



Mass transfer and reaction kinetics of sulfuryl fluoride absorption with aqueous sodium hydroxide solutions^{*}

Yong NIE^{†1}, Xiao-jiang LIANG¹, Mei-zhen LU¹, Feng-wen YU¹, Da-yong GU², Min MIN³, Jian-bing JI¹

⁽¹⁾College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, China)

⁽²⁾Shenzhen International Travel Health Care Center, Shenzhen 518033, China)

⁽³⁾Center for Biorefining and Department of Bioproducts and Biosystems Engineering, University of Minnesota, Saint Paul, MN 55108, USA)

[†]E-mail: ny_zjut@zjut.edu.cn

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Abstract: The mass transfer and reaction kinetics of sulfuryl fluoride (SO₂F₂) absorption with aqueous sodium hydroxide (NaOH) solutions were studied in an experimental double-stirred cell. Results showed that SO₂F₂ absorption with NaOH was followed by a reaction model employing a fast pseudo-first-order. The second-order rate constant for SO₂F₂ absorption with aqueous NaOH solutions was determined to be 1.44 m³/(mol·s) at 298 K. Three models were used in this chemical absorption process, and in each case, the same expression of enhancement factor was obtained. A comparison was made between the experimental enhancement factor and the value calculated from the model, and the maximum relative deviation was less than 4.2%. The proposed model expression gave a reasonable fit with the experimental values, indicating that mass transfer correlations are valid for scaling up design.

Key words: Sulfuryl fluoride, Sodium hydroxide, Mass transfer, Reaction kinetics, Absorption, Double-stirred cell
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1 Introduction

Sulfuryl fluoride (SO₂F₂) was commercially introduced as a fumigant beginning in 1961 (Tsai, 2010). As a gaseous fumigant, SO₂F₂ has been widely used for pest control in buildings, construction materials, and agricultural related products, such as soil, timber, and food (Derrick *et al.*, 1990; Athanassiou *et al.*, 2012; Chayaprasert *et al.*, 2012; Cao *et al.*, 2014), owing to its strong dispersivity in different materials and nearly no residues left after treatment (Meikle and Stewart, 1962).

With the wide application of SO₂F₂ in fumiga-

tion, its greenhouse effect and toxicity were gradually recognized and became the focus of attention. SO₂F₂ is a strong greenhouse gas with global warming potential of 4780 (relative to CO₂ for the 100 year time horizon), and the concentration of SO₂F₂ in the global atmosphere has been increasing 5% each year since 1978 (Papadimitriou *et al.*, 2008; Mühle *et al.*, 2009). In addition, SO₂F₂ gas was marked as an inhalation hazardous material, and long term exposure can cause damage to a human's central nervous system and inhalation system, etc. (Tsai, 2010). However, SO₂F₂, after fumigation, is released directly into the atmosphere at present. Therefore, it is increasingly important to find a reasonable way to remove SO₂F₂ effectively after fumigation.

To achieve this result, our research group previously developed a two-step method based on dielectric barrier discharge (DBD) plasma followed with a chemical absorption, in which the results showed

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that SO_2F_2 could be removed efficiently using this two-step method (Nie *et al.*, 2013a); however, high energy consumption of the DBD plasma process limits its future industrial applications.

Recently, a new approach of using chemical absorption alone for the removal of SO_2F_2 has been developed (Nie *et al.*, 2013b). SO_2F_2 is nearly insoluble in water in neutral conditions; however, SO_2F_2 can be rapidly hydrolyzed in aqueous alkaline media due to the fact that nucleophilic hydroxyl ions will attack the S atom and replace one of the F ions (Cady and Misra, 1974). Therefore, using aqueous NaOH solution as the absorbent could enhance the absorption rates of SO_2F_2 in comparison with using only water.

The present work involves an investigation of mass transfer and reaction kinetics in the absorption of gaseous SO_2F_2 with aqueous NaOH solution in an experimental double-stirred cell, including a zone of mass transfer and reaction kinetics, enhancement factor, etc. The results can provide the theory base for the industrial design of a chemical absorber to remove SO_2F_2 after fumigation.

