



산업안전보건연구원
Occupational Safety & Health Research Institute

Prediction of Flash Point for Binary Mixtures

위험성연구팀

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팝업 ZONE

01 02 03 04 05 06 07 08

건설근로자 안전교육 실시안내

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[자세히 보기](#)

전 체

공지사항

입찰공고

보도자료

신간자료

- [공지] 2009년 석면 조사기관 분석정도관리 ... 2009-09-10
- [공지] 반월·시화 지역산업보건센터 서류심사 ... 2009-09-10
- [공지] 직업병 (톨루엔 중독사망) 발생경보 발령 2009-09-04
- [공지] 2009년 하반기 특수건강진단 분석정... 2009-08-27
- [공지] 직업병 (혼합유기용제 중독사망) 발생경... 2009-08-26

KOSHA

전자민원안내

안전인증·검사신청/확인

공단에서 수행하는 안전인증
/ 검사업무에 대한
신청 및 처리상황을
확인 할 수 있습니다.

GO

기술상담및질의답변

산업재해를확인/조치

안전인증·검사신청/확인

교육신청/확인

사이버감사실

나의민원조회

KOSHANET (안전보건정보서비스)

KOSHA-CODE, MSDS 등
DATA BASE, 교육원 통신교육센터,
참여마당, 안전보건 커뮤니티,
메일 등 회원제 서비스

관련사이트 바로가기

- 01 공단본부 [GO](#)
- 02 산업안전보건연구원 [GO](#)
- 03 산업안전보건교육원 [GO](#)
- 04 지역본부/지도원 [GO](#)

노동부/관련기관 바로가기

 **건설업 대형재해사례**

 **안전보건자료 쇼핑몰**

 **건설업 KOSHA클럽**



KOSHA
자주찾는자료

 **윤리경영**

안전사업

> 클린사업장조성사업

보건사업

> 석면작업관리

교육/인증사업

> 외국인용안전교육자료

□ 구성성분 물질의 자료이용

5. 폭발·화재시 대처방법

구 분	제 품	벤 젠	톨 루 엔	나프탈렌
인 화 점	-2°C	-11	4	79
발 화 점	-	538	480	526
폭발범위 (상)	-	8.0%	7.1%	-
(공기중) (하)	-	1.5%	1.3%	-

고고, 전고에 비해서 고질 고고 일고고 개량고고 고고 내고고 고고고고고 고고고고고 하는 것이다.

Prediction of flash point(1)

Question 1

Octane

FP: 15°C

+

Heptane

FP: -5°C

혼합물의 인화점은?

예상대로



Flash Point between Individual Components

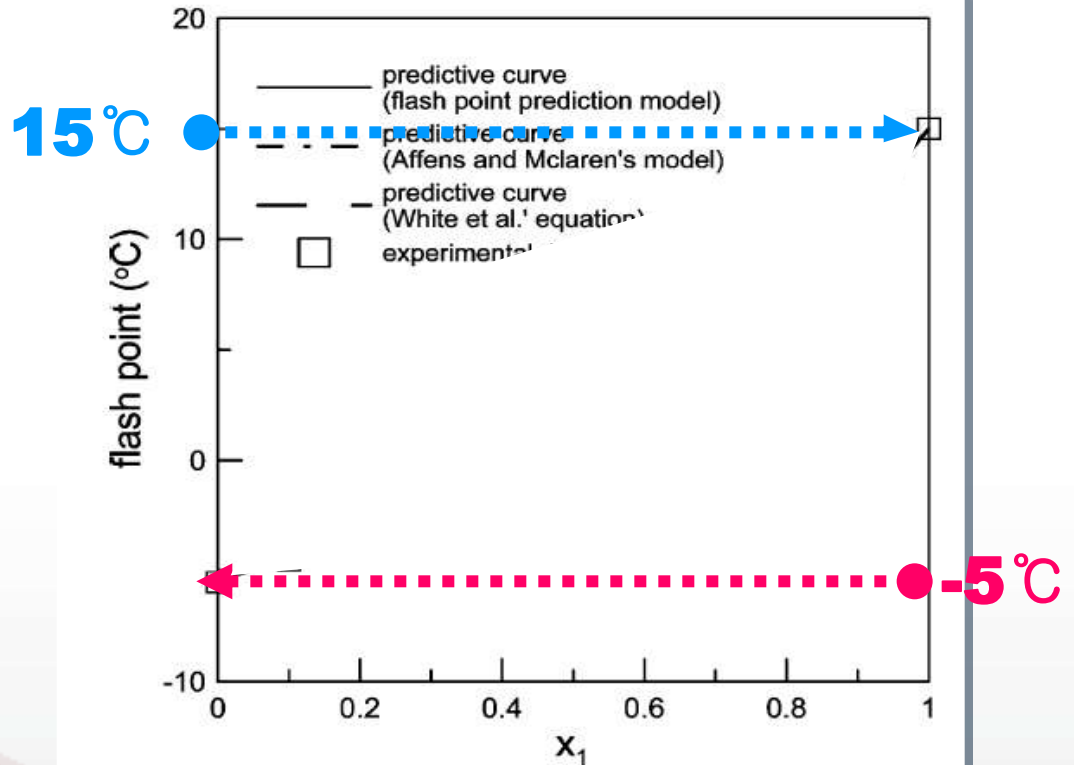


Fig. 1. Comparison of the flash point-prediction curves with experimentally-derived data for octane (1) + heptane (2) solution.

