# Designing Chemical Products

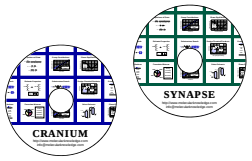
*Dr. Kevin G. Joback*
*Molecular Knowledge Systems, Inc.*
*http://www.molecularknowledge.com*

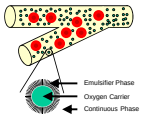
# 化学製品の設計

*Dr. Kevin G. Joback*
*Molecular Knowledge Systems, Inc.*
*http://www.molecularknowledge.com*

## Molecular Knowledge Systems

- Located in New Hampshire, USA
- Company Started in 1989
- Computer Software
- Consulting



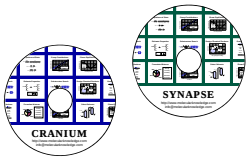



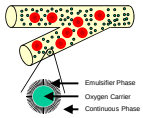

2000-11-15-01



## Molecular Knowledge Systems

- 米国ニューハンプシャー州に位置
- 1989年開業
- コンピュータソフトウェア
- コンサルティング

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## Designing Chemical Products

### Some example projects we have worked on

- Artificial Blood
- Refrigeration Lubes
- Degreasing Solvents
- Non-MMH Rocket Fuels
- Aircraft Deicing Fluids
- Soil Consolidants
- Sonar Fill Fluids
- Phase Change Materials
- CO2 Absorption Solvents
- Hydraulic Energy Storage
- Windshield Washer Fluid
- Pour Point Depressant

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## 化学製品の設計

### 携わったプロジェクトの事例

- 人工血液
- 冷凍機油
- 脱脂溶剤
- 非MMHロケット燃料
- 航空機除氷液
- 土の圧密
- ソナー充填流体
- 相変化物質
- 二酸化炭素吸収剤
- 油圧エネルギ貯蔵
- フロントガラス洗浄液
- 流動点降

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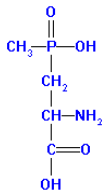
## Our Core Knowledge

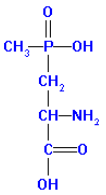


- Thermal Conductivity
- Liquid Viscosity
- Surface Tension
- Heat Capacities
- Vapor Pressure
- Liquid Density
- Flash Point

**Structure Property Relationships**



## 核となる知識



- 熱伝導率
- 液体粘度
- 表面張力
- 熱容量
- 蒸気圧
- 液体密度
- 引火点

**構造物性相関**



## Designing Chemical Products

### Three Main Steps

1) Identifying physical property constraints
2) Generating candidate structures and mixtures
3) Testing if candidates satisfy constraints

Experimental Approach

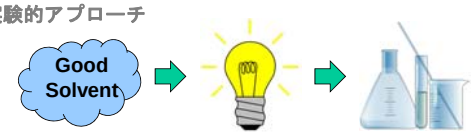



## 化学製品の設計

### ３つの主な手順

1) 物性の制約条件を識別
2) 分子構造と混合物の候補を生成
3) 候補が制約条件を満たしているかをテスト

実験的アプローチ






## Designing Chemical Products

### Three Main Steps

1) Identifying physical property constraints
2) Generating candidate structures and mixtures
3) Testing if candidates satisfy constraints

Computational Approach

$T_b > 100$ °C
$T_m < -40$ °C
$\rho > 1000$ kg/m$^3$

$CH_3\text{-}O\text{-}CH_2\text{-}CH_3$
$CH_3\text{-}S\text{-}CH_2\text{-}CH_3$
$CH_3\text{-}NH_2\text{-}CH_2\text{-}CH_3$
$CH_3\text{-}CO\text{-}CH_2\text{-}CH_3$

$\sum n_i \Delta_{i,Tb}$
$\sum n_i \Delta_{i,Tm}$



## 化学製品の設計

### ３つの主な手順

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計算論的アプローチ

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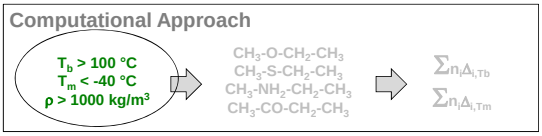
Computational Approach



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### ３つの主な手順

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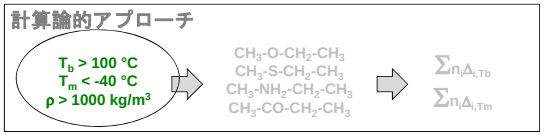
計算論的アプローチ






## Step 1: Identify Constraints

### Do not focus on chemicals or ingredients. Focus on physical properties.

> "People don't need drills. People need holes."
>
> *- Basic Marketing*

> "People don't need chemicals. People need the properties those chemicals possess."
>
> *- Kevin G. Joback*



## Step 1: 制約条件の識別

### 化学物質や成分には焦点を当てない 物性に焦点を当てる

> 「人が欲しいのはドリルではなく、穴である」
>
> *- Basic Marketing*

> 「人が欲しいのは化学物質ではなく、その物質が有する物性である」
>
> *- Kevin G. Joback*



## Example: Windshield Washer Fluid

US Patent 07,585,828
Example Formulation

Why are these ingredients in this product?

| Ingredient | Weight % |
|---|---|
| 1. Methanol (solvent) | 34.750 |
| 2. Chromatech Yellow | 0.005 |
| 3. XD-56 Antifoam | 0.020 |
| 4. Formasil 593 | 0.200 |
| 5. Water | 65.025 |



## 例：フロントガラス洗浄液

米国特許番号　07,585,828
配合例

なぜこれら成分がこの製品に含まれるのか？

| Ingredient | Weight % |
|---|---|
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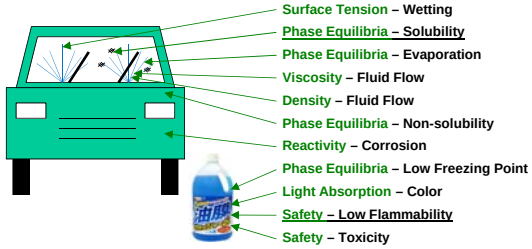
## Example: Windshield Washer Fluid

