

deposition of a catalyst for enhanced reaction control. For example, plural sub-wells **54** can be formed at the bottom of a surface feature and/or the top of a surface feature, and catalyst **56** can be deposited (for example by washcoating) over the plural sub-wells. Optionally, areas **55** of a thermally conductive material can be deposited over the surface features and/or sub-wells for further enhanced surface area.

Reactions

[**0176**] In some aspects, the invention provides a method of conducting a reaction, comprising: flowing at least one reactant into a microchannel, and reacting the at least one reactant in the presence of a catalyst within the microchannel to form at least one product. In some embodiments, the reaction consists essentially of a reaction selected from: acetylation, addition reactions, alkylation, dealkylation, hydrodealkylation, reductive alkylation, amination, ammoxidation, ammonia synthesis, aromatization, arylation, autothermal reforming, carbonylation, decarbonylation, reductive carbonylation, carboxylation, reductive carboxylation, reductive coupling, condensation, cracking, hydrocracking, cyclization, cyclooligomerization, dehalogenation, dimerization, epoxidation, esterification, exchange, Fischer-Tropsch, halogenation, hydrohalogenation, homologation, hydration, dehydration, hydrogenation, dehydrogenation, hydrocarboxylation, hydroformylation, hydrolysis, hydrometallation, hydrosilation, hydrolysis, hydrotreating (HDS/HDN), isomerization, methylation, demethylation, metathesis, nitration, polymerization, reduction, reformation, reverse water gas shift, Sabatier, sulfonation, telomerization, transesterification, trimerization, and water gas shift. Combustion is another preferred reaction. Hydrocarbon steam reforming is especially preferred (such as methane, ethane or propane steam reforming among others).

EXAMPLES

Steam Methane Reforming Reactions in Microreactors with Wall Surface Features

[**0177**] The effect of surface features on the reactor performance was explored for the methane steam reforming reaction. The intent of the features was to increase the conversion per length, especially at low catalyst activity. The surface features increase the available surface area for catalyst, they allow a solution derived catalyst to be washcoated uniformly, and they reduce external mass transport limitations in the bulk microchannel and thus allow the reactor to operate closer to the intrinsic potential of the catalyst activity.

[**0178**] In this example, the surface features have rectangular cross section shape; are on either one or both sides of the microchannel; the depth of the surface features are of the same order as the main flow channel gap; and the surface features are placed at a specified angle relative to the main flow direction

Part of the dimensions defining the problems are kept the same for all the examples

[**0179**] Channel gap: 0.0125"

[**0180**] Channel width: 0.18"

[**0181**] Depth of the grooves: 0.010" (0.005" and 0.015" also evaluated) placed on both sides of the microchannel

[**0182**] Run Width or span of the grooves: 0.015"

[**0183**] Distance between adjacent grooves (edge to edge distance): 0.015"

[**0184**] 5 grooves placed in series (length approximately 0.15")

The per channel flowrate for all computations was 0.238 kg/hr of a mixture of 3:1 steam to methane at 25 atm.

SMR Kinetics

Methane steam reforming (SMR) reaction in a microchannel reactor is the focus of this example.



Also, the water gas shift (WGS) reaction, which is modestly exothermic, was also considered because of the importance of CO₂ formation on the SMR catalyst.



The following kinetics were assumed for all the CFD simulation results reported in this example (where the subscript "1" refers to the SMR reaction and the subscript "2" refers to the WGS reaction). The following rate expressions for the reaction kinetics are used throughout this example,

$$r_1 = k_1 P_{\text{CH}_4}^6 \left(1 - \frac{P_{\text{CO}} P_{\text{H}_2}^3}{K_1 P_{\text{CH}_4} P_{\text{H}_2\text{O}}} \right)$$

$$r_2 = k_2 (P_{\text{CO}} P_{\text{H}_2\text{O}} - P_{\text{H}_2} P_{\text{CO}_2} / K_2)$$

The reaction rates are in kmol/m²-cat.sec, and the pressures P_i in the above equations are in bar. The reaction rate constants follow the Arrhenius form as follows:

$$k_1 = A_1 \exp(-E_1/RT)$$

$$k_2 = A_2 \exp(-E_2/RT)$$

The activation energy for the SMR reaction was assumed to be E₁=1.7E8 J/Kmol; and for the WGS reaction, E₂=6.713E+7 J/Kmol. The pre-exponential factors were assumed to be A₁=2.126E+04 and A₂=1.222.

[**0185**] In these reaction rate expressions, the reverse reactions are taken into account through the respective chemical equilibrium constants

$$K_1 = \exp(-2683/T + 30.114)$$

$$K_2 = \exp(4400/T - 4.036)$$

[**0186**] The parameters in the kinetics are results of best fitting of the model predictions using experimental data for an SMR catalyst based on a 5 wt % Rh dispersed on a MgO stabilized alumina. It should be pointed out that, this set of kinetics is not necessarily typical for all SMR catalysts, but is illustrative of the comparative impact of reactor geometry and design on performance.

[**0187**] This set of kinetics is referred as the baseline kinetics. The impact of reduced activity from this baseline level is also evaluated

Boundary Conditions

[**0188**] The following conditions were imposed on the boundaries.

[**0189**] Inlet: total mass flow rate F=6.48E-5 kg/s; 3 to 1 molar ratio of steam to methane; Temperature is same as that of the wall.