Hong-Jang Liaw, "A mathematical model for predicting the flash point of binary solutions"

Prediction of flash point(2)

Question2

Octane
FP: 15°C

+

Ethanol
FP: 13°C

혼합물의 인화점은?

Min 5°C

Minimum Flash Point Behavior

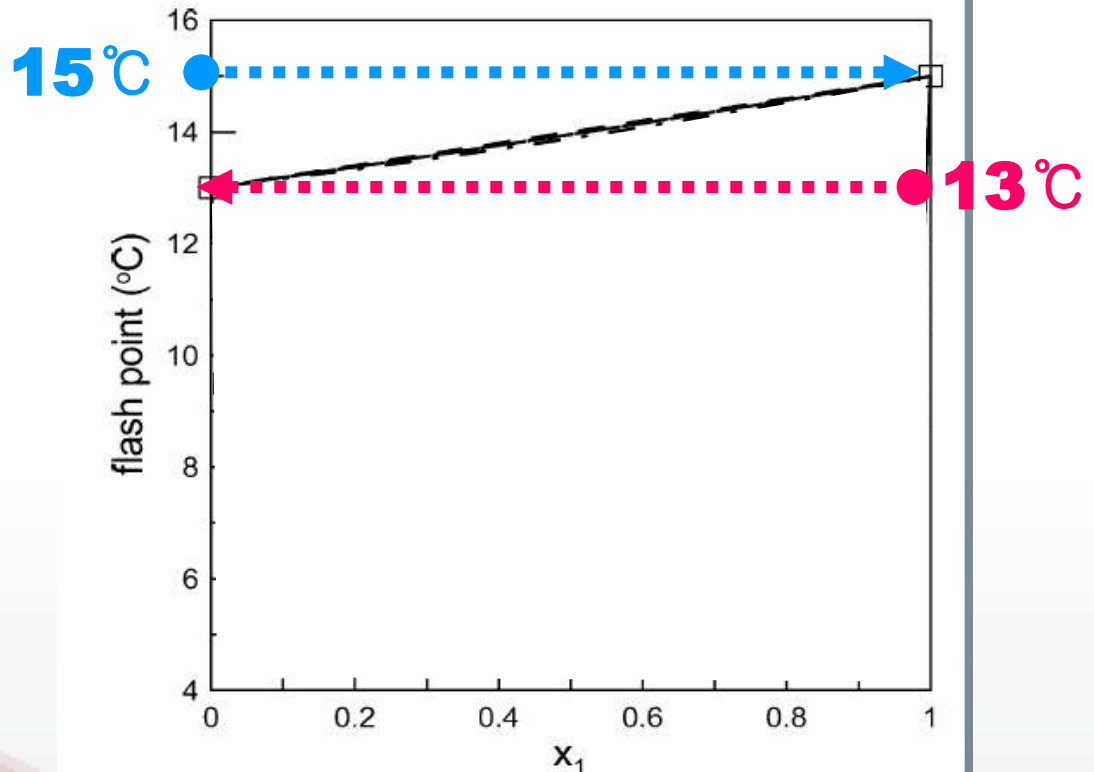


Fig. 5. Comparison of the flash point-prediction curves with experimentally-derived data for octane (1) + ethanol (2) solution.

Horng-Jang Liaw, "A mathematical model for predicting the flash point of binary solutions"

Question 3

Phenol
FP: 83°C

+

Acetophenone
FP: 81°C

혼합물의 인화점은?

