Formulation Design with Organic Conception Diagram

NIHON EMULSION CO.,LTD.

32-7, 5-chome, Koenji-minami Suginami-ku, Tokyo 166-0003, JAPAN
Phone : (81) 3 3314-3211
F ax : (81) 3 3312-7207

Published on November,1998
Revised on March 26,2001

CONTENTS

1. Review of organic conception diagram

It is now described here to make graphs on the organic conception diagram believed to be the most important for researchers of emulsification. Then, characteristic properties of various common organic compounds on the conception diagram are broadly described.

1-1. Profile of organic conception diagram and tables of inorganic groups

1. Numerical figure representing organic properties

The mean value of the increment of the boiling points of linear compounds per one-carbon number around 5 to 10 carbon atoms is 20 °C in Fig. 1 (Boiling Point Curve), which is defined as 20.

2. Numerical figure representing inorganic properties

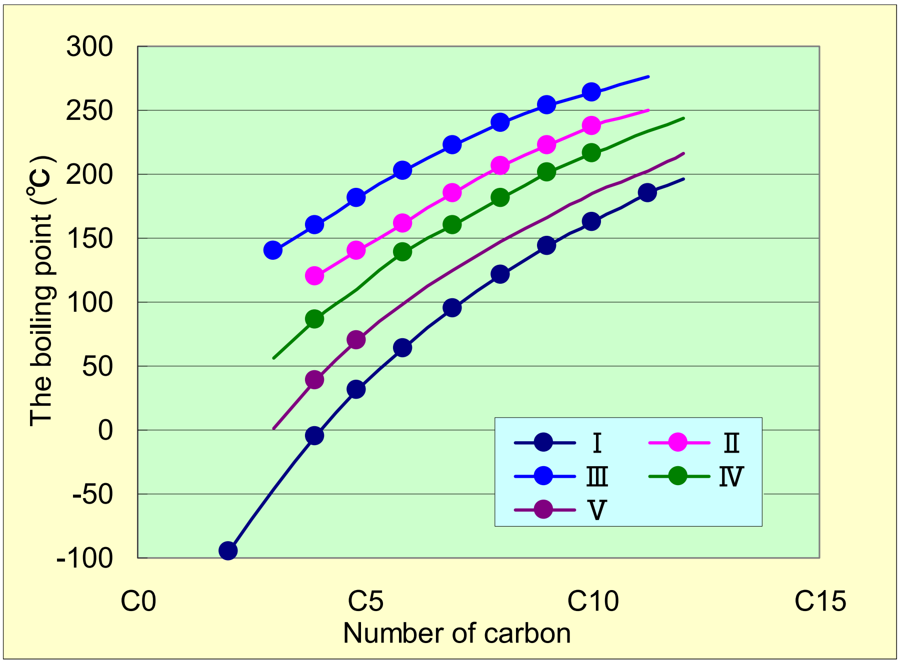
Because the distance between the linear alcohol boiling point curve and the linear paraffin boiling point curve in Fig. 1 (boiling point curve) is represented as about 100 °C in Fig. 1 (boiling point curve) around 5 carbon atoms, the influence of one hydroxyl group is defined as 100.

3. Other substituents

Other substituents are represented as the comparative value of the two values in (I) and (II) and shown in Table 1.

4. Primary subjects for the use of "Table of inorganic groups"

The organic and inorganic values of a compound with a known chemical structure can readily be determined in Table 1. But these values sometimes differ, depending on the determination of the groups. So as to prevent the occurrence of such a difference, those described in detail in references, revised values and specific groups are collectively shown in Table 2.



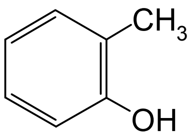
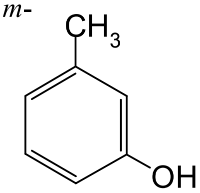
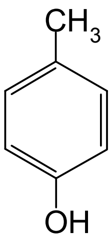
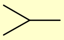
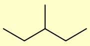
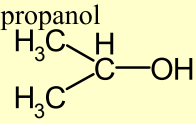
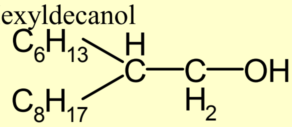
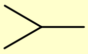
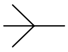
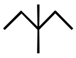
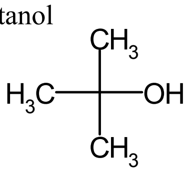
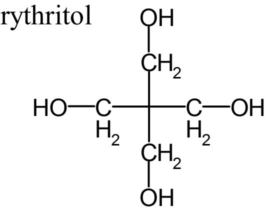
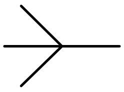
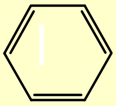
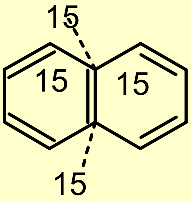
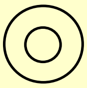
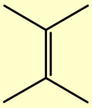
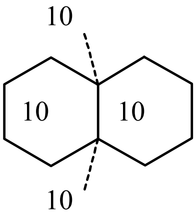
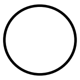
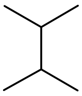
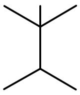
I C_nH_{2n+2}
II C_nH_{2n-1}-OH
III C_nH_{2n+1}-COOH
IV C_nH_{2n+1}-CHO
V C_nH_{2n+1}-OCH

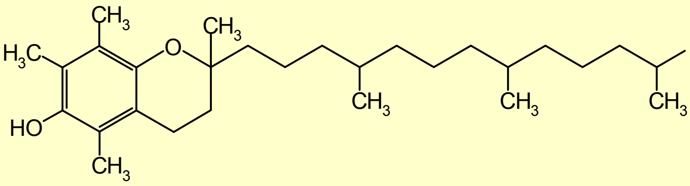
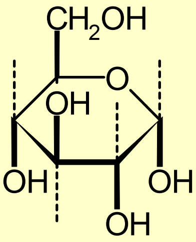
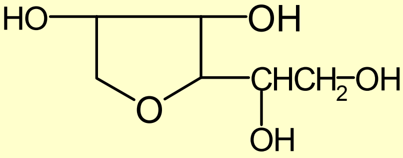
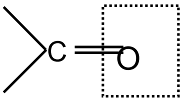
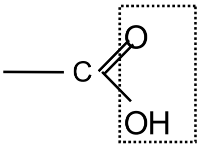
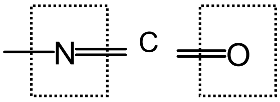
Figure 1, Curve of Boiling Point

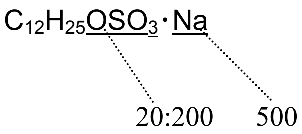
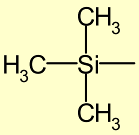
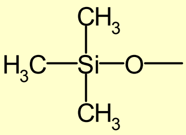
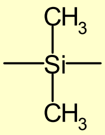
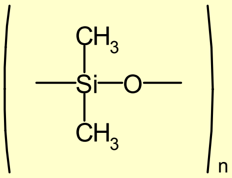
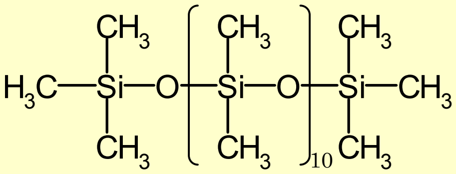
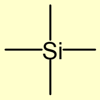
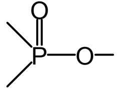
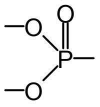
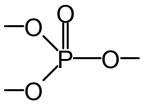
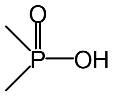
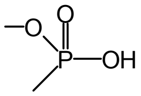
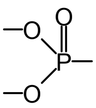
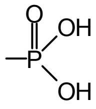
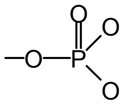
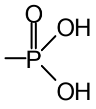
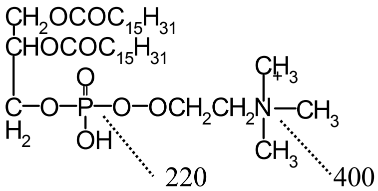
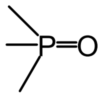
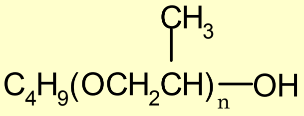
Table 1, of Inorganic Groups

Inorganic Group	Value	Organic and Inorganic Group	Value	
	Inorganic		Organic	Inorganic
Light Metals	500<	R_4Bi-OH	80	250
Heavy Metals, Amine and NH4 salt	400<	R_4Sb-OH	60	250
-AsO_3H_2, >AsO_2H	300	R_4As-CH	40	250
-SO_2-NH-CO-, -N=N-NH_2	260	R_4P-OH	20	250
$\Rightarrow N^+$-OH, -SO_3H, -$NHSO_2$-NH	250	-O-SO_3H	20	220
-CO-NHCO-NHCO-	250	>SO_2	40	170
->S-OH, -CONH-CONH-CONH-, -SO_2NH-	240	>SO	40	140
-CS-NH-, -CONH-CO-	230	-CSSH	100	80
=N-OH-, -NHCONH-	220	-SCN	90	80
=N-NH-, -CONH-NH_2	210	-CSOH, -COSH	80	80
-CONH-	200	-NCS	90	75
->N->O	170	-Bi<	80	70
-COOH	150	-NO_2	70	70
Lactone cyclization	120	-Sb<	60	70
-CO-O-CO-	110	-As<, -CN	40	70
Anthrathene nucleus, Phenanthrene nucleus	105	-P<	20	70
-OH	100	-CSS ϕ	130	50
>Hg (Organic bond)	95	-CSO ϕ, -COS ϕ	80	50
-NH-NH, -O-CO-O-	80	-NO	50	50
-N< (-NH_2, -NH ϕ, -N ϕ_2) Amine	70	-O-NO_2	60	40
>CO	65	-NC	40	40
-COO ϕ, Naphthalene nucleus, Quinoline nucleus*	60	-Sb=Sb-	90	30
>C=NH	50	-As=As-	60	30
-O-O-	40	-P=P-, -NCO	30	30
-N=N-	30	-O-NO, -SH, -S-	40	20
-O-	20	-I	80	10
Benzene nucleus (Aromatic single ring), Pyridine nucleus	15	-Br	60	10
Ring (non-aromatic single ring)	10	=S	50	10
Triple bond	3	-Cl	40	10
Double bond	2	-F	5	5
-(OCH_2CH_2)-, Sugar ring-O-	75	*iso* ramification>-	-10	0
	(20)	*tert* ramification->-	-20	0

Table 2, Preliminary knowledge of “ Inorganic Group “

A	Additional Remarks and Value of Special Group for “ Inorganic Group “	Abbreviation	Value
1	Positional Isomers and Stereoisomers are at identical values (with close boiling points) ・ Cresol *o-*  *m-*  *p-*  		Same Value
2	*iso* ramification (end group  , C-linkage ) ・ Isopropanol  ・ 2-Hexyldecanol  		Organic Value -10
3	*tert* ramification ( , C-linkage ) ・ *tert*-Butanol  ・ Pentaerythritol  		Organic Value -20
4	Aromatic ring and aromatic group-like ring (15 for single ring; each increment of 15 on the top and bottom of attached aromatic rings) ・ Benzene  ・ Naphthalene  	 	: 15
5	Non-aromatic ring (10 for any ring-like geometric shape; 10 for attached rings with H bond; no addition in the presence of substituent; ring with 2 substituents on the same carbon atom is not defined as iso.) ・ Decahydronaphthalene  	  	: 10 : 20 : 10

6	General ether bond (20 for ring-attached furan ring and pyran ring -O-) ・ Diethylether $C_2H_5—O—C_2H_5$ ・ Vitamin E 	- O -	: 20
7	Specific ether (so temperature reversible as 75 for the ether bond of ethylene oxide around ambient temperature or below the cloud point and 20 for the same above the cloud point) 1) POE (n) Cetyl Ether $C_{16}H_{33}$-O-$CH_2CH_2(OCH_2CH_2)_{n-1}$-OH 20 75 In occasion of monohydric alcohol, as 20 for the first ether bond, as 75 for other ether bonds. 2) POE (n) Monostearate $C_{17}H_{35}CO$・$OCH_2CH_2(OCH_2CH_2)_{n-1}$-OH 60 75 In occasion of higher fatty acid, as the ester bond for the first molecule.	- O -	: 75
8	Sugar ring ether (75 for furanose type, pyranose type and bound oxygen in polysaccharide) ・ Glucose  ・ Sorbitan 	- O -	: 75
9	Carbon-containing inorganic group (the carbon, in for example the carbonyl group, carboxyl group and amide group is added to the organic value) ・ carbonyl group  ・ Carboxyl group  ・ Amido group 		

B	Besides " Inorganic Group "	Abbreviation	Value
1	Sulfate ester (-O · SO_3H) conventionally allocated as 350 is revised on the basis of CMC and others ・ Sodium Lauryl Sulfate  $C_{12}H_{25}\underline{OSO_3}\cdot\underline{Na}$ 		20 : 220
2	Organic silicone compound -Si- (defined as organic value 20 like Si = C)  OV : IV 60 : 0  OV : IV 60 : 20  OV : IV 50 : 0  OV : IV 50 : 20  OV: IV 120: 20 500 : 200 260 : 720		20 :
3	Phosphate ester >P=O : 80  : 100  : 120  : 140  :180  : 200  : 220  : 280  : 300  : 380 ・ Hydrogenated Soy Lecithin  OV: IV 800 : 740		: 80
4	Ether bond of propylene oxide: 20 ・ POP (n mol.) Butyl Ether  $C_4H_9(OCH_2\overset{CH_3}{CH})_n{-}OH$	- O -	: 20

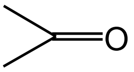
1-2. Calculation and location of organic compounds on the basis of the table of inorganic groups

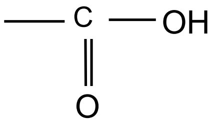
Because it is indicated that the two factors representing the properties of organic compounds, namely organic value and inorganic value, can be calculated, unknown compounds or compounds designed for practical blend examples can be expressed on graphs.

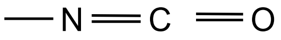
Calculation examples of three compounds are depicted in the organic conception diagram of Fig. 2. The terms in the conception diagram are defined as follows.

1. Substance field as area between longitudinal axis and crosswise axis
2. Crosswise axis is defined as organic axis
3. Longitudinal axis is defined as inorganic axis
4. Plotting of compound in the substance field is referred to as locate (location)

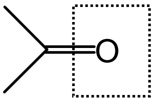
For location, it is noted that an organic value of an the inorganic group is to be added; the carbon group in the carbon-containing inorganic groups in the left column of the table, for example, carbonyl group, carboxyl group and amide group is to be added to organic value;

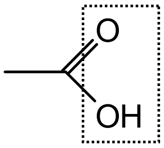


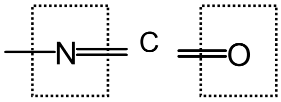




in other words, like methylene group, it is defined that the inorganic value is derived from the binding state shown in the square including inorganic elements.







