JASS 2008 - Joint Advanced Student School, Saint Petersburg, 9. - 19.3.2008
Modelling and Simulation in Multidisciplinary Engineering

Gasdynamic Optimization of a Transonic Nano-particle Reactor - Numerical Investigation of Active/Passive Shock Control

Giglmaier M.
Technische Universität München,
Lehrstuhl für Fluidmechanik – Fachgebiet Gasdynamik,
D-85747 Garching Germany

Content

JASS 2008 - Joint Advanced Student School, Saint Petersburg, 9. - 19.3.2008
Modelling and Simulation in Multidisciplinary Engineering

Gasdynamic Optimization of a Transonic Nano-particle Reactor - Numerical Investigation of Active/Passive Shock Control

Giglmaier M.
Technische Universität München,
Lehrstuhl für Fluidmechanik – Fachgebiet Gasdynamik,
D-85747 Garching Germany

Content

Abstract

A novel method of nano-particle production by shock-induced ignition of a precursor and aerodynamic quenching, developed within a DFG (Deutsche Forschungsgemeinschaft) founded project [2], is the focus of the present study. The reduction of the shock/boundary layer interaction in order to obtain homogeneous post-shock conditions is necessary for a narrow size distribution of the produced particles. Due to a required mixing length and a smooth supersonic nozzle, the boundary layer in our nano-particle reactor thickens up and reaches about 20% of the channel hight. Additionally, due to the multiple boundary layer interactions the single shock disintegrates into a so called pseudo-shock. Thereby, oblique shocks form an aerodynamic nozzle with regions of compressions and expansions which results in inhomogeneous downstream conditions. These effects can be reduced by active and passive control techniques which are compared within this investigation.

1 Introduction

Gas-phase synthesized nanoparticles are broadly used in industry, science and measurement technology. Today flame synthesis and hot-wall synthesis are the most widely used methods for industrial production with an annual volume of several million tons. It is remarkable, that the morphology of the synthesized particles does not vary significantly. Most of them are aggregates with a fractal dimension of 1.8 – 1.9 and a geometric standard deviation of the size distribution in the range of 1.5 – 1.7. Former studies indicate that a homogeneous flow field and high heating and quenching rates are of major importance in order to achieve narrow size distribution and low aggregation [1].

In contrast to conventional methods the gas mixture is instantaneously heated by a stationary shock in an overexpanded supersonic nozzle flow. An overview of the principle of operation is given in Fig. 1. Following the injection of the precursor gas (2) the flow accelerates to supersonic flow speed and the reaction is initiated by shock heating (4).A chemical process leads to the generation and growth of nano-particles in the reaction chamber (5). After an adjustable reaction time depending on the gas velocity and the reactor length, the reaction is terminated due to rapid expansion and, therefore, cooling of the gas in a convergent-divergent nozzle flow (6). The total enthalpy of the flow is finally reduced by injecting water into the supersonic flow at the second nozzle exit (7) [2].