Max 89°C

Maximum Flash Point Behavior

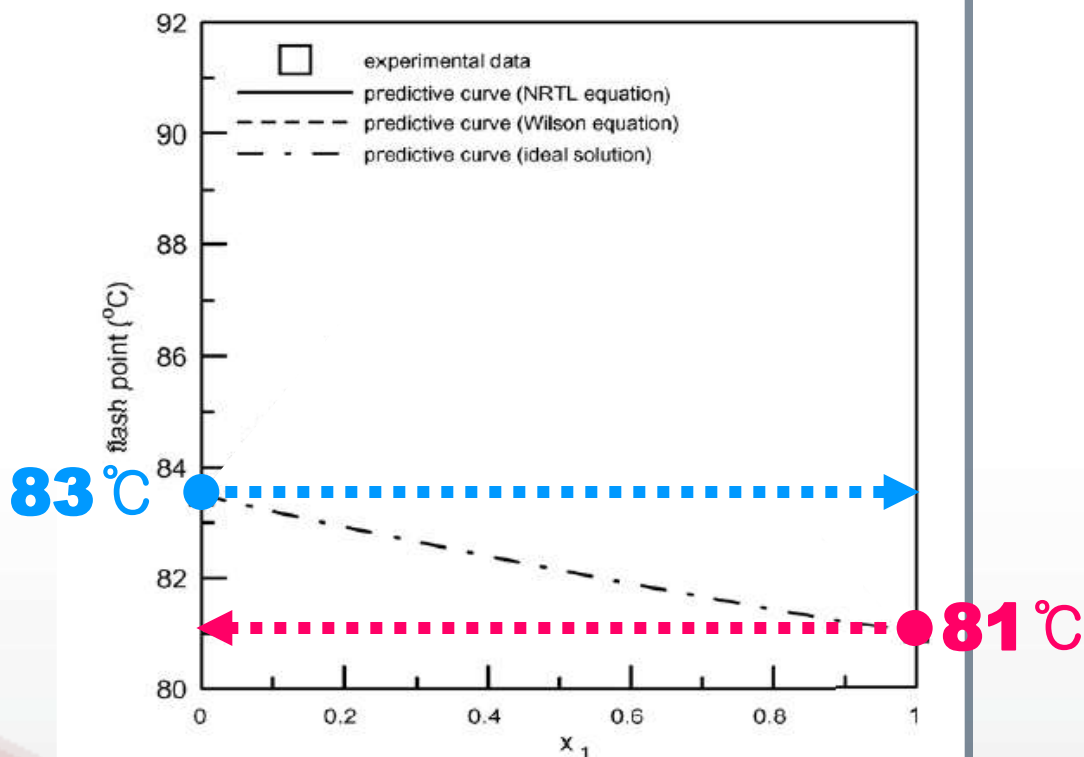


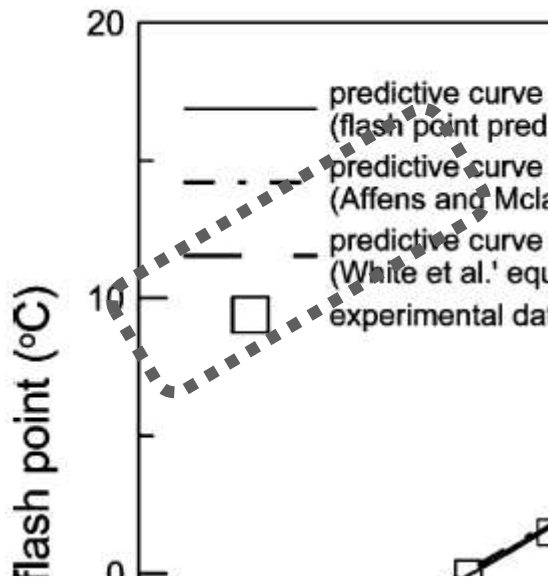
Fig. 5. Variation of flash point with composition for phenol (1) + acetophenone (2).

Horng-Jang Liaw, "Binary mixtures exhibiting maximum flash-point behavior"

Max. FPB vs. Min. FPB

이렇게 물질에 따라 혼합할 때 인화점이 다른 이유는?

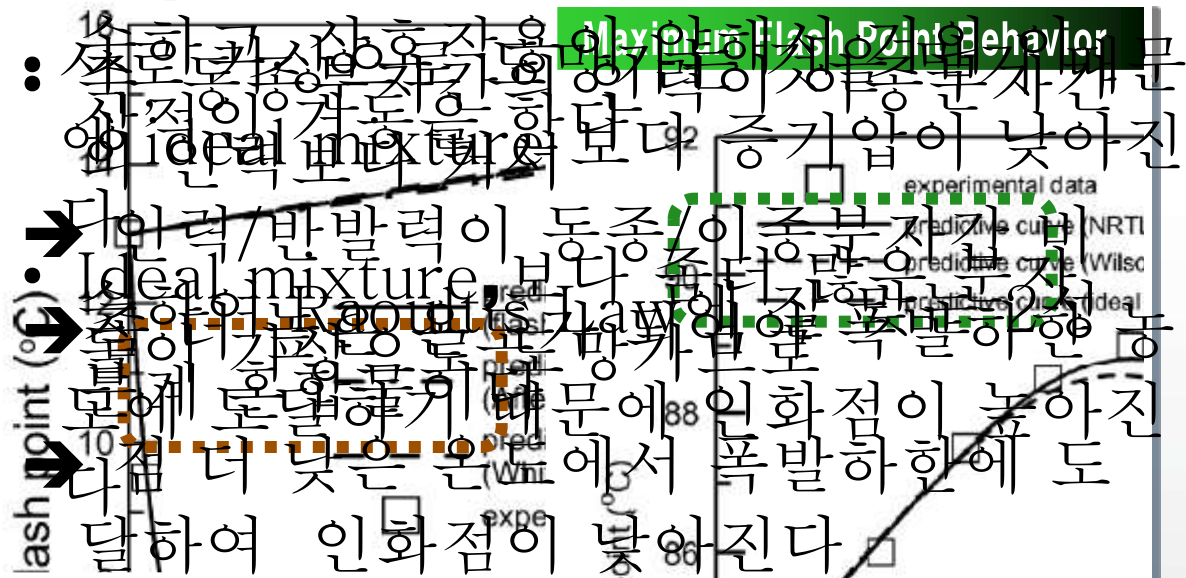
Max. nor min. Flash Point Behavior



Minimum Flash Point Behavior

- Hydrocarbon과 Alcohol은 극성이
- 동종분자끼리 혼합할 때 인화점이 낮아진다
- Heptane과 Octane은 분자구조가 비

Maximum Flash Point Behavior



2성분계에서 두 물질이 아주 이상적인 거동

Ideal Solution

3.2. Reduced model under an ideal solution assumption

For the ideal solution, the activity coefficients of the liquid phase are equal to unity, and the flash point-prediction model may be reduced to a simpler form. Under this condition, the vapor-liquid equilibrium equation, Eq. (5), was able to be reduced to Raoult's law for this study, this being described as:

