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Kinetic Modeling of the Reaction of HCl and Solid Lime at Low Temperatures

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Calcium hydroxide is a commonly used sorbent in the dry-scrubbing of hydrogen chloride from flue gases. In this study the kinetic parameters for the reaction between gaseous HCl and solid Ca(OH)_2 have been obtained at low temperatures in a fixed-bed laboratory reactor. The influence of the operating temperature (323–400 K), HCl concentration (150–1000 ppm), and humidity (0–11% M) was studied. The experimental results show that in the first few seconds a very fast chemical reaction occurs, with a reaction rate constant per unit surface area of solid larger than 10^{-3} ms^{-1} . This reaction was found to be first order relative to HCl concentration and its mechanism is apparently independent of the presence of moisture. However, the relative humidity of the gas has a major impact on the progress of the reaction: when no moisture is present the reaction stops after a short period of time (2–3 min), with very low maximum solid reactant conversions (<5%). For the experiments with humidified gas an almost complete conversion of Ca(OH)_2 was obtained after about 40 min of reaction time. For this case the grain model with product layer diffusion limitations is in very good agreement with the experimental results. The diffusion coefficient in the product layer obtained through this model varied from 10^{-13} to $10^{-11} \text{ m}^2 \text{ s}^{-1}$ and the activation energy for this parameter was estimated at $\approx 19 \text{ kJ mol}^{-1}$ for the range of temperatures studied. A simple linear relationship describes well the effect of relative humidity of the gas on the diffusion coefficient in the solid product layer. In the presence of humidity, the very high conversions of the solid reactant show a good potential applicability to continuous dry-scrubbing of HCl at low temperatures.

Introduction

Hydrogen chloride emissions are formed during combustion of fossil fuels such as chlorine-rich coals and in incineration of many wastes. Recently, due to increasingly severe legal emission limits and high costs associated with traditional scrubbing processes, there has been a great effort in research to develop new processes that are both efficient and cost-effective.

Dry-scrubbing of acid gases is a relatively recent technology for the removal of toxic acidic components from gaseous effluents, whereby finely divided dry powder is injected into the flue gas stream. Calcium based sorbents are widely used due to their low cost and high sorbent capacity for removal of SO_2 , HF, and HCl. According to Weinell et al.,¹ there is a high potential for dry-scrubbing of HCl using Ca(OH)_2 at low temperatures and high humidity levels: their experimental results show almost full conversion of lime below 420 K in the presence of moisture. Also, the use of dry-scrubbing at low temperatures allows the recovery of energy from flue gases by lowering temperatures through heat recovery boilers and economizers to 400 K.² However, the literature data on the reaction of HCl with Ca(OH)_2 below 400 K is scarce.

The kinetics of the reaction



was studied by Karlsson et al.³ in the temperature range 420–670 K in a fixed-bed laboratory reactor where the solid particles of Ca(OH)_2 were dispersed in a sand layer. Their results reveal a high HCl removal efficiency but the Ca(OH)_2 conversions were lower than 40%, thus indicating a poor utilization of this reactant. These authors propose a first-order reaction relative to both reactants. Carminati et al.⁴ conducted experiments in a pilot-plant with injection of an aqueous suspension of Ca(OH)_2 in a hot flue gas containing HCl ("spray-dryer" process). Their acid removal efficiencies were higher than 75% for the lowest temperature (450 K) with feed ratios $\text{Ca(OH)}_2/\text{HCl}$ between 7 and 8 times the stoichiometric ratio. These authors suggest a complex reaction order relative to HCl, presumably higher than one. Weinell et al.¹ achieved almost complete conversions of Ca(OH)_2 in a differential fixed-bed reactor at low temperatures (330–420 K) in the presence of humidity (4–15% M). According to these authors, the reaction was governed by diffusion in the solid phase, and the high conversions observed in the presence of humidity were due to the formation of a partially liquid product phase. Recently Duo et al.⁵ suggest that the rate-limiting step for this reaction is altered with the reaction progress, changing from chemical reaction control to product layer diffusion