### Focus on physical properties





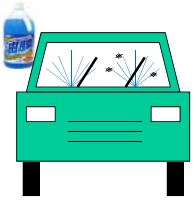

## 例：フロントガラス洗浄液

### 物性に焦点を当てる




## Step 1: Identify Constraints

### The required physical properties place constraints on the molecular structure of the solvent

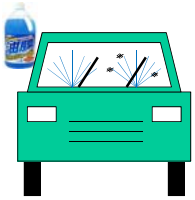


1. Non-reactive with metal – no -COOH group
2. Environmentally friendly – no –Cl, -F, -Br
3. Must wet glass surface – hydrocarbon
4. Rapid evaporation rate – low Mw
5. Low freezing point – -OH group
6. Low flammability – -OH, -Cl, -F
7. Low toxicity – water soluble
8. Low viscosity – low Mw



## Step 1: 制約条件の識別

### 必要な物性が溶剤の分子構造に制約条件を課す



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## Example: Ball Point Pen Ink

### US Patent 05,466,281 Example Formulation

| Ingredient | Weight % |
|---|---|
| 1. Sunsperse black LHD-9303 | 20.00 |
| 2. Ammonia as 20% NH3 | 0.10 |
| 3. Cobratec TT-25-EG | 0.25 |
| 4. Ethylene glycol | 74.12 |
| 5. Surfynol 104E | 0.18 |
| 6. Xanthan gum | 0.20 |
| 7. Proxel GXL | 0.15 |
| 8. Joncryl 58 | 5.00 |

Why are these ingredients in this product?



## 例：ボールペンのインク

### 米国特許番号　05,466,281 配合例

| Ingredient | Weight % |
|---|---|
| 1. Sunsperse black LHD-9303 | 20.00 |
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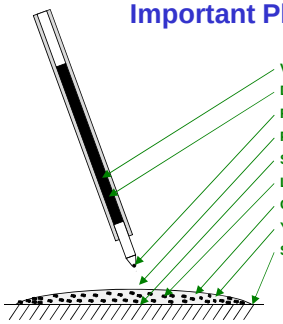
なぜこれら成がこの製品に含まれるのか？

## Example: Ball Point Pen Ink

### Important Physical Properties

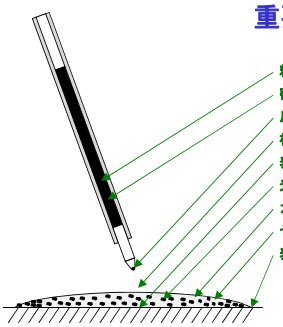


- Viscosity - Suspension
- Density – Fluid Flow
- Reactivity – Corrosion
- Phase Equilibria – Drying
- Surface Tension – Adhesion
- Light Absorption – Color
- Glass Transition Temp – Film Forming
- Young's Modulus – Stress Strain
- Surface Tension – Wetting



## 例：ボールペンのインク

### 重要な物性

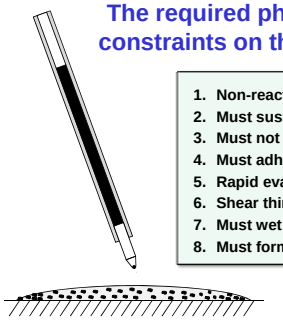


- 粘度 – 懸濁液
- 密度 – 流体の流れ
- 反応度 – 腐食
- 相平衡 – 乾燥
- 表面張力 – 粘着
- 光吸収 – 色
- ガラス転移温度 – 皮膜形成
- ヤング率-応力 – ひずみ
- 表面張力 – 濡れ性



## Step 1: Identify Constraints

### The required physical properties place constraints on the mixture's ingredients



1. Non-reactive with metal – corrosion inhibitor
2. Must suspend pigment particles – thickener
3. Must not degrade for many years – biocide
4. Must adhere particles to paper – polymer
5. Rapid evaporation rate – low Mw solvent
6. Shear thinning viscosity – thickener
7. Must wet paper surface – surfactant
8. Must form a tough film – polymer



## Step 1: 制約条件の識別

### 必要な物性が混合物の成分に制約条件を課す

1. Non-reactive with metal – corrosion inhibitor
2. Must suspend pigment particles – thickener
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## Designing Chemical Products

### Three Main Steps

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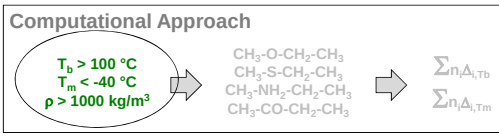
Computational Approach






## 化学製品の設計

### 3 つの主な手順

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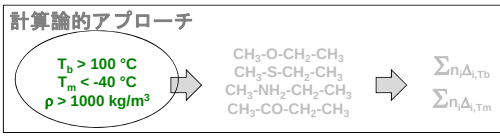
計算論的アプローチ



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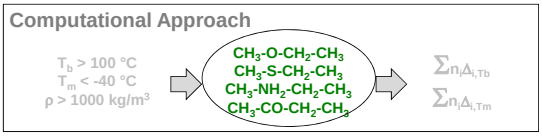




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### ３つの主な手順

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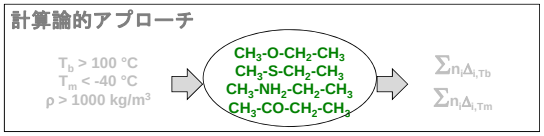




## Designing Chemical Products

### Generating Candidates
### Pure Components and Mixtures

1) Generating Structures: the molecular structure of pure component candidates
2) Generating Mixtures: the components and concentration of mixture candidates



## 化学製品の設計

### 候補生成
### 純物質と混合物

1) 分子構造生成：純物質候補の分子構造
2) 混合物生成：混合物候補の成分と濃度



## Designing Chemical Products

### Generating Candidates
### Pure Components and Mixtures

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## 化学製品の設計

### 候補生成
### 純物質と混合物

1) 分子構造生成：純物質候補の分子構造
2) 混合物生成：混合物候補の成分と濃度

## Step 2: Generating Structures

**Groups are small pieces of molecular structure. Begin by compiling groups.**

| | | |
|---|---|---|
| –$CH_3$ | –$CH_2$– | >CH– |
| –COO– | –OH | –CO– |
| –$NH_2$ | –NH– | >N– |
| –O– | -Br | –F |
| –Cl | –COOH | –SH |