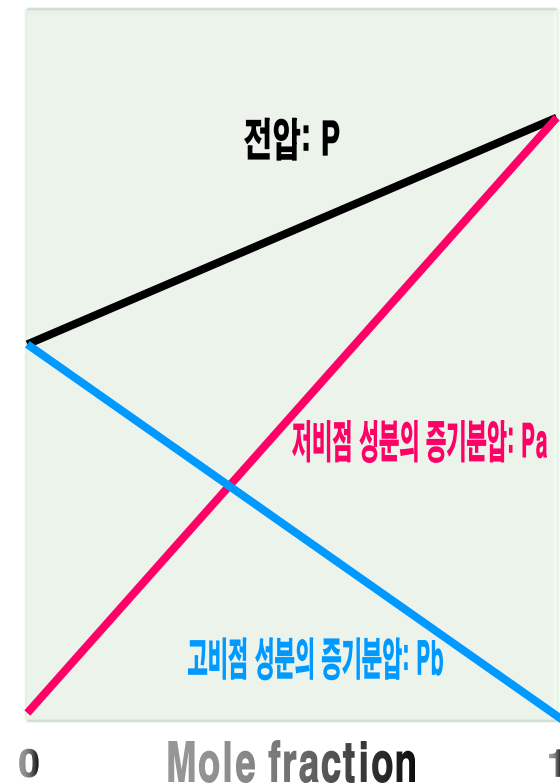
$$y_i = \frac{x_i P_i^{\text{sat}}}{P} \quad (8)$$

Therefore, the modified equation of Le Chatelier, Eq. (6), was reduced to:

$$1 = \sum \frac{x_i P_i^{\text{sat}}}{P_{i,\text{fp}}^{\text{sat}}} = \frac{x_1 P_1^{\text{sat}}}{P_{1,\text{fp}}^{\text{sat}}} + \frac{x_2 P_2^{\text{sat}}}{P_{2,\text{fp}}^{\text{sat}}} \quad (9)$$

this being the equation used by White et al. (1997) to estimate the flash point of aviation-fuel mixtures, JP-4/JP-8 and JP-5/JP-8. The Antoine equation, Eq. (7), was still deemed by us to be useful to estimate P_i^{sat} and $P_{i,\text{fp}}^{\text{sat}}$ for this reduced model. Therefore, the reduced

이상용액의 증기압 곡선

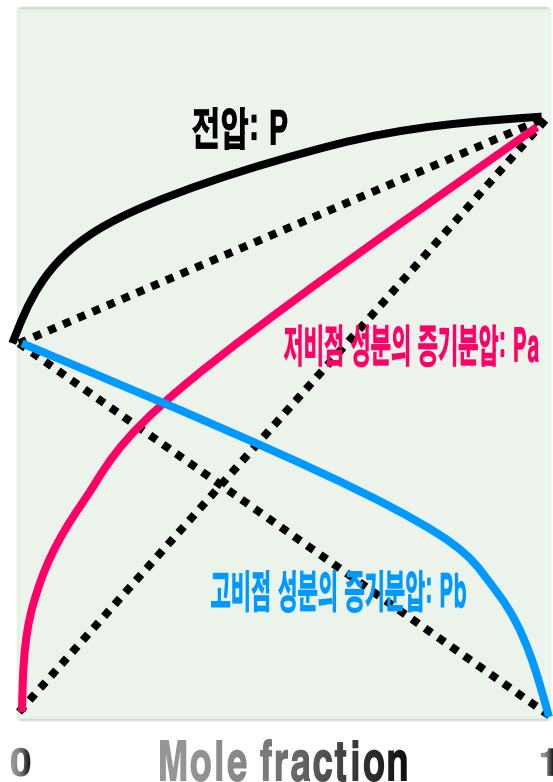


Non-ideal Solution

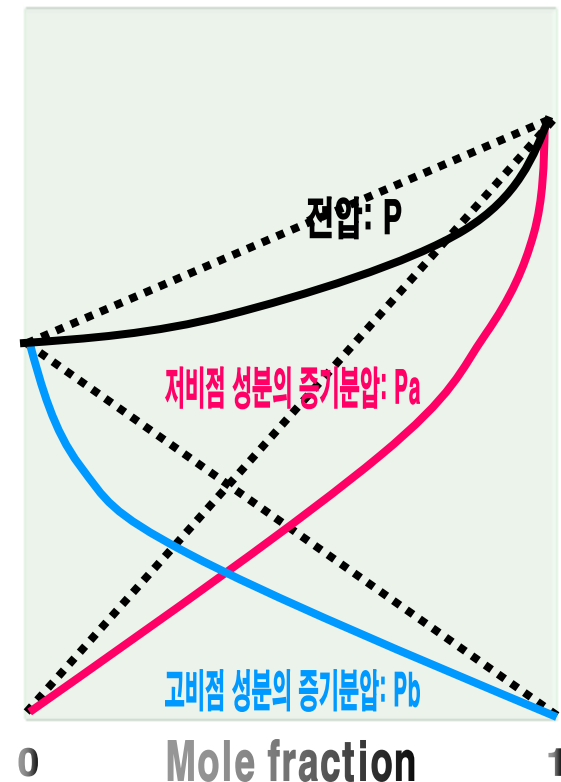
$$y_i = \frac{x_i \gamma_i p_i^{sat}}{P}$$

2성분계 비이상적인 거동

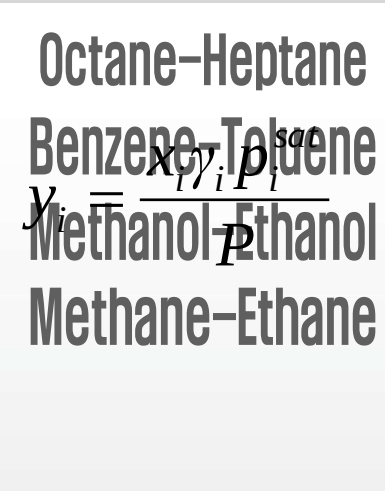
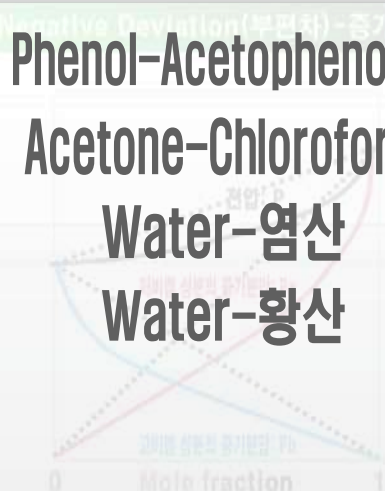
Positive Deviation(정편차)-증기압 ↑



