

# **GAS-PHASE KINETIC MODELLING IN THE $\text{AlCl}_3\text{-CO}_2\text{-H}_2\text{-HCl}$ SYSTEM IN VIEW OF THE CHEMICAL VAPOR DEPOSITION OF $\text{Al}_2\text{O}_3$**

P. Tan\*, J. Müller, D. Neuschütz

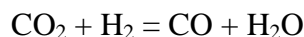
Materials Chemistry, Rheinisch-Westfälische  
Technische Hochschule Aachen,  
D-52056 Aachen, Germany  
\* now with Portovesme s.r.l., I-09010  
Portoscuso, Italy.

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 $\text{AlOCl}$  formation; water gas shift reaction

## **ABSTRACT**

For a specific set of conditions applied in experimental hot-wall reactor investigations to deposit  $\alpha\text{-Al}_2\text{O}_3$  from precursor gas mixtures containing  $\text{AlCl}_3$ , kinetic modelling of the gas-phase reactions was carried out on the basis of rate parameters collected or estimated by Catoire and Swihart.

Calculations are presented for upward flow rates of 20 and 0.41 slh through a vertical tube reactor (27 mm i.d.) with a 450 mm isothermal zone (1050 °C) and with varying concentrations of  $\text{AlCl}_3$ ,  $\text{CO}_2$ ,  $\text{H}_2$  and  $\text{HCl}$  in the feed gas. The results show that  $\text{AlCl}_3$  decomposes by reacting with  $\text{CO}_2$  and  $\text{H}_2$  to form  $\text{AlOCl}$  as the major intermediate species. The water gas shift reaction



is found to take place very slowly at short residence times, but much faster with lower gas flow-rates. The  $\text{H}_2\text{O}$  generation apparently increases with the  $\text{AlOCl}$  content in the gas phase.

The results may be helpful in understanding the complex reaction mechanisms involved in alumina CVD