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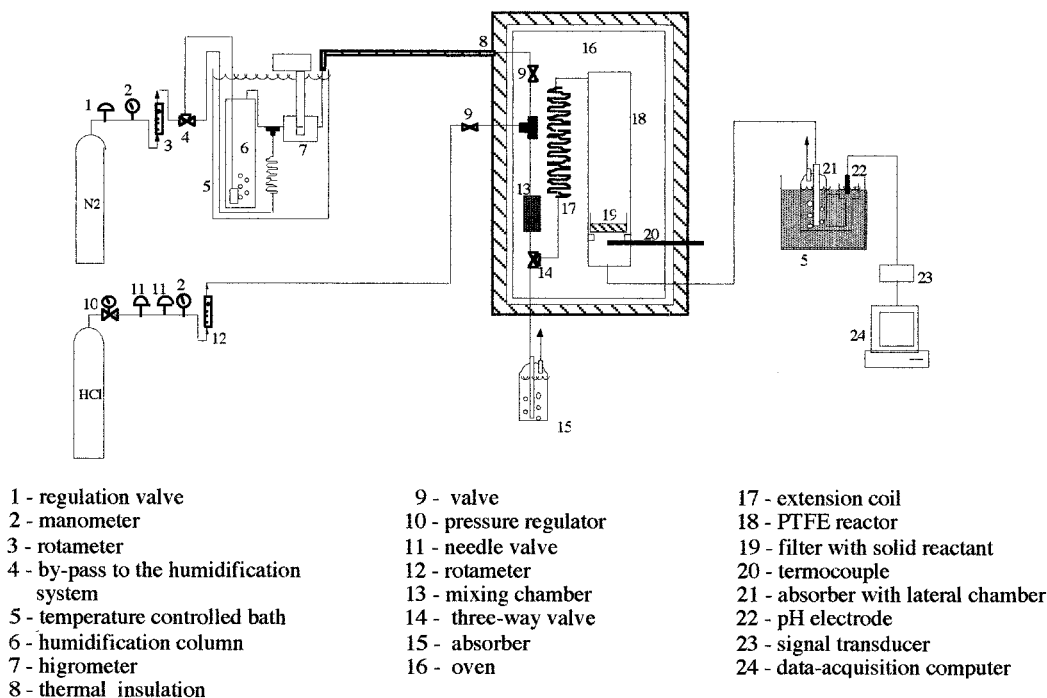


Figure 1. Schematic diagram of the experimental equipment.

control. They propose a crystallization and fracture model for the formation of the solid product. The stopping of the reaction before complete conversion of the sorbent has been experimentally observed in the case of $\text{Ca}(\text{OH})_2$ ¹ as well as for other Ca-based sorbents.^{6–9} According to Duo et al.⁵ the crystallization and fracture model may explain this phenomenon: the reaction stops when the energy required to break the crystalline structure of the product is superior to the energy released by the reaction. Jozewicz and Gullett¹⁰ investigated the nature of the solid product of this reaction in the absence of humidity and concluded that in the range 100–600 °C a solid solution of $\text{Ca}(\text{OH})_2$ and $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$ was formed.

The aim of this project is to study the dry-scrubbing of HCl at low temperatures (<400 K) and controlled humidity levels, using a continuous reactor with dry injection of $\text{Ca}(\text{OH})_2$ as sorbent. A prior step necessary for an optimized design of any continuous reactor and of the operating conditions is the determination of the kinetic parameters for this reaction. This is the main subject of the present paper.

Experimental Section

The kinetics of the reaction between HCl and solid lime was studied in a fixed-bed laboratory reactor. The parameters investigated were the temperature, HCl concentration, and humidity. A thin layer of $\text{Ca}(\text{OH})_2$ (approximately 20 mg) supported on a glass microfiber filter was placed in the reactor. A gas stream of HCl in N_2 is passed through the reactor at controlled concentration, humidity level, and temperature. The evolution of the effluent gas concentration is obtained by absorbing the HCl in water by means of an appropriate external circulation air-lift absorption vessel,¹ and the pH of the resulting solution is monitored on-line with a computerized data acquisition system. Preliminary experiments showed that practically all the HCl is retained in the absorber, even for high absorption times (45 min). The solid obtained at the end of the experi-

ment is dissolved in distilled water and chemically analyzed for chlorides by an appropriate spectrophotometric method.¹¹

The experimental apparatus is shown schematically in Figure 1. The laboratory reactor is a cylinder made of PFA, 0.3 m high and with external and internal diameters of 0.05 and 0.03 m, respectively. It is placed inside a highly precise gas chromatograph temperature controlled oven. The solid reactant layer is prepared by placing a few drops of a lime suspension in ethanol in a 0.025-m diameter GFA filter. This suspension is previously submitted to ultrasounds in order to deagglomerate the solid particles. The GFA filter with the $\text{Ca}(\text{OH})_2$ layer, once dried and weighted, is placed in a PFA basket, which is introduced in the reactor and positioned at approximately 0.05 m from its bottom, so that the inlet gas flow may stabilize before contacting with the solid reactant. A type K thermocouple placed immediately below the basket measures the temperature as closely as possible to the reaction zone. To prevent the contact of the corrosive HCl with the thermocouple, this is placed inside a glove finger made of stainless steel coated with a thin layer of PFA.

