

Turnover frequency (TOF) is defined as the maximum number of chemical conversions of substrate molecules  $N_{CH_4}$  per unit time over a single catalytic site:

$$TOF = \frac{N_{CH_4}}{N_{Ni} \cdot t}, \quad (1)$$

where  $N_{Ni}$  is number in surface nickel sites

The following transformations could be done:

$$TOF = \frac{N_{CH_4} \cdot N_A}{N_{Ni_{surf}} \cdot t \cdot N_A} = \frac{v_{CH_4}}{v_{Ni} \cdot t} = \frac{v_{CH_4} \cdot V}{v_{Ni} \cdot t \cdot V} = \frac{C_{CH_4}}{C_{Ni} \cdot t}, \quad (2)$$

where  $N_A$  is Avohadro's number  $6.02 \times 10^{23}$ ,

$v_{CH_4}$  is amount of substance of methane, mol,

$v_{Ni}$  is amount of substance of surface nickel, mol,

$V$  is volume, L,

$C_{CH_4}$  is methane concentration, mol L<sup>-1</sup>

$C_{Ni}$  is surface nickel concentration, mol L<sup>-1</sup>

Since

$$C_{Ni_{surf}} = N_{Ni} \cdot \rho_{cat}, \quad (3)$$

and

$$W_0 = \frac{C_{CH_4}}{t}, \quad (4)$$

then

$$TOF = \frac{C_{CH_4}}{N_{Ni} \cdot \rho_{cat} \cdot t}, \quad (5)$$

$$TOF = \frac{W_0}{N_{Ni} \cdot \rho_{cat}}, \quad (6)$$

where  $N_{Ni}$  is surface nickel concentration, mol g<sup>-1</sup> of catalyst

$\rho_{cat}$  is density of catalyst, g L<sup>-1</sup>

$W_{CH_4}$  is reaction rate, mol L<sup>-1</sup> s<sup>-1</sup>