

**PREDICTION OF ASPHALTENE MOLECULAR WEIGHT FROM
ASPHALTENE SOLUBILITY IN TOLUENE/HEPTANE SYSTEM**

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ABSTRACT

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Asphaltenes are defined as n-alkane insoluble and are the heaviest portion in crude oil. Asphaltene precipitation from crude oil during production, transportation, and the processing processes can cause serious problems in the petroleum industry. Because of the lack of information about asphaltenes, the complicated asphaltene reactions such as asphaltene dissolution and precipitation are poor. Molecular weight is one of the most important properties because it can be related to the other thermodynamic properties. Moreover, it can be used as the property for constructing the structure of asphaltene. In this study, the solubilities of Cold Lake reservoir asphaltene in binary solvents of toluene-heptane were used to predict asphaltene molecular weights. The solubilities obtained from both non-agitated and agitated systems were virtually the same after the equilibrium was reached. Single and three component solubility parameter models were developed from Scatchard-Hildebrand and Hansen solubility theory in order to predict the molecular weights. The results showed that the molecular weight of Cold Lake asphaltene were in the range of 850 to 1020 Daltons for the single component and 978-2009 for the three-component model. Furthermore, the different polarity fractions of Cold Lake asphaltene were examined. The higher polar fractions had higher molecular weight. Possible asphaltene structures could be predicted from these predicted molecular weights and elemental analysis data.

บทคัดย่อ

ตรีณัฐ สายทอง: การศึกษาการละลายและมวลโมเลกุลของอัสฟัลทีน (Asphaltene Solubility and Molecular Weight) อ. ที่ปรึกษา: ศาสตราจารย์ เอช สก๊อต ฟอกเลอร์, รองศาสตราจารย์ สุเมธ ชวเดจ 60 หน้า ISBN 974-17-2312-1

อัสฟัลทีนเป็นองค์ประกอบน้ำมันดิบหนึ่งที่ถูกแบ่งแยกโดยใช้คุณสมบัติการละลาย อัสฟัลทีนสามารถสกัดออกจากน้ำมันดิบโดยใช้สารประกอบจำพวกแอลเคน ปัญหาที่เกิดจากอัสฟัลทีนตกตะกอนและอุดตันในบ่อน้ำมันเป็นปัญหาที่สำคัญที่จะต้องได้รับการแก้ไข แต่เนื่องจากการขาดข้อมูล ความรู้ ความเข้าใจในคุณสมบัติพื้นฐานของอัสฟัลทีนเป็นผลให้ไม่สามารถเข้าใจและอธิบายปรากฏการณ์ที่ซับซ้อน เช่น การละลายของอัสฟัลทีนได้ งานวิจัยนี้จึงมีจุดมุ่งหมายที่จะศึกษาคุณสมบัติพื้นฐานของอัสฟัลทีน คือ มวลโมเลกุล โดยใช้ข้อมูลจากการละลายของอัสฟัลทีนในตัวทำละลายผสมของเฮกเซนและโทลูอีน และแบบจำลองที่ใช้ในการคำนวณค่ามวลโมเลกุลของอัสฟัลทีนมี 2 ชุด คือ แบบจำลองแบบหนึ่งพารามิเตอร์ และแบบจำลองแบบสามพารามิเตอร์ ซึ่งถูกพัฒนามาจากทฤษฎีของฮิลคิبران และแฮนเซน ตามลำดับ จากผลการศึกษาแสดงว่า ค่ามวลโมเลกุลของอัสฟัลทีนอยู่ในช่วง 850-1020 เมื่อใช้แบบจำลองแบบหนึ่งพารามิเตอร์ และ 978-2009 สำหรับแบบจำลองแบบสามพารามิเตอร์ นอกจากนี้ค่ามวลโมเลกุลของอัสฟัลทีนที่มีความเป็นขั้วสูงจะมีค่าสูงกว่าค่ามวลโมเลกุลของอัสฟัลทีนที่มีความเป็นขั้วต่ำ ซึ่งค่ามวลโมเลกุลของอัสฟัลทีนที่ได้นี้อาจเป็นประโยชน์ในการหาโครงสร้างที่เป็นไปได้ของอัสฟัลทีนเมื่อนำมาประกอบกับข้อมูลที่ได้จากการวิเคราะห์องค์ประกอบของอัสฟัลทีน

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LIST OF SYMBOLS

A	Heat of vaporization per unit mass (kJ/g) or Slope of a plot of the heat of vaporization as a function of the molecular weight of aromatic hydrocarbons series
b	A weighting factor, with a recommend value of 0.25
$C_{A,s}$	Solubility of asphaltenes in solvent mixture (g/dm ³)
K	Equilibrium ratio ($K = X_S / X_L$)
E_{coh}	Cohesion energy
$F_{d,i}$	Molar attraction constant (J ^{0.5} *cm ³ /mol)
MW	Molecular weight of asphaltenes (g/mol)
R	Gas constant (J/mol.K)
T	Temperature (K)
ΔU^{vap}	The internal energy of vaporization (kJ/mol)
v^l	Liquid phase molar volume of asphaltenes (m ³ /mol)
v_m	Liquid phase molar volume of solvent mixture (m ³ /mol)
V_m	The liquid phase molar volume (m ³ /mol)
X_L	Liquid mole fraction of asphaltenes
X_S	Solid mole fraction of asphaltenes
δ	The solubility parameter (MPa ^{0.5})
δ_l	Solubility parameter of asphaltenes (MPa ^{0.5})
δ_m	Solubility parameter of solvent mixture (MPa ^{0.5})
δ_t	The total solubility parameter or Hildebrand solubility parameter (MPa ^{0.5})
δ_d	The dispersion solubility parameter (MPa ^{0.5})
δ_p	The polar solubility parameter (MPa ^{0.5})
δ_h	The hydrogen bonding solubility parameter (MPa ^{0.5})
ρ	The density of asphaltenes (kg/m ³)

w	Weight fraction of asphaltene in toluene solution
ϕ_T	Volume fraction of precipitant ($V_T / (V_S + V_T)$)
ϕ_S	Volume fraction of solvent ($V_S / (V_S + V_T)$)
V_T	Precipitant volume at the onset point of asphaltene precipitation
V_S	Solvent volume at the onset point of asphaltene precipitation