## Step 2: 分子構造の生成

**小片の分子構造のグループ**
**グループの収集から開始**

| | | |
|---|---|---|
| –$CH_3$ | –$CH_2$– | >CH– |
| –COO– | –OH | –CO– |
| –$NH_2$ | –NH– | >N– |
| –O– | -Br | –F |
| –Cl | –COOH | –SH |



## Step 2: Generating Structures

**Eliminate groups based on reactivity, corrosivity, odor, safety, ...**

| | | |
|---|---|---|
| –$CH_3$ | –$CH_2$– | >CH– |
| –COO– | –OH | –CO– |
| –$NH_2$ | –NH– | >N– |
| ~~–O–~~ | ~~-Br~~ | –F |
| ~~–Cl~~ | ~~–COOH~~ | ~~–SH~~ |



## Step 2: 分子構造の生成

**反応度、腐食性、臭気性、安全性を基に**
**グループを除去・・・**

| | | |
|---|---|---|
| –$CH_3$ | –$CH_2$– | >CH– |
| –COO– | –OH | –CO– |
| –$NH_2$ | –NH– | >N– |
| ~~–O–~~ | ~~-Br~~ | –F |
| ~~–Cl~~ | ~~–COOH~~ | ~~–SH~~ |



## Step 2: Generating Structures

**Exhaustively generate all combinations. Combinations of 2 groups, 3 groups, …**

| 2 Groups | 3 Groups | 4 Groups |
|---|---|---|
| -$CH_3$ -$CH_3$ | -$CH_3$ -$CH_3$ -$CH_3$ | -$CH_3$ -$CH_3$ -$CH_3$ -$CH_3$ |
| -$CH_3$ -$CH_2$- | -$CH_3$ -$CH_3$ -$CH_2$- | -$CH_3$ -$CH_3$ -$CH_3$ -CH2- |
| -$CH_3$ >CH- | -$CH_3$ -$CH_3$ >CH- | -$CH_3$ -$CH_3$ -$CH_3$ >CH- |
| -$CH_3$ -OH | -$CH_3$ -$CH_3$ -OH | -$CH_3$ -$CH_3$ -$CH_3$ -OH |
| -$CH_3$ -NH- | -$CH_3$ -$CH_3$ -NH- | -$CH_3$ -$CH_3$ -$CH_3$ -NH- |
| -$CH_3$ >N- | -$CH_3$ -$CH_3$ >N- | -$CH_3$ -$CH_3$ -$CH_3$ >N- |
| ⋮ | ⋮ | ⋮ |



## Step 2: 分子構造の生成

**全ての組合せを徹底的に生成**
**2 つのグループ、 3つのグループ・・・の組合せ**

| 2 Groups | 3 Groups | 4 Groups |
|---|---|---|
| -$CH_3$ -$CH_3$ | -$CH_3$ -$CH_3$ -$CH_3$ | -$CH_3$ -$CH_3$ -$CH_3$ -$CH_3$ |
| -$CH_3$ -$CH_2$- | -$CH_3$ -$CH_3$ -$CH_2$- | -$CH_3$ -$CH_3$ -$CH_3$ -CH2- |
| -$CH_3$ >CH- | -$CH_3$ -$CH_3$ >CH- | -$CH_3$ -$CH_3$ -$CH_3$ >CH- |
| -$CH_3$ -OH | -$CH_3$ -$CH_3$ -OH | -$CH_3$ -$CH_3$ -$CH_3$ -OH |
| -$CH_3$ -NH- | -$CH_3$ -$CH_3$ -NH- | -$CH_3$ -$CH_3$ -$CH_3$ -NH- |
| -$CH_3$ >N- | -$CH_3$ -$CH_3$ >N- | -$CH_3$ -$CH_3$ -$CH_3$ >N- |
| ⋮ | ⋮ | ⋮ |

## Step 2: Generating Structures

**Delete infeasible combinations.**
**Feasible combinations must satisfy:**

$$\frac{b}{2} = n - 1 + r$$

b = number of bonds
n = number of groups
r = number of rings

-$CH_3$ -$CH_3$ -$CH_3$ -CH3
b = 4 n = 4 r = 0

$$\frac{4}{2} = 4 - 1 + 0$$

✗



## Step 2: 分子構造の生成

**実現不可能な組合せの削除**
**実現可能な組合せは方程式を満たす：**

$$\frac{b}{2} = n - 1 + r$$

b = number of bonds
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-$CH_3$ -$CH_3$ -$CH_3$ -CH3
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✗



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**Delete infeasible combinations.**
**Feasible combinations must satisfy:**

$$\frac{b}{2} = n - 1 + r$$

b = number of bonds
n = number of groups
r = number of rings

-$CH_3$ -$CH_3$ -$CH_3$ >N-
b = 6 n = 4 r = 0

$$\frac{6}{2} = 4 - 1 + 0$$ ✓

$CH_3$-N-$CH_3$
$CH_3$



## Step 2: 分子構造の生成

**実現不可能な組合せの削除**
**実現可能な組合せは方程式を満たす：**

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r = number of rings

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b = 6 n = 4 r = 0

$$\frac{6}{2} = 4 - 1 + 0$$ ✓

$CH_3$-N-$CH_3$
$CH_3$



## Step 2: Generating Structures

**Delete infeasible combinations.**
**b/2 ≠ n – 1 + r**

| 2 Groups | 3 Groups | 4 Groups |
|---|---|---|
| -$CH_3$ -$CH_3$ | -$CH_3$ -$CH_3$ -$CH_3$ | -$CH_3$ -$CH_3$ -$CH_3$ -$CH_3$ |
| -$CH_3$ -$CH_2$- | -$CH_3$ -$CH_3$ -$CH_2$- | -$CH_3$ -$CH_3$ -$CH_3$ -CH2- |
| -$CH_3$ >CH- | -$CH_3$ -$CH_3$ >CH- | -$CH_3$ -$CH_3$ -$CH_3$ >CH- |
| -$CH_3$ -OH | -$CH_3$ -$CH_3$ -OH | -$CH_3$ -$CH_3$ -$CH_3$ -OH |
| -$CH_3$ -NH- | -$CH_3$ -$CH_3$ -NH- | -$CH_3$ -$CH_3$ -$CH_3$ -NH- |
| -$CH_3$ >N- | -$CH_3$ -$CH_3$ >N- | -$CH_3$ -$CH_3$ -$CH_3$ >N- |
| ⋮ | ⋮ | ⋮ |



