

Abstract Submitted  
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**On the coverage dependence of Arrhenius parameters in thermal desorption of interacting adsorbates** NAYELI ZUNIGA-HANSEN, University of Denver, LEONARDO E. SILBERT, Southern Illinois University Carbondale, M. MERCEDES CALBI, University of Denver — In temperature programmed desorption (TPD) the “compensation effect” is a linear relationship between the activation energy,  $E_a$ , and the preexponential factor,  $\nu_n$ , of the Arrhenius equation. From the Arrhenius plot  $\ln \frac{-\dot{\theta}}{\theta}$  vs.  $\frac{1}{T}$ , we can extract the activation energy and the preexponential factor to test the validity of linearity. A linear relationship has been demonstrated to be valid *when the kinetic parameters are independent of the surface coverage*. In the presence of adsorbate-adsorbate interactions this analysis fails because the second order effects come into play. The compensation effect arises from the assumption that the second order terms in the derivative of the plot sum to zero. Some authors refer to this as a “forced” compensation effect and show that it can yield misleading results. Therefore this effect has not been completely understood. We use kinetic Monte Carlo simulations on ordered and disordered surface configurations to investigate the coverage dependence of the kinetic parameters to verify whether the compensation effect provides reliable information for our system, we do this over a range of binding and interaction energies.

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