Negative Deviation(부편차)-증기압 ↓

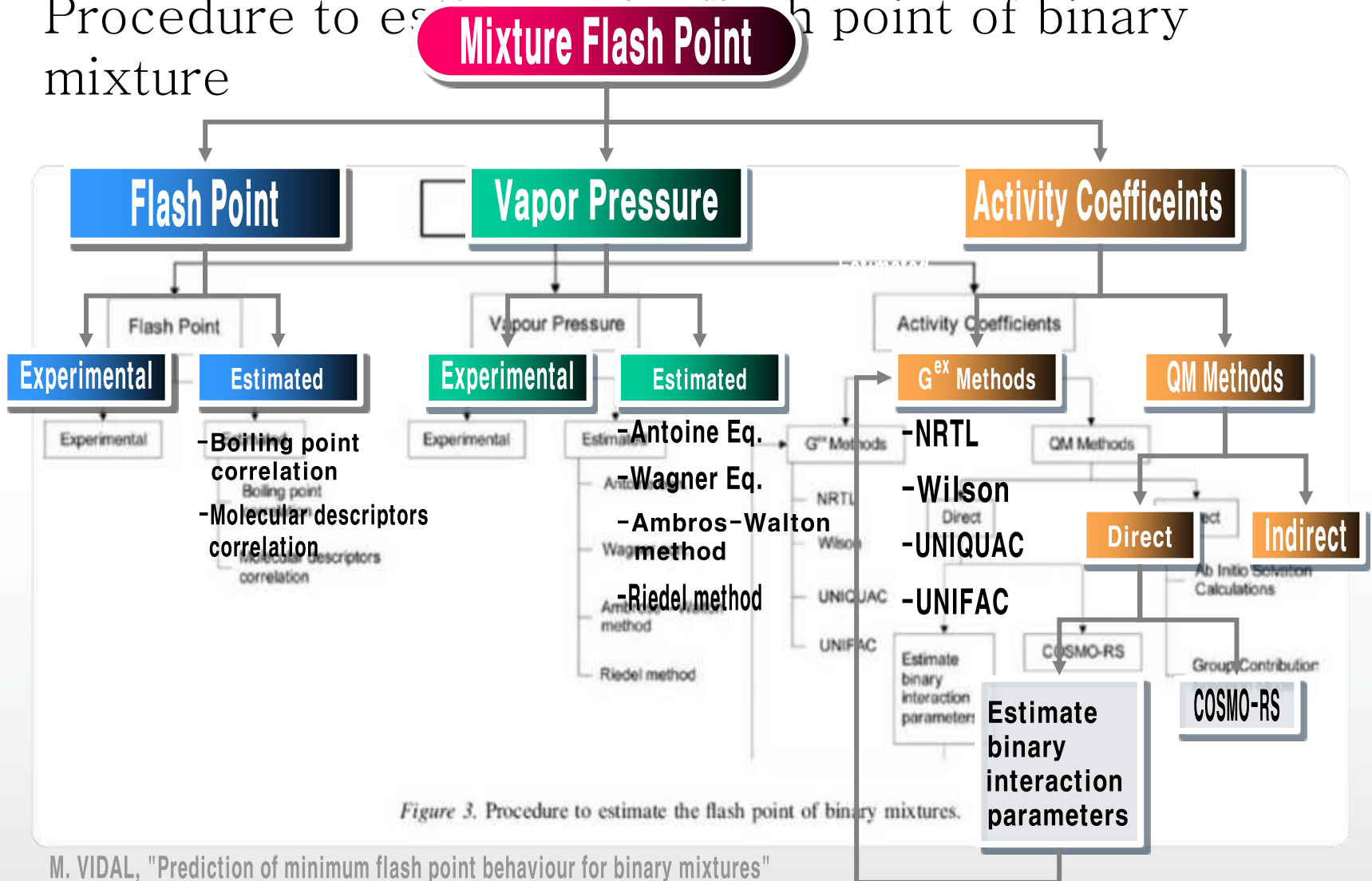


Comparison of Ideal & non-ideal Soln

	Positive Deviation(정편차)-증기압 ↑	Ideal Solution과 유사	Negative Deviation(부편차)-증기압 ↓
증 기 압	이상용액에 비해 크게 나타남	이상용액과 비슷 or 크게 벗어나지 않음	이상용액에 비해 작게 나타남
인 력	동종분자간 인력 > 이종분자간 인력	구조가 비슷하여 동종/이종 인력이 비슷	동종분자간 인력 < 이종분자간 인력
활동도계수	$\gamma_A > 1, \gamma_B > 1$	$\gamma_A = 1, \gamma_B = 1$	$\gamma_A < 1, \gamma_B < 1$
2성분계	Octane-Ethanol Water-Ethanol Ethanol-Benzene Acetone-CS₂계 	Octane-Heptane Benzene-Toluene Methanol-Ethanol Methane-Ethane 	Phenol-Acetophenone Acetone-Chloroform Water-염산 Water-황산 

Procedure to estimate

Procedure to estimate the flash point of binary mixture



인화성 액체와 물의 혼합물인 경우

한쪽은 불에 타는 물질이고 한쪽은 불에 타지 않는 물질

Ethanol-Water 계

물과 에탄올 모두 **positive deviation(정편차)**이 보이므로
실제로는 **증기압이 더 커지지만...**

➔ 물이 불연성이므로 기상으로 증발한 물분자는 **기상의 에탄올 농도를 희석시키는 역할**을 하기 때문에

➔ **Min. FPB 현상은 보이지 않으나**, Raoul't law에 의한 예상치 보다 **낮은 인화점을** 갖게 된다.