The test gas at the inlet of the reactor is made up by mixing two gaseous streams: commercial HCl type N26 with a minimum 99.6% purity (maximum H_2O content: 10 ppm) and N_2 (purity level 99.95% minimum; maximum H_2O content: 10 ppm) with a controlled humidity level. The HCl flow rate is varied with appropriate needle valves and measured by a PFA microrotameter. The N_2 stream is optionally diverted to the humidification system, which is basically a bubbling column with height and internal diameter of 0.38 and 0.05 m, respectively, filled with distilled water. The effluent gas stream temperature and humidity are measured in situ with a hygrometer (Protimeter I-220 Rotronic). The humidification column and the hygrometer are placed inside a thermostated water bath with regulated temperature according to the desired humidity level. All the tubing leading from the humidification

column to the inlet of the oven is thermally insulated to prevent any water condensation. The two gaseous streams are mixed inside the oven and homogenized in a plenum chamber made of PFA with 0.03-m internal diameter and 0.1-m height, totally filled with glass spheres of 0.006-m diameter. Before entering the reactor the gas stream is passed through an 8-m coil of PFA tubing to promote homogenizing both in temperature and composition.

The HCl concentration of the effluent gas at the outlet of the reactor is determined by absorbing it in a system similar to the one described by Weinell et al.,¹ which avoids undesirable interaction between gas bubbles and the pH electrode. The gas flows through a two-compartment external circulation air-lift absorber filled with 2.5×10^{-4} m³ of distilled water. The gas bubbles up through the main chamber of the absorber causing a rapid recirculation of the liquid due to the different densities of the solutions present in the two compartments. A pH electrode immersed in the bubble-free lateral compartment is connected to a data acquisition unit (signal transducer, A/D acquisition interface, and microcomputer) which continuously registers the pH of the homogenized solution. The absorption system is immersed in a thermostated bath which is kept at a temperature 10 °C above that of the humidification system, since at lower temperatures an aqueous phase is formed due to the occurrence of a maximum boiling point azeotrope for the system HCl/H₂O.¹²

The Solid Reactant

Calcium hydroxide *pro-analysis* (Riedel-de-Haen) was chosen to avoid any competing reaction with impurities. A scanning electron microscope (SEM) analysis revealed that practically all the solid particles are in the form of agglomerates of 30–100 μm (Figure 2a). In an attempt to destroy the agglomerates, a Ca(OH)₂ suspension in ethanol was submitted to ultrasounds during approximately 15 min. This suspension was then analyzed by SEM and it was verified (Figure 2b) that, although not complete, the deagglomeration lead to submicrometer individualized particles (0.05–1 μm).

An X-ray sedimentometry technique was used to determine the solid reactant particle size distribution. A bimodal distribution was obtained, indicating the presence of some larger particles, but with a clearly dominant contribution of the smaller particles to the total mass (Figure 3). The mean mass diameters were respectively 40 and 2 μm and the particle size distribution by weight of the smaller particles agrees with an essentially submicrometer particle distribution by number,¹³ as observed in the SEM analysis.

The pore size distribution of the solid reactant was investigated through mercury porosimetry together with the determination of the N₂ adsorption/desorption isotherms at 77 K. The results show that the agglomerates have predominantly macropores of 10^3 – 10^4 Å (Figure 4). Taking into account that the individualized particles are essentially submicrometric, we conclude that the macropores should be spaces between agglomerated particles, and thus the individualized particles are nonporous. The low specific surface area results obtained by the BET method ($S \approx 10$ m² g⁻¹) are in agreement with these conclusions. The mean radius of the individualized particles was estimated as 0.15 μm , assuming that they were spheric and taking into account the values for S and true density of Ca(OH)₂.