2 Materials and methods

2.1 Materials

Sulfuryl fluoride (99.9%) in a cylinder was obtained from the Hangzhou Maoyu Electronic Chemicals Co., Ltd., China. Air in a cylinder was obtained from the Hangzhou Jingong Specialty Gases Co., Ltd., China. Sodium hydroxide (96%) and potassium biphthalate (99.9%) were obtained from the Sinopharm Chemical Reagent Co., Ltd., China.

2.2 Apparatus and procedure

The experimental setup is illustrated in Fig. 1, in which the SO_2F_2 absorption was conducted in an experimental double-stirred cell. The detailed description of the double-stirred cell used for the absorption measurements is available elsewhere (Shi and Zhong, 2005; Zhang *et al.*, 2007). The cell has a water jacket through which water from a constant temperature bath is circulated to maintain the desired temperature of 298 K. The stirred cell is a glass cylinder with an 8.0 cm inner diameter and a length of 15.5 cm, which is equipped with four vertical baffles

and two stirring blades. The stirring blades are driven by a separate DC motor in the gas and liquid phases.

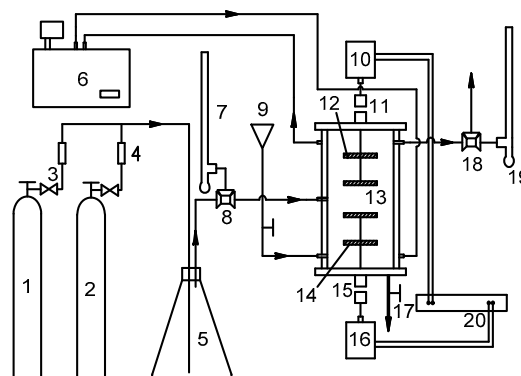


Fig. 1 Experimental apparatus for SO_2F_2 absorption in an experimental double-stirred cell

1: SO_2F_2 ; 2: air cylinder; 3: gas control valve; 4: flow meter; 5: buffer; 6: water bath; 7, 19: soap-film meter; 8, 18: three-way cock; 9: entrance of liquid; 10, 16: DC motor; 11, 15: magnetic force gearing; 12, 14: stirring blade; 13: absorber; 17: liquid control valve; 20: stirrer-speed controller

A mixture of SO_2F_2 and air with a SO_2F_2 concentration ranging from 0.2% to 0.5% in volume was fed into the stirred cell at a fixed gas flow rate of 100 ml/min. Gaseous SO_2F_2 was absorbed by the aqueous NaOH solution in the cell. The NaOH solution was prepared by adding the solid NaOH to distilled water to obtain the desired NaOH concentration, calibrating with a potassium biphthalate solution. Most of the experiments were performed with an aqueous NaOH solution volume V_L of 200 ml.

The inlet and outlet gas concentrations of SO_2F_2 for the cell were analyzed by a gas chromatography (GC) equipped with a Gaspro plot column and a flame photometric detector (7890A, Agilent Technologies, USA). The sensitivity of the GC for SO_2F_2 analysis was 5×10^{-7} in volume. The experimental absorption rate N_A can be calculated from

$$N_A = G(C_{\text{Gin}} - C_{\text{Gout}})/A, \quad (1)$$

where C_{Gin} and C_{Gout} are the inlet and outlet gas concentrations of the cell, respectively; A is the effective interfacial area of the cell, which is influenced slightly by the stirring with a constant gas-liquid interface of 0.00264 m^2 ; and G is the total gas flow rate.

All of the experiments for SO₂F₂ absorption were carried out at atmospheric pressure.

2.3 Physical properties of the NaOH-SO₂F₂ system

The liquid and gas phase diffusivities of SO₂F₂ can be predicted from the model developed by Wilke and Chang (1955) and Wilke and Lee (1955), respectively. The solubility of SO₂F₂ in the water (H) can be calculated (Derrick *et al.*, 1990; Tsai, 2010). In addition, the liquid phase diffusivity of NaOH is obtained from Tan *et al.* (1990). Some of the parameters for the NaOH-SO₂F₂ system are listed as follows: the temperature is 298 K; the molecular diffusivity for SO₂F₂ in the air and water ($D_{\text{SO}_2\text{F}_2\text{-air}}$ and $D_{\text{SO}_2\text{F}_2\text{-water}}$) are 1.24×10^{-5} m²/s and 1.19×10^{-9} m²/s, respectively; the molecular diffusivity for NaOH in the water ($D_{\text{NaOH-water}}$) is 3.09×10^{-9} m²/s; and H is 7.27×10^{-5} mol/(L·kPa).