## Step 2: 分子構造の生成

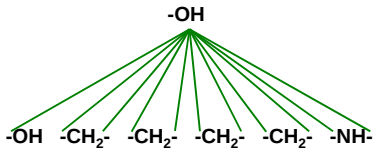
**実現不可能な組合せの削除**
**b/2 ≠ n – 1 + r**

| 2 Groups | 3 Groups | 4 Groups |
|---|---|---|
| -$CH_3$ -$CH_3$ | -$CH_3$ -$CH_3$ -$CH_3$ | -$CH_3$ -$CH_3$ -$CH_3$ -$CH_3$ |
| -$CH_3$ -$CH_2$- | -$CH_3$ -$CH_3$ -$CH_2$- | -$CH_3$ -$CH_3$ -$CH_3$ -CH2- |
| -$CH_3$ >CH- | -$CH_3$ -$CH_3$ >CH- | -$CH_3$ -$CH_3$ -$CH_3$ >CH- |
| -$CH_3$ -OH | -$CH_3$ -$CH_3$ -OH | -$CH_3$ -$CH_3$ -$CH_3$ -OH |
| -$CH_3$ -NH- | -$CH_3$ -$CH_3$ -NH- | -$CH_3$ -$CH_3$ -$CH_3$ -NH- |
| -$CH_3$ >N- | -$CH_3$ -$CH_3$ >N- | -$CH_3$ -$CH_3$ -$CH_3$ >N- |
| ⋮ | ⋮ | ⋮ |

## Step 2: Generating Structures

Groups must now be connected.
Enumeration of all bonds

-OH -OH -$CH_2$- -$CH_2$- -$CH_2$- -$CH_2$- -NH-

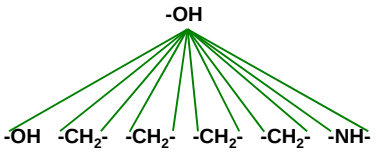





## Step 2: Generating Structures

この時点でグループは結合しているに違いない
全ての結合手の列挙

-OH -OH -$CH_2$- -$CH_2$- -$CH_2$- -$CH_2$- -NH-

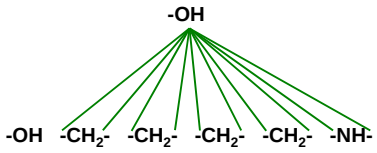





## Step 2: Generating Structures

Eliminate infeasible bonds
Eliminate duplicate structures

-OH -OH -$CH_2$- -$CH_2$- -$CH_2$- -$CH_2$- -NH-

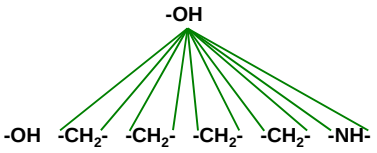





## Step 2:　分子構造の生成

実現不可能な結合手の除去
重複した分子構造の除去

-OH -OH -$CH_2$- -$CH_2$- -$CH_2$- -$CH_2$- -NH-

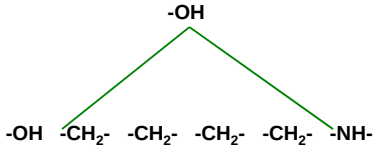





## Step 2: Generating Structures

Eliminate infeasible bonds
Eliminate duplicate structures

-OH -OH -$CH_2$- -$CH_2$- -$CH_2$- -$CH_2$- -NH-

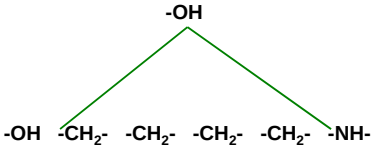





## Step 2:　分子構造の生成

実現不可能な結合手の除去
重複した分子構造の除去

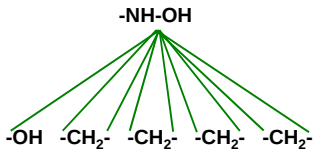
-OH -OH -$CH_2$- -$CH_2$- -$CH_2$- -$CH_2$- -NH-



## Step 2: Generating Structures

**Repeat the procedure for each bonded substructure**

| -OH | -OH | $-CH_2-$ | $-CH_2-$ | $-CH_2-$ | $-CH_2-$ | -NH- |
|---|---|---|---|---|---|---|

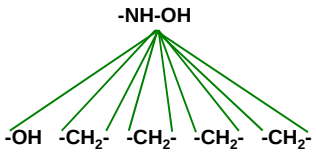





## Step 2: 分子構造の生成

**結合した部分構造ごと手順を繰り返す**

| -OH | -OH | $-CH_2-$ | $-CH_2-$ | $-CH_2-$ | $-CH_2-$ | -NH- |
|---|---|---|---|---|---|---|






## Step 2: Generating Structures

**Finally we have enumerated all candidate molecular structures**

| -OH | -OH | $-CH_2-$ | $-CH_2-$ | $-CH_2-$ | $-CH_2-$ | -NH- |
|---|---|---|---|---|---|---|

$HO-CH_2-CH_2-CH_2-CH_2-NH-OH$

$HO-CH_2-CH_2-CH_2-NH-CH_2-OH$

$HO-CH_2-CH_2-NH-CH_2-CH_2-OH$



## Step 2: 分子構造の生成

**最後に分子構造候補全てを列挙**

| -OH | -OH | $-CH_2-$ | $-CH_2-$ | $-CH_2-$ | $-CH_2-$ | -NH- |
|---|---|---|---|---|---|---|

$HO-CH_2-CH_2-CH_2-CH_2-NH-OH$

$HO-CH_2-CH_2-CH_2-NH-CH_2-OH$

$HO-CH_2-CH_2-NH-CH_2-CH_2-OH$



## Designing Chemical Products

**Generating Candidates**
**Pure Components and Mixtures**

1) Generating Structures: the molecular structure of pure component candidates
2) Generating Mixtures: the components and concentration of mixture candidates