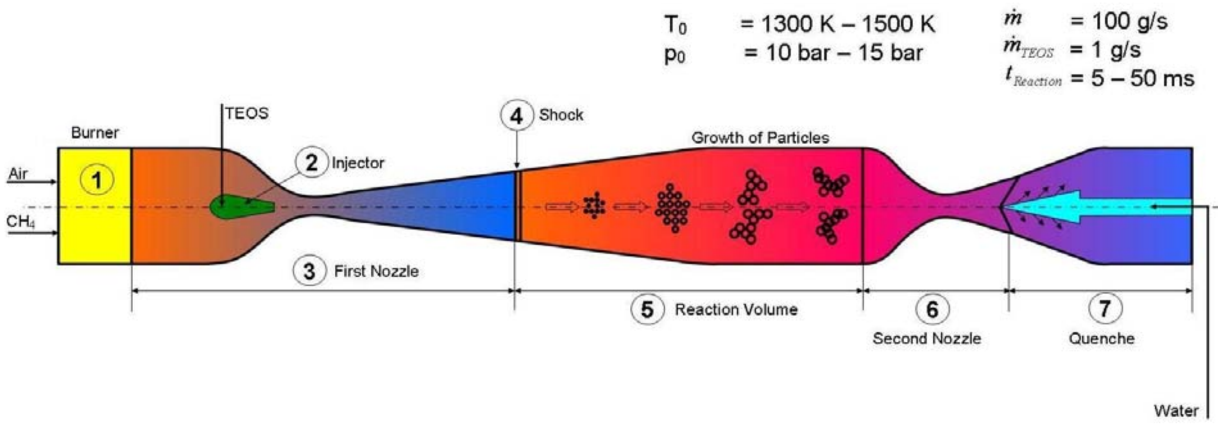

Fig. 1: Sketch of the nano-particle reactor

2 The inviscid process

To achieve particles with a narrow size distribution homogeneous conditions have to be provided. It is important to ensure perfect mixing of the precursor and homogeneous conditions across each cross-section. The heat increase due to the stationary shock provides ignition conditions. The basic layout of the first nozzle is defined by the pre-shock Mach number, the design mass flow rate and the distance from the injection position of the precursor to the shock location. The minimum of the distance follows from the required mixing length of the precursor with air. The maximum allowable length is prescribed by the ignition delay time of the precursor under the given thermal conditions. By neglecting viscid effects and the reactive heat addition, the throat area of the second nozzle can be calculated by the total pressure loss across the shock. Therefore, a 2-D Euler simulation is shown in Fig. 2.

