

การสร้างแบบจำลองทางคณิตศาสตร์ของปฏิกริยาออกซิเดชัน
ของก๊าซซัลเฟอร์ไดออกไซด์ในพลูมโดยใช้วิธีมอนติคาร์โล



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Modeling of Sulfur Dioxide Oxidation in Plume
Using the Monte Carlo Method

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มุกิตา ตวีวิทยากุมิ : การสร้างแบบจำลองทางคณิตศาสตร์ของปฏิกิริยาออกซิเดชันของก๊าซซัลเฟอร์ไดออกไซด์ในพวยมโดย

ใช้วิธีมอนติคาร์โล (MODELING OF SULFUR DIOXIDE OXIDATION IN PLUME USING THE MONTE CARLO METHOD)

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การวิจัยนี้ประกอบด้วยการสร้างแบบจำลองทางคณิตศาสตร์ของปฏิกิริยาออกซิเดชันของก๊าซซัลเฟอร์ไดออกไซด์ในพวยมโดย
ใช้วิธีมอนติคาร์โลสำหรับแหล่งกำเนิดแบบจุดและลักษณะภูมิประเทศเป็นที่ราบ แบบจำลองทางคณิตศาสตร์แบบกายภาพและเคมีนี้สามารถ
ประมวลผลการแพร่กระจายแบบเกาส์เซียนและการเปลี่ยนแปลงทางปฏิกิริยาเคมีของก๊าซซัลเฟอร์ไดออกไซด์ ปฏิกิริยาเคมีของ Brimblecombe
และ Spedding (1974) ปฏิกิริยาเคมีของ Freiberg (1974) ในสภาพแวดล้อมที่มีแอมโมเนียมาก และ แอมโมเนียจำกัด และ ปฏิกิริยาเคมีของ
Ibusuki, Ohsawa และ Takeuchi (1990) ในสภาพแวดล้อมที่มีแอมโมเนียมาก ทั้ง 3 ปฏิกิริยานี้เป็นปฏิกิริยาที่ใช้ในการศึกษาวิเคราะห์
ความไวทางปฏิกิริยาเคมีด้วยแบบจำลองทางคณิตศาสตร์ โดยทำการแปรเปลี่ยนตัวแปรต่าง ๆ ดังนี้ คือ ความเสถียรของบรรยากาศ
ความชื้นสัมพัทธ์ อุณหภูมิ ความเข้มข้นของเหล็ก และ แอมโมเนีย ในการศึกษาความเข้มข้นของซัลเฟตที่วัดได้ในอากาศบริเวณบางนา
ถูกเปรียบเทียบกับความเข้มข้นของซัลเฟตที่ประมวลผลได้จากปฏิกิริยาเคมีของ Freiberg (1974) และ Alkezweeny และ Powell (1977) ด้วย

ผลการศึกษาของการเกิดซัลเฟตของปฏิกิริยาเคมีทั้ง 3 แบบ พบว่า ปฏิกิริยาเคมีของ Freiberg (1974)
ทั้งในสภาพแวดล้อมที่มีแอมโมเนียมาก และ แอมโมเนียจำกัด มีซัลเฟตเกิดขึ้นที่ความชื้นสัมพัทธ์สูง แต่ปฏิกิริยาเคมีของ Brimblecombe และ
Spedding (1974) และ ปฏิกิริยาเคมีของ Ibusuki et al. (1990) ในสภาพแวดล้อมที่มีแอมโมเนียมาก กลับพบว่า มีการเกิดซัลเฟตได้น้อยมาก
ในทุกสถานการณ์