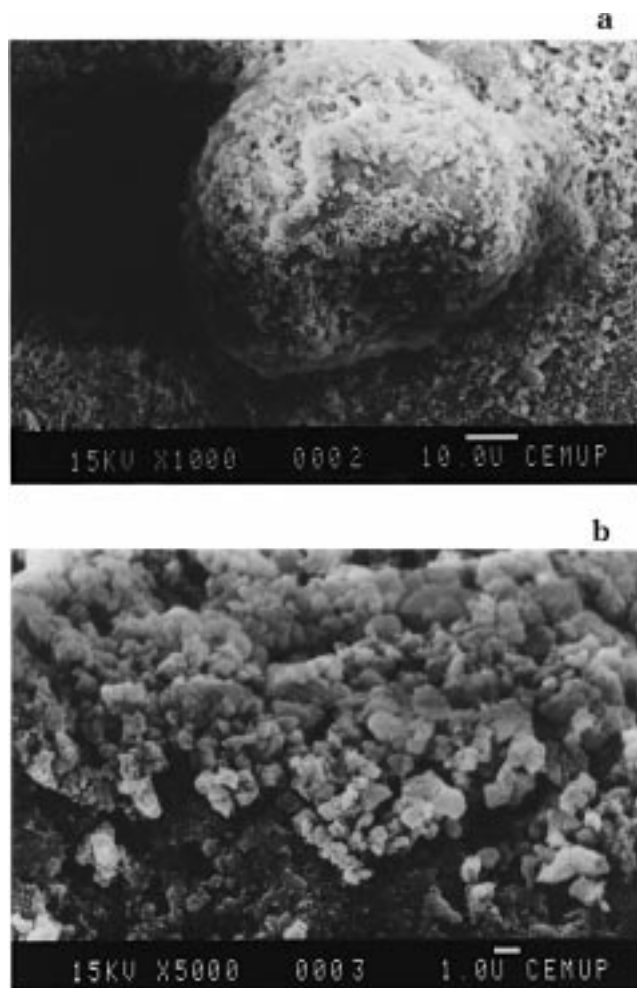


Figure 2. SEM photographs of the solid reactant particles. (a) Agglomerate. (b) Individualized particles.

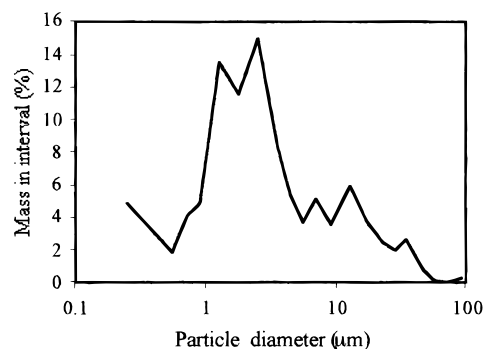


Figure 3. Size distribution for the solid reactant particles.

Again, this value is in general agreement with the SEM observations.

Experimental Results

Preliminary experiments were carried out in order to establish the operating conditions that minimize external mass transfer limitations: at the higher values of temperature and HCl concentration, the total gas flow rate was varied from 1.7×10^{-5} to 1.3×10^{-4} N m³ s⁻¹ at a fixed Q/m ratio. No significant differences were found in the experimental curves of HCl concentration at the outlet of the reactor. Therefore we concluded that in this range of flow rates the external mass diffusion resistance was negligible. The total gas flow rate used

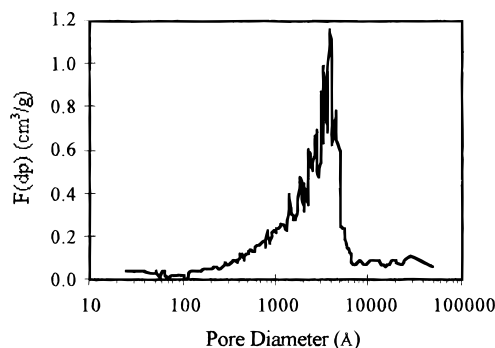


Figure 4. Pore size distribution of the solid reactant ($F(d_p) = \Delta V_p / (\Delta \log d_p)$ with d_p in Å).