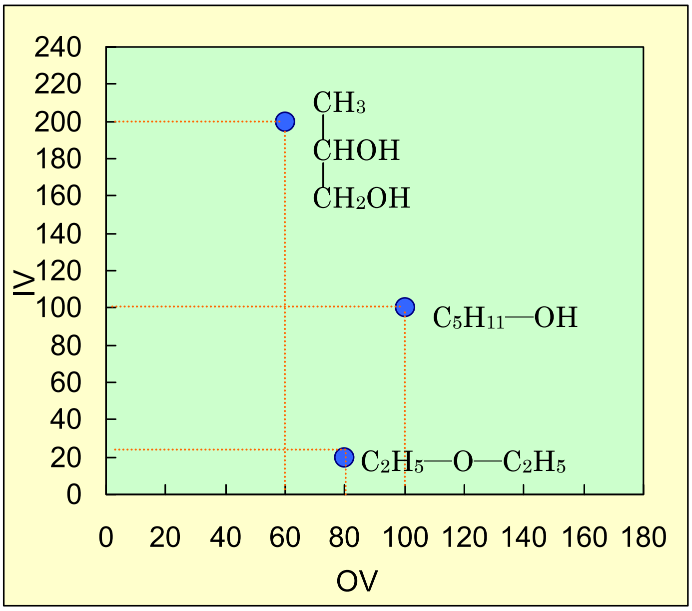
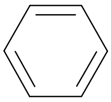
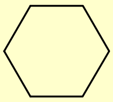
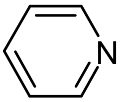
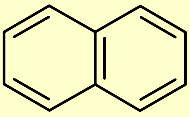
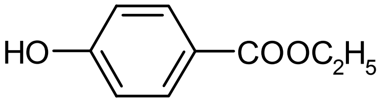
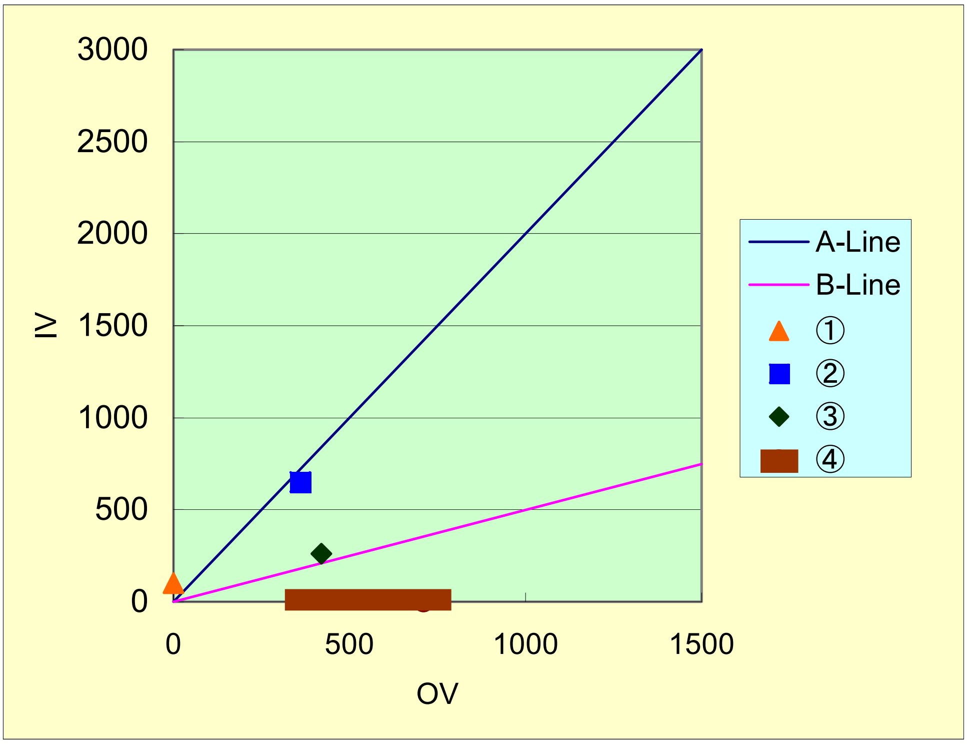


Figure 2, Organic Conception Diagram

Table 3, The practice of Organic Compound for OV : IV

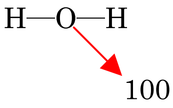
Example	Organic Compound	OV	IV
1	Methane CH_3	20 (20 X 1)	0
2	Ethane C_2H_6	40 (20 X 2)	0
3	Ethanol C_2H_5—OH	40 (20 X 2)	100 (100 X 1)
4	Propionaldehyde C_2H_5CHO	60 (20 x 3)	65
5	Benene 	120 (20 X 6)	15
6	Cyclohexane 	120 (20 X 6)	10
7	Pyridine 	100 (20 X 10)	85
8	Naphtalene 	200 (20 X 10)	60
9	Chloroform $CH{\cdot}Cl_3$	140 (20 + 40 X3)	30
10	Acetone $(CH_3)_2$=CO	60 (20 X 3)	65
11	Ethyl Parraben 	180 (20 X 9)	175 (100 + 15 + 60)



① Water

OV=0

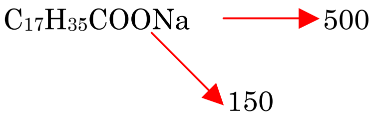
IV=100



② Sodium Stearate

OV=C_{18} X 20 = 360

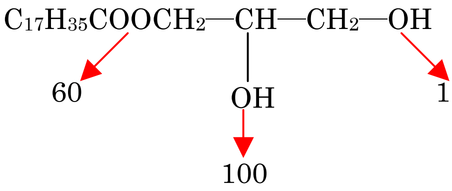
IV=150 + 500 = 650



③ Glyceryl Monostearate

OV=C_{21} X 20 = 420

IV=100 X 2 + 60 = 260



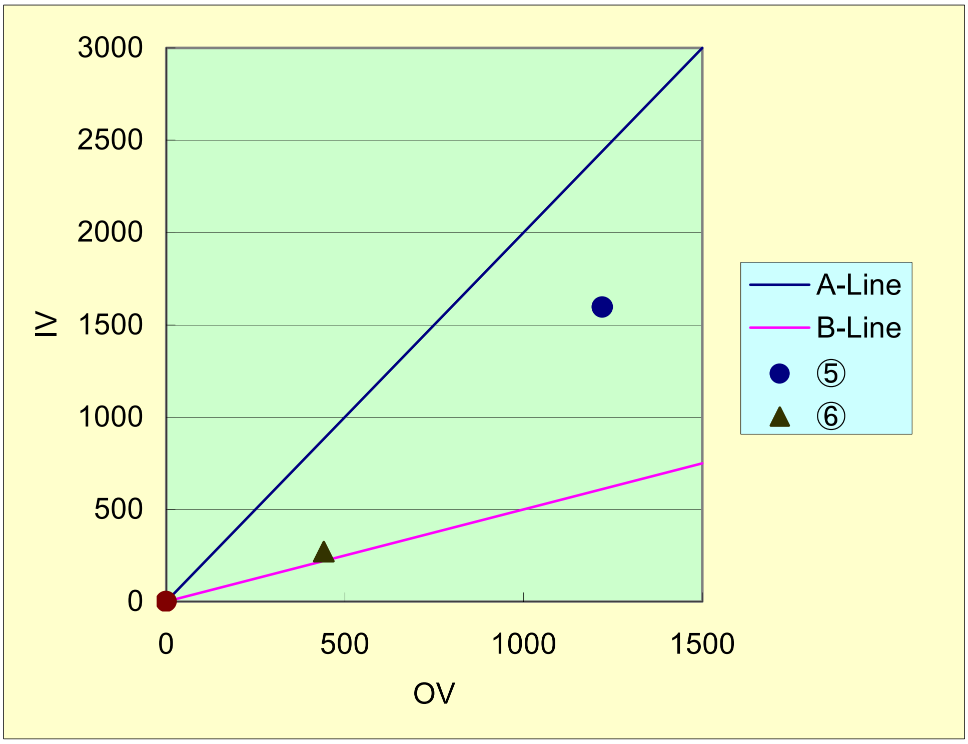
④ Liquid Paraffin

$C_{16}H_{34}$ ～ $C_{38}H_{74}$
(Including iso-paraffin)

OV=(C_{16} ～ C_{38} X 20) –50 = 270 ～ 710

IV=0

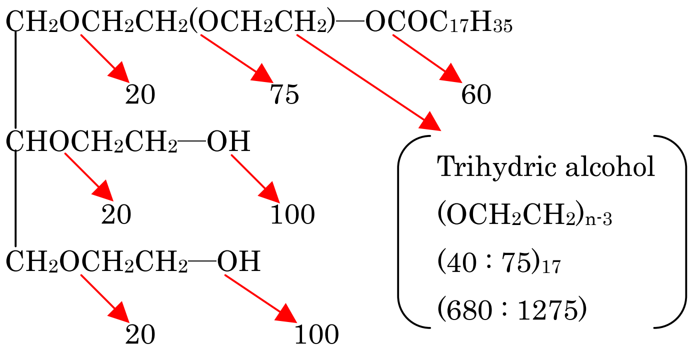
Figure 3, Organic Conception of Typical Cosmetic Ingredients



⑤ POE (20mol) Glyceryl Monostearate

OV=C_{27} X 20 + 680 = 540 + 680 = 1220

IV=20 X 3 + 100 X 2 + 1275 + 60 = 1595



⑥ POE (3mol) Cetyl Ether

OV=C_{18} X 20 + 80 = 360 + 80 = 440

IV=20 + 150 + 100 = 270

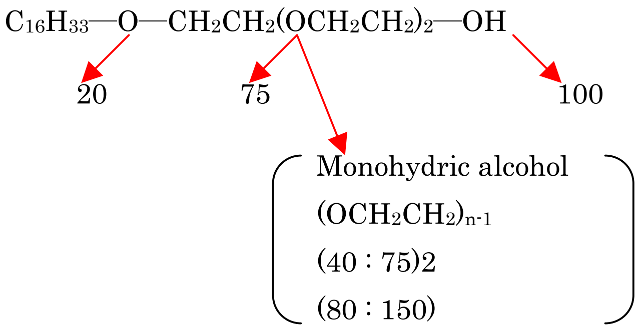
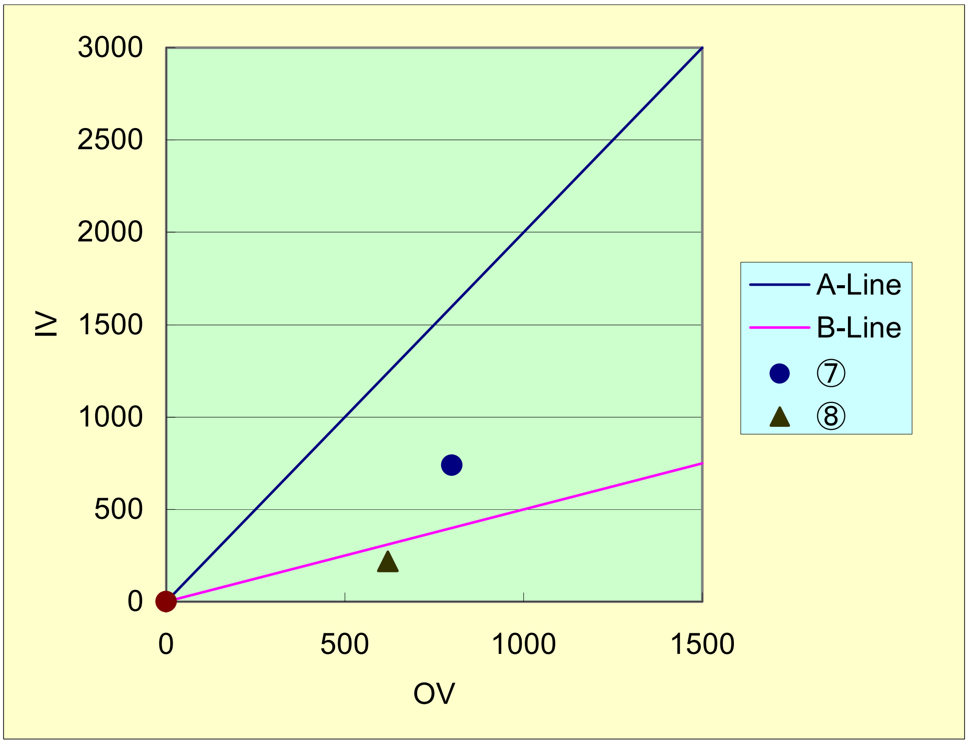


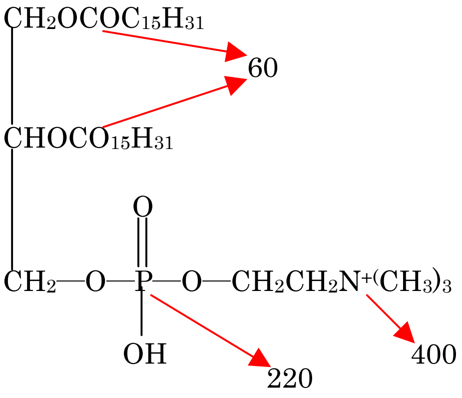
Figure 4, Organic Conception of Typical Non-Ion Surfactant



⑦ Hydrogenated Soybean Phospholipid

OV=C40 X 20 = 800

IV=60 X 2 + 220 + 400 =740



⑧ Methyl Polysiloxane

OV=120 + 50 X 10 = 620

IV=20 + 20 X 10 = 220

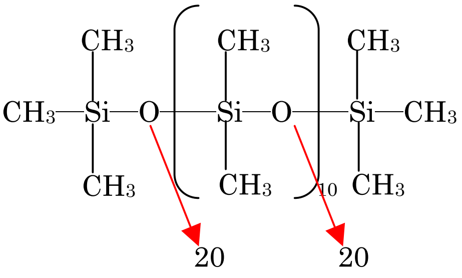


Figure 5, Organic Conception of Cosmetic Ingredients

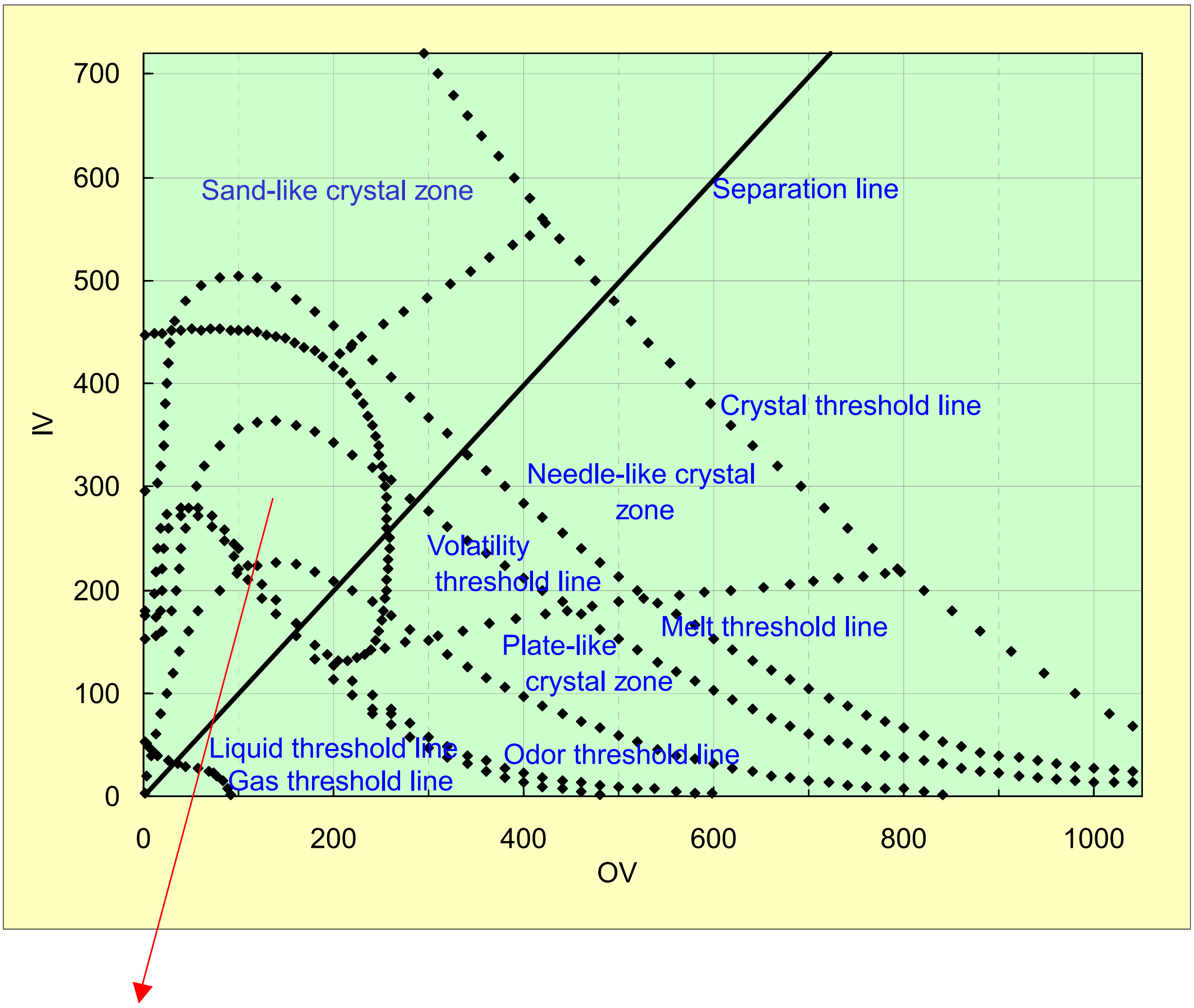
1-3. Specific performance observed on organic conception diagram

1-3-1. Properties and conception diagram of organic compounds

As shown in Fig. 6, threshold lines of gas, liquid, odor, volatility, melted state and crystal are sequentially shown around the origin.

Simple location of a compound on the organic conception diagram enables the prediction of approximate physical properties of the compound.

Alternatively, the organic value (carbon number) and inorganic value (number of substituents) of a substance can be estimated by the location of individual properties of the substance in appropriate fields in the conception diagram. Hence, the zone of the chemical structure can appropriately be suggested.



Zone of concomitant presence of plate-like and needle-like crystals

Figure 6, Organic Conception diagram (2)

1-3-2. Properties shown in organic conception diagram

1.Identical ratio line (inorganic value/organic value = I. O. B.) and miscibility

The line between the coordinate of Compound A and the origin as shown in Fig. 7 is referred to as the identical ratio line. Substances on the line can miscible well to each other.

However, the solubility of a substance more apart above or below the line is so reduced that the substance is more slightly soluble.

