

## Prova orale 1

- a) Si richiede che il candidato discuta il processo NH<sub>3</sub>-SCR per l'abbattimento di NO<sub>x</sub> in gas esausti da applicazioni veicolari su catalizzatori commerciali a base di Cu, con particolare riferimento al meccanismo catalitico del processo.
- b) Office EXCEL: Utilizzo della funzione "if" per l'azzeramento di dati negativi da una lista in Office Excel. Utilizzo delle funzioni massimo, minimo e media per l'analisi dei dati.
- c) Potassium-promoted ruthenium supported on CaO is a very efficient catalyst for ammonia decomposition, surpassing the performance of other Ru-supported solids. At an optimum Ru loading of 3% wt, catalysts with a K/Ru atomic ratio of 0.9 showed the best catalytic performance under a wide range of operating conditions, P = 1–40 bar, T = 250–550 °C and WHSV = 9000–30000 mL g<sup>-1</sup> h<sup>-1</sup>. Although NH<sub>3</sub> conversion levels decrease considerably upon increasing the reaction pressure (X550 °C, 40 bar = 0.8), high pressure ammonia decomposition offers the possibility of CO<sub>x</sub>-free compressed hydrogen and hydrogeN productivities and TOFs 40 times bigger than when applying atmospheric pressure. Extensive characterization by CO chemisorption and HR-TEM demonstrates that potassium promotion increases metal dispersion by decreasing the Ru particle size. Electronic effects derived from the close proximity between K and Ru result in a decrease in the reaction apparent activation energy, as shown by a detailed kinetic analysis.

## Prova orale 2

- a) Si richiede che il candidato discuta il processo di adsorbimento di  $\text{NO}_2$  su catalizzatori SCR commerciali a base Cu-zeolite, con particolare riferimento alla relazione tra questo processo e quello di  $\text{NH}_3$ -SCR per l'abbattimento di  $\text{NO}_x$ .
- b) Office EXCEL: regressione lineare e polinomiale di una serie di dati.
- c) An operando experimental method for monitoring relative variations in half-cycle rates of the Cu redox-cycle model of selective-catalytic-reduction (SCR) is demonstrated, along with a kinetic model for predicting the same. Conversion inflections (CI) can occur at SCR onset within Cu/SCR catalysts; transient CI involves initial conversion growth to an intermediate value greater than exists at steady state (SS) before degrading to the SS value. While similar CI has been reported for Fe/SCR catalysts as being due to  $\text{NH}_3$  inhibition, Cu/SCR CI is inconsistent with a similar origin. Rather, Cu/SCR CI is due to imbalances in the redox-half-cycle rates, and will occur when reduction is faster than oxidation. The temporal CI shape varies with the redox-cycle kinetic parameters and model formulation, and can be used to study the same. We demonstrate the first measurements of dynamic halfcycle rate balancing at SCR onset, use CI and onset transients to study variations in half-cycle rates under Standard, Fast and  $\text{NO}_2$  SCR, and present the first redox-cycle model showing CI. The new operando method and model provides a basis for better understanding the SCR redox process, and determining the individual halfcycles kinetic model formulation and parameters.