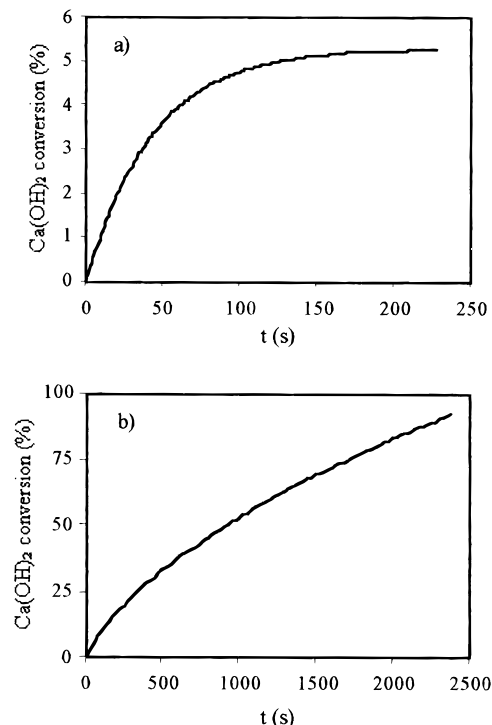


Figure 5. Typical curves for the experimental conversion of solid reactant vs time. (Operating conditions: 50 °C, 600 ppm HCl). (a) 0% H₂O; (b) 6% H₂O.

in the subsequent experiments was therefore 6.7×10^{-5} N m³ s⁻¹, close to the average value of the range tested.

The experimental results reveal two distinct periods for this reaction: during the first 10–20 s the reaction is very fast, with almost complete conversion of HCl. After this initial period, the reaction rate decreases with time, suggesting solid product diffusion limitations. However, the rate of decrease is much higher in the dry situation than in the presence of moisture. For the dry case, the reaction stops after a short period of time (2–3 min), with maximum conversions of Ca(OH)₂ of only around 5% (Figure 5a). In the presence of moisture and at lower temperatures, almost complete ($\approx 98\%$) conversions of Ca(OH)₂ have been achieved after 40 min of reaction (Figure 5b). Thus, the presence of water affects the final lime conversion values. Figure 6 shows that this influence is stronger at lower temperatures, indicating that relative humidity should be the parameter most responsible for these differences. Similar results are also described by Weinell et al.¹

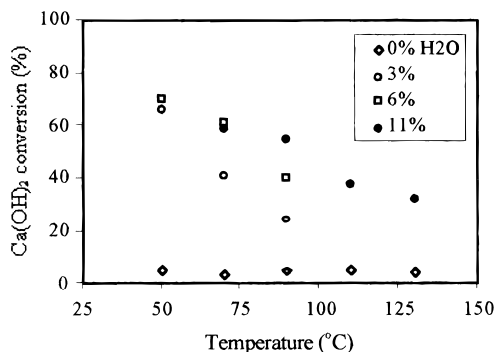


Figure 6. Influence of temperature and humidity level on the solid conversion after 20 min of reaction for 600 ppm HCl.

Kinetic Parameters

The experimental results have been modeled by the “grain model” for gas–solid reactions in porous media. This model, described in detail by Szekely et al.,¹⁴ assumes that the porous solid is made up of small nonporous grains, and each of these grains is converted according to the unreacted core model. The grain model is appropriate since the SEM observations and pore characterization reveal nonporous particles aggregated into macroporous clusters. A single n th order irreversible reaction is concerned, represented by the general form



In agreement with our previous observations, it will be assumed that the grains are spherical with uniform initial radius R_p and that the reaction proceeds without external mass transfer limitations. The effective diffusivity of HCl in the pores of the solid has been estimated,¹⁵ and, according to the Weisz-Prater criteria,¹⁶ the internal mass transfer limitations can be neglected. Thus, the only possible rate-limiting steps are chemical reaction or diffusion through the product layer, as it has been considered by other authors.^{1,5,17} In the initial or early stages of the reaction no continuous product layer has been formed, so the chemical reaction should be the rate-controlling step.⁵

Chemical Reaction Control. For chemical reaction control, assuming a reaction of order n , the time required for the conversion X of solid reactant is given by

$$t_{\text{CRC}} = \frac{1}{K_C} [1 - (1 - X)^{1/3}] \quad (1)$$

with

$$K_C = \frac{bk_s C_A^n}{\rho_B R_p} \quad (2)$$

where k_s is the reaction rate constant, ρ_B is the molar density of the solid product B, R_p is the radius of the unreacted grain, and C_A is the concentration of the gas to which the solid particles are exposed. In the present case, due to the high HCl conversions, this concentration cannot be considered uniform throughout the solid bed. A material balance over a differential slice of the solid layer gives

$$QC_A|_{z+dz} = QC_A|_z - (-r_A) dS_B \quad (3)$$

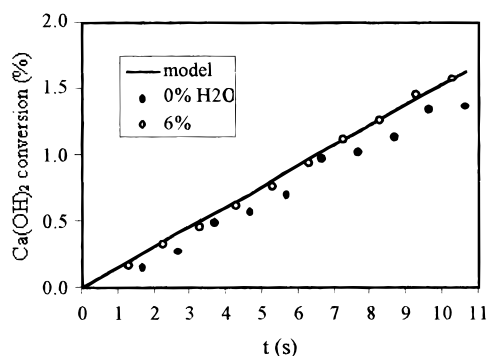


Figure 7. Experimental data for the chemical regime in experiments with and without humidity (operating conditions: 50 °C, 600 ppm HCl).

