From- A Flavor-Receptor Ellipsoid Model for the Prediction of Flavor Sensory Thresholds

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Abstract

A flavor or odor threshold is the minimum energy of stimulus in a solid or liquid state that is needed to cause a minimal sensory response. A sensory threshold force is derived from a dimensional analysis of momentum about a fixed center of mass. Lyderson critical property increments (in lieu of molecular simulation) are then used to compute this force from molecular structure and boiling point data. A constant ratio, δ, of total rotational energy over angular momentum is found to correlate to the chemical functional group contribution for sensory thresholds over six orders of magnitude. A model based on the rotation of the inertial ellipse can be applied to molecules containing multiple functional groups and exhibiting chemical diastereoselectivity.

Introduction

Sensory or odor activity is strongly dependent on molecular properties. The strength and characteristics of odorants are related to functional group structure and polarity and to various physical properties. Among these are surface activity, vapor pressure, polarity, lipophilicity and solubility. The ability to elicit an odor response in humans is usually limited to molecules of molecular weights below 300 daltons.

Molecular geometry, shape and size also influence odor qualities. The interaction of odorant with specific and non-specific receptors in the olfactory membrane is responsible for odor stimulation and recognition. The affinity constants of odorants for the receptor are inversely related to their concentration. The concentration threshold for the perceptual detection of flavors varies over ten orders of magnitude. The olfactory **threshold** or minimum concentration of detection in a specified environment has both a molecular and physiological foundation.

Beyond the traditional taste senses of salty, bitter, sweet, and sour are the olfactory senses which are responsible for our recognition of flavors. Flavors are generally volatile, and by definition this indicates that the chemical component is in a vapor state when it is sensed. The olfactory receptors in the nasal passage are sensitive to these flavor compounds. During the ingestion of food or beverage the volatile flavors pass up the rear of the nasal passage (retronasal) and come in contact with the receptors.

Several theories describe how flavor compounds interact with these receptors. The exact mechanism is presently unknown but certainly involves both a physical and chemical interaction with the receptor. Physical interaction assumes a certain level of energy provided by the flavor molecule is required to interact and stimulate the receptor. The receptor may bind these flavors, or the flavor may dissolve in a membrane matrix and interact with the receptor. Some of the flavors may chemically interact and this chemical interaction is responsible for the other sensations such as the trigeminal senses. These sensations are associated with chemical irritation, astringency and dryness.

The individual flavor when sensed, can be described in terms different from the taste sensations. Terms such as fruity, caramelized, vegetable, earthy, chemical (sulfury, terpene-like), spicy, and floral are used. A flavor material dissolved in some food or beverage matrix is said to have a threshold concentration level. This is usually defined as the minimum concentration in a solid or liquid state that is required to just sense the flavor. Below the threshold, a finite concentration of the chemical is ignored by the sensory system, at least from a conscious level. (Subliminal levels may occur for some flavorings). Above the threshold value the flavor can be considered a stimulus which gives a flavor response which is related to the concentration of the flavor in the solid or liquid state. At some intermediate concentration the flavor may have an optimal taste level. At higher levels the response to the flavor may become an exaggerated or negative impact, suggesting a saturation of the receptors, which makes the response independent of concentration.

Presently, flavor thresholds are determined experimentally and statistically for each flavor. Unfortunately the threshold value of a flavor measured in water may not relate to the threshold of the flavor dissolved in another more complicated food matrix. This matrix may contain other flavors and tastes, which interact with the flavor compound to either increase or decrease its threshold value. The mechanism for this change in threshold is unknown, but it can be assumed to be related to differences in the response of receptors that have been adapted to the same or to other flavors/tastes in the matrix. The principle of adaptation of flavors to alter response is well known in sensory evaluation.

Is it possible to predict flavor threshold values from the structure of a flavor molecule? Given the above uncertainty of measuring experimentally a value, the prediction of that value seems even more remote. However, prediction or models can usually give values of the right order of magnitude under the most ideal conditions. It is the definition of "ideal condition" and the realization of the "non-ideality" of flavor interactions, which make theoretical predictions more reliable than experimental values. The reason for this reliability is that physical models are not influenced by outside variables, which occur during experimental measurement. The question then becomes; Are theoretical threshold values applicable to the real world?

The answer depends on the success of the model to the applications needed. Within a confined framework the model may be accurate but have no value beyond. For example, the activity coefficients of solutions can be theoretically calculated and, in many cases, can be used to predict the vapor-liquid equilibrium curves needed for distillation processes. If the liquid is non-ideal, various models are available to correct for the non-ideality and still be useful. At some large level of non-ideality, experimental data is needed to correct the theory. What type of experimental data is useful is actually predicted from the model. For example, knowledge of the boiling point or composition of a liquid azeotrope is sufficient. In the case of a flavor model perhaps knowledge of some experimental factor will be helpful to enhance the predictability of the model. As the framework of the model is established the relationship of real factors and model factors will become apparent.

Next: Threshold Energy and Threshold Force