

การพัฒนาระบบฐานข้อมูลสำหรับการค้นหาและประมาณค่าสมบัติของแก๊สและของเหลว

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วิทยานิพนธ์เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิศวกรรมศาสตรมหาบัณฑิต

ภาควิชาวิศวกรรมเคมี

บัณฑิตวิทยาลัย จุฬาลงกรณ์มหาวิทยาลัย

พ.ศ. 2539

ISBN 974 - 633 - 921 - 4

ลิขสิทธิ์ของบัณฑิตวิทยาลัย จุฬาลงกรณ์มหาวิทยาลัย

I17069701

DEVELOPMENT OF A DATABASE SYSTEM FOR SEARCHING AND
ESTIMATING PROPERTIES OF GASES AND LIQUIDS

Mr. Thanit Swasdisevi

A Thesis Submitted in Partial Fulfillment of the Requirements

for the Degree of Master of Engineering

Department of Chemical Engineering

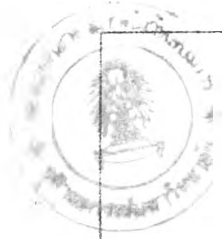
Graduate School

Chulalongkorn University

1996

ISBN 974 - 633 - 921 - 4

พิมพ์ต้นฉบับบทคัดย่อวิทยานิพนธ์ภายในกรอบสี่เหลี่ยมนี้เพียงแผ่นเดียว



ชนิด สวัสดิ์เสวี : การพัฒนาระบบฐานข้อมูลสำหรับการค้นหาและประมาณค่าสมบัติของแก๊ส
และของเหลว (DEVELOPMENT OF A DATABASE SYSTEM FOR SEARCHING AND
ESTIMATING PROPERTIES OF GASES AND LIQUIDS) อ.ที่ปรึกษา : ดร. ธวัชชัย ชรินพาณิชกุล,
182 หน้า, ISBN 974 - 633 - 921 - 4

จุดประสงค์ของงานวิจัยนี้คือการพัฒนาฐานข้อมูลสำหรับการค้นหาและประมาณค่าสมบัติของแก๊ส
และของเหลว โปรแกรมนี้สามารถทำงานได้บนวินโดวส์ที่ใช้กับเครื่องคอมพิวเตอร์ส่วนบุคคล โปรแกรมประกอบด้วย
สารจำนวน 150 สารในฐานข้อมูล แบบจำลองฐานข้อมูลแบบรีเลชันนอล(relational database model) ถูกนำมาใช้เพื่อเก็บ
ข้อมูลเพราะโครงสร้างของแบบจำลองไม่ซับซ้อนและเข้าถึงฐานข้อมูลได้ง่าย โปรแกรมออกแบบมาสำหรับเชื่อมโยงกับ
โปรแกรมอื่นที่พัฒนาขึ้นมาด้วยภาษาซีพลัสพลัส(C++ language) หลักการโปรแกรมแบบเน้นวัตถุถูกนำมาใช้กับ
โปรแกรมดังนั้นโปรแกรมจึงสามารถเชื่อมโยงกับโปรแกรมอื่นได้ง่าย สมการของซอฟว์-เรดลิก-ควอง(Soave-Redlich-
Kwong equation) และ สมการของเพ็ง-โรบินสัน(Peng-Robinson equation) นำมาใช้เพื่อทำนายสมบัติของแก๊สและ
ของเหลวเพราะสมการเหล่านี้สามารถใช้ได้ในสภาวะที่กว้าง

ผลการทำนายเมื่อนำไปเปรียบเทียบกับผลจาก ไฮซิม(HYSIM) และ ข้อมูลอ้างอิง(reference data) แสดงให้เห็น
ว่า โปรแกรมสามารถทำนายสมบัติของสารได้อย่างถูกต้อง เปรอร์เซ็นต์ส่วนเบี่ยงเบนเป็นดังนี้ ความดันไอมีส่วนเบี่ยงเบน
น้อยกว่า 2 เปรอร์เซ็นต์ ความร้อนของการระเหยมีส่วนเบี่ยงเบนน้อยกว่า 7 เปรอร์เซ็นต์ คอมเพรสซิบิลิตีแฟกเตอร์
(compressibility factor) มีส่วนเบี่ยงเบนน้อยกว่า 10 เปรอร์เซ็นต์ ปริมาตรต่อโมลมีส่วนเบี่ยงเบนน้อยกว่า 10 เปรอร์เซ็นต์
การเปลี่ยนแปลงของเอนทัลปี(enthalpy changes) และการเปลี่ยนแปลงของเอนโทรปี(entropy changes) มีส่วนเบี่ยงเบน
น้อยกว่า 5 เปรอร์เซ็นต์ สัมประสิทธิ์ฟูกาซิตี(fugacity coefficient) มีส่วนเบี่ยงเบนน้อยกว่า 4.5 เปรอร์เซ็นต์ สมดุลระหว่าง
ไอและของเหลว มีส่วนเบี่ยงเบนน้อยกว่า 5 เปรอร์เซ็นต์ ความหนืดของของเหลว มีส่วนเบี่ยงเบนน้อยกว่า 8 เปรอร์เซ็นต์

ภาควิชา วิศวกรรมเคมี
สาขาวิชา วิศวกรรมเคมี
ปีการศึกษา 2538

ลายมือชื่อนิติ
ลายมือชื่ออาจารย์ที่ปรึกษา
ลายมือชื่ออาจารย์ที่ปรึกษาร่วม

C617029 : MAJOR CHEMICAL ENGINEERING

KEY WORD: PROPERTIES OF GASES AND LIQUIDS/ DATABASE SYSTEM

THANIT SWASDISEVI : DEVELOPMENT OF A DATABASE SYSTEM FOR SEARCHING AND ESTIMATING PROPERTIES OF GASES AND LIQUIDS

THESIS ADVISOR : TAWATCHAI CHARINPANITKUL, Dr. Eng. 182 pp.