2.4 Mass transfer coefficients

The gas-side and liquid-side mass transfer coefficients in the cell, k_{GA} and k_{LA}^0 (where the superscript 0 represents without chemical reaction and the subscript A represents SO₂F₂), are calculated from the empirical correlations of Shi *et al.* (1996) as follows:

$$k_{\text{LCO}_2}^0 = 1.635 \times 10^{-6} n_{\text{L}}^{0.56}, \quad (2)$$

$$k_{\text{GSO}_2} = 5.878 \times 10^{-8} n_{\text{G}}^{0.70}, \quad (3)$$

$$k_{\text{LA}}^0 = k_{\text{LCO}_2}^0 (D_{\text{A}} / D_{\text{CO}_2})^{2/3}, \quad (4)$$

$$k_{\text{GA}} = k_{\text{GSO}_2} (D_{\text{A}} / D_{\text{SO}_2})^{2/3}, \quad (5)$$

where $k_{\text{LCO}_2}^0$ is the liquid-side mass transfer coefficient for carbon dioxide (CO₂) without chemical reaction at 298 K, k_{GSO_2} is the gas-side mass transfer coefficient for sulfur dioxide (SO₂) at 298 K, n_{L} is the liquid phase stirrer speed, n_{G} is the gas phase stirrer speed, D_{A} , D_{CO_2} , and D_{SO_2} are the molecular diffusivities for SO₂F₂, CO₂, and SO₂, respectively.

In this study, the value of k_{GA} for SO₂F₂ is 3.157×10^{-6} kmol/(m²·s·kPa) at 300 r/min and 298 K, and k_{LA}^0 is 1.918×10^{-5} m/s at 150 r/min and 298 K.

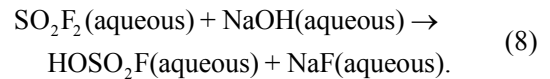
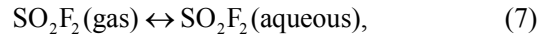
2.5 Interfacial concentration of SO₂F₂ in liquid phase

The interfacial concentration of SO₂F₂ in the liquid phase C_{Ai} is a key factor affecting the reaction kinetics for the absorption of SO₂F₂ in the liquid phase. At a low SO₂F₂ concentration, C_{Ai} can be estimated using Henry's law. In the experimental double-stirred cell, the complete mixing coefficients for the gas and liquid phases were all close to 1 with a liquid stirring speed of 150 r/min and a gas stirring speed of 300 r/min (Gu, 1986). Thus, the partial pressure P_{A0} (where the subscript 0 represents without chemical reaction) of the bulk gas stream at the outlet of the cell was used to calculate the interfacial concentration of SO₂F₂ as follows:

$$C_{\text{Ai}} = H(P_{\text{A0}} - N_{\text{A}} / k_{\text{GA}}). \quad (6)$$

2.6 Absorption process of SO₂F₂ into the aqueous NaOH solution

The absorption process of SO₂F₂ into the aqueous NaOH solution consists of the following two steps:



3 Results and discussion

3.1 Determination of the mass transfer and the reaction kinetics zone

To study the chemical absorption process, the zone of the mass transfer and reaction kinetics should be determined firstly. Generally, the kinetics zones are classified based on the magnitude of the reaction rate, and kinetics zones are mainly used to indicate the influences of the chemical reaction on the process of gas-liquid mass transfer and reaction. Table 1 shows how to determine the kinetics zone, according to the effect of factors influencing absorption and reaction on each kinetics zone using the film theory (Tan *et al.*, 1990).