As in the case of solvents, low-molecular substance (B) is with a wider range of solubility even when the angle α is large. But the range of the solubility of a high-molecular substance (A) is narrower.

2.Distance from the origin

The distance of Compound C from the origin in Fig. 7 can be determined as follows.

$$C = \sqrt{X^2 + Y^2}$$

3.The angle (tan α) from the organic axis can be expressed as follows.

I.O.B. value　angle α = ° ′

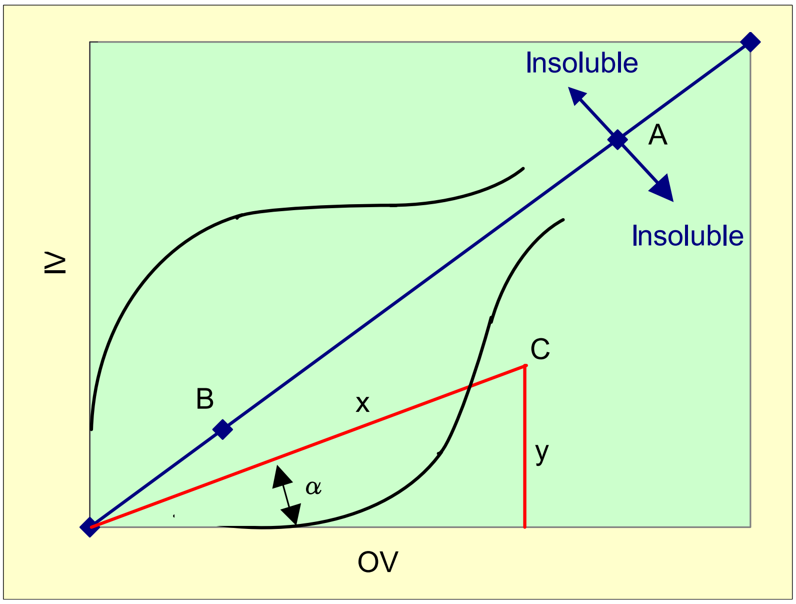


Figure 7, Properties of Organic Conception diagram

2. Properties of detergents on conception diagram

2-1. Positions on conception diagram and grouping of compounds

Location of routine organic compounds on the conception diagram indicates the presence of a zone of a group of similar compounds on the basis of their positions (angle and distance from the origin). The conception diagram of these similar compounds and the table of the list of representative raw materials belonging to them are shown below.

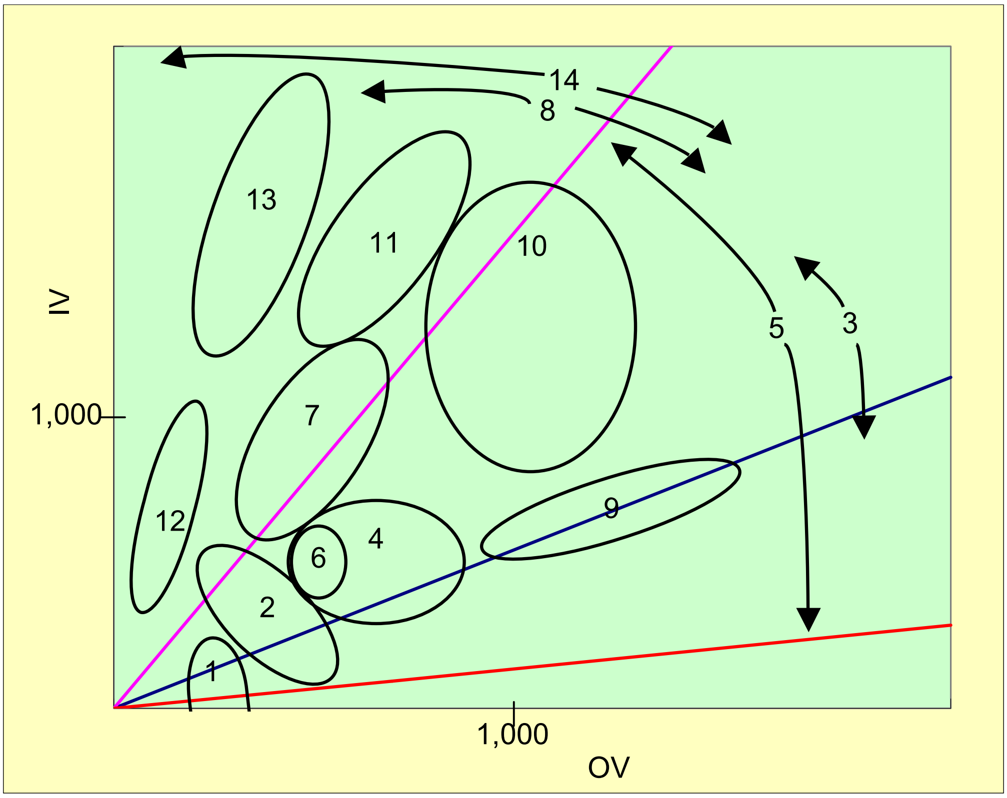


Figure 8,　Conception diagram of similar compounds

No.	α (about)	Surfactant	No.	α (about)	Dying etc
1	0° ～ 40°	Oil-soluble solvents	9	25° ～ 35°	Oil-soluble dyes, dispersion dyes
2	10° ～ 75°	Plasticizers	10	35° ～ 65°	Organic pigments
3	23° ～ 45°	W/O-SAA(HLB 3～6)	11	65° ～ 75°	Alcohol-soluble dyes
4	25° ～ 55°	Cation SAA	12	75° ～ 85°	Introfier, emollient NMF
5	10° ～ 60°	Nonion SAA	13	75° ～ 85°	Water-soluble dyes
6	40° ～ 55°	Foaming auxiliary agents	14	55° ～ 85°	Water-soluble polymers (protective colloids)
7	55° ～ 75°	Anion SAA, rinse agents			
8	55° ～ 75°	O/W-SAA(HLB 8～18)			

Table 4, List of Similar Chemical Substance

No.	α (about)	Similar chemical name	Chemical name of typical Ingredients	OV	IV	α
1	0° - 40°	Oil-soluble solvents	Isopentane	90	0	0°
			n-Hexane	120	0	0°
2	10° - 75°	Plasticizers	Di-(2-ethylhexyl)Adipate	420	120	16°
			Di-(2-ethylhexyl)Phthalate	460	135	16°
3	23° - 45°	W/O-SAA(HLB 3～6)	Diglyceryl Diisostearate	820	340	23°
			Sorbitan Sesqui-oleate	660	427	33°
4	25° - 55°	Cation SAA	Stearyl Trimethyl-A*-Chloride	460	410	41°
			Di-Stearyl Dimethyl-A*-Chloride	800	410	27°
5	10° - 60°	Nonion SAA	Glyceryl Monostearate	420	250	31°
			POE (20mol) Cetyl Ether	1120	1545	54°
6	40° - 55°	Foaming auxiliary agents	Lauroyl Diethanolamide	320	400	51°
			POE (8mol) Nonyl Phenyl Ether	590	660	48°
7	55° - 75°	Anion SAA, rinse agents	Sodium Stearate	360	650	61°
			Sodium Lauryl Sulfate	260	720	70°
8	55° - 75°	O/W-SAA(HLB 8～18)	POE (30) Cholesteryl Ether	1720	2377	54°
			POE(60)Glyceryl Monoisostearate	2810	4595	59°
9	25° - 35°	Oil-soluble dyes, dispersion dyes	Orange SS	340	205	31°
			Yellow AB	320	175	29°
10	35° - 65°	Organic pigments	Permatone Red	430	270	32°
			Phtalocyanine	640	1084	59°
11	65° - 75°	Alcohol-soluble dyes	Alizanine cyanine Green F	560	1900	73°
			Quinizarin Green SS	560	405	36°
12	75° - 85°	Introfier, emollient NMF	Sodium Lactate	60	750	85°
			Ethyleneglycol	40	200	78°
13	75° - 85°	Water-soluble dyes	Amaranth	400	2500	81°
			Tartrazine	320	2452	82°
14	55° - 85°	Water-soluble polymers (protective colloids)	Hydroxyethyl Cellulose	(200 : 500)n		68°
			Polyvinyl alcohol	(40 : 100)n		68°

A* Ammonium

2-2. Cloud points of polyoxyethylene-series detergents

When the temperature of aqueous solutions (0.5, 1.0, 2.0 %) of polyoxyethylene (abbreviated as POE)-series nonionic detergents is gradually elevated, the aqueous solutions rapidly turn opaque. The temperature is referred to as cloud point or cloud temperature.

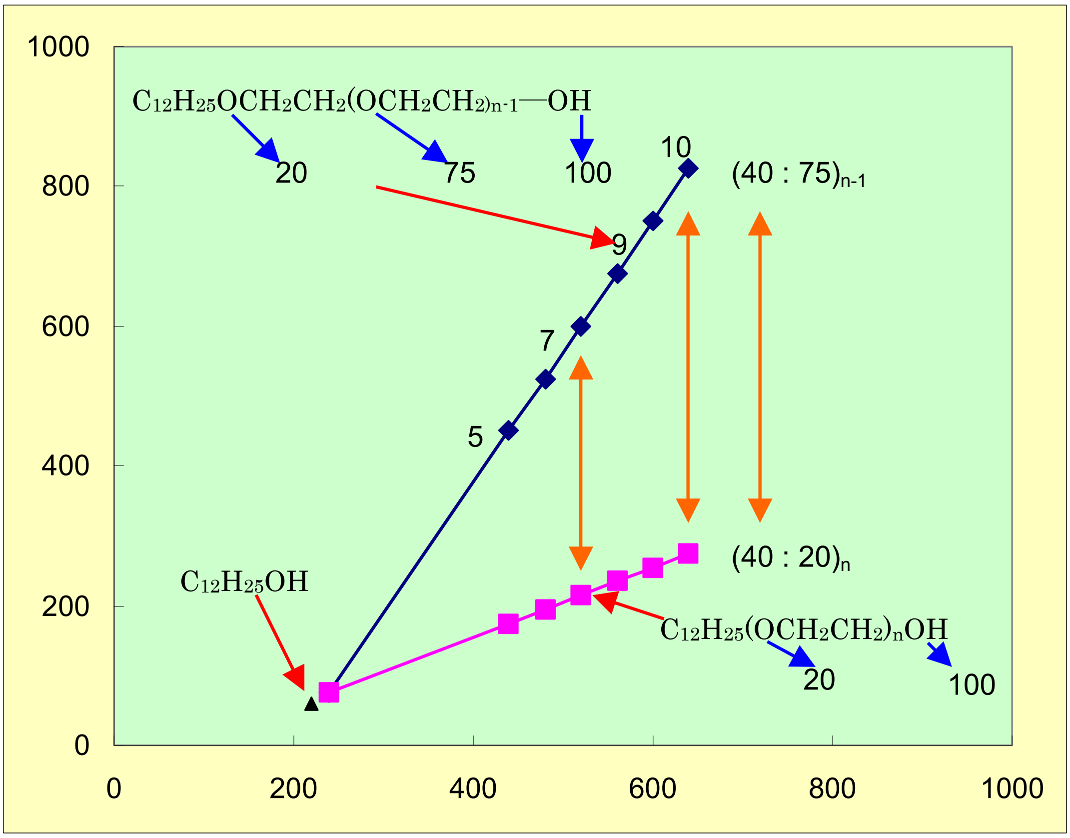


Figure 9, Cloud point of nonionic detergents

1. While the solubilities of general organic compounds are increased at higher temperatures, POE-series detergents hardly coordinate with H_2O due to the properties of oxygen in polyoxyethylene group, so that micelles are rapidly associated together and fall into an opaque state in dispersion.

2. At a temperature below the cloud point, the phenomenon is so temperature reversible that the transparent state is again resumed rapidly.

— (OCH2CH2) — (40 : 75) $\rightleftarrows$ [Cloud point] (40 : 20)

2-3. Organic conception diagram and HLB

1. Mr. Oda has found that because the organic value in the organic conception diagram totally coincides with detergent lipophilicity and the inorganic value coincides with hydrophilicity, the ratio (IV/OV) of the inorganic value of an appropriate detergent to the organic value is calculated on the basis of the chemical structure and that the IOB value × 10 represents a numerical figure with the same meaning of HLB defined by Griffin.

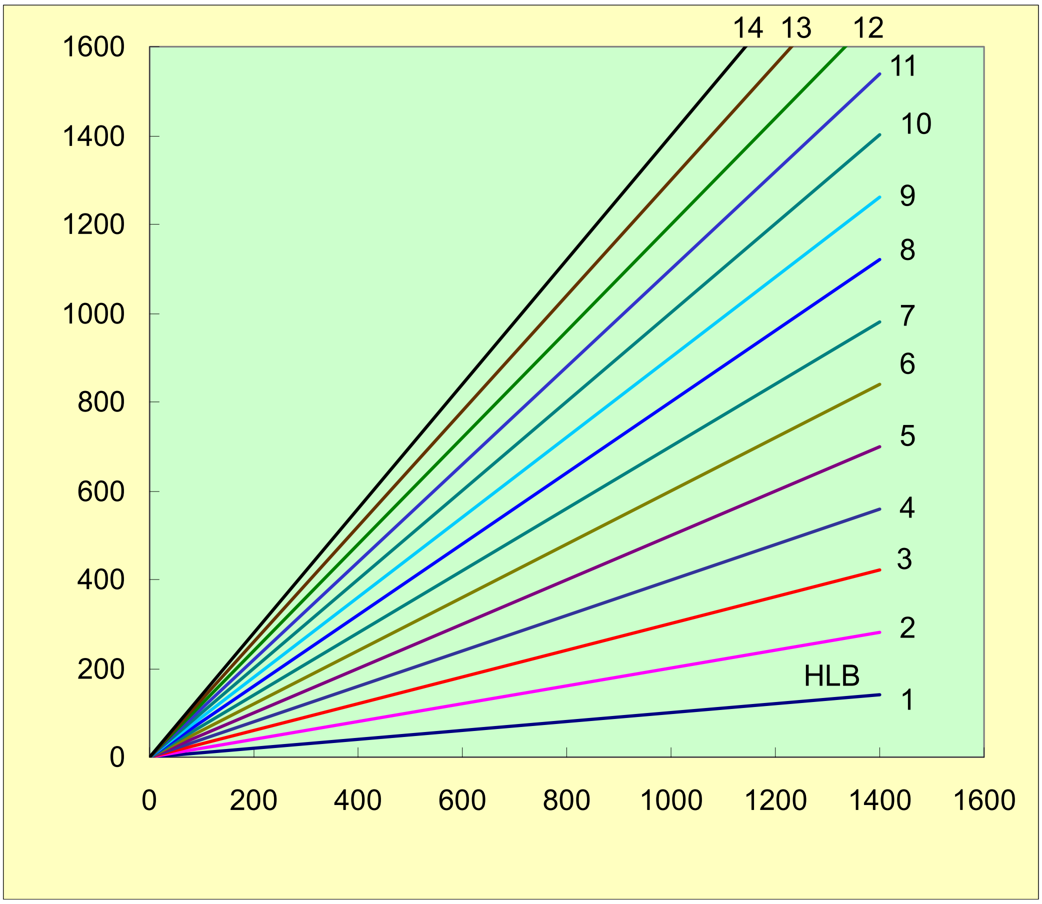


Figure 10, HLB of Oda type and Conception diagram

3. Examination of formulation on organic conception diagram

In this chapter, how to compose formulation is described. Practically, the composition of formulation is the most essential for researchers responsible for emulsification works in practice. More specifically, important subjects concerning emulsification, such as how to select emulsifier, component quality for formulation and component quantity for formulation, are described. Essential subjects for practical examinations are described below.

3-1. How to select emulsifier (Emulsification and solubilization based on conception diagram)

3-1-1. Conception diagram and emulsion type

Depending on the balance (value α) between the organic and inorganic values of an emulsifier, the resulting water/oil emulsion forms O/W (oil in water) or W/O (water in oil).

Generally, emulsifiers are in W/O around line B (around $\alpha = 30$ °); alternatively, emulsifiers are in O/W around line A (around $\alpha = 60°$). Thus, these are referred to as emulsifiers for W/O and O/W, respectively.

When fluid paraffin and water for example are emulsified using sodium oleate ($\alpha = 61°05'$. 360:652), the resulting emulsion is in O/W type (Fig. 11). When fluid paraffin and water for example are emulsified using glycerin monostearate ($\alpha = 31°45'$. 420:260; generally a mixture of several species), the resulting emulsion is in W/O type (Fig. 12). The phenomena mean that larger quantities of emulsifiers are present around line A or B. According to the conception diagram, then, type A emulsion means that large quantities of emulsifiers are present around line A, while type B emulsion means that large quantities of emulsifiers are present around line B.

