**References:**

1. Eren et al, Structure of Copper−Cobalt Surface Alloys in Equilibrium with Carbon Monoxide Gas, J. Am. Chem. Soc. 2018, 140, 6575−6581.

**2. E. Iglesia, Appl. Catal., A 1997, 161, 59−78.**

**The Kinetic Monte Carlo Model for Fischer-Tropsch process on Co catalyst**

1. Construct a hexagonal lattice.

2. CO – as one unit – may adsorb on a lattice site.

3. H2 – may dissociate and adsorb on two adjacent vacant sites.

4. If two adjacent H sites are nearest neighbour to CO occupied site then they will react and form H2O. H2O desorbs leaving two vacant sites (previously occupied by H atoms).

5. Simultaneously, another set of two adjacent H atoms (which are also nearest neighbour to the CO occupied site in step 4) react with C to form CH2. The reaction is also possible if only one H occupied site is adjacent to the CO occupied site in step 4. In this case only CH will be formed.

6. Adjacent CH3, CH2, CH units will be taken as a chain. If CH or CH2 occupied site is adjacent to an H occupied site, then CH2 or CH3 may be formed. Whether such reaction takes place or not depends on the valences of CHn occupied site keeping in view the overall alkane or possible alkene chain. If this reaction happens then the site which was previously occupied by H will be vacated after the reaction.

7. Adjacent CH3, CH2, CH units will be taken as a chain. Depending on the composition, and if all valences are satisfied, an alkane or alkene unit may desorb. On such desorption the sites earlier occupied by CHn type units will be vacated.

This model is based on reference 2. As per this reference pure Co surface can act as catalyst for CO + H2 reaction. The products formed in such pure Co catalysed reaction are a mixture of alkanes and alkenes.