where Q is the total gas flow rate, $(-r_A)$ is the reaction rate per unit surface area of the solid, and dS_B represents the differential surface area of solid particles present in slice dz . Assuming a uniform distribution of the particles in the layer,

$$dS_B = S(m/L) dz \quad (4)$$

where m is the total mass of solid in the layer, S is the specific surface area, and L the layer depth. Thus, for chemical reaction control

$$\frac{dC_A}{C_A^n} = -\frac{k_s S}{L} \frac{m}{Q} dz \quad (5)$$

The value of C_A considered in eq 2 was the mean integrated value given by

$$\bar{C}_A = \frac{\int_0^L C_A dz}{L} \quad (6)$$

The time period of the chemical reaction control regime was estimated through statistical analysis of the parameters of linear regressions made to the initial experimental results of t vs $(1 - (1 - X)^{1/3})$ by varying the number of experimental points considered within this regime. The slope of this linear regression is the experimental value of $1/K_c$. The results obtained show that this time period is generally less than 20 s but depends on the experimental conditions. For the same temperature and HCl concentration, the experiments with moisture have a period of chemical regime 2–3 times longer than the experiments in the absence of moisture, but the experimental data points in the chemical regime are almost coincidental for these two situations (Figure 7). Therefore the chemical reaction mechanism seems to be the same for both dry and humid conditions, which indicates that the reaction does not occur in the liquid phase in the presence of moisture. Figure 7 also shows that the experimental data points in the dry case are slightly below those for the experiments with moisture. This behavior was systematically observed for other experimental conditions and might be explained by a stronger influence of the product layer diffusion limitations in the absence of water.

The reaction order and the reaction rate constants were determined by nonlinear least-squares analysis,¹⁸ by minimizing the residuals between the experimental results of K_c and those given by eq 1. The results

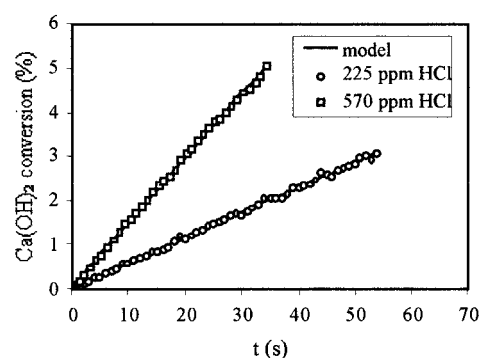


Figure 8. Experimental data and grain model for chemical reaction control (operating conditions: 50 °C, 6% H₂O).

indicate a first-order reaction, in agreement with Karlsson et al.³ but not with Carminati et al.,⁴ who have found a complex reaction order. We found that the model is not sensitive to the reaction rate constant for high values of this parameter ($k_s > 10^{-3} \text{ ms}^{-1}$). In fact, for first-order reactions the integral in eq 6 is solved giving

$$\bar{C}_A = C_{A_{in}} \frac{Q/m}{k_s S} \left\{ 1 - \exp\left(-\frac{k_s S}{Q/m}\right) \right\} \quad (7)$$

where $C_{A_{in}}$ is the inlet gas concentration. This equation together with eq 2 gives

$$K_c = \frac{bC_{A_{in}}(Q/m)}{\rho_B R_p S} \left\{ 1 - \exp\left(-\frac{k_s S}{Q/m}\right) \right\} \quad (8)$$

Equation 8 shows that the exponential term is practically equal to zero for high k_s values, and therefore K_c is insensitive to k_s . Our experimental results are well modeled by eqs 1 and 8 as can be seen in Figure 8. No experimental values of the reaction rate constant can be confidently obtained from the present data, but we can conclude that this constant is higher than 10^{-3} ms^{-1} , indicating a very fast chemical reaction.