## 化学製品の設計

**候補の生成**
**純物質と混合物**

1) 分子構造生成：純物質候補の分子構造
2) 混合物生成：混合物候補の成分と濃度

## Step 2: Generating Mixtures

**Begin by collecting chemicals into component categories**

| Category: Solvent 1 | Category: Solvent 2 | Category: Water |
|---|---|---|
| Propylene glycol | Propylene glycol | Water |
| Isopropanol | Isopropanol | |
| Methanol | Methanol | |
| Glycerol | Glycerol | |
| Ethanol | Ethanol | |



## Step 2: 混合物生成

**化学物質収集から始め 成分のカテゴリーに分類**

| Category: Solvent 1 | Category: Solvent 2 | Category: Water |
|---|---|---|
| Propylene glycol | Propylene glycol | Water |
| Isopropanol | Isopropanol | |
| Methanol | Methanol | |
| Glycerol | Glycerol | |
| Ethanol | Ethanol | |



## Step 2: Generating Mixtures

**Specify each category's concentration: minimum, maximum and increment**

| Category | Min, wt% | Max, wt% | Increment |
|---|---|---|---|
| Solvent 1 | 0 | 60 | 10 |
| Solvent 2 | 0 | 60 | 10 |
| Surfactant | 0.001 | 0.010 | 0.001 |
| Colorant | 0.05 | 0.10 | 0.05 |
| Water | 20 | 70 | q.s. |

**q.s. = quantum sufficit (amount needed)**



## Step 2: 混合物生成

**各カテゴリーの濃度を指定： 最低限、最大限、増加量**

| Category | Min, wt% | Max, wt% | Increment |
|---|---|---|---|
| Solvent 1 | 0 | 60 | 10 |
| Solvent 2 | 0 | 60 | 10 |
| Surfactant | 0.001 | 0.010 | 0.001 |
| Colorant | 0.05 | 0.10 | 0.05 |
| Water | 20 | 70 | q.s. |

**q.s. = quantum sufficit (amount needed)**



## Step 2: Generating Mixtures

**First all concentrations are generated for the component categories**

| Candidate 0001 | | Candidate 0002 | | ••• | Candidate 0253 | |
|---|---|---|---|---|---|---|
| Solvent 1 | 30.000 | Solvent 1 | 40.000 | | Solvent 1 | 50.000 |
| Solvent 2 | 0.000 | Solvent 2 | 0.000 | | Solvent 2 | 30.000 |
| Surfactant | 0.001 | Surfactant | 0.001 | | Surfactant | 0.004 |
| Colorant | 0.050 | Colorant | 0.050 | | Colorant | 0.100 |
| Water | 69.949 | Water | 59.949 | | Water | 19.899 |

**Constraint: concentration must total 100%**



## Step 2: 混合物生成

**まず最初に、成分のカテゴリーにつき 全ての濃度が生成される**

| Candidate 0001 | | Candidate 0002 | | ••• | Candidate 0253 | |
|---|---|---|---|---|---|---|
| Solvent 1 | 30.000 | Solvent 1 | 40.000 | | Solvent 1 | 50.000 |
| Solvent 2 | 0.000 | Solvent 2 | 0.000 | | Solvent 2 | 30.000 |
| Surfactant | 0.001 | Surfactant | 0.001 | | Surfactant | 0.004 |
| Colorant | 0.050 | Colorant | 0.050 | | Colorant | 0.100 |
| Water | 69.949 | Water | 59.949 | | Water | 19.899 |

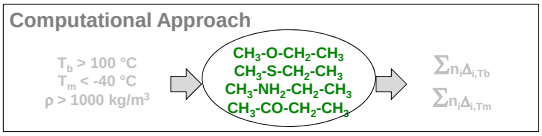
**制約条件：総濃度　100%**

## Designing Chemical Products

### Three Main Steps

1) Identifying physical property constraints
2) Generating candidate structures and mixtures
3) Testing if candidates satisfy constraints

Computational Approach

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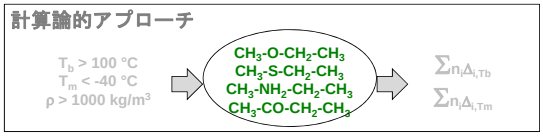
## 化学製品の設計

### ３つの主な手順

1) 物性の制約条件を識別
2) 分子構造と混合物の候補を生成
3) 候補が制約条件を満たしているかテスト

計算論的アプローチ

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## Designing Chemical Products

### Three Main Steps

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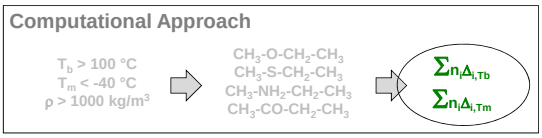
Computational Approach

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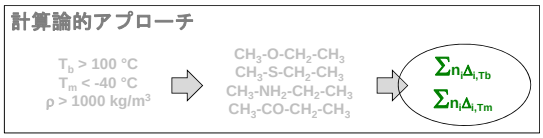


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## Step 3: Evaluating Candidates

### Three Main Categories of Property Estimation Techniques

- ❑ Group Contribution Techniques
- ❑ Equation Oriented Techniques
- ❑ Mixture Estimation Techniques

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## Step 3: 候補を評価

### 物性推算法の３つの主なカテゴリー

- ❑ グループ寄与法
- ❑ 方程式指向法
- ❑ 混合物技法

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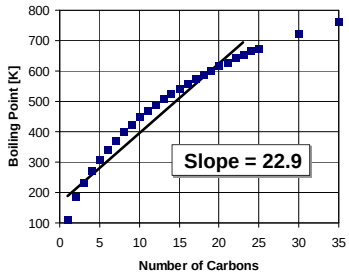
- ❑ 混合物技法