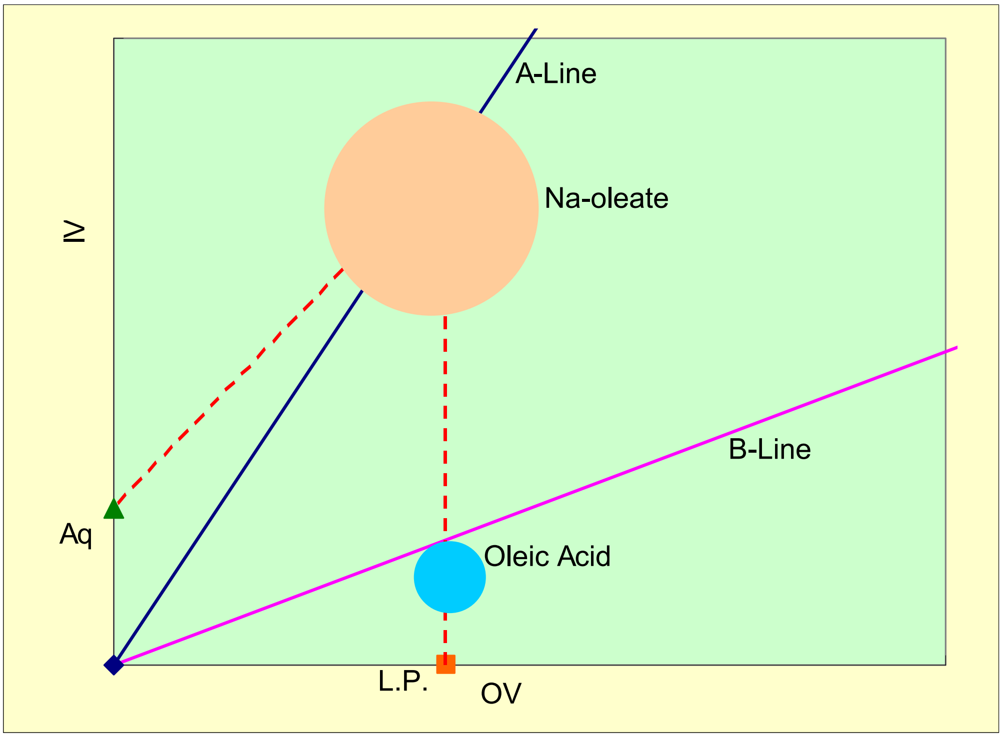


Figure 11, Type A emulsion

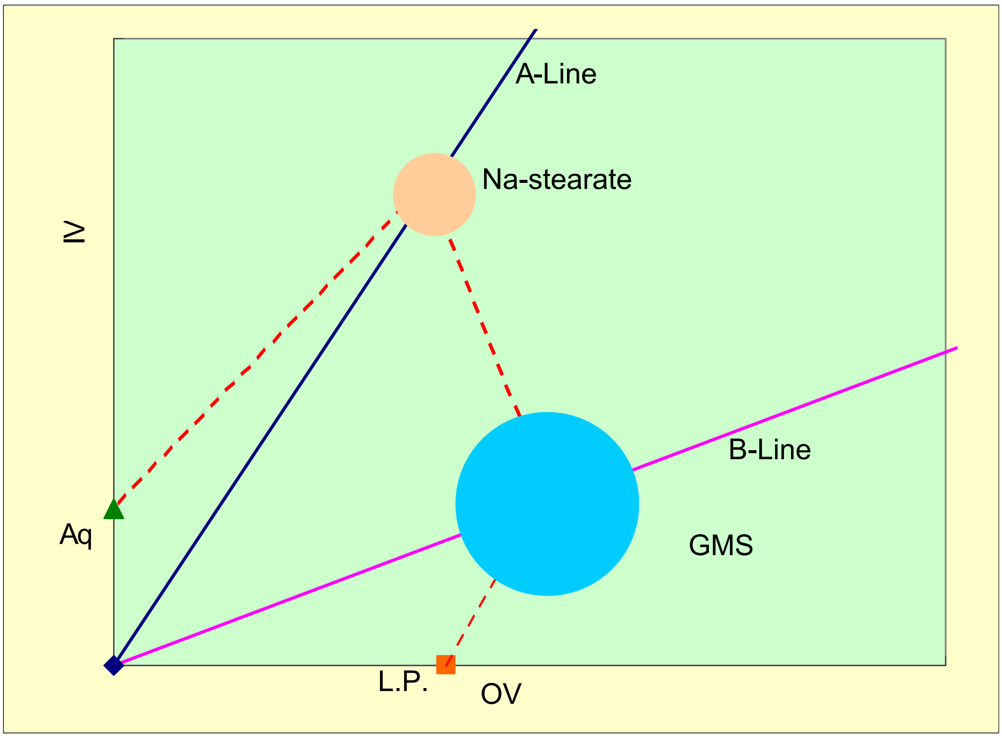


Figure 12, Type B emulsion

3-1-2. Conception diagram and phase inversion

1. When an emulsifier around line B is added gradually to type A emulsion until the quantity exceeds the quantity of an emulsifier around line A, the emulsion falls in phase inversion to type B (shown in Fig. 13).

2. When acid is added to type A emulsion of fluid paraffin, water and fatty acid soda soap, the soap is converted to fatty acid (shown in Fig. 14). Consequently, the coordinate of the original soap as an emulsifier moves on the conception diagram. In such manner, the emulsion is decomposed and separated.

Those described above correspond to the addition of another emulsifier to the emulsion system, which leads to chemical modification. These coincide with the modification of the quality and quantity of emulsifier.

Because the emulsion is separated or falls into a state readily separable because of such a reason, it is thus suggested that no addition of any substance except oil and water to an emulsion for the stabilization of the emulsion is significant.

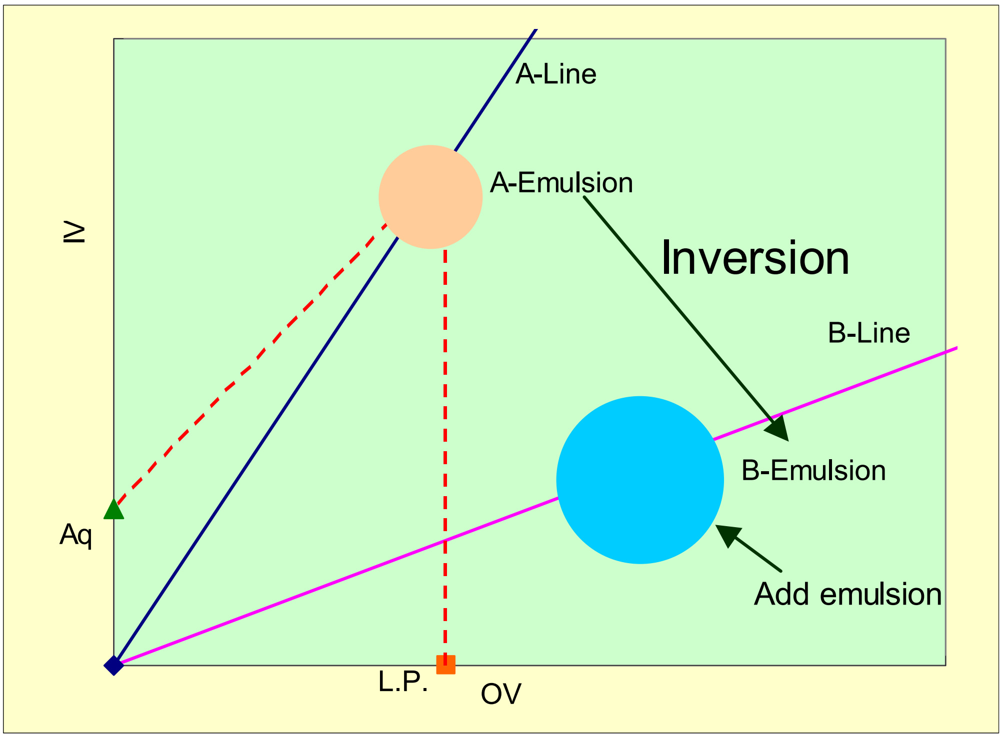


Figure 13, Phase inversion with additive

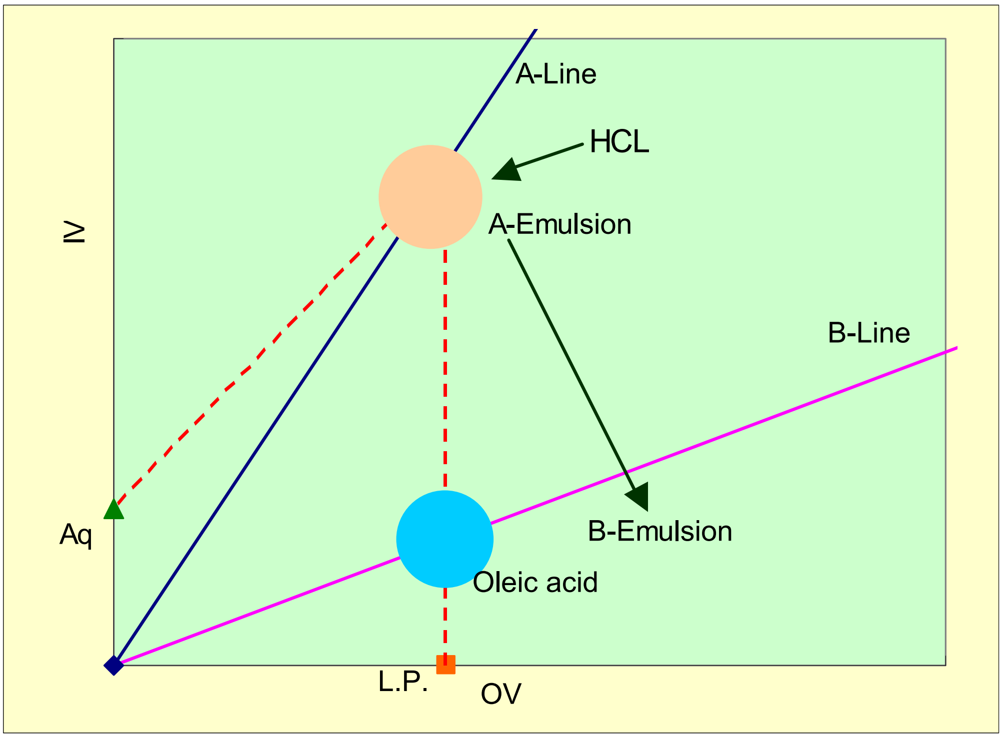


Figure 14, Phase inversion by chemical modification

3-1-3. Relation between emulsion stability and component coordinate

Emulsion with POE-series detergent as emulsifier sometimes incurs creaming or separation due to temperature change (high temperature or low temperature). As a preventive measure of the phenomenon, a part of the emulsifier is essentially modified. Specifically, a part of the emulsifier used in the formulation is simply substituted with an emulsifier with the same α value [on the same ratio line but with a different distance from the origin (a higher molecular or lower molecular emulsifier)] on the conception diagram, which works to prepare a stable system. This essentially serves for the efficient recovery of stable emulsion (how to select emulsifier). This suggests the relation between the temperature resistance of emulsion and the length of the coordinate of emulsifier, namely emulsifier quality. When the quality of a part of emulsion composed of plural components is modified, the tendency of the stability of the emulsion against temperature change can be predicted on the basis of the positions on the conception diagram. One of the examples is shown in Fig. 15.

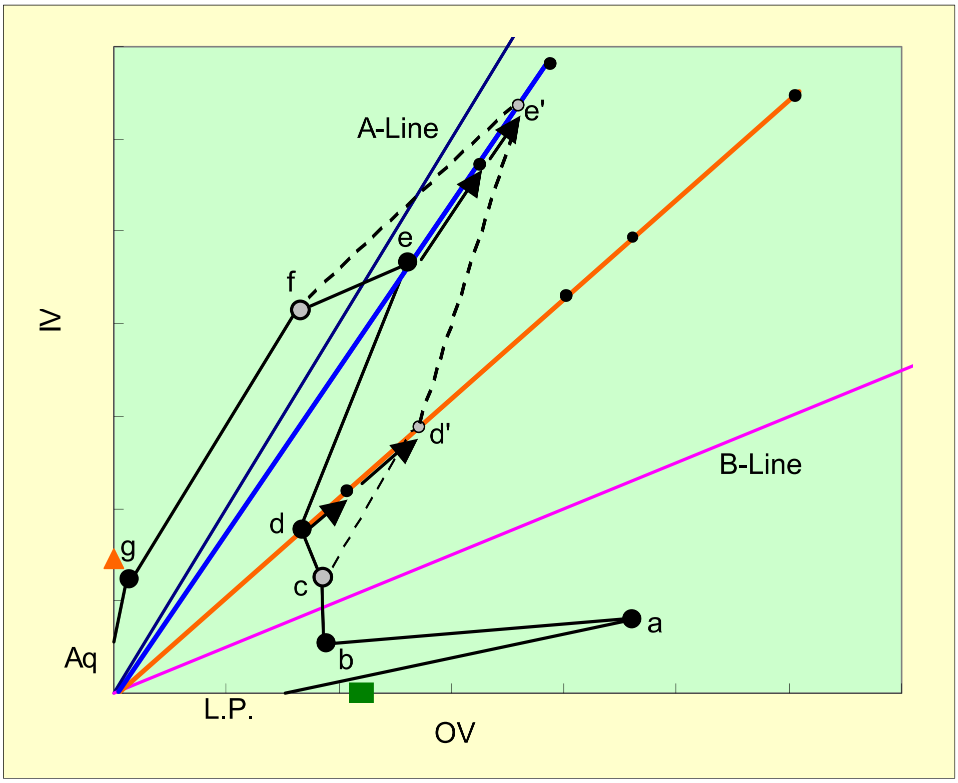


Figure 15, How to select emulsifier

3-2. Role of component quality for emulsification

The role of the quality of a component composing a formulation is thoroughly understood as one of the factors significantly influencing various properties of emulsion. Thus, component designation and representative examples of emulsion types with quality differences are described below.

3-2-1. Definition of trisectional lines dividing organic property (oil) and inorganic property (water)

In the conception diagram, trisectional lines can be drawn; one is line B with α = 30 ° and the other is line A with α = 60 °. However, components within the α range of 0 to 90 ° are not necessarily used for preparing a practical formulation. Depending on the purpose, components with a narrow α range on the conception diagram are sometimes used for preparing a formulation. In such a case, trisectional lines are drawn between a component with the minimum α value and a component with the maximum α value among the components; then, line B is drawn at the 1/3-fold angle while line A is drawn at the 2/3-fold angle. These examples are shown below.