Product Layer Diffusion Control. For product layer diffusion control with a constant diffusion coefficient D_s , the time required for a certain conversion X of solid is given by

$$t_{PLDC} = \frac{3}{K_p} \left\{ \frac{\alpha - [(1 - X)(1 - \alpha) + \alpha]^{2/3}}{\alpha - 1} - (1 - X)^{2/3} \right\} \quad (9)$$

with

$$K_p = \frac{6bD_s C_A}{\rho_B R_p^2} \quad (10)$$

where α is the volume expansion ratio (ratio between the molar volumes of the solid product and the reactant). For the present reaction $\alpha = 2.37$, where it was assumed that the reaction product is $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$.

In this regime C_A will be not only a function of the position in the solid layer but also a function of time. Assuming that C_A varies exponentially with bed depth

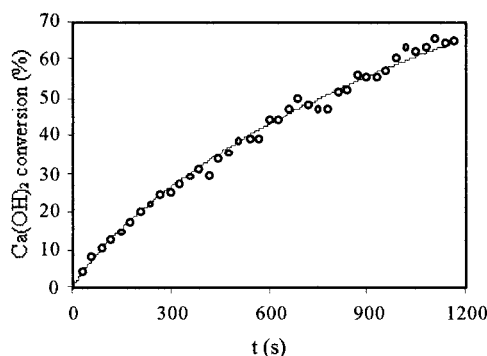


Figure 9. Experimental results and the grain model (operating conditions: 50 °C, 600 ppm HCl, 6% H₂O).

as with chemical reaction control, we have for each time t

$$\bar{C}_A = \frac{C_{A_{in}}}{C_{A_{out}}} \left(1 - \frac{C_{A_{out}}}{C_{A_{in}}} \right) \quad (11)$$

where $C_{A_{in}}$ is the inlet gas concentration (independent of t) and $C_{A_{out}}$ is the outlet gas concentration, which depends on t according to the following equation:

$$C_{A_{out}} = C_{A_{in}} - \frac{2m/M}{Q} \frac{dX}{dt} \quad (12)$$

Simultaneous Chemical Reaction and Product Layer Diffusion Control. Reactions are likely to have a combination of the limiting mechanisms at intermediate conversions. In this case the time required for a certain conversion of solid is the sum of two parcels, each corresponding to a single limiting mechanism:

$$t = t_{CRC} + t_{PLDC} \quad (13)$$

For the experiments without moisture this model cannot explain the observed behavior. The reaction stops after a very short period of time and this cannot be justified by a pore blocking phenomena due to the initial pore dimension of the agglomerates and the assumed volume expansion ratio for this system. Duo et al.⁵ proposed a crystallization and fracture model to describe the mechanism of the solid product layer formation in gas–solid reactions of Ca-compounds with HCl. According to this model, solid products are formed in clusters of molecules through crystallization and, if the volume expansion ratio is greater than 1, the product layer has to be fractured so that the reaction can proceed. Thus, the reaction stops when the energy required to fracture the crystals is greater than the chemical potential available.

In the case of the experiments with moisture this abrupt stopping of the reaction is not observed, and this might be due to the formation of an aqueous phase in the presence of moisture that breaks the crystalline structure of the solid product and enables the progress of the reaction. As can be seen in Figure 9, a very good agreement was found between the results of the experiments with moisture and the grain model given by eq 13. The diffusion coefficient in the solid product layer D_s is the only parameter in this equation set, and it was determined by nonlinear least-squares using the same optimizer as before. The diffusivities obtained are in

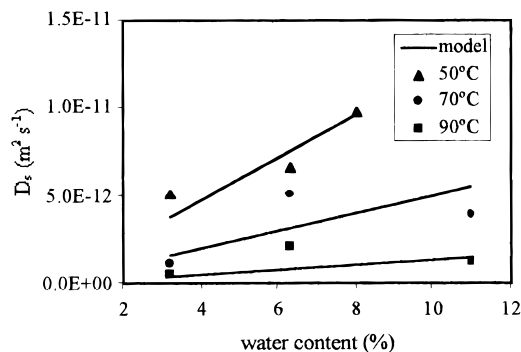


Figure 10. Adjusted D_s and the model described by eq 14.

