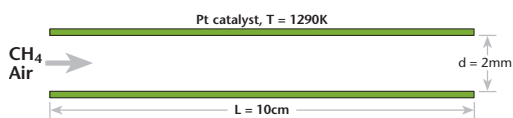


In many industrial applications, such as wafer processing by chemical vapor deposition (CVD), combustion of solids, chemical etching, and catalytic combustion, reactions occur on wall surfaces. During the last few years, detailed mechanisms for certain surface reactions, including rate constants, began appearing in the literature. Although there is a strong need to simulate such problems numerically, especially in conjunction with flow field simulations that include gas-phase reactions, the stiffness of the reaction systems and the complex mass/energy interactions between the surface species and gas phase species often make such problems difficult to solve.

The new surface reaction model in FLUENT 6.1 allows for arbitrary, complex reaction mechanisms, involving any number of gas phase and/or surface species, and reactions between different gas species, gas and surface species, and different surface species. Surface reactions are fully coupled with the flow simulation, so that the distribution (coverage) of different surface species and the deposition rate of bulk species on a wall can be tracked. In addition to dealing with reactions on actual walls, the model can also account for surface reactions on unresolved walls in a porous medium. Moreover, there is full flexibility in the problem setup – different reaction mechanisms can be defined in different fluid or porous zones.

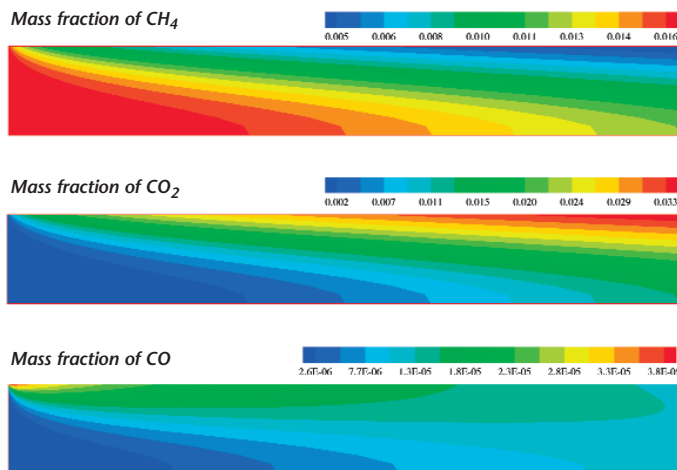
To illustrate the new capabilities in FLUENT, a tubular catalytic reactor, which represents a single pore of an actual monolithic catalyst, was simulated. The tubular reactor is 10cm long and 2mm in diameter. The inner tube surface is coated with platinum (Pt), which serves as a catalyst to initiate and/or accelerate reactions. A 22-step reaction mechanism¹ was used in the simulation. The system involves seven gas phase species (CH_4 , O_2 , H_2 , H_2O , CO , CO_2 , and N_2) and eleven site (surface) species ($\text{H}(\text{s})$, $\text{O}(\text{s})$, $\text{OH}(\text{s})$, $\text{H}_2\text{O}(\text{s})$, $\text{C}(\text{s})$, $\text{CO}(\text{s})$, $\text{CO}_2(\text{s})$, $\text{CH}_3(\text{s})$, $\text{CH}_2(\text{s})$, $\text{CH}(\text{s})$, and $\text{Pt}(\text{s})$). Both gas phase species and surface species can be depleted or created as a result of surface reactions. This causes the concentrations of gas phase species and the coverage of site species to change along the pipe. The results show that methane is oxidized quickly after it enters the pipe, and that CO and CO_2 are produced. Changes in site species coverage include increases in $\text{H}_2\text{O}(\text{s})$, $\text{H}(\text{s})$, and $\text{OH}(\text{s})$, and decreases in $\text{CO}_2(\text{s})$ and $\text{C}(\text{s})$. The coverage of some surface species, such as platinum and oxygen, remains relatively constant. Due to the effective numerical algorithm in FLUENT for reaction simulations such as this, convergence of this example was rapid and well-behaved. ■



Schematic of the problem, with the diameter greatly exaggerated

reference

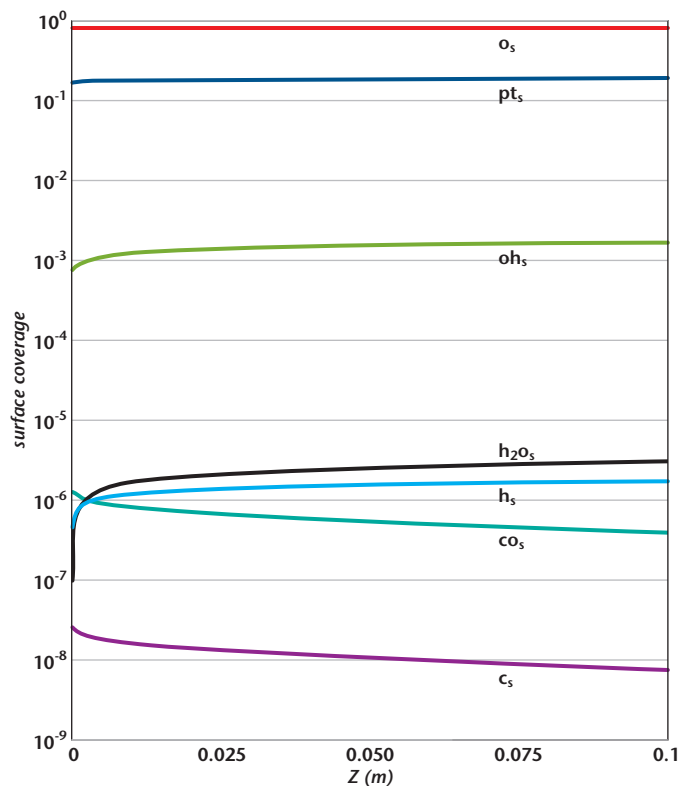
1 Deutschmann O., Maier L.I., Riedel U., Stroemman A.H., and Dibble R.W., "Hydrogen Assisted Catalytic Combustion of Methane on Platinum," Catalysis Today 59, p. 141-150, 2000.



Contours of mass fraction of the major gas species; diameter exaggerated for clarity

Surface Reactions in Catalytic Tubes

By Genong Li, Fluent Inc.



Surface coverage profiles along the length of the tubular reactor