

[0217] Models predict that the intrachannel uniformity of coating is poor (>20% variability) for all fluid properties. Where the coating at the top of the coated section is quite thin and a much thicker coating is present at the bottom of the microchannel. These results have been verified experimentally, where the measured catalyst composition at the bottom edge of the catalyst channel is more than 20% thicker (or higher weight loading) than the catalyst at the top of the microchannel. In some cases, no catalyst was observed at the top of the microchannel.

[0218] It should also be noted, that it is possible to reduce the intrachannel non-uniformity by coating to a vertical height much higher than the desired level such that the desired coating or reactor region length falls within the near-asymptotic region of the axial coating profile. This would work reasonably well if the drying time were long enough such that the coating would not set up (dry in place) a poor coating profile. It would be possible to wash away the uneven catalyst that was retained above the desired coating location. This would be possible if a second fluid were filled and drained from the opposite end of the microchannel reactor or device. The second fluid would solubilize the uneven coating and remove the material. Several fill and drain steps may be required to wash out the undesired catalyst.

[0219] Model parameters used in FIG. 5 showing the axial profile of coating thickness as a function of time.

[0220] Viscosity: 0.006135 Pa-s

[0221] Density: 1100 kg/m<sup>3</sup>

[0222] Liquid surface tension: 0.07 N/m

[0223] Liquid contact angle: 75 degrees

[0224] Hydraulic diameter: 1 mm

[0225] Washcoating Uniformity Modeling with the Use of Capillary Features to Retain the Liquid on the Microchannel Walls

[0226] An improvement to uniform liquid retention on the walls of a microchannel that is coated after assembly is enabled by the use of small features created into or out of the microchannel walls. The features are referred to as capillary features and make use of capillary forces to hold or retain a fluid sufficiently uniformly along the length of the microreactor walls as well as from channel to channel.

[0227] It should be noted that surface forces, when dominating over gravitational forces, should be sufficient to increase the catalyst interchannel and intrachannel uniformity. Surface forces include adhesion and chemical reaction. An example of adhesion is a sticky fluid that has relatively strong attractive forces with the microchannel wall. The use of polymeric, adhesive, or other adhesion-prone fluids may improve the catalyst uniformity within a microchannel.

[0228] Capillary-Feature Liquid Uptake Model Results

[0229] A 1-D capillary feature liquid retention model was developed assuming that the groove cross-section is rectangular and the groove is oriented such that gravity acts parallel to the groove width and is orthogonal to the length and depth of the groove. The resulting third order non-linear differential equation describing this 1-D system was solved using Mathcad 2001i (MathSoft, Cambridge, Mass.). In

order to solve the differential equation, the following boundary conditions were assumed: the liquid depth in the groove is approximately equal to the depth of the groove along the bottom-most edge with respect to gravity and the angle between the liquid and the solid along the bottom and top edges is equal to the thermodynamic contact angle for that liquid/solid/gas interface system.

[0230] The model is used to predict the shape of the liquid meniscus in the groove (for example see FIGS. 6a and 6b), and to explore the effect of several variables over a wide range of conditions on liquid retention. The variables found to have the greatest effect on the allowable catalyst uptake are groove depth, groove width to depth ratio, contact angle, and gravity factor ratio. The gravity factor ratio is defined as shown in Equation 1 below, where  $\rho$  is the liquid density,  $g$  is the gravitational constant (i.e. 9.81 m/s<sup>2</sup>), and  $\sigma$  is the liquid surface tension. The gravity factor ratio for water at room temperature and pressure is about 1.

[0231] A general form of the equation for predicting active material uptake in milligrams active material/inch<sup>2</sup> (milligrams/6.45 cm<sup>2</sup>) on a surface with capillary features is given in equation 2 below.

$$\text{gravity factor ratio} = \frac{\frac{\rho g}{\sigma}}{\left[1.344E5 \frac{\text{kg} \cdot \text{sec}}{\text{m}}\right]} \quad (\text{Eq. 1})$$

$$\begin{aligned} \text{Active material uptake (mg/6.45 cm}^2\text{)} = \\ 10 * (\rho_{\text{liquid}}) * (w_{\text{catalyst}}) * f_{\text{area}} * [+2.13119 - 0.040174 * (\text{contact} \\ \text{angle}) + 0.025326 * (\text{groove depth}) - 0.69857 * (\text{height/depth}) + \\ 7.70816E-004 * (\text{contact angle}) * (\text{groove depth}) + \\ 0.013161 * (\text{contact angle}) * (\text{height/depth}) - 8.42001E- \\ 003 * (\text{groove depth}) * (\text{height/depth})] \quad (\text{Eq. 2}) \end{aligned}$$

[0232] Where  $\rho_{\text{liquid}}$  is the density of the liquid in grams/cm<sup>3</sup>,  $w_{\text{catalyst}}$  the mass fraction of active material in the liquid solution,  $f_{\text{area}}$  is the fraction of area which is covered by the capillary features, contact angle is in degrees, groove depth is in microns (10<sup>-6</sup> m), and height/depth ratio is unitless.

[0233] The model equation in Equation Z is valid only over the range 25-125 micron groove depth, 0.5-10 groove width to depth ratio, contact angles of 10-80 degrees, and gravity factors (Equation 1) of 0.1-10.

[0234] In addition, the height/depth ratio must satisfy the following criterion (where contact angle is given in degrees):

$$\text{height/depth} < [1.122E-03 * (\text{contact angle})^2 + 8.265E-03 * (\text{contact angle}) + 2.155]$$

[0235] Table 1 compares predictions using the above correlation to those obtained using the full model.

[0236] Where rib is defined as a flat wall, neither recessed or protruded, along the microchannel length. It is anticipated that less liquid washcoat solution will be retained on the top of the rib as gravity draining will occur.