Characteristics of the flash point in water-ethanol mixture

예한올 제올의 인화점 특성 평가
 Characteristic of the flash point in water-ethanol mixture
 최은영, 이근원, 최이락

Background & Objective
 Water-ethanol mixture is a common solvent used in various industries. However, its flash point is not well understood, which is a critical safety parameter. This study aims to determine the flash point of water-ethanol mixtures and compare it with the ideal curve and experimental data.

Methods
 The flash point was determined using a closed-cup method. The experimental data were compared with the ideal curve and the experimental data of pure ethanol.

Results & Discussion
 The flash point of water-ethanol mixtures decreases as the ethanol concentration increases. The experimental data show that the flash point is lower than the ideal curve and higher than the experimental data of pure ethanol.

Conclusion
 The flash point of water-ethanol mixtures is lower than the ideal curve and higher than the experimental data of pure ethanol. This indicates that the flash point of water-ethanol mixtures is not simply the sum of the flash points of the components.

인화점 특성 평가 Flash point in water-ethanol mixture

이근원, 최이락
산업안전보건연구원

Conclusion

Water-ethanol 계의 인화점은 저농도 ethanol 영역에서 **인화점이 낮아지고**, 이는 저농도 주류에서 인화점이 예상보다 낮게 나타남을 알 수 있다.

또한, 위험물안전관리법에 의해 완제품 주류의 경우 62 vol. % 이하는 비위험물로 분류되나, 19.5 vol. % 소주는 인화점이 37.5 °C로 자동차 연료인 경유(인화점 38 °C)와 비슷하므로 이보다 높은 농도의 ethanol 제품은 경유보다 인화점이 낮다는 것을 알 수 있었다.

Methods

Table 2. Experimental apparatus and test methods

구분	인화점(Flash Point)	폭발한계(Flammability Limits)
장비명	Fully automated flash-point tester TAGA	Flammability Range Apparatus
제조사	Peltronix (미국)	The Cliftworth Technology (영국)
시험규격	KGS M 2010-2904 (개정 2010. 4월 29일 제정)	ASTM E 681-04 (Standard test method for determination of flammability of chemicals, vapors, and gases)

Results & Discussion

Comparison of the flash point prediction curve with experimental data

Figure 1. Comparison of the flash point-ideal curve with experimental data for water-ethanol.

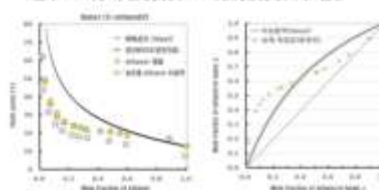


Figure 1. Comparison of the flash point-ideal curve with experimental data for water-ethanol.

폭발한계

Table 2

구분	인화점(Flash Point)	폭발한계(Flammability Limits)
장비명	Fully automated flash-point tester TAGA	Flammability Range Apparatus
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Conclusion

Water-ethanol 계의 인화점은 저농도 ethanol 영역에서 인화점이 낮아지고, 이는 저농도 주류에서 인화점이 예상보다 낮게 나타남을 알 수 있다.

References

1. GHS, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100.
2. GHS, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100.
3. GHS, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100.
4. GHS, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100.



Figure 1. Comparison of the flash point-ideal curve with experimental data for water-ethanol.

Figure 2. Comparison of the equilibrium curve with experimental data.

Question Can we treat mixtures as pure compounds and use the available methodologies to evaluate the risks associated with them?

Answer The answer to this question is generally NO.

The behavior of mixtures can be **extremely different** compared to the behavior of the individual components, and making such assumptions can be **very dangerous**.

감사합니다!!!

The flash point values of the individual mixture components can be obtained from experimental measurements or from correlations with boiling point or with molecular descriptors. A correlation of the flash point for organics compounds with their boiling points was developed by Satyanarayana and Rao (1992) and is presented in equation (7).

$$T_f = a + \frac{b(c/T_b)^2 e^{-c/T_b}}{(1 - e^{-c/T_b})^2} \quad (7)$$

where T_f is the flash point temperature (K), a , b , and c are constants provided in Satyanarayana and Rao (1992), and T_b is the boiling point temperature (K).

The equation was fit for over 1200 compounds with less than 1% absolute error with experimental data (based on K). The larger deviations, of approximately 10°C, were found for the phosphorous chemical group. A comparison of this correlation with other correlations is presented (Satyanarayana and Rao, 1992).

