Towards 3D-Simulation of Gas Phase Reactions Involved in the Deposition of α-Al_2O_3

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The objective of increasing the efficiency of gas turbines is directly associated to the raise of the gas temperature at the turbine inlet (at present 1230ºC to 1350ºC). The resultant higher load at the turbine blades, must be faced through introduction of new concepts related to cooling and material selection.

Nowadays superalloys, like some nickel-based alloys, are the main choice as structural materials for turbine blades. These superalloys are protected against hot gas corrosion and hot temperature oxidation, as well as against heat failure, by a layer system. Eventhough, at local temperatures over 1000ºC, a higher interdiffusion between this hot gas corrosion protective layer (MCrAlY-layer, where M = Ni or Co, 50-100 u.m) and the superalloy takes place, this can lead to premature layer breakdown. One basic approach to avoid this is the growth of an intermediate layer in the interphase MCrAlY-layer-superalloy as a diffusion barrier.

In the frame of this project, we aspire to grow an intermediate α-Al_2O_3 layer in the interphase between the MCrAlY-layer and the superalloy as diffusion barrier. The CVD deposition of α-Al_2O_3 from $AlCl_3$-H_2-CO_2 composites is a technical process which is frequently used nowadays, for example, to get hard metal tool coating as corrosion protective layer. However, it is shown in the literature how the α-Al_2O_3 CVD-deposition on superalloys, as for example, CMSX4, is problematic due to undesired reactions that take place between the substrate and the growing layer (whisker growth). This complex phenomena can be well understood by using numerical simulation of the processes involved.

In the present work, we simulate CVD model reactors, in order to investigate the deposition process and the influene of the fluid mechanical, thermodynamic and chemical parameters on this process. The CHEMKIN-code has been coupled to a 3D-CFD-code to determine the flow and temperature fields in the reactor. For validation, a model geometry has been defined and studied in order to get a description of the process in terms of thermofluid mechanics and chemical reactions. It consists of a rectangular substrate placed on a holder, both lying on an horizontal reactor.

The generated grid used for simulation is a conform, block-structured hexahedral mesh, with approximately 200.000 elements. The dimensions are 900 mm length (axial direction) and 28 mm diameter (radial direction). The substrate and the holder have dimensions of 2.5x8x14 mm and 14x16x500 mm in the vertical, tangential and axial direction respectively.

The substrate is placed in the middle of the reactor, where the temperature is maximum. The temperature profile is assumed to be parabolic, equal to 350 K in both ends and 1400 K at the center of the reactor. The substrate is supposed to be at uniform temperature in the vertical direction. Previous to the integration of the chemical reactions in the CFD-code, some results for a 3D cold configuration were first obtained and will be presented. Results following Catoire and Swihart, of the gas phase rections in a plug flow reactor have been reproduced.

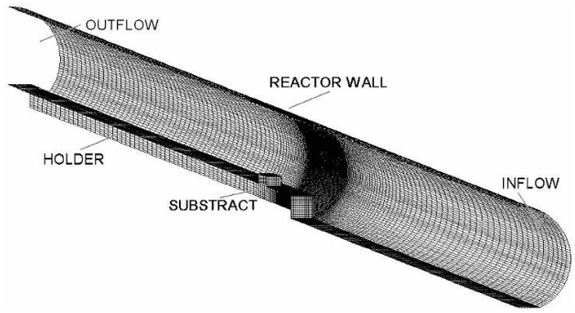

Fig 1. Schema of the reactor

We can see in figure 2 how the velocity vectors represent a typical laminar profile, with the highest values of the velocity gradient and the shear strain over the substrate.

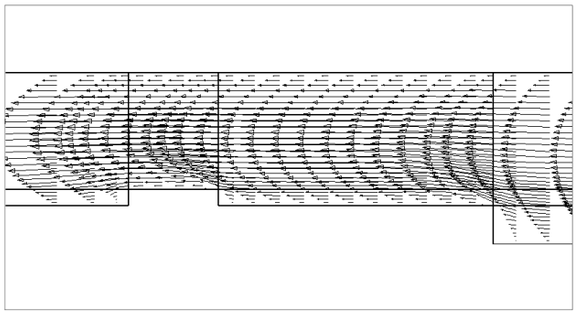

Fig. 2. Vector velocity representation over the substrate

The temperature values have been plotted one milimeter over the substrate in figure 3. The substrate is situated between the vertical lines at *z = 0.457* and *z = 0.457 m* and we can appreciate the temperature gradient of the gas on it, colder at the beginning, when the flow comes in contact with the substrate, and warmer as the gas is at the end of the substrate.

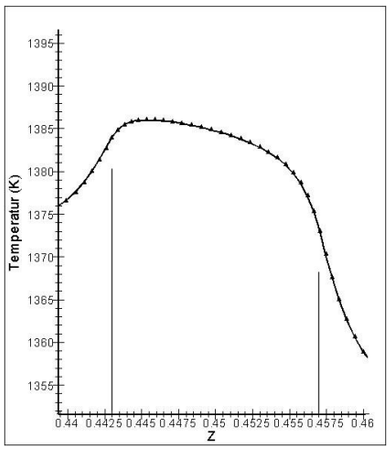

Fig. 3. Temperature plot over the substrate