ผลการวิเคราะห์ความไวทางปฏิกิริยาเคมีของปฏิกิริยาเคมีแบบ Freiberg (1974) ในสภาพแวดล้อมที่มีแอมโมเนียมาก และ
แอมโมเนียจำกัด พบว่า อัตราการเกิดซัลเฟตจะเพิ่มขึ้น เมื่อความชื้นสัมพัทธ์ ความเข้มข้นของเหล็ก และ แอมโมเนียเพิ่มขึ้น และ
เมื่ออุณหภูมิลดลง ในสภาพแวดล้อมที่มีแอมโมเนียมาก และ แอมโมเนียจำกัด จะพบว่า ปริมาณซัลเฟตจะเกิดขึ้นในกรณีแรกมากกว่า
ในกรณีที่สองสำหรับที่เงื่อนไขเดียวกัน ในการทดลองแปรเปลี่ยนความเสถียรของบรรยากาศ พบว่า ปริมาณซัลเฟตที่เกิดขึ้นมีค่าต่ำมากในความ
เสถียรของบรรยากาศแบบไม่เสถียร และ แบบสะเทิน ในทางกลับกัน ปริมาณซัลเฟตที่เกิดขึ้นมีค่าสูงมากในความเสถียรของบรรยากาศ
แบบเสถียรเนื่องจากเป็นปฏิกิริยาเคมีแบบอันดับที่สอง

ปริมาณซัลเฟตต่อซัลเฟอร์ไดออกไซด์ที่วัดได้ที่จุดตรวจวัดบริเวณบางนา และ ที่ความเร็วลมเท่ากับ 2 เมตร ต่อ วินาที
เปรียบเทียบกับปริมาณซัลเฟตต่อซัลเฟอร์ไดออกไซด์ที่ได้จากปฏิกิริยาเคมีของ Freiberg (1974) ให้ข้อสรุปว่า ปฏิกิริยาเคมีของ Freiberg (1974)
อาจมีความสำคัญในการออกซิไดซ์ซัลเฟอร์ไดออกไซด์ให้กลายเป็นซัลเฟต หากในสภาวะแวดล้อมมีปัจจัย เช่น ความชื้นสัมพัทธ์ ความเข้มข้น
ของแอมโมเนีย และ เหล็กที่สูง และ อุณหภูมิที่ต่ำ



ภาควิชา วิศวกรรมสิ่งแวดล้อม

สาขาวิชา วิศวกรรมสุขาภิบาล

ปีการศึกษา 2537.....

ลายมือชื่อนักศึกษา มุกิตา ตวีวิทยากุมิ

ลายมือชื่ออาจารย์ที่ปรึกษา

ลายมือชื่ออาจารย์ที่ปรึกษาร่วม

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KEY WORD: SULFUR DIOXIDE OXIDATION / MATHEMATICAL MODEL / MONTE CARLO

MUTITA TRIWITTAYAPOOM : MODELING OF SULFUR DIOXIDE OXIDATION IN PLUME USING THE MONTE CARLO METHOD. THESIS ADVISOR : SANGSANT PANICH, Ph.D. 167 pp. ISBN 974-584-825-5

This research succeeds in modeling of sulfur dioxide oxidation in plume using the Monte Carlo method for a single point source and flat terrain. The physico-chemical mathematical model is capable of simulating the Gaussian dispersions and chemical transformations of sulfur dioxide. The mathematical model was also used to assess sensitivity analysis of Brimblecombe and Spedding (1974)'s reaction rate, Freiberg (1974)'s reaction rate in ammonia-rich environment and in ammonia-deficient environment and Ibusuki, Ohsawa and Takeuchi (1990)'s reaction rate in ammonia-rich environment, which effects sulfate formation by varying parameters such as atmospheric stability class, relative humidity, temperature, iron and ammonia concentrations. In this study, the measured sulfate concentration in Bang Na was compared with the simulated sulfate concentrations calculated from Freiberg (1974)'s reaction rate and Alkezweeny and Powell (1977)'s first order reaction rate.

In comparison with yields of three chemical reactions, it is found that no yield occurs for Brimblecombe and Spedding (1974)'s reaction rate. Only at relative humidity of 99%, Freiberg (1974)'s reaction rate in both of ammonia-rich environment and ammonia-deficient environment plays a significant role in sulfate formation for every atmospheric stability class, temperature, iron concentration or ammonia concentration variations. Ibusuki et al. (1990)'s reaction rate in ammonia-rich environment does not cause significant yield for each atmospheric stability class, nor as a result of the temperature decrease or the relative humidity increase or the ammonia concentration increase or iron concentration increase.

