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MODELING OF RESOLE TYPE PHENOLIC RESIN FORMATION

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พิมพ์ต้นฉบับบทคัดย่อวิทยานิพนธ์ภายในกรอบสี่เหลี่ยมนี้เพียงแผ่นเดียว

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พัฒนาแบบจำลองทางจลนพลศาสตร์เพื่อทำนายปฏิกิริยาการเกิดฟีนอลิกเรซินชนิดรีโซล โดยใช้โซเดียมไฮดรอกไซด์เป็นตัวเร่งปฏิกิริยาในเครื่องปฏิกรณ์แบบแบทช์ (Batch reactor) แบบจำลองที่เสนอ (Proposed model) พัฒนาโดยการลดรูปสมการสมดุลไอออนของแต่ละองค์ประกอบจากแบบจำลองของ Zavitsas และเพิ่มสมการการคำนวณความเข้มข้นของน้ำเริ่มต้นในระบบ เปรียบเทียบแบบจำลองดังกล่าวกับแบบจำลองแบบง่าย (Simple model) ซึ่งเป็นแบบจำลองการเกิดรีโซลโดยไม่คำนึงถึงสมดุลต่างๆ ในระบบ และแบบจำลองของ Zavitsas (Zavitsas' model) ซึ่งคำนึงถึงสมดุลของฟีนเตไอออน (Phenate ion) และสมดุลของฟอร์มัลดีไฮด์ในระบบ ทำการประมาณค่าพารามิเตอร์ในแบบจำลองทั้งสามด้วยวิธีซิมเพล็กซ์ (Simplex method) โดยเปรียบเทียบข้อมูลจากการทดลองในวารสารในช่วงอุณหภูมิ 30 ถึง 90 องศาเซลเซียส และความเข้มข้นของฟีนอลเริ่มต้นในช่วง 0.5 ถึง 5.375 โมลต่อลิตร ผลการเปรียบเทียบพบว่า แบบจำลองที่เสนอให้การคำนวณที่สอดคล้องกับการทดลองมากที่สุด และค่าคงที่ปฏิกิริยาที่ความเข้มข้นสูงมีค่ามากกว่าที่ความเข้มข้นต่ำเนื่องจากอิทธิพลของปริมาณตัวทำละลายที่มีต่อค่าคงที่ปฏิกิริยา จากนั้น หากความสัมพันธ์ระหว่างค่าคงที่ปฏิกิริยากับความเข้มข้นของน้ำเริ่มต้นในระบบ โดยในการศึกษาใช้ความสัมพันธ์ 2 ความสัมพันธ์ในการเปรียบเทียบได้แก่ ความสัมพันธ์เชิงเส้นตรง (Linear relationship) และ ความสัมพันธ์ของ Born (Born's relationship) ผลการศึกษา พบว่าแบบจำลองที่เสนอและความสัมพันธ์เชิงเส้นตรงระหว่างค่าคงที่ปฏิกิริยากับความเข้มข้นของน้ำเริ่มต้นในระบบสามารถทำนายปฏิกิริยาการเกิดรีโซลได้ใกล้เคียงข้อมูลจากการทดลองในวารสารได้ดีที่สุด



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A kinetic model was developed to predict the behavior of resole type phenolic resin formation under NaOH-catalyzed condition in batch reactor. The proposed model was developed by reducing the ionization equilibrium equation for each component of Zavitsas' model and adding an equation for calculating initial water concentration. The proposed model was compared with two models : a simple model in which equilibrium was not considered in the system and Zavitsas' model where phenate ion and formaldehyde equilibrium were included. Parameters in these three models were estimated and compared with experimental data from literatures in the range of 30 to 90 °C and initial phenol concentration of 0.5 to 5.375 mole/l by Simplex method. The proposed model was found to be in best agreement in comparing with the experimental data. Rate constants in concentrated systems were found to be higher than those in dilute systems due to the influence of solvent quantity on rate constants. Two relationships between rate constant and initial water concentration were studied : linear relationship and Born's relationship. The results show that the proposed model with the linear relationship of rate constants and initial water concentration was the best model to predict resole resin formation.



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ลายมือชื่ออาจารย์ที่ปรึกษา..... *สุวิธาม อัครกวีเอก*

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