ISBN 974 - 633 - 921 - 4

The objective of this research is to develop a database system for searching and estimating properties of gases and liquids. A program can be run on Windows platform used with a personal computer. The program contains 150 compounds in its database. Relational database model is used to store data because the structure of this model is not complicated but easy to access. The program is designed for linking to other programs which are developed in the C++ language. The concept of object-oriented programming is used in the program; therefore it can be linked with other programs easily. Soave-Redlich-Kwong and Peng-Robinson equations are used to predict the properties of gases and liquids because these equations can be used within a wide range of condition.

The results of prediction compared with those from HYSIM and reference data show that the program is able to predict the properties of gases and liquids accurately. Percent deviation is as follows: the deviation of vapor pressure is less than $\pm 2\%$, the deviation of heat of vaporization less than $\pm 7\%$, the deviation of compressibility factor less than $\pm 10\%$, the deviation of molar volume less than $\pm 10\%$, the deviation of enthalpy changes and entropy changes less than $\pm 5\%$, the deviation of fugacity coefficient less than $\pm 4.5\%$. the deviation of vapor-liquid equilibria less than $\pm 5\%$, the deviation of liquid viscosity less than $\pm 8\%$.

ภาควิชา.....วิศวกรรมเคมี.....

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ลายมือชื่ออาจารย์ที่ปรึกษาร่วม.....

ACKNOWLEDGMENTS

The author would like to express his gratitude to Dr. Tawatchai Charinpanitkul, his advisor, for his greatest guidance, valuable help, suggestions and supervision during this study. He is also grateful to Professor Piyasan Prasertdam, Dr. Deacha Chatsiriwech, Dr. Somprasong Srichai for serving as chairman and members of the thesis evaluating committee, respectively.

Finally, the author would like to give his greatest thanks to his colleagues for their continuous support and encouragement throughout this study.

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NOMENCLATURE

- A = Helmholtz energy (j/mol)
- C_p = heat capacity (j/(mol K))
- DBMS = database management system (-)
- G = Gibbs free energy (j/mol)
- H = enthalpy (j/mol)
- H⁰-H = enthalpy departure (j/mol)
- K = equilibrium constant (-)
- k = interaction parameter
- L = moles of liquid (mole)
- P = pressure (bar)
- P_{ant} = vapor pressure estimated by Antoine equation
- P_{wag} = vapor pressure estimated by Wagner equation
- P_{exp} = reference values of vapor pressure
- P_d = dew point pressure (bar)
- P_b = bubble point pressure (bar)
- P_c = critical pressure (K)
- P_{vp} = vapor pressure (bar)
- R = universal gas constant (bar cm³/(mol K))
- S = entropy (j/mol K)
- S⁰-S = entropy departure (j/mol)
- T = temperature (K)
- T_c = critical temperature (K)
- T_r = reduced temperature (K)
- T_{min} = minimum temperature (K)
- T_{max} = maximum temperature (K)
- u = constant of cubic equation (-)
- V = molar volume (cm³/mol)
- V_c = critical volume (cm³/mol)

w = constant of cubic equation (-)

x = mole fractions of liquid (-)

y = mole fractions of vapor (-)

Z = compressibility factor (-)

z = mole fractions of feed (-)

Symbols

f = fugacity (bar)

Δ_{wag} = Percent deviation of vapor pressure estimated by Wagner equation between T_{min} and T_{max} (%)

Δ_{ant} = Percent deviation of vapor pressure estimated by Antoine equation between T_{min} and T_{max} (%)

Δ_{owag} = Percent deviation of vapor pressure all through range of temperature estimated by Wagner equation (%)

Δ_{oant} = Percent deviation of vapor pressure all through range of temperature estimated by Antoine equation (%)

$\Delta H_{exp.}$ = heat of vaporization of reference data (j/mol)

H_{vR} = heat of vaporization calculated by Riedel method (j/mol)

H_{vC} = heat of vaporization calculated by Chen method (j/mol)

H_{vV} = heat of vaporization calculated by Vetere method (j/mol)

H_{vP} = heat of vaporization calculated by Pitzer method (j/mol)

ϕ = fugacity coefficient (-)

ω = acentric factor (-)

γ = activity coefficient (-)

% Riedel = Percent deviation of heat of vaporization calculated by Riedel method compared with reference data (%)

% Vetere = Percent deviation of heat of vaporization calculated by Vetere method compared with reference data (%)

% Chen = Percent deviation of heat of vaporization calculated by Chen method compared with reference data (%)

% Pitzer = Percent deviation of heat of vaporization calculated by Pitzer method compared with reference data (%)

Subscript

i = component

ij = binary component

k = number of component

P = pressure

T = temperature

Superscript

V = vapor phase

L = liquid phase

id = ideal state

- = partial property

o = reference state

sat = saturated condition