1. Oil of α=0° in formulation and water of α=90°

B-Line=30° , A-Line=60° (Figure 16)

2. Cetyl alcohol of α minimum of oil

(Cetyl alcohol : OV:IV=320:100, α=17° 21’)

(a) Move organic pole to α=17° 21’
As long as (90° — 17° 21’)=72° 39’, divide into third
72° 39’ / 3 = 24° 13’
(b) B-Line=24° 13’ + 17° 21’ (moving of organic pole) = 41° 34’
A-Line = B-Line (41° 34’) + 24° 13’ = 65° 47’ (Figure 17)

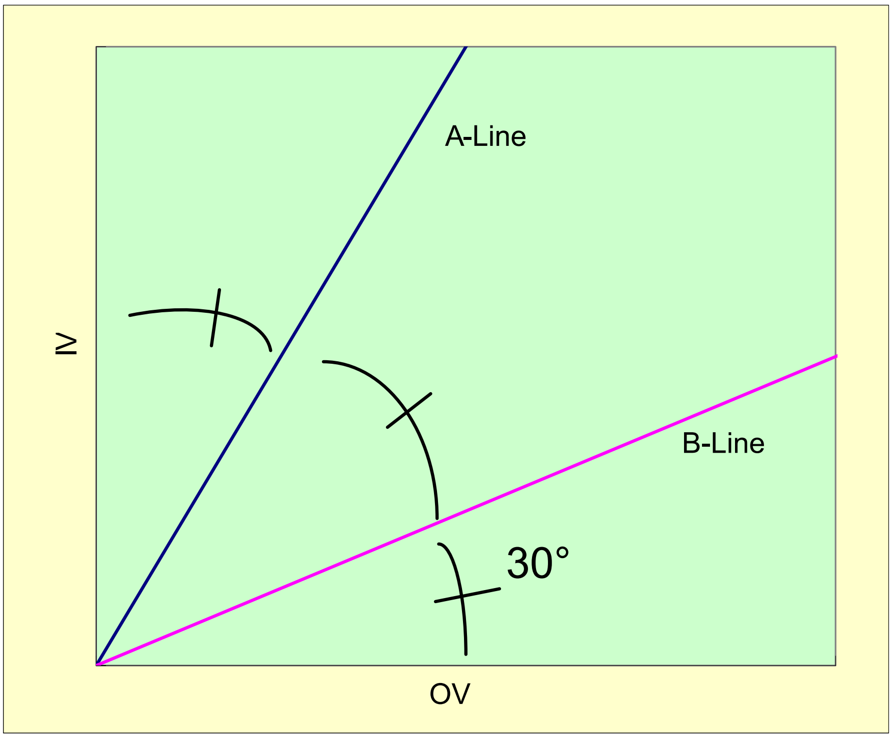


Figure 16, Dvision into third line between water and hydrocarbon

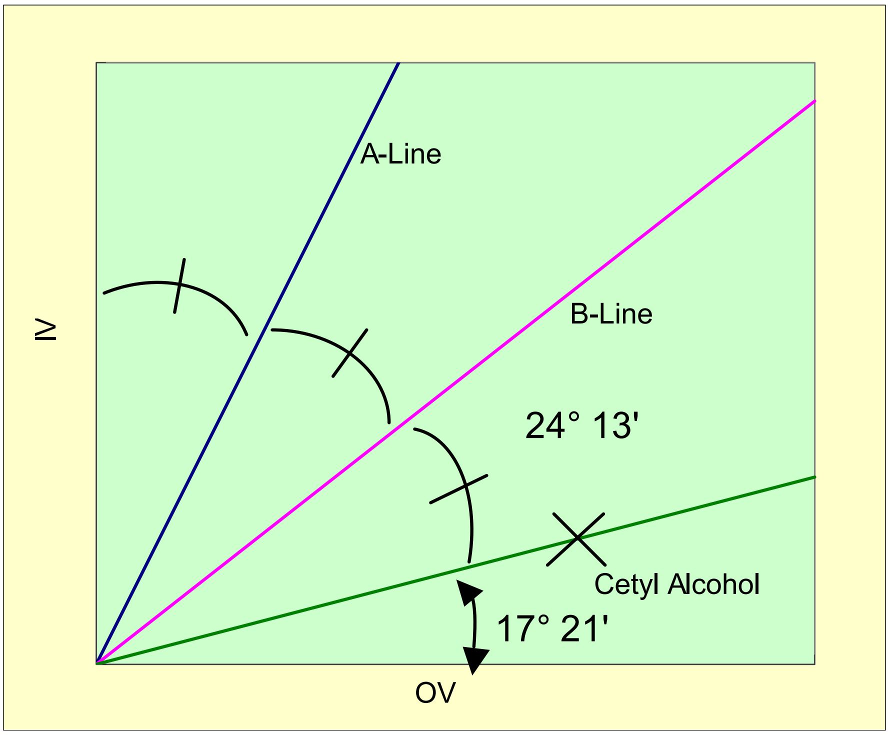


Figure 17, Dvision into third line between water and cetyl alcohol

As shown in Fig. 17, the organic axis transfers, depending on the α value of an oil used, so the positions of the trisectional lines also transfer. The transfer of these trisectional lines is advantageous for the objective formulation in that the range for the selection of numerous components can be so narrowed that appropriate components can readily be found.

The trisectional lines thus drawn play important roles for the properties of the resulting emulsion, the determination of formulation and component selection and the like.

3-2-2. Composition and definition of oil phase and water phase

	Abbreviation
① (Oil phase : oil phase) or its quantity	(O : W)
② Emulfier on oil phase	O_{SAA}
③ Emulfier on water phase	W_{SAA}
④ (② : ③)	(O_{SAA} : W_{SAA})

2. Type A emulsion and O_{SAA} : W_{SAA} (Fig. 18)

Emulsifiers are mostly present around line A. Among all the components, all components present in the region around line A, from an emulsifier with the second smallest α value [meaning that components with α values larger than the α value of the component (emulsifier) are referred to as emulsifiers] to oil with the smallest α value, are defined as oil-phase emulsifiers (O_{SAA}).

Components present above the line A to the inorganic axis of water are defined as aqueous phase emulsifiers (W_{SAA}).

As described above, emulsifiers present around the line A are divided on the line A and defined as O_{SAA}:W_{SAA}.

3. Type B emulsion and O_{SAA}:W_{SAA} (Fig. 19)

Type B emulsion can be considered like the type A emulsion. More specifically, components present around line B including a component with the second smallest α value to the α value of oil are defined O_{SAA}. Then, components present above the line B and immediately before water are defined W_{SAA}.

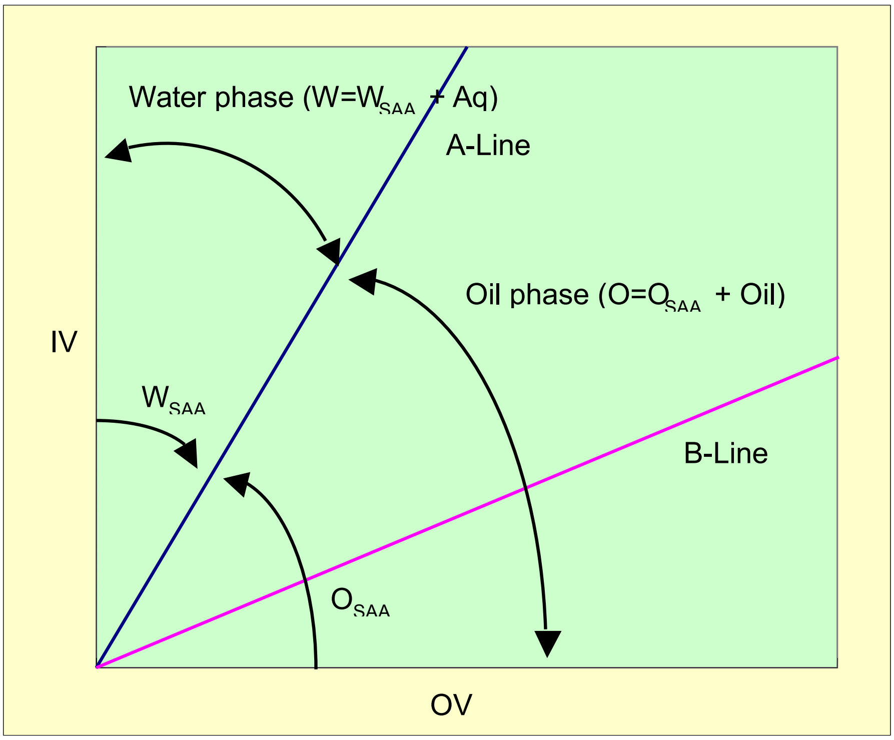


Figure 18, Located regions of type A emulsion and O_{SAA}:W_{SAA}

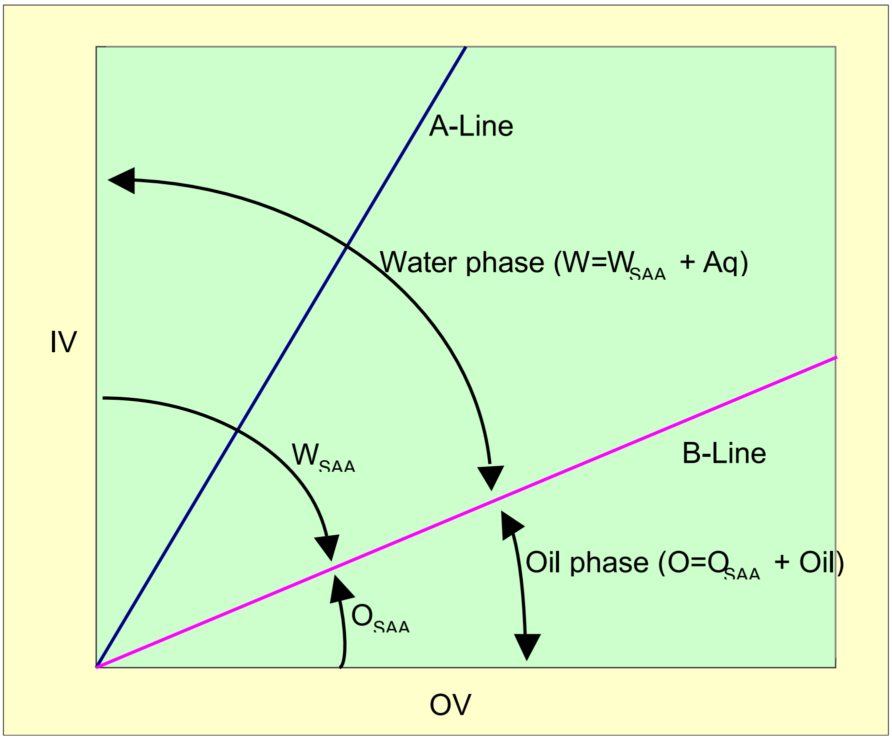


Figure 19, Located regions of type B emulsion and O_{SAA}:W_{SAA}

4. Content of water phase and oil phase

Fig. 18 and Fig. 19 are explained as follows:-

Oil phase : O_{SAA} and Oil (Oil : content of minimum of α value)

Water phase : W_{SAA} and Aq (Water : content of minimum of α value)

So, $O + W = 100$ (%)

$O = (O_{SAA} + Oil)$

$W = (W_{SAA} + Aq)$

So, O : W is as follows:-

A type emulsion : $O = Oil + O_{SAA}$ (0° to A-Line), $W = W_{SAA}$ (A-Line < 90°) + Aq

B type emulsion : $O = Oil + O_{SAA}$ (0° to B-Line), $W = W_{SAA}$ (B-Line < 90°) + Aq

3-2-3. Component quality-influencing emulsion type

Individual components in emulsion formulation are now located on the conception diagram. These components are distributed, variously, depending on the types.

When these coordinates are lined together in the order of α value, the individual components are likely to be classified in a number of types.

Among several emulsifiers, then, the position of an emulsifier with the longest distance from the origin on the coordinate axis is determined on the side of line A or the side of line B. An emulsifier present around line A is expressed as lA, while an emulsifier present around line B is expressed as lB.

It is said generally that an emulsion composition containing an emulsifier of a long distance around line A or B is likely to be stable. Thus, typical types are illustrated.

1. Example lA and l : s type (shown in Fig. 20)

a. (With respect to lA)

Because an emulsifier of the longest distance from the origin is around line A among formulation components, the formulation is referred to as lA type.

b. (With respect to l : s)

The distance (χ) of O_{SAA} with the minimum α value from the origin is longer than the distance (y) of W_{SAA} with the maximum α value among aqueous phase components.

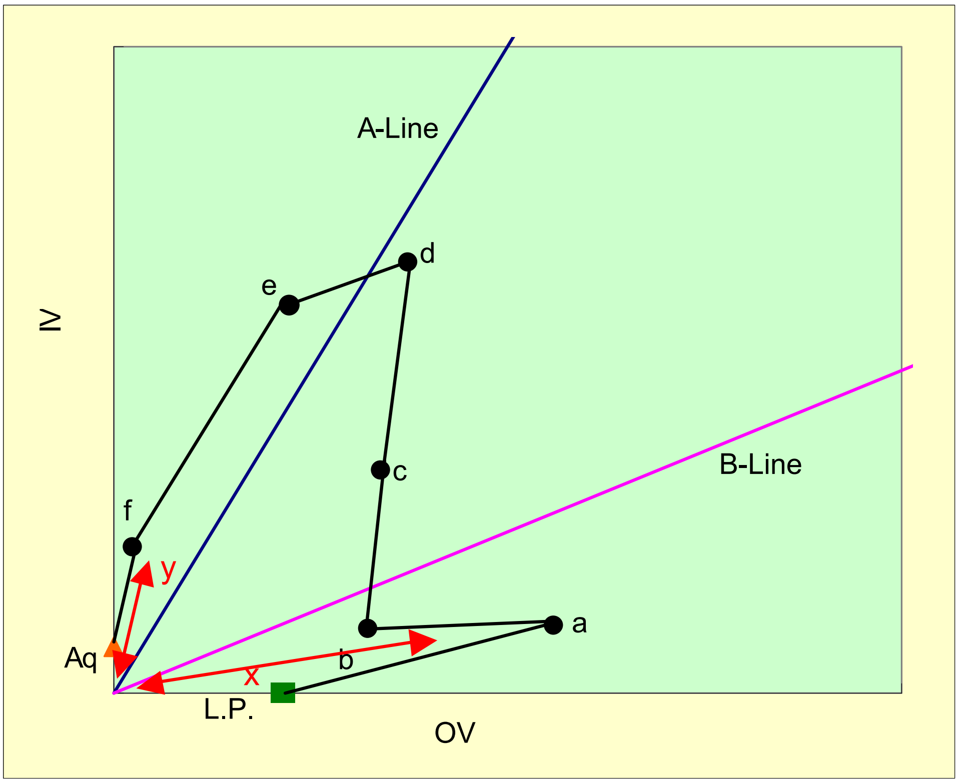


Figure 20, lA and l : s type

Characteristics of this type

This type of the A type is so highly hydrophilic that the type is dispersed well in water and foams well. Due to l : s , the type can add slight emollient property to facial detergents, shampoos, etc.

This type of the B type is most commonly used as base cosmetics and is very stable thermally due to the lA . Due to the l : s , furthermore, products with no white shade, even after spreading, can be developed.

Example of cosmetic

A type : Creansing wash, Pearl shampoo and lotion

B type : Milky cream, Cream and Basic cosmetic

2. Example ｌA and ｓ：ｌ type (shown in Fig. 21)

a. (With respect to ｌA)

It is same as example 1.

b. (With respect to ｓ：ｌ)

The distance (χ) of the O_{SAA} with the minimum α value from the origin in oil phase components is shorter than the distance (y) of W_{SAA} with the maximum α value in aqueous phase components.

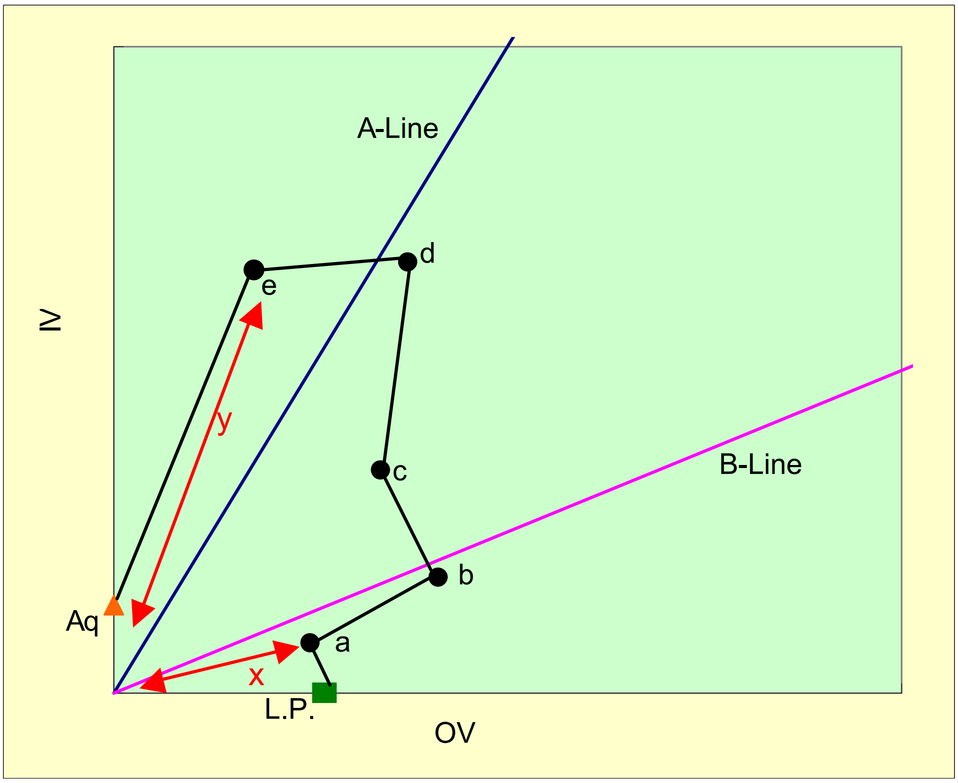


Figure 21, ｌA and ｓ：ｌ type

Characteristics of this type

This ｌA and ｓ：ｌ of the A type is the most hydrophilic and foams most among all the types. Due to ｓ：ｌ the type can cause stitches and cramps due to the strong defeating power in facial detergents, shampoos, etc.

This type of the B type is commonly used as base cosmetics like ｌA and ｌ：s and is the most thermally stable. Additionally, this type of ｓ：ｌ is absorbed well into the skin when used, so products with a refreshing feeling and with a whitened shade after spreading can be developed.

Example of cosmetic

A type : Washing and Shampoo

B type : Basic cosmetic

3. Example ｌB and ｌ：ｓ type (shown in Fig. 22)

a. (With respect to ｌB)

Because an emulsifier of the longest distance from the origin among formulation components is present around line B, the emulsion is defined as ｌB type.

b. (With respect to ｌ：ｓ)

It is same as example 1.