Table 1 Factors influencing the gas-liquid absorption and reaction

Parameter instruction	Zone of mass transfer and reaction kinetics							
	A	B	C	D	E	F	G	H
Concentration of reactant NaOH in bulk of liquid, C_{BL}	+	-	+	+	?	?	+	+
Intensity of pressure of SO_2F_2 in bulk of gas, P	+	+	+	+	?	?	+	+
Interfacial areas, A	+	+	+	+	+	+	+	-
Liquid volume, V_L	-	-	-	-	+	+	+	+
Liquid-side mass-transfer coefficient, k_L	+	-	+	-	?	?	+	-
Gas-side mass-transfer coefficient, k_G	+	+	+	+	?	?	+	-
Second-order rate constant, k_2	-	-	+	+	?	?	+	+

A: instantaneous reaction; B: instantaneous reaction in diffusion film; C: fast reaction; D: fast pseudo- m th-order reaction; E: moderately fast reaction; F: moderately fast pseudo- m th-order reaction; G: slow reaction in bulk liquid; H: very slow reaction in bulk liquid; '+': effected by factor; '-': not effected by factor; '?': may be effected by factor, but the rate equation will not be changed

Based on the above method, the zone determining experiments for the absorption of SO_2F_2 into aqueous NaOH solutions were designed as shown in Table 2. The basic conditions of the experiments are as follows: $T=298$ K, $P_{in}=0.5$ kPa (the inlet partial pressure of SO_2F_2 , equivalent to a regular SO_2F_2 application rate of 20 g/ m^3 used in container fumigation), $n_G=300$ r/min, $n_L=150$ r/min, $V_L=200$ ml, and $C_{BL}=47.8$ mmol/L (bulk concentration, where the subscript B represents NaOH). In our testing, the bulk concentration C_{BL} of NaOH was much higher than the interfacial concentration of SO_2F_2 in the liquid phase C_{Ai} . Thus, the bulk concentration of NaOH was considered to be a constant during the absorption process of SO_2F_2 .

Table 2 Determination of zone of mass transfer and reaction kinetics

Parameter	Absorption rate ($\times 10^{-5}$ mol/($m^2 \cdot s$))
$V_L=150$ ml	1.04
$V_L=200$ ml	1.08
$n_L=150$ r/min	1.08
$n_L=100$ r/min	1.05
$C_{BL}=47.8$ mmol/L	1.08
$C_{BL}=57.4$ mmol/L	1.25
$C_{BL}=66.9$ mmol/L	1.36

As can be seen from Table 2, firstly, the variation of liquid volume V_L has a slight effect on the absorption rate of SO_2F_2 , according to Table 1, the zones of E to H can be excluded. Secondly, the liquid-side mass transfer coefficient can be changed by changing the liquid stirring speed, the variation of

liquid stirring speed n_L has an insignificant effect on the absorption rate of SO_2F_2 (Table 2); therefore, the zones of A and C in Table 1 can be excluded. Thirdly, the variation of concentration of the reactant NaOH in bulk of liquid C_{BL} has a great effect on the absorption rate of SO_2F_2 , according to Table 1; therefore, the zone of B can be excluded. Thus, the kinetics zone for the absorption of gaseous SO_2F_2 with NaOH solution belongs to D, a fast pseudo- m th-order reaction.

3.2 Determination of fast pseudo-first-order reaction and second-order rate constant k_2

Based on the Dankwerts theory (Dankwerts, 1970), the absorption rate for a fast pseudo- m th-order reaction is given by

$$N_A = \sqrt{2k_{m+1}D_A C_{Ai}^{m+1} C_{BL} / (m+1)}, \quad (9)$$

where m is the reaction order.

A plot of N_A versus C_{Ai} can give the reaction order m for SO_2F_2 . Fig. 2 shows the effect of the bulk concentration of NaOH on the SO_2F_2 absorption rate as a function of the interfacial concentration of SO_2F_2 in the liquid phase. There was a linear relationship between the SO_2F_2 absorption rate N_A and the interfacial concentration of SO_2F_2 in the liquid phase C_{Ai} . Thus, the results confirmed that the hydrolysis reaction for SO_2F_2 was a fast pseudo-first-order reaction ($m=1$). In addition, as illustrated in Fig. 2, the SO_2F_2 absorption rate N_A had a positive relationship with both C_{Ai} and C_{BL} .

