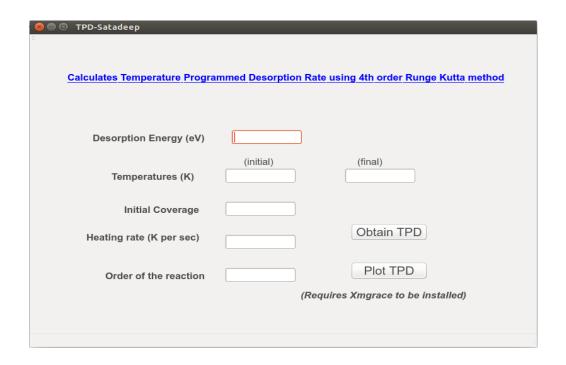# Temperature programmed desorption rate

May 23, 2018

The rate of desorption is calculated using Polanyi-Wigner equation given by

$$r_d = -\frac{d\theta}{dt} = \frac{k_0 \theta^n}{\beta} exp\left(-\frac{E_d}{K_B T}\right) \tag{1}$$

where $k_0 (= 10^{13} s^{-1})$ is the temperature-independent frequency factor, β is the heating rate, k_B is the Boltzmann factor, n is the order of the reaction, θ is the coverage and E_d is the desorption energy.

1   How to use the APP in ubuntu:

1. Download TPD.run and give permission chmod +x TPD.run

2. ./TPD.run in shell

3. It will appear as follows:

4. Fill up the boxes as shown below (for example)

TPD-Satadeep

Calculates Temperature Programmed Desorption Rate using 4th order Runge Kutta method

Desorption Energy (eV)   1.0

	(initial)	(final)
Temperatures (K)	100	1000

Initial Coverage   0.3

Hit this button

Heating rate (K per sec)   10

[Obtain TPD] ➡ Will generate the file: "Coverage.dat"

Order of the reaction   2   [Plot TPD]

(Requires Xmgrace to be installed)

Hit this button to plot the TPD in xmgrace