the range 10^{-13} – 10^{-11} m² s⁻¹, as expected for gas diffusion in solids. It was found that the diffusivities for this system depend not only on the temperature but also on the relative humidity of the gas. Assuming that the dependence on temperature is of the Arrhenius type, some preliminary tests showed that the dependence on the relative humidity could be well described by a simple linear relationship. Thus, the following model was tested:

$$D_s = \exp(-E_{act}/RT) K \frac{[H_2O]}{[H_2O]_{sat}} \quad (14)$$

where $[H_2O]_{sat}$ is the concentration at saturation (mol H₂O/mol gas), which can be estimated from Antoine's equation by¹⁹

$$[H_2O]_{sat} = \frac{10^{[7.96681 - 16668.21/(228 + T)]}}{760 - 10^{[7.96681 - 16668.21/(228 + T)]}} \quad (15)$$

The residuals between the obtained values of D_s and those predicted by eq 14 were minimized to obtain the optimum values of E_{act} and K (Figure 10). The estimated value for the activation energy of 19 kJ mol⁻¹ is between the results reported by Weinell et al.¹ and Duo et al.,⁵ 10–15 and 36.5 kJ mol⁻¹, respectively.

Conclusions

The reaction of gaseous HCl with solid lime was studied in a laboratory fixed-bed reactor. The experimental results confirm the high capacity of Ca(OH)₂ to react with HCl, with almost complete gas conversion even for very low contact times. In the absence of moisture, the low conversion of the solid reactant makes the process unsuitable for dry-scrubbing at low temperatures. In the presence of moisture, very high conversions of the solid reactant can be achieved but only for long reaction times (≈ 40 min).

The reaction was found to be first order relative to HCl concentration in the range of temperatures studied. The chemical reaction mechanism seems to be independent of humidity. No experimental values of the reaction rate constant could be obtained, but there is evidence that this reaction is very fast even at temperatures as low as 320 K, with a value of $k_s > 10^{-3}$ ms⁻¹.

In the absence of moisture the progress of reaction is limited by the solid product formation, resulting in maximum solid reactant conversions of around 5% after low reaction times. This behavior might be explained by the crystallization and fracture hypothesis of Duo et al.⁵

In the presence of moisture, very good agreement was found between the experimental results and the grain model for reactions with solid product diffusion limitations. In this case the reaction does not stop, and practically complete conversion of the solid reactant was obtained. Assuming that the crystallization and fracture model of Duo et al.⁵ explains the experimental results under dry conditions, the different behavior observed in the presence of moisture might be caused by the formation of an aqueous phase which dissolves the crystals of the solid product and therefore enables the progress of the reaction. However, since there are no significative differences between the dry and wet experiments for the first moments of reaction, the hypothesis that the reaction in the presence of humidity occurs in the liquid phase is not probable.

The diffusion coefficient in the solid product was estimated by applying the grain model to the experimental results in the presence of humidity. The values obtained for the diffusivity are in the range expected for gas diffusion in solids (10^{-13} – 10^{-11} m² s⁻¹) and are dependent on temperature through an Arrhenius type equation (activation energy ≈ 19 kJ mol⁻¹) and on the relative humidity of the gas through a simple linear relation.

The results so far obtained suggest that very high removal efficiencies of HCl by dry lime injection may only be achieved in a continuous reactor with small residence times under controlled humidity and in the absence of solid product diffusion limitations. The concept of such a reactor is presently under study.

Acknowledgment

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Nomenclature

b = stoichiometric coefficient for solid reactant B
 C_A = concentration of gaseous reactant A (mol m⁻³)
 D_s = diffusion coefficient in the solid product layer (m² s⁻¹)
 E_{act} = activation energy (J mol⁻¹)
 k_s = reaction rate constant per unit surface area of the solid (ms⁻¹)
 K = parameter in eq 14 (m² s⁻¹)
 K_c = inverse of time required for complete conversion in chemical reaction control (s⁻¹)
 K_p = inverse of time required for complete conversion in product layer diffusion control for $\alpha = 1$ (s⁻¹)
 L = solid layer depth (m)
 m = mass of solid reactant (g)
 M = molar mass (g mol⁻¹)
 n = reaction order
 Q = gas flow rate (N m³ s⁻¹)
 $-r_A$ = reaction rate per unit surface area of the solid (mol m² s⁻¹)
 R = ideal gas constant (J mol⁻¹ K⁻¹)
 R_p = radius of unreacted nonporous grain (m)
 S_B = surface area (m²)
 S = specific surface area (m² g⁻¹)

t = time (s)

T = temperature (°C or K)

X = solid reactant conversion

Greek Symbols

α = volume expansion ratio

ρ = molar density (mol m⁻³)

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