## Group Contribution Techniques

**Normal Paraffins Homologous Series**




$CH_3-[CH_2]_n-CH_3$

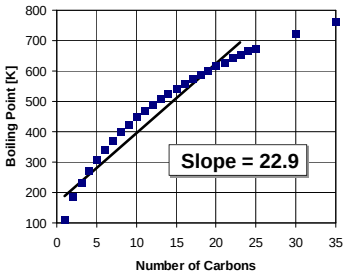
**Contribution**

**-CH2- = 22.9**



## グループ寄与法

**ノルマルパラフィン同族列**



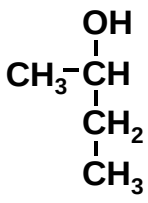

$CH_3-[CH_2]_n-CH_3$

**Contribution**

**-CH2- = 22.9**



## Group Contribution Techniques



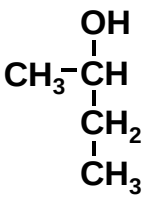

1) Select Technique
2) Dissect Structure
3) Get Contributions
4) Insert into Model

| Group | ΔTb |
|---|---|
| -CH3 | 23.6 |
| -CH3 | 23.6 |
| -CH2- | 22.9 |
| >CH- | 21.7 |
| -OH | 92.9 |
| Tb (est) | 382.8 K |
| Tb (lit) | 372.7 K |

$Tb = 198.1 + \Sigma\Delta_i$



## グループ寄与法




1) 推算法の選択
2) 構造の解体
3) 寄与
4) モデルに挿入

| Group | ΔTb |
|---|---|
| -CH3 | 23.6 |
| -CH3 | 23.6 |
| -CH2- | 22.9 |
| >CH- | 21.7 |
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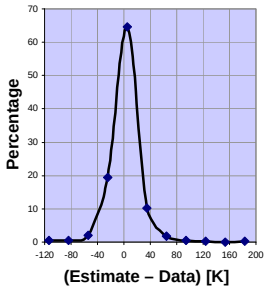
## Boiling Point, Estimation Errors




Estimates generated using Joback's method

**Statistics**

| | |
|---|---|
| Observations | 559 |
| Avg Error | 0.97 K |
| Avg Abs Err | 15.1 K |
| Avg % Error | 4.8 % |
| Max Error | 197.4 K |

**Outliers, Errors**

| | |
|---|---|
| N-Methylformamide | -128.5 K |
| Acetamide | -122.6 K |
| Fluorine | 113.1 K |
| Cyanogen | 197.4 K |

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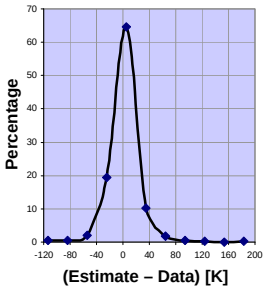
## 沸点、推算エラー

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## Step 3: Evaluating Candidates

### Three Main Categories of Property Estimation Techniques

- ❑ Group Contribution Techniques
- ❑ Equation Oriented Techniques
- ❑ Mixture Estimation Techniques

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## Step 3: 候補を評価

### 物性推算法の 3つの主なカテゴリー

- ❑ グループ寄与法
- ❑ 方程式指向法
- ❑ 混合物技法

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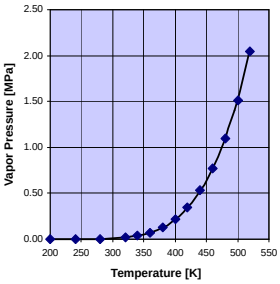
## Equation Oriented Techniques

$$\ln\left(\frac{P_{vp}}{P_c}\right) = T_{br}\frac{\ln(P_c)}{1-T_{br}}\left(1-\frac{1}{T_r}\right)$$

**Required Properties**

- Tc – Critical Temperature
- Pc – Critical Pressure
- Tb – Boiling point

**Vapor Pressure - Heptane**

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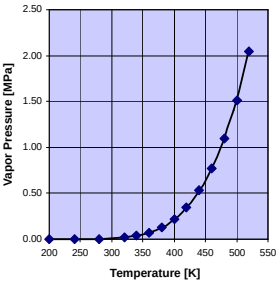
## 方程式指向法

$$\ln\left(\frac{P_{vp}}{P_c}\right) = T_{br}\frac{\ln(P_c)}{1-T_{br}}\left(1-\frac{1}{T_r}\right)$$

**必要な物性**

- Tc – 臨界温度
- Pc – 臨界圧力
- Tb – 沸点

**Vapor Pressure - Heptane**

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## Step 3: 候補を評価

### 物性推算法の 3 つの主なカテゴリー

- ❑ グループ寄与法
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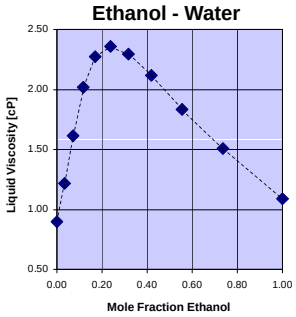
## Mixture Techniques

$$\ln(\eta_m) = x_1 \ln(\eta_1) + x_2 \ln(\eta_2) + x_1 x_2 G$$

**Mixture Functions**

- ❑ Pure Data Inputs
- ❑ Reduces to Pure
- ❑ Molecular Forces
- ❑ Characteristics



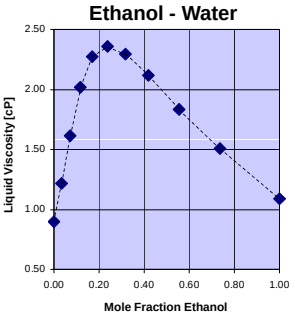



## 混合物技法

$$\ln(\eta_m) = x_1 \ln(\eta_1) + x_2 \ln(\eta_2) + x_1 x_2 G$$

**混合物機能**

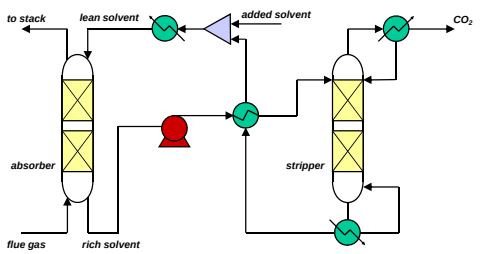
- ❑ 純物質データ入力
- ❑ 純粋成分値に還元
- ❑ 分子間力
- ❑ 特性