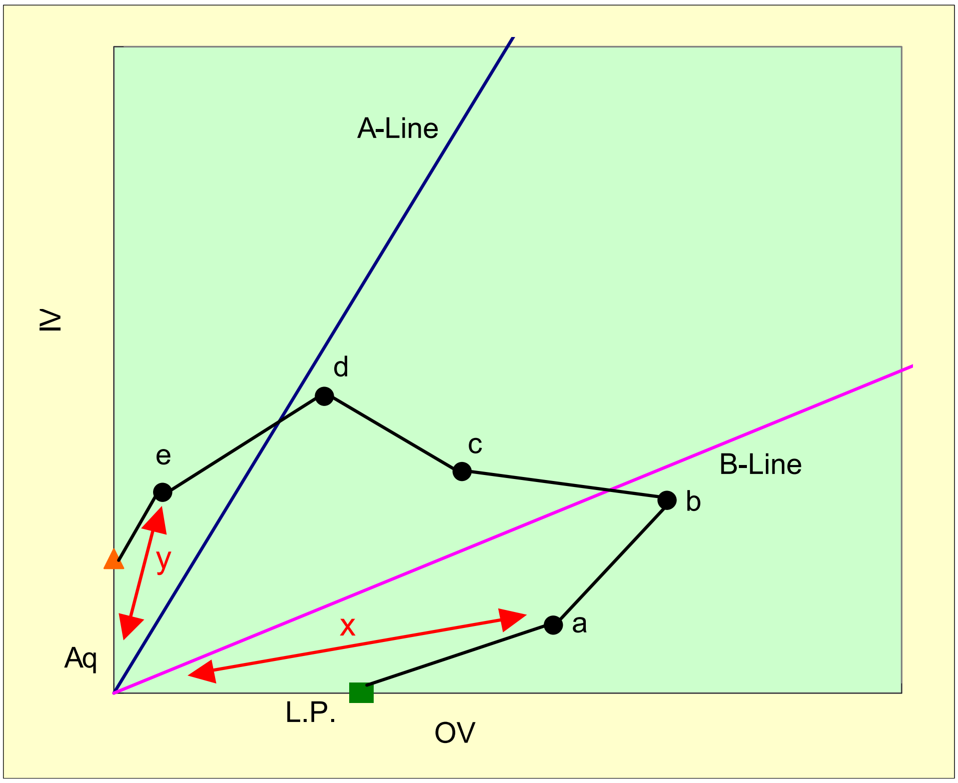


Figure 22, ｌB and ｌ ：ｓ type

Characteristics of this type

This type of the type A is the least hydrophilic and dispersible in water with the lowest foaming potency. The type is generally at high viscosity but is the most emollient in detergents such as facial detergent and shampoo.

From this type of the type B, furthermore, products with the strongest oily feeling and water repellence can be developed.

Example of cosmetic

A type : Remover of make up

B type : Sun care cosmetic, Hand cream and W/O emulsion

4. Example lB and s : l type (shown in Fig. 23)

a. (With respect to lB)

It is same as example 3.

b. (With respect to s : l)

It is same as example 2.

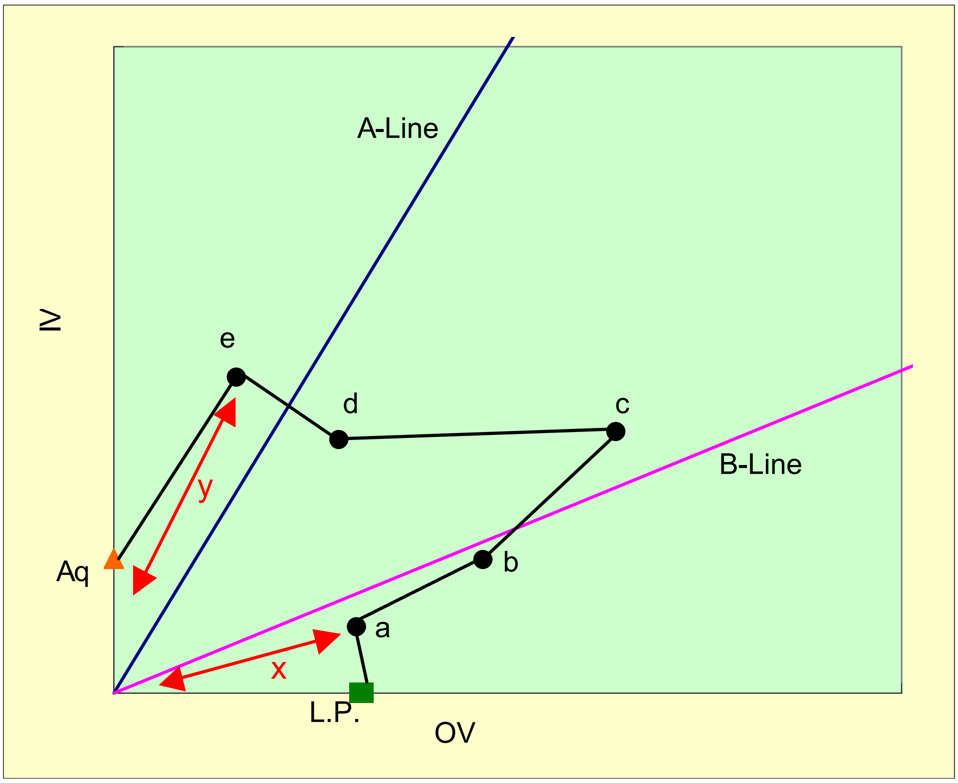


Figure 23, lB and s : l type

Characteristics of this type

This type of the type A is better than the lB l : s in terms of hydrophilicity and foaming property. This type is most commonly used in detergents such as shampoo and facial detergents.

This type of the type B is more thermally stable than the lB l:s but poorer in terms of oily touch. The water repellence is similarly great.

Example of cosmetic

A type : Rinse in shampoo

B type : Sun tan cosmetic, Hand cream and W/O emulsion

As has been described above, representative examples are shown in Figs. 20 to 23 but combinations of emulsion types (Types A and B) as described above are shown in Table 6. More specifically, the combinations are composed of three major elements in emulsification.

1. Emulsion type (under influence of quantities of emulsifiers around trisectional lines)
2. Peak length of emulsifier (under influence of lengths of emulsifiers present around trisectional lines)
3. Comparison of the distances of emulsifiers in the two phases from the origin.

Table 6, Emulsion types

Emulsion type	Peak of Emulsifer	Trend of O_{SAA} : W_{SAA}
A	lA	l：s
		s：l
	lB	l：s
		s：l
B	lA	l：s
		s：l
	lB	l：s
		s：l

Formulation of emulsion is included in this table.

3-3. How to blend quantities of components for emulsification

It is shown in 3-2 that various types of emulsions can be recovered by emulsifier quality. However, the quantity is also a significant factor, along with the quality.

It is now described as to how to blend quantities of emulsifiers, which is the most significant factor for formulation researchs.

3-3-1. Meanings of oil phase quantity and aqueous phase quantity and calculation methods

Oil phase quantity (oil phase) and aqueous phase quantity (aqueous phase) are represented by O:W, respectively. The ratio is generally expressed as shown below.

Example : In case of oil phase quantity : aqueous phase quantity = 10:90, O:W = 10:90.

O and W can be set free but these are variable within the range of 100 % in total.

Oil phase quantity (O) inclusive of all the components in the oil phase therefore includes emulsifiers in the oil phase.

Aqueous phase quantity (W) inclusive of all the components in the aqueous phase therefore includes water and emulsifiers in the aqueous phase.

O = Oil + emulsifiers in oil phase (O_{SAA})

W = Water (Aq) + emulsifiers in aqueous phase (W_{SAA})

Then, O + W = 100. Emulsion is thus formed.

An example of how to calculate quantities of emulsifiers is now described.

Table 7 shows the ratio of oil phase and aqueous phase and quantities of emulsifiers then. Using the table, the quantities are predetermined. Furthermore, how to use the table is described below. Based on the table, oil, O_{SAA} and W_{SAA} are calculated so the remaining portion is occupied by water. Using water, the balance is set to 100, so emulsion can be formulated.

(i) Example 1

(A) Condition

(a) Oil phase : Water phase → O : W = 40 : 60

(b) Emulsion type → 5A

(B) Calculation

(a) Calculation of O_{SAA}, W_{SAA} and Oil content, water

According to Fig.7, O<W, 5A, O : W = 40 : 60

$O_{SAA} : W_{SAA} = 6.0 : 3.2$

This means, emulsifer of oil phase is 6.0% and emulsifer of water phase is 3.2%

So, as oil quantity = $(O-O_{SAA})$,

= 40 - 6.0 = 34% (oil content is 34%)

By the way, this oil means the smallest of α value in formulation.

Water quantity = $W-W_{SAA}$

=60 – 3.2 = 56.8%

Oil	34.0%
O_{SAA}	6.0%
W_{SAA}	3.2%
Aq	56.8%
Total	100.0%

As has been described above, the components can be calculated and determined.

However, not any single emulsifier is satisfactory enough for practical stabilization of emulsion. Depending on the angle of trisectional line, emulsifiers at an α interval of about 10 ° on the conception diagram are preferably used. The blending is now described below.

(b) Calculation of blend ratio of O_{SAA}:W_{SAA}

(b-1) Calculation of blend ratio of O_{SAA}:W_{SAA} for type A emulsion

For type A, O_{SAA} (6.0 %) is allocated in a 2-geometric series of emulsifiers of the number used in the zone of the organic axis to the line A.

For example, three emulsifiers (a, b, c) as shown in Fig. 24 are defined as a ratio of 1:2:4 on the organic axis. In total, then, the emulsifiers occupy 6.0 %.

Because the quantity (6 %/7) of allocated emulsifier a with the minimum α value among O_{SAA} is at about 0.8 %, the quantities of other allocated O_{SAA} are b = 1.7 % and c = 3.5 % in total of 6.0 % (a = 0.8 %).

W_{SAA} (3.2 %) in aqueous phase is allocated in a 2-geometric series of emulsifiers of the number used in the zone from the inorganic axis to the line A.

For example, W_{SAA} are composed of two species (a, b) and sequentially allocated at a ratio of 1:2 from the inorganic axis. Then, W_{SAA} occupies 3.2 % in total. Because the quantity (3.2 %/3) of allocated emulsifier a with the maximum α value among W_{SAA} is at about 1.1 %, the quantity of the other allocated W_{SAA} is b = 2.1 % in total of 3.2 % (a = 1.1 %).

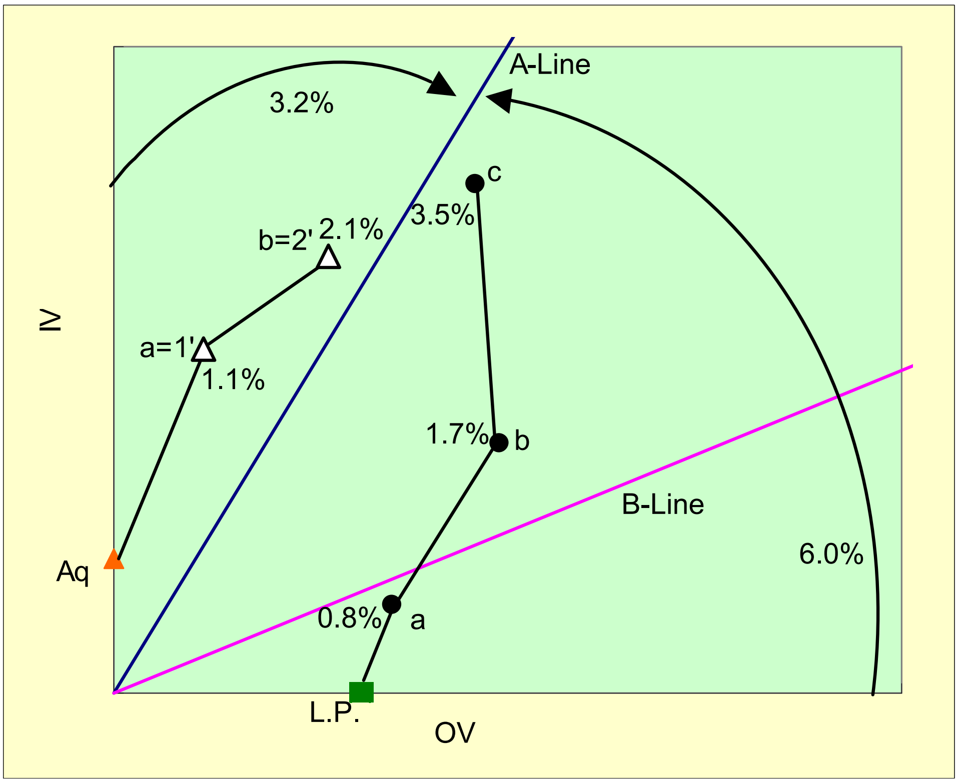


Figure 24, Allocation of the quantities of O_{SAA}:W_{SAA} in type A emulsion

(b-2) Calculation of blend ratio of O_{SAA}:W_{SAA} for type B emulsion

For type B, O_{SAA} (6.0 %) is allocated in a 2-geometric series of emulsifiers of the number used on the organic axis to the line B.

For example, three emulsifiers (a, b, c) as shown in Fig. 25 are defined as a ratio of 1:2:4 from the organic axis. In total, then, the emulsifiers occupy 6.0 %.

Because the quantity (6 %/7) of allocated emulsifier a with the minimum α value among O_{SAA} is at about 0.8 %, the quantities of other allocated O_{SAA} are b = 1.7 % and c = 3.5 % in total of 6.0 % (a = 0.8 %).

W_{SAA} (3.2 %) in aqueous phase is allocated in a 2-geometric series of emulsifiers of the number used on the inorganic axis to the line B.

For example, W_{SAA} are composed of four species (a, b, c, d) and sequentially allocated at a ratio of 1:2:4:8 from the inorganic axis. Then, W_{SAA} occupies 3.2 % in total.

Because the quantity (3.2 %/15) of allocated emulsifier a with the maximum α value among W_{SAA} is at about 0.2 %, the quantities of other allocated W_{SAA} are b = 0.4 %, c = 0.8 % and d = 1.8 % in total of 3.2 % (a = 0.2 %).

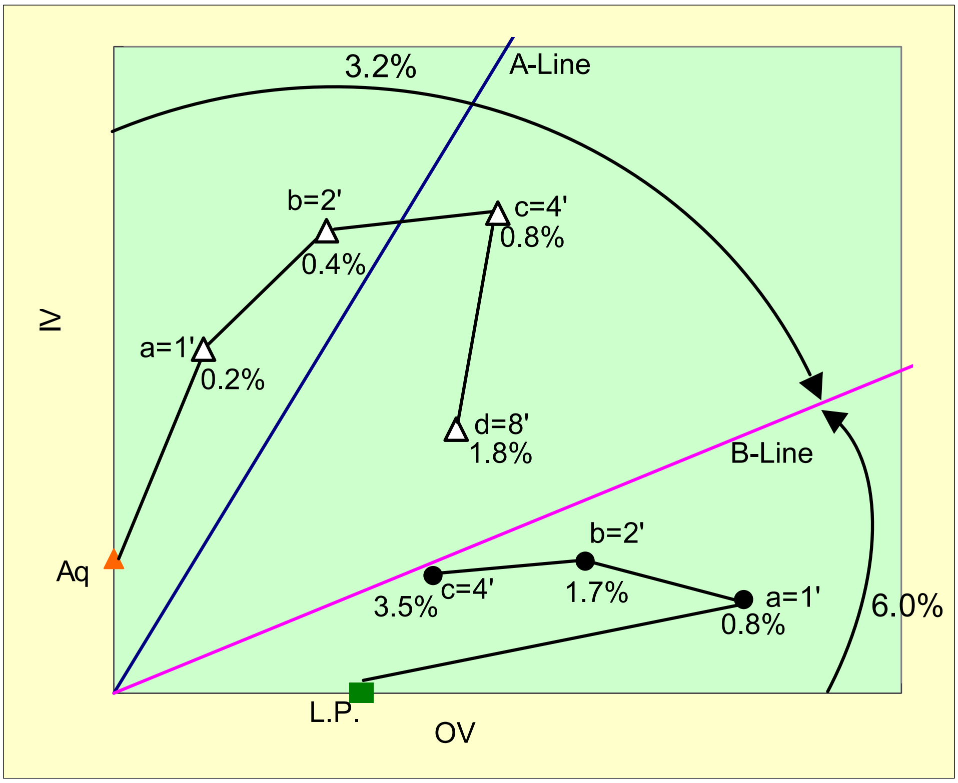


Figure 25, Allocation of the quantities of O_{SAA}:W_{SAA} in type B emulsion

3-3-2. Change of ratio of oil phase quantity and aqueous phase quantity and calculation of emulsifiers

Oil phase and aqueous phase individually contain O_{SAA}:W_{SAA} at various quantities; when the quantities of O_{SAA} and W_{SAA} are defined, the emulsified state and properties of the resulting emulsion can be predicted.

