates from which sodas are made, with the addition of other ingredients such as water, sugar, preservatives, colorants, and thickeners.
- Most manufacturers of soda use commercially prepared concentrates or concentrates manufactured by the SDLC or its proxy; thus, they can be considered as bottling companies.
- Cola concentrates are used in cola sodas; lemon-lime sodas use essential oils from lemon, lime, neroli, and orange; whereas orange sodas are made from concentrates containing orange oil as the major component.
- Cutting-edge scientific processes, such as solvent-assisted flavor evaporation and solid-phase microextraction, using high-tech equipment such as gas chromatograph-mass spectroscope and high-performance liquid chromatography, are routinely employed in the formulation, evaluation, and manufacture of the flavor industry.
- The main molecular entities in essential oils exist as complex mixtures of isomers and closely related substances, creating a challenge in their analysis and the ability of the chemist to mix them accurately to create new formulas.

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