[0190] Outlet: pressure. 345 psia (2.38 MPa) was assumed for all cases unless specified otherwise.

[0191] Wall: no slip velocity; constant temperature.

Imposing mass flow rate at the inlet of the reactor section is easy to implement, but this might cause some concerns if the inlet is located right at the leading edge of the catalyst structure because of a known entrance length effect where flow full develops into a laminar flow profile. To avoid this effect in the calculations, a microchannel inlet is placed a certain length upstream of the catalyst structure. No reaction was modeled in this entrance section. The actual length of this entrance is a matter of numerical experiment to make sure that the laminar flow is indeed fully developed when reaching the catalyst structure. In general, an entrance length twenty times of that of the flow gap is sufficient for fully developed laminar flow.

[0192] The methane conversion rate is used to compare the reactor performance of different configurations. Also, for the purpose of comparison, a baseline case is modeled which is a straight channel of the same dimensions as those for the cases with surface features in terms of channel length, channel width and gap size. The reactor performance with surface features is quantitatively measured using the following enhancement factor,

$$E\_factor = \frac{(x_{withSF} - x_{baseline})}{x_{baseline}};$$

X in the above equation is the methane conversion rate. It is calculated based on the mass flow rate of methane flowing in and out of the reactor. Although, a uniform methane concentration at the inlet of the reactor is assumed, it is not the case at the outlet of the reactor. In general, methane concentration is not completely uniform over the channel cross-section at the outlet. The total flow rate of methane at the outlet is integrated over the outlet area to calculate the average conversion.

A) Surface Grooves Placed at a 90 Degree Angle to the Flow Direction or Substantially Horizontal to the Flow Direction

[0193] The modeling results show that there is no convective mixing between the fluid within the grooves and the fluid in the main channel. For the trajectories of fluid particles released inside the grooves, they form closed circle confined to the groves in which they are released. The fluid rolls or rotates only within the surface feature. Under the reactive environment, the chemical reactions take place on the surface of the grooves which lead to concentration gradients of the species. Mass diffusion occurs across the interface of the grooves and the main flow channel. Within each groove, the pressure difference is so small that no transverse fluid movement is observed. The E-factor was computed, as shown in Table 1.

TABLE 1

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	Methane conversion		E_factor
C.	baseline	case A	case A
850	24.2%	22.7%	−6.1%
700	5.4%	6.3%	17.8%

For this geometry, a surprising result was noted in that if the kinetics were sufficiently fast (at the higher temperature), the surface features may actually have a deleterious effect (a negative enhancement feature). If the kinetics are sufficiently fast and the only flow rotation is within the surface feature, then moving or translating the respective catalyst area from the wall of the bulk flow channel (or empty channel) to a farther distance (end or bottom or valley of the surface feature) adds more mass transfer resistance and inhibits performance. When the kinetics are slow, as seen by the lower temperature results, the longer mass transfer distance from wall to surface feature valley is more than offset by the added surface area of the surface feature and the increase in reaction time for molecules within the surface feature. This pattern did not use advection to bring the reactants into the active surface features.

B) Surface Grooves at an Oblique Angle with the Flow Direction—on both Opposite Walls of the Channel—Symmetry—Converging Flows within the Grooves

[0194] In this example, SFG0 (V-shaped, or chevron) surface features (or grooves) were simulated via CFD on opposing walls of a main channel in the "cis A" configuration. The SFG0 pattern consists of a repeated similar chevron pattern and acts to bring more fluid into the active surface features than the horizontal groove pattern. As such, the effectiveness factor is always positive thus the features always act to bring more reactants within the active surface features.

[0195] Three angles were evaluated, 30, 45 and 60 degrees. The positive angle means that the apex of the V-shaped grooves point to the downstream of the flow (or are pointed with the flow direction), and the flows within the two branches of the V-shape grooves converge at the middle of the main flow channel.

[0196] Imaginary massless fluid particles released near the side walls of the flow channel enter the grooves and move transversely toward the center of the channel. The flow of the fluid within each leg (or branch) of the groove is driven by the pressure difference, its maximum is observed near the side walls of the main flow channel—the most upstream location for this particular groove. A secondary flow pattern inside the grooves is driven by the momentum exchange at the interface between the sweeping flow in the main channel and the flow inside the grooves. By superposing the secondary flow onto the dominating transverse flow inside the grooves a spiraling flow pattern is seen. This flow pattern benefits the degree of the chemical conversion taking placing on the walls of the grooves due to the longer effective reaction time. The flows in two connecting branches of the groove converge at the center of the channel where a strong lifting flow is formed into the main flow channel. This lifting flow occurs over a section of the groove and reaches its maximum strength near the center of the channel width. This strong lifting flow near the center of the channel prevents the fluid in the main flow channel from being sucked into the grooves.

[0197] The modeling results show that the methane concentration distribution is symmetric referring to the middle plane. But a certain level of un-even distribution of methane in the transverse direction is observed. This will lead to an un-even reaction rate distribution which in turn will cause un-even heat load. However, this un-even heat load will be relieved effectively considering the heat conduction along the transverse direction within the channel walls. Similarly, an un-even product (H2) distribution in the transverse direction is observed.