To determine the forward second-order rate constant k_2 for the hydrolysis reaction of SO_2F_2 , the

mass transfer model described in Eq. (9) was used. The values for the second-order rate constant can be derived from Fig. 2, and the average value of the rate constant k_2 calculated at 298 K was $1.44 \text{ m}^3/(\text{mol}\cdot\text{s})$. Cady and Misra (1974) found that the rate constant k_2 for the hydrolysis reaction of SO_2F_2 was $0.418 \text{ m}^3/(\text{mol}\cdot\text{s})$, which is smaller than that in this study. The possible reason for this phenomenon is the difference of the measuring method. In our case, the overall dynamic processes of SO_2F_2 absorption and the subsequent hydrolysis reaction were taken into account. However, in the experiments of Cady and Misra (1974), the process of SO_2F_2 absorption was not considered, and the hydrolysis reaction of SO_2F_2 was restricted in the liquid solution, in which SO_2F_2 was dissolved in advance; therefore, maybe some of the SO_2F_2 evaporated from the solution during the hydrolysis reaction, and resulted in the deviation for the determination of the forward second-order rate constant k_2 .

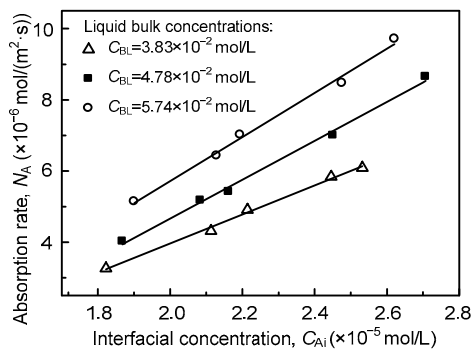


Fig. 2 Effect of the bulk concentration of NaOH on the SO_2F_2 absorption rate as a function of the interfacial concentration of SO_2F_2 in the liquid phase

3.3 Enhancement factor E

The enhancement factor E determines the mass transfer rate for a chemical absorption process, which is very important for the industrial absorber design. In this section, the comparison between the experimental value and the model value for the enhancement factor is conducted.

Generally, the experimental value of the enhancement factor for a fast reaction can be obtained by

$$N_A = Ek_{LA}^0 C_{Ai}, \quad (10)$$

where N_A , k_{LA}^0 , and C_{Ai} are experimental values, as shown in Fig. 3. The experimental value of the enhancement factor increases with the increase of the bulk concentration C_{BL} of NaOH.

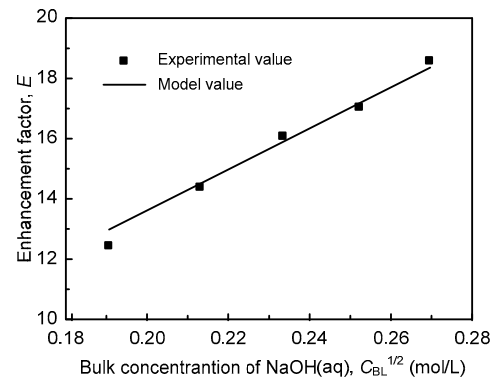


Fig. 3 Comparison of experimental and model values for the enhancement factor

For the aim of modeling the enhancement factor of a fast pseudo-first-order reaction, three widely used mass transfer models based on the film, penetration, and surface renewal theories, respectively, are applied to predict the enhancement factor here as follows (Tan *et al.*, 1990):

$$\text{Film theory model: } E = Ha / \tanh Ha, \quad (11)$$

$$\text{Penetration theory model: } E = Ha + \pi / (8Ha), \quad (12)$$

$$\text{Surface renewal theory model: } E = \sqrt{1 + Ha^2}, \quad (13)$$

where Ha is the dimensionless Hatta number, defined as follows:

$$Ha = \sqrt{k_2 D_A / (k_{LA}^0)^2 C_{BL}^{1/2}}. \quad (14)$$

In terms of the above three models, when $Ha > 3$, the mathematical expression of the enhancement factor could be the same equation as follows (Dankwerts, 1970):

$$E = Ha = \sqrt{k_2 D_A / (k_{LA}^0)^2 C_{BL}^{1/2}}. \quad (15)$$

According to the above experimental value of the enhancement factor, Eq. (15) could be used as the model expression of the enhancement factor, and the

corresponding mathematical expression in this study is

$$E = 68.08C_{BL}^{1/2}. \quad (16)$$

The corresponding model values are also shown in Fig. 3. The proposed model expression based on the three mass transfer models gives a reasonable fit with the experimental values: the average relative deviation is 1.7%, and the maximum relative deviation is 4.2%.

