

trast the predicted values for wall shear stress and dynamic pressure in regions where the treatment was not successful to those regions where treatment was successfully applied. These simulations used as boundary conditions the same temperature, flow rates, stream composition, and flow input/output configuration as was used in the respective device aluminidization process. Comparisons utilized autopsy results of aluminized and heat treated devices. It was determined from these studies that there could be established a threshold value for both wall shear stress and dynamic pressure whereby for flow conditions in which both shear and dynamic pressure were below the threshold values, good treatment should take place; and when the threshold value of either variable was exceeded, the treatment could be flawed.

[0107] Metric Thresholds

[0108] Wall shear stress is expressed as $\tau = \mu |\nabla u|$ or the product of the fluid viscosity μ and the magnitude of the local velocity gradient, expressed in units of force per channel wall unit surface area. This quantity reflects the magnitude of the molecular frictional forces at the interface between a very thin fluid layer and the channel wall itself.

[0109] The dynamic pressure (or equivalently the momentum flux) is given by the expression

$$p = \frac{1}{2} \rho u^2$$

[0110] where p denotes the fluid density and u the local fluid velocity magnitude. It is a measure of the force imparted by the change in momentum when a jet plume strikes the side of a channel and is also expressed in terms of force per unit area. CFD simulations of a number of combustion test devices were performed to determine if there was any definitive correlation between poor aluminide coating and critical values in either wall shear stress or dynamic pressure.

[0111] Based on a detailed analysis of the tested devices, the following thresholds were established:

[0112] Wall Shear Stress: To ensure drag forces do not impair the formation of aluminide coating, the wall shear stress should not exceed 50 Pa if the aluminidization gases are flowing through a jet orifice. Allowable wall shear stress should not exceed 200 Pa if the aluminidization gases are not impinging on the wall of a microchannel as through a jet orifice.

[0113] Wall Dynamic Pressure: To ensure momentum impact erosion does not impair the adequate formation of aluminide coating, the wall dynamic pressure should not exceed 10 Pa if the aluminidization gases are flowing through a jet orifice. Substantially higher wall dynamic pressure is allowed in the absence of a jet orifice. Allowable wall dynamic pressure should not exceed 100 Pa if the aluminidization gases are not impinging on the wall of a microchannel as through a jet orifice.

[0114] Practical Application

[0115] The metrics presented above are used to determine the flow configuration and individual inlet flow rates that will imply good aluminidization treatment from a fluidics

standpoint. Generally there are a combination of possible input and output flow paths for a device. CFD predictions are used to determine those inflow/outflow combinations and the individual inlet flow rates that will result in globally maintaining the wall shear stress below 50 Pa, and the wall dynamic pressure below 10 Pa throughout the entire device if flow of at least one of the aluminidization gases is through a jet orifice. The maximum allowable inlet flow rate that satisfies these two criteria and the associated flow configuration becomes the recommended procedure for aluminidizing the device based on the metrics developed here. Examples of the aluminide coating resulting from this guidance produced aluminide coatings without visual defects.

[0116] A surprising discovery of this invention is that flowing (nonstatic, see previous discussion on preferred pressures) aluminidizing gas at rates below the threshold rates discussed above produced defect-free, highly uniform (less than 10% variation in thickness) aluminide coatings.

[0117] FIG. 3 schematically illustrates an application in which a metal substrate **42** has a first layer of aluminide **44**, a layer of alumina with sintering aid(s) **46**, and a layer of alumina **48**. In preferred embodiments, the outermost layer further comprises an additional catalytically active material **49**.

[0118] II. Washcoats

[0119] Washcoats are coatings that are applied to a channel wall by exposing a channel wall to a liquid based coating composition. The coating composition may contain a suspension of particles (typically a metal oxide or mixture of metal oxide and metal particles) or a sol.

[0120] Washcoat Uniformity Using a Fill and Drain Method Without Capillary Features

[0121] Process Description

[0122] A fill and drain method of applying washcoat solution to the substantially planar and flat walls of a microchannel include slowly filling a liquid solution to a parallel array of microchannels at a point that exposes the desired coating location to the washcoat solution. After the channels are filled, either completely or to an intermediate level, the solution is allowed to drain from one end of the device. Fluid is left behind on the microchannel walls. A second fluid, such as a nitrogen gas, may then be used to purge the microchannels and remove excess material.

[0123] A fill and drain method has been applied to washcoating an aqueous coating composition onto aluminidized Inconel™ walls of a microchannel reactor and has not demonstrated sufficient uniformity.

[0124] Modeling Approach

[0125] Notation

[0126] Fluidic Properties

[0127] μ viscosity (molecular)

[0128] ρ density

[0129] σ surface tension (relative to ambient gas)

[0130] ν viscosity (dynamic) $\nu = \mu/\rho$

[0131] \vec{v}, \vec{u} velocity vector