1. Oil phase quantity + aqueous phase quantity = 100 %.

2. O_{SAA}: W_{SAA} can be set free. Therefore, 4 variable O_{SAA}:W_{SAA} ratios of O: W were given.

3. As to O:W, the SAA quantity in one of the phases was defined as 1/10 of the phase quantity, while the SAA quantity in the other phase was a variant.

4. One of the axes X and Y is defined as representing O quantity, while the other is defined as representing W quantity. The bisectional line (45 °) of the inner angle between O: W = 50:50 (center) and the origin is drawn, while the bisectional line of the outer angle is also drawn. Lines are drawn from the 50% points on the axes X and Y; and the cross point is determined (at a distance of 20.7). O: W = 60:40 to 90:10 is determined in the same manner, to draw a locus of the cross point.

5. The resulting loci are numbered individually; Nos. 1, 4, 6 and 7 are emulsification lines; and Nos. 2, 3, 5 and 8 are solubilization lines.

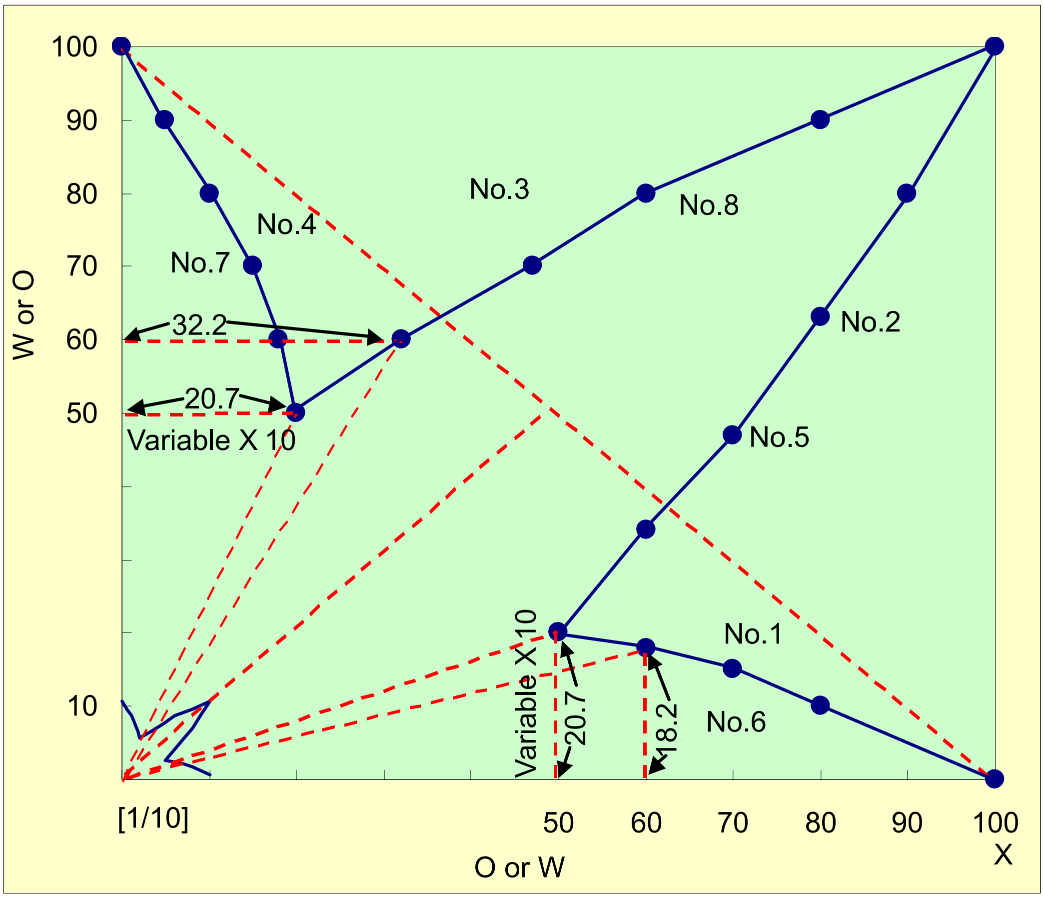


Figure 26, Amount of O_{SAA}:W_{SAA} for O : W

The total of O: W is 100 %; the SAA quantity in one of the phases is 1/10 of the phase; depending on the transfer of O:W, the SAA quantity in the other phase is set as variant. The figure shows that the locus of cross points between inner angle bisectional line and outer angle bisectional line is determined, depending on the change of O:W. 1/10-fold quantity is defined as SAA quantity in the other phase.

The SAA quantity as the variant can be read on the graphs on Fig. 26 or can be determined by the following formula. These are shown in Table 7.

O>W

$Z = X/10Y\ (-X + \sqrt{X^2 + Y^2})$: No.1, No.4 (X, Y exchange), Emulsification

$Z' = 1/10\ (-X + \sqrt{X^2 + Y^2})$: No.2, No.3 (X, Y exchange), Oil soluble line

O<W

$Z = Y/10X\ (-Y + \sqrt{X^2 + Y^2})$: No.6, No.7 (X, Y exchange), Emulsification line

$Z' = 1/10\ (-X + \sqrt{X^2 + Y^2})$: No.5, No.8 (X, Y exchange), Aq soluble line

Table 7-1, Tendency of which changing of quality abd quantity are effected to emulsion and solublization.

①	②	③	④	⑤	Stable at high to low temp			O : W 85 : 15	O : W 80 : 20	O : W 75 : 25	O : W 70 : 30	O : W 65 : 35	O : W 60 : 40	O : W 55 : 45	O : W 50 : 50
					0° -B (Nonion)	B-A (Nonion)	A-90° (Anion)	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SA0A}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}
O>W	1	A	l l:s A s:l	↑	l ↓ s ↑	l ↓ l ↓	s ↑ l ↓	8.5:0.75 4 5	8.0 : 0.984	7.5:1.22	7.0:1.43 10 30	6.5:1.64 26 30	6.0:1.82	5.5:1.96	5.0:2.07 20 28 25
			l l:s B s:l	↑	l ↓ s ↑	s ↓ s ↓	s ↑ l ↓								
		B	l l:s A s:l	↓	l ↓ s ↑	l ↑ l ↑	s ↑ l ↓								
			l l:s B s:l	↓	l ↓ s ↑	s ↑ s ↑	s ↑ l ↓								
	2	A	l l:s A s:l	↑	l ↓ s ↑	l ↓ l ↓	s ↑ l ↓	8.5:7.1 14 13	8.0:6.25	7.5:5.4	7.0:4.62 25 30 20 28	6.5:3.88 23 30 28	6.0:3.22	5.5:2.6	5.0:2.07 20 28 25
			l l:s B s:l	↑	l ↓ s ↑	s ↓ s ↓	s ↑ l ↓								
		B	l l:s A s:l	↓	l ↓ s ↑	l ↑ l ↑	s ↑ l ↓								
			l l:s B s:l	↓	l ↓ s ↑	s ↑ s ↑	s ↑ l ↓								
	3	A	l l:s A s:l	↑	l ↓ s ↑	s ↓ s ↓	s ↑ l ↓	7.1:8.5 14 15	6.25:8.0	5.4:7.5	4.62:7.0 23 26	3.88:6.5 17 24 28	3.22:6.0	2.6:5.5	2.07:5.0 5 15 10
			l l:s B s:l	↑	l ↓ s ↑	l ↓ l ↓	s ↑ l ↓								
		B	l l:s A s:l	↓	l ↓ s ↑	s ↑ s ↑	s ↑ l ↓								
			l l:s B s:l	↓	l ↓ s ↑	l ↑ l ↑	s ↑ l ↓								
	4	A	l l:s A s:l	↑	l ↓ s ↑	s ↓ s ↓	s ↑ l ↓	0.75:8.5 5 10	0.984:8.0	1.22:7.5	1.43:7.0 20 29	1.64:6.5 14 18 25	1.82:6.0	1.96:5.5	2.07:5.0 5 15 10 (Vise)
			l l:s B s:l	↑	l ↓ s ↑	l ↓ l ↓	s ↑ l ↓								
		B	l l:s A s:l	↓	l ↓ s ↑	s ↑ s ↑	s ↑ l ↓								
			l l:s B s:l	↓	l ↓ s ↑	l ↑ l ↑	s ↑ l ↓								

①	②	③	④	⑤	Stable at high to low temp			Dilution tend for oil and water			
					0° -B (Nonion)	B-A (Nonion)	A-90° (Anion)	Rp SAA		SAA X mag.	
								Oil	Aq	Oil	Aq
O≧W	1	A	lA l:s s:l	↓	l ↓ s ↑	s ↑ s ↑	s ↑ l ↓	E	/	E	E
			lB l:s s:l	↑	l ↓ s ↑	l ↓ l ↓	s ↑ l ↓				
		B	lA l:s s:l	↓	l ↓ s ↑	s ↓ s ↓	s ↑ l ↓	E	/	E	E
			lB l:s s:l	↑	l ↓ s ↑	l ↑ l ↑	s ↑ l ↓				
	2	A	lA l:s s:l	↓	l ↓ s ↑	s ↑ s ↑	s ↑ l ↓	E	/	E	E
			lB l:s s:l	↑	l ↓ s ↑	l ↓ l ↓	s ↑ l ↓				
		B	lA l:s s:l	↓	l ↓ s ↑	s ↓ s ↓	s ↑ l ↓	S	/	S	E
			lB l:s s:l	↑	l ↓ s ↑	l ↑ l ↑	s ↑ l ↓				
	3	A	lA l:s s:l	↓	l ↓ s ↑	l ↑ l ↑	s ↑ l ↓	E	/	E	E
			lB l:s s:l	↑	l ↓ s ↑	s ↓ s ↓	s ↑ l ↓				
		B	lA l:s s:l	↓	l ↓ s ↑	l ↓ l ↓	s ↑ l ↓	S	/	S	E
			lB l:s s:l	↑	l ↓ s ↑	s ↑ s ↑	s ↑ l ↓				
	4	A	lA l:s s:l	↓	l ↓ s ↑	l ↑ l ↑	s ↑ l ↓	E	/	E	E
			lB l:s s:l	↑	l ↓ s ↑	s ↓ s ↓	s ↑ l ↓				
		B	lA l:s s:l	↓	l ↓ s ↑	l ↓ l ↓	s ↑ l ↓	E	/	E	E
			lB l:s s:l	↑	l ↓ s ↑	s ↑ s ↑	s ↑ l ↓				

①: Quantity, ②: Locus No., ③: Type of formulation, ④: Type of Emulsifier, ⑤: Stability in formulation for Temp., E:Emilifier, S:Soluble, /:Seperation

High temp. stable with choice of s ↑・s tendency, Low temp. stable with choice of l ↓・l tendency(20℃,25℃)

Viscosity of formulation (vise), 0. water state>5.solution state, 10.oil state, 15.soft milky lotion state, 20.milky lotion state, 25.soft cream state, 30.cream state

Oaspect is a test; which is used SAA of POE ether family - possible narrow distribution of liquid parrafine-.

Table 7-2, Tendency of which changing of quality abd quantity are effected to emulsion and solublization.

①	②	③	④	⑤	Stable at high to low temp			O : W 85 : 15	O : W 80 : 20	O : W 75 : 25	O : W 70 : 30	O : W 65 : 35	O : W 60 : 40	O : W 55 : 45	O : W 50 : 50
					0° -B (Nonion)	B-A (Nonion)	A-90° (Anion)	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SA0A}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}	O_{SAA}:W_{SAA}
O<W	5	A	l l:s A s:l	↙	l ↙ s ↗	l ↗ l ↗	s ↗ l ↙	8.5:7.1 18 20	8.0:6.25	7.5:5.4	7.0:4.62 21 17	6.5:3.88 23 25 28	6.0:3.22	5.5:2.6	5.0:2.07 20 28 25
			l l:s B s:l	↙	l ↙ s ↗	s ↗ s ↗	s ↗ l ↙								
		B	l l:s A s:l	↗	l ↙ s ↗	l ↙ l ↙	s ↗ l ↙								
			l l:s B s:l	↗	l ↙ s ↗	s ↙ s ↙	s ↗ l ↙								
	6	A	l l:s A s:l	↙	l ↙ s ↗	l ↗ l ↗	s ↗ l ↙	8.5:0.75 22 20	8.0:0.984	7.5:1.22	7.0:1.43 25 8	6.5:1.64 23 25 28	6.0:1.82	5.5:1.96	5.0:2.07 20 28 25
			l l:s B s:l	↙	l ↙ s ↗	s ↗ s ↗	s ↗ l ↙								
		B	l l:s A s:l	↗	l ↙ s ↗	l ↙ l ↙	s ↗ l ↙								
			l l:s B s:l	↗	l ↙ s ↗	s ↙ s ↙	s ↗ l ↙								
	7	A	l l:s A s:l	↙	l ↙ s ↗	s ↗ s ↗	s ↗ l ↙	0.75:8.5 0 5	0.984:8.0	1.22:7.5	1.43:7.0 3-6 9	1.64:6.5 6 13	1.82:6.0	1.96:5.5	2.07:5.0 5 15 10
			l l:s B s:l	↙	l ↙ s ↗	l ↗ l ↗	s ↗ l ↙								
		B	l l:s A s:l	↗	l ↙ s ↗	s ↙ s ↙	s ↗ l ↙								
			l l:s B s:l	↗	l ↙ s ↗	l ↙ l ↙	s ↗ l ↙								
	8	A	l l:s A s:l	↙	l ↙ s ↗	s ↗ s ↗	s ↗ l ↙	7.1:8.5 21 25	6.25:8.0	5.4:7.5	4.62:7.0 15 13	3.88:6.5 11 18 22	3.22:6.0	2.6:5.5	2.07:5.0 5 15 10
			l l:s B s:l	↙	l ↙ s ↗	l ↗ l ↗	s ↗ l ↙								
		B	l l:s A s:l	↗	l ↙ s ↗	s ↙ s ↙	s ↗ l ↙								
			l l:s B s:l	↗	l ↙ s ↗	l ↙ l ↙	s ↗ l ↙								

①	②	③	④	⑤	Stable at high to low temp			Dilution tend for oil and water			
					0° -B (Nonion)	B-A (Nonion)	A-90° (Anion)	Rp SAA		SAA X mag.	
								Oil	Aq	Oil	Aq
O≦W	5	A	lA l:s s:l	↙	l ↙ s ↗	s ↗ s ↗	s ↗ l ↙	/	S	E	S
			lB l:s s:l	↗	l ↙ s ↗	l ↙ l ↙	s ↗ l ↙				
		B	lA l:s s:l	↗	l ↙ s ↗	s ↙ s ↙	s ↗ l ↙	/	E	E	E
			lB l:s s:l	↙	l ↙ s ↗	l ↗ l ↗	s ↗ l ↙				
	6	A	lA l:s s:l	↙	l ↙ s ↗	s ↗ s ↗	s ↗ l ↙	/	E	E	E
			lB l:s s:l	↗	l ↙ s ↗	l ↙ l ↙	s ↗ l ↙				
		B	lA l:s s:l	↗	l ↙ s ↗	s ↙ s ↙	s ↗ l ↙	/	E	S	E
			lB l:s s:l	↙	l ↙ s ↗	l ↗ l ↗	s ↗ l ↙				
	7	A	lA l:s s:l	↙	l ↙ s ↗	l ↗ l ↗	s ↗ l ↙	/	E	E	E
			lB l:s s:l	↗	l ↙ s ↗	s ↙ s ↙	s ↗ l ↙				
		B	lA l:s s:l	↗	l ↙ s ↗	l ↙ l ↙	s ↗ l ↙	/	E	S	E
			lB l:s s:l	↙	l ↙ s ↗	s ↗ s ↗	s ↗ l ↙				
	8	A	lA l:s s:l	↙	l ↙ s ↗	l ↗ l ↗	s ↗ l ↙	/	S	E	S
			lB l:s s:l	↗	l ↙ s ↗	s ↙ s ↙	s ↗ l ↙				
		B	lA l:s s:l	↗	l ↙ s ↗	l ↙ l ↙	s ↗ l ↙	/	E	E	E
			lB l:s s:l	↙	l ↙ s ↗	s ↗ s ↗	s ↗ l ↙				

①: Quantity, ②: Locus No., ③: Type of formulation, ④: Type of Emulsifier, ⑤: Stability in formulation for Temp., E:Emilifier, S:Soluble, /:Seperation

High temp. stable with choice of s ↗・s tendency, Low temp. stable with choice of l ↙・l tendency(20℃,25℃)

Viscosity of formulation (vise), 0. water state>5.solution state, 10.oil state, 15.soft milky lotion state, 20.milky lotion state, 25.soft cream state, 30.cream state

Oaspect is a test; which is used SAA of POE ether family - possible narrow distribution of liquid parrafine-.

3-4. Method for using Table 7 (tendency table)

The emulsion type is influenced by the difference in components composing the emulsion. Accordingly, the properties of the emulsified formulation are essentially different.