3.4 Validation of the fast pseudo-first-order reaction

For a bimolecular-second-order reaction, the universal non-steady-state model for the enhancement factor can be expressed by (Tan *et al.*, 1990)

$$E = \frac{Ha\sqrt{1-(E-1)/(rS)}}{\tanh\left[Ha\sqrt{1-(E-1)/(rS)}\right]}, \quad (17)$$

where r represents the ratio of the diffusion coefficients in the liquid phase, and S represents the ratio of the stoichiometric concentrations in the liquid phase. These two dimensionless parameters are given by

$$r = D_B/D_A, \quad (18)$$

$$S = C_{BL}/(bC_{Ai}), \quad b=1, \quad (19)$$

where D_B is the molecular diffusivity for NaOH, and b is the stoichiometric number.

In terms of a second-order reaction, the condition to be regarded as a pseudo-first-order reaction is that: $r^{1/2}S/Ha \geq 10$. Table 3 shows the calculating results based on the experimental data depicted in Fig. 3, and the experiments were performed with P_{in} of 0.36 kPa for the inlet gas stream (equivalent to a SO_2F_2 application rate of 14.4 g/m³).

Table 3 Validation of fast pseudo-first-order reaction

C_{BL} (mol/L)	C_{Ai} (mol/L)	S	Ha	$r^{1/2}S/Ha$
3.89×10^{-2}	2.470×10^{-5}	1575	13.4	189
4.94×10^{-2}	2.370×10^{-5}	2084	15.1	222
5.74×10^{-2}	2.363×10^{-5}	2429	16.3	240
7.03×10^{-2}	2.347×10^{-5}	2995	18.1	267
7.64×10^{-2}	2.330×10^{-5}	3279	18.8	281

As can be seen from Table 3, the condition of $r^{1/2}S/Ha \geq 10$ is satisfied for our test cases. Hence, the results confirmed that the absorption of SO_2F_2 into aqueous NaOH solutions is a fast pseudo-first-order reaction.

4 Conclusions

The mass transfer and reaction kinetics of the absorption of SO_2F_2 with aqueous NaOH solutions were studied in an experimental double-stirred cell. Conclusions can be drawn as follows.

1. SO_2F_2 absorption with NaOH was a fast pseudo-first-order reaction. The second-order rate constant was determined from experimental results and found to be 1.44 m³/(mol·s) at 298 K.

2. Three widely used mass transfer models based on the film, penetration, and surface renewal theories, respectively, were applied in this mass transfer with a chemical reaction process, and the same expression of enhancement factors was obtained. A comparison was made between the experimental enhancement factor and the data calculated from the models, and the maximum relative deviation was less than 4.2%.

Associated with the developed model for the enhancement factor E , mass transfer coefficients, and material balance in the scrubber, the number of the theoretical plate in the scrubber could be calculated accurately, which is the critical index used to determine the performance and effectiveness of the scrubber. Furthermore, the scaling up study for the removal of SO_2F_2 in a rotating zigzag high gravity bed could be carried out to set up mobile equipment.

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中文概要:

本文题目: 氢氧化钠溶液吸收硫酰氟的传质反应动力学

Mass transfer and reaction kinetics of sulfuryl fluoride absorption with aqueous sodium hydroxide solutions

研究目的: 确定氢氧化钠溶液化学吸收硫酰氟的传质反应动力学区域, 建立增强因子模型。

研究方法: 研究气液传质测定设备双搅拌釜中氢氧化钠溶液化学吸收硫酰氟的过程, 并结合实验研究与理论分析建立了增强因子模型。

重要结论: 基于氢氧化钠溶液化学吸收硫酰氟过程的实验研究, 确定了氢氧化钠溶液化学吸收硫酰氟的传质反应动力学区域为快速拟一级反应。得到了 298 K 下其二级反应速率常数为 1.44 m³/(mol·s), 并建立了增强因子模型 $E=68.08C_{BL}^{1/2}$, 为脱除熏蒸后残留硫酰氟的工业化应用提供了理论依据。

关键词组: 硫酰氟; 氢氧化钠; 传质; 反应动力学; 化学吸收; 双搅拌釜