Table 1
Models of activity coefficients and their composition effect in binary systems

Wilson equation

$\ln \gamma_1$ and $\ln \gamma_2$

$$\ln \gamma_1 = -\ln(x_1 + A_{12}x_2) + x_2 \left(\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{A_{21}x_1 + x_2} \right), \quad \ln \gamma_2 = -\ln(x_2 + A_{21}x_1) - x_1 \left(\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{A_{21}x_1 + x_2} \right),$$

$$\text{where } A_{12} = \frac{v_1^L}{v_2^L} \exp \left(-\frac{\lambda_{12} - \lambda_{11}}{RT} \right), \quad A_{21} = \frac{v_1^L}{v_2^L} \exp \left(-\frac{\lambda_{21} - \lambda_{22}}{RT} \right)$$

$\left(\frac{\partial \gamma_1}{\partial x_1} \right)_T$ and $\left(\frac{\partial \gamma_2}{\partial x_1} \right)_T$

$$\left(\frac{\partial \gamma_1}{\partial x_1} \right)_T = \gamma_1 \left\{ -\frac{1-A_{12}}{x_1 + A_{12}x_2} - \left(\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{A_{21}x_1 + x_2} \right) + x_2 \left[-\frac{A_{12}}{(x_1 + A_{12}x_2)^2} (1-A_{12}) + \frac{A_{21}}{(A_{21}x_1 + x_2)^2} (A_{21}-1) \right] \right\},$$

$$\left(\frac{\partial \gamma_2}{\partial x_1} \right)_T = \gamma_2 \left\{ \frac{1-A_{21}}{x_2 + A_{21}x_1} - \left(\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{A_{21}x_1 + x_2} \right) + x_1 \left[\frac{A_{12}}{(x_1 + A_{12}x_2)^2} (1-A_{12}) - \frac{A_{21}}{(A_{21}x_1 + x_2)^2} (A_{21}-1) \right] \right\}$$

γ_1^∞ and γ_2^∞

$$\gamma_1^\infty = \frac{1}{A_{12}} \exp(1-A_{21}), \quad \gamma_2^\infty = \frac{1}{A_{21}} \exp(1-A_{12})$$

NRTL equation

$\ln \gamma_1$ and $\ln \gamma_2$

$$\ln \gamma_1 = x_2^2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \frac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right], \quad \ln \gamma_2 = x_1^2 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \frac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right],$$

$$\text{where } \tau_{12} = \frac{g_{12} - g_{22}}{RT}, \quad \tau_{21} = \frac{g_{21} - g_{11}}{RT}, \quad \ln G_{12} = -\alpha_{12} \tau_{12}, \quad \ln G_{21} = -\alpha_{12} \tau_{21}$$

$\left(\frac{\partial \gamma_1}{\partial x_1} \right)_T$ and $\left(\frac{\partial \gamma_2}{\partial x_1} \right)_T$

$$\left(\frac{\partial \gamma_1}{\partial x_1} \right)_T = \gamma_1 \left\{ -2x_2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \frac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right] + x_2^2 \left[-2\tau_{21} \frac{G_{21}^2}{(x_1 + x_2 G_{21})^3} (1-G_{21}) + \frac{2\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^3} (1-G_{12}) \right] \right\}$$

$$\left(\frac{\partial \gamma_2}{\partial x_1} \right)_T = \gamma_2 \left\{ 2x_1 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \frac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right] + x_1^2 \left[2\tau_{12} \frac{G_{12}^2}{(x_2 + x_1 G_{12})^3} (1-G_{12}) - \frac{2\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^3} (1-G_{21}) \right] \right\}$$

γ_1^∞ and γ_2^∞

$$\gamma_1^\infty = \exp(\tau_{21} + \tau_{12} G_{12}), \quad \gamma_2^\infty = \exp(\tau_{12} + \tau_{21} G_{21})$$

UNIQUAC equation

$\ln \gamma_1$ and $\ln \gamma_2$

$$\ln \gamma_1 = \ln \frac{\Phi_1}{x_1} + \frac{z}{2} q_1 \ln \frac{\theta_1}{\Phi_1} + \Phi_2 \left(l_1 - \frac{r_1}{r_2} l_2 \right) - q_1 \ln(\theta_1 + \theta_2 \tau_{21}) + \theta_2 q_1 \left(\frac{\tau_{21}}{\theta_1 + \theta_2 \tau_{21}} - \frac{\tau_{12}}{\theta_2 + \theta_1 \tau_{12}} \right),$$

$$\ln \gamma_2 = \ln \frac{\Phi_2}{x_2} + \frac{z}{2} q_2 \ln \frac{\theta_2}{\Phi_2} + \Phi_1 \left(l_2 - \frac{r_2}{r_1} l_1 \right) - q_2 \ln(\theta_2 + \theta_1 \tau_{12}) + \theta_1 q_2 \left(\frac{\tau_{12}}{\theta_2 + \theta_1 \tau_{12}} - \frac{\tau_{21}}{\theta_1 + \theta_2 \tau_{21}} \right),$$

$$\text{where } \ln \tau_{12} = -\frac{u_{12} - u_{22}}{RT}, \quad \ln \tau_{21} = -\frac{u_{21} - u_{11}}{RT}, \quad \Phi_1 = \frac{x_1 r_1}{x_1 r_1 + x_2 r_2}, \quad \Phi_2 = \frac{x_2 r_2}{x_1 r_1 + x_2 r_2}, \quad \theta_1 = \frac{x_1 q_1}{x_1 q_1 + x_2 q_2},$$

$$\theta_2 = \frac{x_2 q_2}{x_1 q_1 + x_2 q_2}, \quad l_1 = \frac{z}{2} (r_1 - q_1) - (r_1 - 1), \quad l_2 = \frac{z}{2} (r_2 - q_2) - (r_2 - 1), \quad z = 10$$