The research works will be promoted efficiently when the difference can be deduced from the emulsion type. Hence, general aspects of the relation between the difference in emulsion type and the properties are now reviewed. This can be summarized as the following three points.

1. Emulsion state (opaqueness, solubilized state, viscosity)
2. Properties (hydrophilicity, hydrophobicity, aqueous solubility, water repellence, defoaming, foaming)
3. Thermal stability

The three items are collectively shown in the tendency table. It is now briefly described how to read the table.

3-4-1. How to read Table 7

Table 8, Excerpt of tendency table

Amount	Locus No.*1	Type of formulation *2	Type of Emulsifier *3		Stability in formulation for Temp. *4	Stable at high to low temp. *5			*6 O : W 70 : 30 O_{SAA} : W_{SAA}	Dilution tend for oil and water *7			
						0 – B° (nonion)	B – A (nonion)	A – 90° (anion)		Rp SAA		SAA X magnification	
										Oil	Aq	Oil	Aq
O>W	2	A	lA	l : s	↗	l ↙	l ↙	s ↗	7.0 : 4.62	E	/	E	E
				s : l		s ↗	l ↙	l ↙					
			lB	l : s	↗	l ↙	s ↙	s ↗					
				s : l		s ↗	s ↙	l ↙					
		B	lA	l : s	↙	l ↙	l ↗	s ↗	25 30 20 28	S	/	S	E
				s : l		s ↗	l ↗	l ↙					
			lB	l : s	↙	l ↙	s ↗	s ↗					
				s : l		s ↗	s ↗	l ↙					

For hydrophilic cleansing cream formulation, emulsion types are selected as follows from Table 8.

1. *6 O:W = 70:30
2. *1 Locus No. 2
3. *2 Formulation type of B
4. *3 Emulsifier selection tendency type is l : s of lA.

Collectively, 1 to 4 are expressed as an emulsion type of 2B lA l : s.

The temperature stability (*4, low temperature stability) and properties of the 2B lA l : s are described and explained in Table 8.

1. 5* Length tendency for stabilization at high to low temperatures

a. Emulsifiers (nonion) of `l:s` to emulsifiers between 0 °C to Line B are with symbol (`l` ↓).

This indicates that O_{SAA} with a long distance from the origin is blended as an oil phase component in the formulation, leading to the stable tendency at low temperature (↓).

b. Emulsifiers (nonion) between lines B and A are with symbol `l` ↑.

The blend of W_{SAA} with a long distance from the origin induces stable tendency at high temperature (`l` ↑).

c. Emulsifiers (anion) of `l:s` to emulsifiers between line A to 90 ° are expressed with symbol `s` ↑.

Anion SAA with a shorter distance (`s`) from the origin should be used. As a result, the stabilization at high temperature can be expected.

Provided that nonion SAA is used between line A and 90 °, nonion SAA with a long distance from the origin is necessarily used. As a result, nonion (`l` ↑) can surely be stabilized.

2. Viscosity

The right column of O_{SAA}:W_{SAA} in the tendency table includes the numerical figure 25, which expresses approximately the viscosity of the resulting formulation.

The numerical figures are shown in 7 ranks; and the relation of such numerical figures and appearance is as shown below.

O: aqueous
5: solution
10: oily
15: soft emulsion
20: emulsion
25: soft cream state
30: cream state

Herein, oil is fluid paraffin at a viscosity state of liquid/liquid phase. When a component between the organic axis and line B has a melting point or when oils with variable distances from the origin are selected, the resulting viscosity changes.

As has been described above, it is indicated that the formulation is at a viscosity of 25 (soft cream state).

3. *7 Dilution tendency in oil or water

RpSAA (O_{SAA}:W_{SAA} quantities as they are in the table) shown at6 the most right row in Table 8, exerts S when oil (the oil used for the formulation) is added to the formulation for dilution. This means that dilution is possible and solubilized materials can be formed after dilution.

Alternatively, dilution with Aq (water) is represented with dash /. The formulation is separated with water of the same quantity or more. In other words, the formulation is immiscible with water.

Finally, the column of SAA × magnification means whether or not the dilution tendency changes at the same increment ratios of essential emulsifiers O_{SAA}:W_{SAA} = 7.0:4.62 shown in the formulation. When oil (the oil used in the formulation) is added to the formulation for dilution, the formulation falls in S. This means that dilution is possible and solubilized materials can be formed after dilution. Additionally, the formulation falls in E after dilution with water. This means that dilution is possible and emulsions are formed after dilution.

Furthermore, the column of dilution tendency in Table 7 shows that Nos. 2 and 3B can be solubilized with oil and turn transparent and that Nos. 5 and 8A can be solubilized with water and turn transparent.

3-4-2. Solubilization and emulsification tendency

For preparing liquid/liquid as transparent, a liquid material should be selected as O_{SAA} as much as possible, while solid materials should be suppressed at a small quantity relative to the circle phase. Then, the solid materials should turn liquid around ambient temperature.

The general relation between the size and appearance of liquid drop is shown in Table 9.

Diameter of Liquid Drop	Appearance
1 μ m	Milky white (Emulsion)
↓	↓
It make smaller	It is occurred blue color.
↓	↓
Under 0.1 μ m	Transparent micro emulsion

Table 9, Appearance and size of liquid drop

In Fig. 26, Nos. 1, 4, 6 and 7 loci at trace quantities of SAA in one of the phases O_{SAA}:W_{SAA} express opaque emulsion, while Nos. 2, 3, 5 and 8 loci with less difference in the ratio of O_{SAA}:W_{SAA} are likely to express semi-solubilization in pale bluish white.

As shown in Fig. 27 of the relation with oil length, additionally, the substitution of fluid paraffin ($\alpha = 0\,^\circ$; L-Oil) with benzine ($\alpha = 0^\circ$, S-Oil) causes ready transparency; like vegetable oil, L-oil in particular causes opaqueness even at the slight increase of α.

Generally, an oil with larger α and at a given length is more readily soluble. Longer emulsifiers are at high solubilization efficiency.

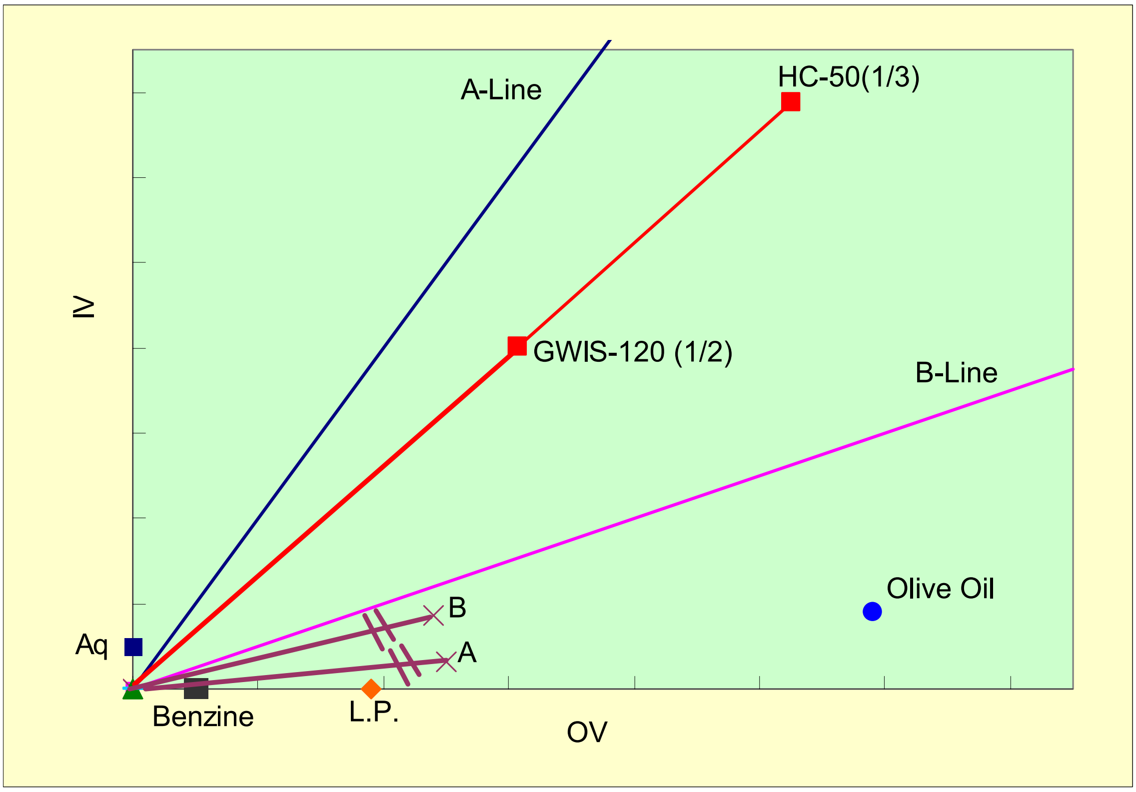


Figure 27, Soluble phenomenon with organic conception

1. With respect to to-be-solubilized materials in terms of oil length, the substitution of fluid paraffin with benzine of S-Oil readily causes transparency; the substitution with long L-Oil such as olive oil in particular causes opaqueness even at the slight increase of α.
2. Generally, an oil with larger α and at a given length is more readily soluble.
3. Longer emulsifiers (with larger molecular weights) are at high solubilization efficiency.

3-4-3. Oil soluble character, water soluble character and bubble character

According to the table 7, strength of oil soluble character and water soluble character are shown in table 10.

Table 10, Type of Emulsifier and Character

Condition	Oil soluble character ≒ Disappearance character of bubble	Water soluble character ≒ Appearance character of bubble
① O>W, O<W	(O>W) > (O<W)	(O<W) > (O>W)
② No. O>W W>O	1>2>3>4 6>5>8>7	4>3>2>1 7>8>5>6
③ Formulation Type	B	A
④ Maximum Emulsifier	lB	lA
⑤ Type of Choice Tendency	l : s	s : l
⑥ O : W	85 : 15 > 50 : 50	15 : 85 > 50 : 50
⑦ Example of Order	Big ▲ 1BlB l : s 1BlB s : l 1BlA l : s 1BlA s : l ▼ Small	Big ▲ 7AlA s : l 7AlA l : s 7AlB s : l 7AlB l : s ▼ Small

The formulation type of emulsion; which you want to get is decided in accordance with table 10.

3-4-4. Determination of known formulations on conception diagram

The emulsion types of formulations with known components (Table 11) are determined on the conception diagram. The procedures are described below.

Table 11, Judgment of known formulation

Substance name	%	OV	IV	α	Analysis
1. Liquid Paraffin	28.55	300 - 400	0	0°	Oil =28.55
2. Cetyl Octanoate	0.9	470	60	7°	O=35
3. Cetanol	1.85	320	100	17°	O_{SAA}=6.45
4. POE (2mol) Stearyl ether	3.7	440	195	23°	B
5. POE (8mol) Distearate	0.85	1040	645	31°	
6. POE (11mol) Stearyl ether	0.4	800	870	47°	W_{SAA}=1.6 W=65
7. POE (20mol) Laury ether	0.2	1040	1545	56°	A
8. PEG-600	0.1	480	1025	64°	
9. Sodium-Stearoyl-glutamate	0.05	460	1000	65°	
10. Purified Water	64.5	0	100	90°	
	100.0%				

1. Determination of type A or B

The organic and inorganic values of each component are calculated; then, the α values are determined. Then, a formulation is prepared by aligning individual components in the order of α to the total 100 %. By drawing lines A and B, then, type A or B can be determined by determining where a larger quantity of the emulsifier is blended, on line A or B.

2. Determination of ｌA or ｌB and ｌ : s or ｓ : ｌ

Based on the type B emulsion, oil phase : aqueous phase can be identified; O_{SAA} and W_{SAA} quantities can be determined. Additionally, ｌA or ｌB and ｌ : s or ｓ : ｌ can be determined as well.

3. Calculation of oil phase quantity : aqueous phase quantity

Because the emulsion type is determined on the drawn lines A and B as described above in I, the oil phase quantity and aqueous phase quantity can readily be calculated.

$O:W = 35:65$, $O_{SAA}:W_{SAA} = 6.45:1.6$

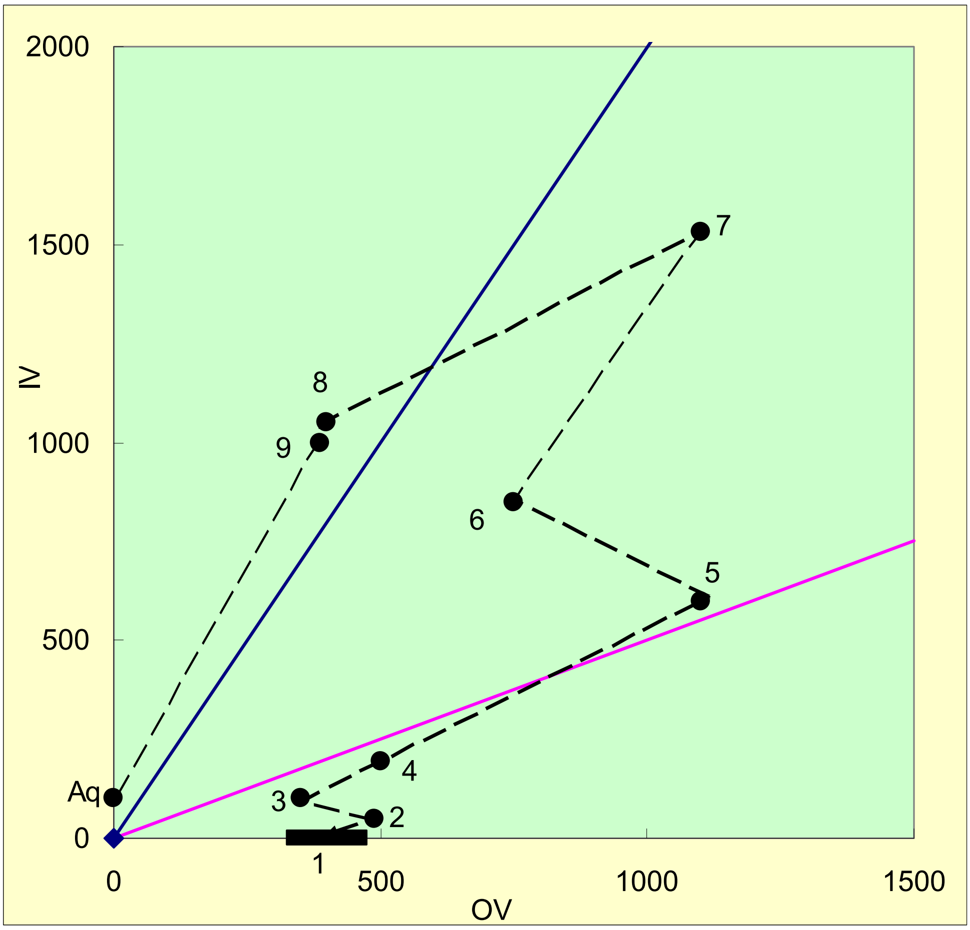


Figure 28, Conception diagram of Formulation

4. Determination of formulation number

Because O:W is calculated and O_{SAA}:W_{SAA} is also determined, a formulation number corresponding to them can be found on the basis of the W_{SAA}:O_{SAA} ratio in Table 7.

O : W

1.6/6.45 = 0.248 → 6B 35:65 → Approximately 1.64/6.5 = 0.252

O_{SAA}:W_{SAA}

6.5 1.6

By the procedures, the emulsion type of the formulation can be determined, which indicates the properties and performance specific to the type as shown in Table 7.

Using Table 7, the conception diagram of Fig. 28 can be described and shown in the determination results of Table 12.

Table 12, Result [6BlA s : l] 35 : 65 and 3.45 : 1.6

Subject	Results	Reason
① A or B	B Type	More emulsions around line B
② lA or lB	lA	E-720 (No. 7 under component name) around line A is of the longest distance from the origin among formulation components.
③ l : s or s : l	s : l	The distance of No. 2 (under component name) with the minimum α from the origin among oil phase components is longer than the distance of No. 9 (under component name) with the maximum α from the origin among aqueous phase components.
④ Calculation of O : W	O : 35 W : 65	Sum of 4 components within the zone of 0° to line B Sum of 6 components above line B
⑤ Calculation of OSAA : WSAA	O_{SAA} = 6.45% W_{SAA} = 1.6%	Sum of 3 components except fluid paraffin in oil phase Sum of 5 components except water in aqueous phase
⑥ Number of locus	6	See Table 7

4. Conclusion

As shown in Table 7, the definition of the change of the relation of O_{SAA}:W_{SAA} in quantity ratio with oil phase : aqueous phase can eliminate useless experiments for the objective emulsion state (what is the purpose of the use, emulsion type, properties, performance, etc.). Additionally, the objective emulsion can easily be developed just when it is shown that the tendency of the change of the emulsified state is in a close relation with the combination of the change of the SAA quantity ratio and quality type.