## Example: $CO_2$ Absorption Solvent

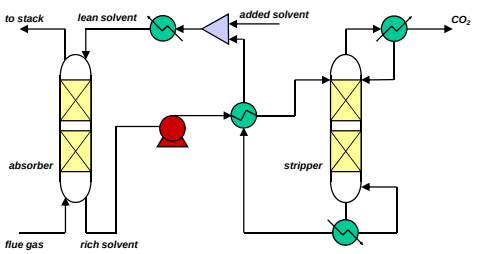
### Absorption, Heat Exchange, Distillation





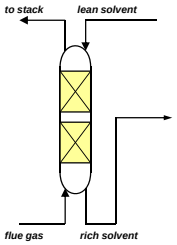

## 例：二酸化炭素吸収剤

### 吸収、熱交換、蒸留



# Example: $CO_2$ Absorption Solvent

**Absorber**




Packed Column: Percentage of packing wetted by the solvent is important

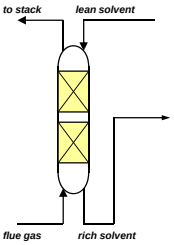
Wilcox, Rochana, Kirchofer, Glatz and He. Energy and Environmental Science, volume 7, page 1769, 2014.

2000-11-15-01



# 例：二酸化炭素吸収剤

**吸収装置**




充填塔：溶剤による充填材の濡れ状態の割合が重要

Wilcox, Rochana, Kirchofer, Glatz and He. Energy and Environmental Science, volume 7, page 1769, 2014.

2000-11-15-01



# Example: $CO_2$ Absorption Solvent

**Percentage of packing wetted by the solvent**

$$\frac{a_w}{a_t} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{\rho L}{a_t \mu}\right)^{0.1}\left(\frac{L^2 a_t}{g}\right)^{-0.05}\left(\frac{\rho L^2}{\sigma a_t}\right)^{0.2}\right\}$$

$a_t$ = total area
$a_w$ = wetted area
L = liquid velocity
ρ = solvent density

$\sigma_c$ = critical surface tension
σ = solvent surface tension
g = gravitational constant
μ = solvent viscosity

2000-11-15-01



# 例：二酸化炭素吸収剤

**溶剤による充填材の濡れ状態の割合**

$$\frac{a_w}{a_t} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{\rho L}{a_t \mu}\right)^{0.1}\left(\frac{L^2 a_t}{g}\right)^{-0.05}\left(\frac{\rho L^2}{\sigma a_t}\right)^{0.2}\right\}$$

$a_t$ = 全面積
$a_w$ = 濡れ面積
L = 流体速度
ρ = 溶剤密度

$\sigma_c$ = 臨界表面張力
σ = 溶剤表面張力
g = 重力定数
μ = 溶剤粘度

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# Example: $CO_2$ Absorption Solvent

**For 30 wt% Monoethanolamine (MEA) in Water**

$$\frac{a_w}{a_t} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{\rho L}{a_t \mu}\right)^{0.1}\left(\frac{L^2 a_t}{g}\right)^{-0.05}\left(\frac{\rho L^2}{\sigma a_t}\right)^{0.2}\right\}$$

Temp = 313.5 K
$\sigma_c$ = 0.061 N/m
$a_t$ = 500 $m^2/m^3$
L = 0.006 m/s
g = 9.81 $m/s^2$

μ = 0.00091 Pa·s
ρ = 953.6 $kg/m^3$
σ = 0.065 N/m
Estimated values

$$\frac{a_w}{a_t} = 0.462$$

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# 例：二酸化炭素吸収剤

**For 30 wt% Monoethanolamine (MEA) in Water**

$$\frac{a_w}{a_t} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{\rho L}{a_t \mu}\right)^{0.1}\left(\frac{L^2 a_t}{g}\right)^{-0.05}\left(\frac{\rho L^2}{\sigma a_t}\right)^{0.2}\right\}$$

Temp = 313.5 K
$\sigma_c$ = 0.061 N/m
$a_t$ = 500 $m^2/m^3$
L = 0.006 m/s
g = 9.81 $m/s^2$

μ = 0.00091 Pa·s
ρ = 953.6 $kg/m^3$
σ = 0.065 N/m
推算値

$$\frac{a_w}{a_t} = 0.462$$

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## Step 1: Identify Constraints

A more extensive design would have constraints on the percentage of wetted surface area, the potential for flooding, the energy usage, and many more. For this example we simply create a constraint on the percentage of wetted surface area.

$$\frac{a_w}{a_t} > 0.462$$

**Constraint:**
**Better than MEA**

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## Step1：制約条件の識別

より広範な設計は、濡れ表面積の割合、フラッディングの可能性、エネルギー使用量、その他多くの制約条件がある。この例では、濡れ表面積の割合の制約条件を作成してみる。

$$\frac{a_w}{a_t} > 0.462$$

**Constraint:**
**Better than MEA**

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## Step 2: Generate Candidates

We chose the following design groups

**-CH3 -CH2- >CH- >C< -OH**
**-NH2 >NH >N-**

**We chose a fixed amount of solvent in water:**
**30% Water Mixtures**

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## Step 2：候補の生成

以下の設計グループを選択

**-CH3 -CH2- >CH- >C< -OH**
**-NH2 >NH >N-**

**水中の一定量の溶剤：**
**３０％水混合溶液**

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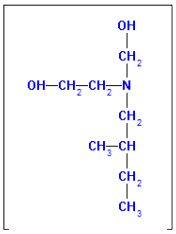
## Step 3: Evaluate Candidates

$$\frac{a_w}{a_t} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{\rho L}{a_t \mu}\right)^{0.1}\left(\frac{L^2 a_t}{g}\right)^{-0.05}\left(\frac{\rho L^2}{\sigma a_t}\right)^{0.2}\right\}$$



**$T_b$ = Joback's Technique (GCT)**
**$T_c$ = Joback's Technique (GCT)**
**$P_c$ = Joback's Technique (GCT)**

**σ = Sastri + Rao Technique (EOT)**
**μ = Joback's Technique (GCT)**
**ρ = Rackett Equation (EOT)**

First estimates are generated. Estimates are then inserted into the wetting equation.