The results of sensitivity analysis of Freiberg (1974)'s reaction rate in ammonia-rich environment and in ammonia-deficient environment indicate that the sulfate formation increases with increasing relative humidity, iron and ammonia concentrations and with decreasing temperature. Between ammonia-rich environment and ammonia-deficient environment, the yield in the first condition is much more than that in the latter condition for the same given condition. In the cases of varying atmospheric stability class, the sulfate production is very low in the unstable and neutral atmospheric stabilities, vice versa, the conversion of sulfur dioxide to sulfate is very high in the stable atmosphere due to the nature of second order reaction rate.

The measured yield during the dry season at the location of Bang Na with wind velocity of 2 m/s and Freiberg (1974)'s yields in some cases provide the comparable yields, which indicate that Freiberg (1974)'s reaction rate may become important if relative humidity, ammonia and iron concentrations are high with low temperature in the environment.

ภาควิชา..... วิศวกรรมสิ่งแวดล้อม..... ลายมือชื่อนิสิต..... มุทิตา ทวีวิทิตายปoom.....
สาขาวิชา..... วิศวกรรมสุขาภิบาล..... ลายมือชื่ออาจารย์ที่ปรึกษา.....
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Nomenclature

C	concentration of the non-gaseous pollutant	(g/m ³)
d	stack diameter	(m)
g	gravitational acceleration	(m/s ²)
Δh	plume rise	(m)
H	effective height	(m)
K _d	diffusion coefficient	(m ² /s)
K _n	dissociation constant of ammonia	(mole/m ³)
K _o	rate constant of the reaction	(m ³ /mole-min)
K _s	first dissociation constant of sulfurous acid	(mole/m ³)
K _w	dissociation constant of water	(mole/m ³) ²
K _x	diffusion coefficient in x direction	(m ² /s)
K _y	diffusion coefficient in y direction	(m ² /s)
K _z	diffusion coefficient in z direction	(m ² /s)
m	m th order with respect to oxidizing agent or inert substance or catalyst concentration	(-)
n	n th order with respect to sulfur dioxide concentration	(-)
P	probability of sulfur dioxide to sulfate transformation of each sulfur dioxide quantum	(-)
P1	probability of sulfur dioxide to sulfate transformation of the first sulfur dioxide quantum	(-)
P2	probability of sulfur dioxide to sulfate transformation of the second sulfur dioxide quantum	(-)

Nomenclature (Continued)

P_{total}	probability of sulfur dioxide to sulfate transformation of the both sulfur dioxide quanta	(-)
Q	sulfur dioxide emission rate	(g/s)
RH	relative humidity	(-)
t	time	(s or min)
T	temperature	(°C)
T_a	absolute temperature of ambient atmosphere	(K)
T_s	absolute flue gas exit temperature	(K)
\bar{u}	average wind velocity	(m/s)
V_s	stack gas exit velocity	(m/s)
x	distance downwind from the source	(m)
y	distance horizontally from the plume center line	(m)
z	distance vertically from the plume center line	(m)
β_n	Ostwald's constant for ammonia	(-)
β_s	Ostwald's constant for sulfur dioxide	(-)
λ_z	pressure-lowering coefficient for ammonium sulfate	(m ³ /mole)
σ_y	horizontal dispersion coefficient	(m)
σ_z	vertical dispersion coefficient	(m)
[]	molar concentration of the component	(mole/m ³)
subscript [] _o	initial condition	(-)
subscript [] _{react}	reacting condition	(-)
subscript [] _{remaining}	remaining condition	(-)
subscript () _{acc}	accumulation condition	(-)

Nomenclature (Continued)

subscript () _{in}	input condition	(-)
subscript () _{out}	output condition	(-)