$\left(\frac{\partial \gamma_1}{\partial x_1} \right)_T$ and $\left(\frac{\partial \gamma_2}{\partial x_1} \right)_T$

$$\left(\frac{\partial \gamma_1}{\partial x_1} \right)_T = \gamma_1 \left\{ \frac{1}{\Phi_1} \frac{d\Phi_1}{dx_1} - \frac{1}{x_1} + \frac{z}{2} q_1 \left(\frac{1}{\theta_1} \frac{d\theta_1}{dx_1} - \frac{1}{\Phi_1} \frac{d\Phi_1}{dx_1} \right) + \left(l_1 - \frac{r_1}{r_2} l_2 \right) \frac{d\Phi_2}{dx_1} - \frac{q_1}{\theta_1 + \theta_2 \tau_{21}} \left(\frac{d\theta_1}{dx_1} + \tau_{21} \frac{d\theta_2}{dx_1} \right) \right. \\ \left. + q_1 \frac{d\theta_2}{dx_1} \left(\frac{\tau_{21}}{\theta_1 + \theta_2 \tau_{21}} - \frac{\tau_{12}}{\theta_2 + \theta_1 \tau_{12}} \right) + \theta_2 q_1 \left[\frac{\tau_{12}}{(\theta_2 + \theta_1 \tau_{12})^2} \left(\frac{d\theta_2}{dx_1} + \tau_{12} \frac{d\theta_1}{dx_1} \right) - \frac{\tau_{21}}{(\theta_1 + \theta_2 \tau_{21})^2} \left(\frac{d\theta_1}{dx_1} + \tau_{21} \frac{d\theta_2}{dx_1} \right) \right] \right\},$$

$$\left(\frac{\partial \gamma_2}{\partial x_1} \right)_T = \gamma_2 \left\{ \frac{1}{\Phi_2} \frac{d\Phi_2}{dx_1} + \frac{1}{x_2} + \frac{z}{2} q_2 \left(\frac{1}{\theta_2} \frac{d\theta_2}{dx_1} - \frac{1}{\Phi_2} \frac{d\Phi_2}{dx_1} \right) + \left(l_2 - \frac{r_2}{r_1} l_1 \right) \frac{d\Phi_1}{dx_1} - \frac{q_2}{\theta_2 + \theta_1 \tau_{12}} \left(\frac{d\theta_2}{dx_1} + \tau_{12} \frac{d\theta_1}{dx_1} \right) \right. \\ \left. + q_2 \frac{d\theta_1}{dx_1} \left(\frac{\tau_{12}}{\theta_2 + \theta_1 \tau_{12}} - \frac{\tau_{21}}{\theta_1 + \theta_2 \tau_{21}} \right) + \theta_1 q_2 \left[\frac{\tau_{21}}{(\theta_1 + \theta_2 \tau_{21})^2} \left(\frac{d\theta_1}{dx_1} + \tau_{21} \frac{d\theta_2}{dx_1} \right) - \frac{\tau_{12}}{(\theta_2 + \theta_1 \tau_{12})^2} \left(\frac{d\theta_2}{dx_1} + \tau_{12} \frac{d\theta_1}{dx_1} \right) \right] \right\},$$

$$\text{where } \frac{d\Phi_1}{dx_1} = \frac{r_1 r_2}{(x_1 r_1 + x_2 r_2)^2}, \quad \frac{d\Phi_2}{dx_1} = -\frac{r_1 r_2}{(x_1 r_1 + x_2 r_2)^2}, \quad \frac{d\theta_1}{dx_1} = \frac{q_1 q_2}{(x_1 q_1 + x_2 q_2)^2}, \quad \frac{d\theta_2}{dx_1} = -\frac{q_1 q_2}{(x_1 q_1 + x_2 q_2)^2}$$

γ_1^∞ and γ_2^∞

$$\ln \gamma_1^\infty = \ln \frac{r_1}{r_2} + \frac{z}{2} q_1 \ln \frac{r_2 q_1}{r_1 q_2} + \left(l_1 - \frac{r_1}{r_2} l_2 \right) - q_1 \ln \tau_{21} + q_1 (1 - \tau_{12}), \quad \ln \gamma_2^\infty = \ln \frac{r_2}{r_1} + \frac{z}{2} q_2 \ln \frac{r_1 q_2}{r_2 q_1} + \left(l_2 - \frac{r_2}{r_1} l_1 \right) - q_2 \ln \tau_{12} + q_2 (1 - \tau_{21})$$



The screenshot shows the COSMO-RS Manual website. The header features the SCM logo, the text "Scientific Computing & Modelling", and the tagline "Quality Software. Quantum Science". A navigation bar includes links for Home, Products, Try & Buy, Downloads, Documentation, Support, News, About SCM, and Contact. A search bar is located on the left, and a dropdown menu for "Contents ADF COSMO-RS Manual" is visible. The main content area displays the "ADF COSMO-RS Manual" title and a search box. A sidebar on the left lists various sections: Overview, ADF, ADF-GUI, BAND, BAND-GUI, COSMO-RS (selected), References, Installation, Release Notes, Basis Sets, Multiplet Energies, Publications, Theses, Old Versions, and Developer. The main content area lists the Table of Contents, including Introduction, COSMO-RS (Theory, Combinatorial term, Temperature dependent hydrogen bond interaction, Calculation of properties), COSMO result files (ADF COSMO calculation, Accuracy), The COSMO-RS program (Running the COSMO-RS program, COSMO-RS parameters, Compounds, Temperature, Pressure, Properties, Analysis), COSMO-RS command line utilities, and References.

Antoine Eq. & Reidel Eq.