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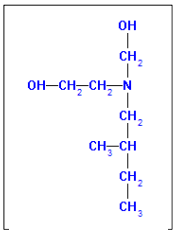
## Step 3：候補の評価

$$\frac{a_w}{a_t} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{\rho L}{a_t \mu}\right)^{0.1}\left(\frac{L^2 a_t}{g}\right)^{-0.05}\left(\frac{\rho L^2}{\sigma a_t}\right)^{0.2}\right\}$$



**$T_b$ = Joback's Technique (GCT)**
**$T_c$ = Joback's Technique (GCT)**
**$P_c$ = Joback's Technique (GCT)**

**σ = Sastri + Rao Technique (EOT)**
**μ = Joback's Technique (GCT)**
**ρ = Rackett Equation (EOT)**

先ず推算値が生成され、
次に推算値は方程式に挿入される。

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## Step 3: Evaluate Candidates

**Mixtures: 30 wt% Candidate + 70 % Water**

$$\frac{a_w}{a_t} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{\rho L}{a_t \mu}\right)^{0.1}\left(\frac{L^2 a_t}{g}\right)^{-0.05}\left(\frac{\rho L^2}{\sigma a_t}\right)^{0.2}\right\}$$

**μ = Arrhenius Equation (Mix)**
**ρ = Weight Fraction Average (Mix)**
**σ = Weight Fraction Average (Mix)**



## Step 3：候補の評価

**Mixtures: 30 wt% Candidate + 70 % Water**

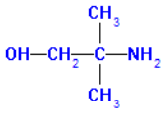
$$\frac{a_w}{a_t} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{\rho L}{a_t \mu}\right)^{0.1}\left(\frac{L^2 a_t}{g}\right)^{-0.05}\left(\frac{\rho L^2}{\sigma a_t}\right)^{0.2}\right\}$$

**μ = Arrhenius Equation (Mix)**
**ρ = Weight Fraction Average (Mix)**
**σ = Weight Fraction Average (Mix)**



## Step 3: Evaluate Candidates

**2-Amino-2-methylpropanol**



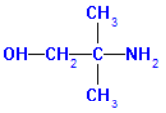
| Pure Component Ests | Mixture Estimates |
|---|---|
| μ = 0.04760 Pa·s | μ = 0.00092 Pa·s |
| ρ = 844.2 kg/m³ | ρ = 947.5 kg/m³ |
| σ = 0.043 N/m | σ = 0.062 N/m |

$$\frac{a_w}{a_t} = 0.476$$



## Step 3：候補の評価

**2-Amino-2-methylpropanol**



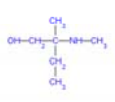
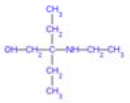
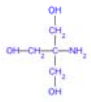
| Pure Component Ests | Mixture Estimates |
|---|---|
| μ = 0.04760 Pa·s | μ = 0.00092 Pa·s |
| ρ = 844.2 kg/m³ | ρ = 947.5 kg/m³ |
| σ = 0.043 N/m | σ = 0.062 N/m |

$$\frac{a_w}{a_t} = 0.476$$



## Interesting Candidates

**Some designed candidates and their $a_w/a_t$ values**

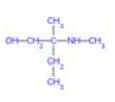
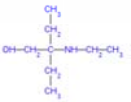
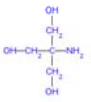




**0.490** **0.492** **0.399**



## 興味ある候補

**いくつかの設計された候補**

**0.490** **0.492** **0.399**

## Designing Chemical Products

### Three Main Steps

1) Identifying physical property constraints
2) Generating candidate structures and mixtures
3) Testing if candidates satisfy constraints

Computational Approach

$T_b$ > 100 °C
$T_m$ < -40 °C
ρ > 1000 kg/m³

$CH_3$-O-$CH_2$-$CH_3$
$CH_3$-S-$CH_2$-$CH_3$
$CH_3$-$NH_2$-$CH_2$-$CH_3$
$CH_3$-CO-$CH_2$-$CH_3$

$\sum n_i \Delta_{i,Tb}$
$\sum n_i \Delta_{i,Tm}$

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## 化学製品の設計

### ３つの主な手順

1) 物性の制約条件を識別
2) 分子構造と混合物の候補を生成
3) 候補が制約条件を満たしているかをテスト

Computational Approach

$T_b$ > 100 °C
$T_m$ < -40 °C
ρ > 1000 kg/m³

$CH_3$-O-$CH_2$-$CH_3$
$CH_3$-S-$CH_2$-$CH_3$
$CH_3$-$NH_2$-$CH_2$-$CH_3$
$CH_3$-CO-$CH_2$-$CH_3$

$\sum n_i \Delta_{i,Tb}$
$\sum n_i \Delta_{i,Tm}$

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## Designing Chemical Products

### Applicable to many types of chemical products

- ❑ Artificial Blood
- ❑ Refrigeration Lubes
- ❑ Degreasing Solvents
- ❑ Non-MMH Rocket Fuels
- ❑ Aircraft Deicing Fluids
- ❑ Soil Consolidants
- ❑ Sonar Fill Fluids
- ❑ Phase Change Materials
- ❑ CO2 Absorption Solvents
- ❑ Hydraulic Energy Storage
- ❑ Windshield Washer Fluid
- ❑ Pour Point Depressant

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## 化学製品の設計

### 多くの種類の化学製品に適用

- ❑ 人工血液
- ❑ 冷凍機油
- ❑ 脱脂溶剤
- ❑ 非ＭＭＨロケット燃料
- ❑ 航空機除氷液
- ❑ 土の圧密
- ❑ ソナー充填流体
- ❑ 相変化物質
- ❑ 二酸化炭素吸収剤
- ❑ 油圧エネルギ貯蔵
- ❑ フロントガラス洗浄液
- ❑ 流動点降

2000-11-15-01



## Thank You

Thank you again for the opportunity to speak to you today.

**Questions ?**

2000-11-15-01



## Thank You

本日は皆様方にお話する機会を頂きましたこと
重ねて御礼申し上げます。

**Questions ?**

2000-11-15-01