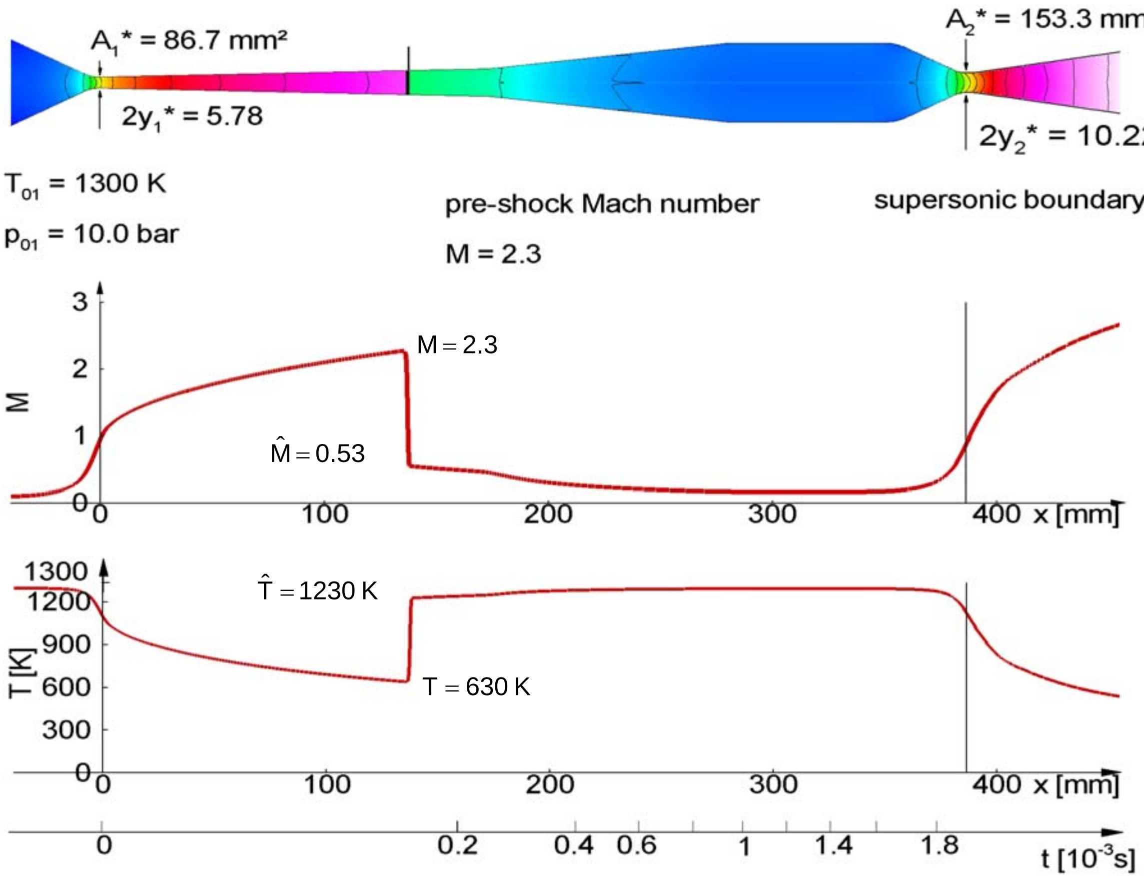

Fig. 2: 2-D Euler simulation of the nano-particle reactor

The mixing length is 150 mm and the ignition temperature of the precursor is 1200 K. Figure 2 shows the Mach number and temperature distribution along the axis. The temperature drops due to the acceleration in the supersonic part of the first nozzle. The position of the stationary shock is defined by the ratio of the critical areas (A_1^*/A_2^*). Due to the shock, the temperature rises up to 1230 K, the ignition temperature. The Mach number depicted in Fig. 2 is nearly constant at each cross section and therefore, the conditions can be assumed constant. The Euler-case can be seen as the desirable thermodynamic solution for the flow.

3 Viscid effects and the influences to the shock

After defining the basic geometry and the starting conditions viscid simulations were done to analyse the influence on the process. The boundary layer is resolved by 20 cells in normal wall direction and $y^+<1$ is ensured [3].

Figure 3 and 4 show geometrically identical nozzles with the same initial- and boundary conditions. The viscous simulation (Fig. 4) shows the effects to the shock boundary layer interaction. The main influence of friction can be seen by comparing the shock-structure and the pre-shock Mach number.

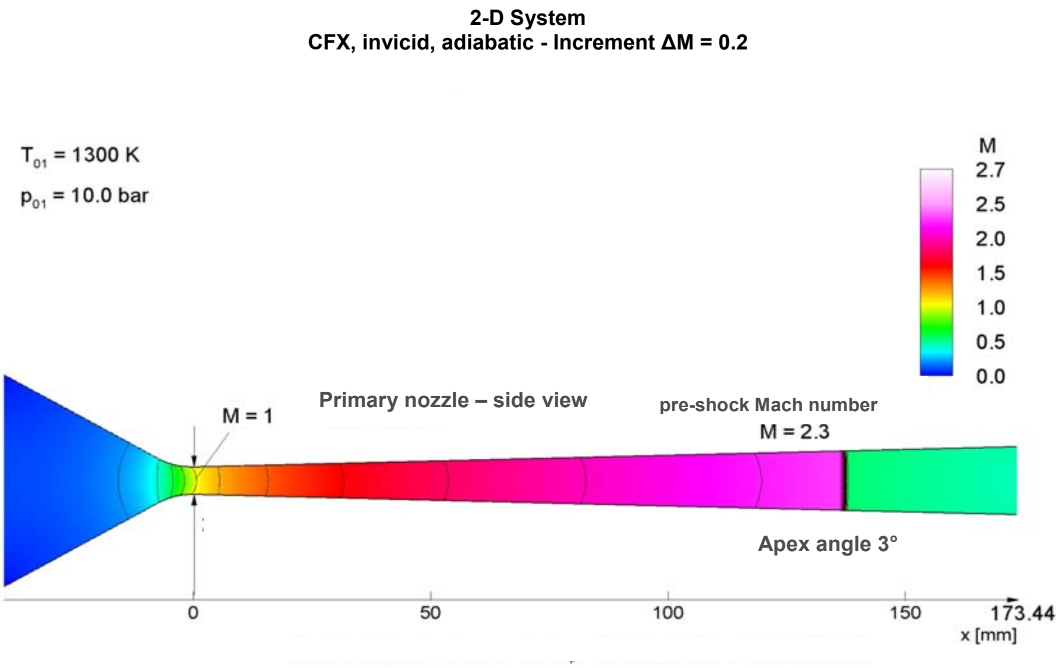

Fig. 3: The Euler case with a normal shock

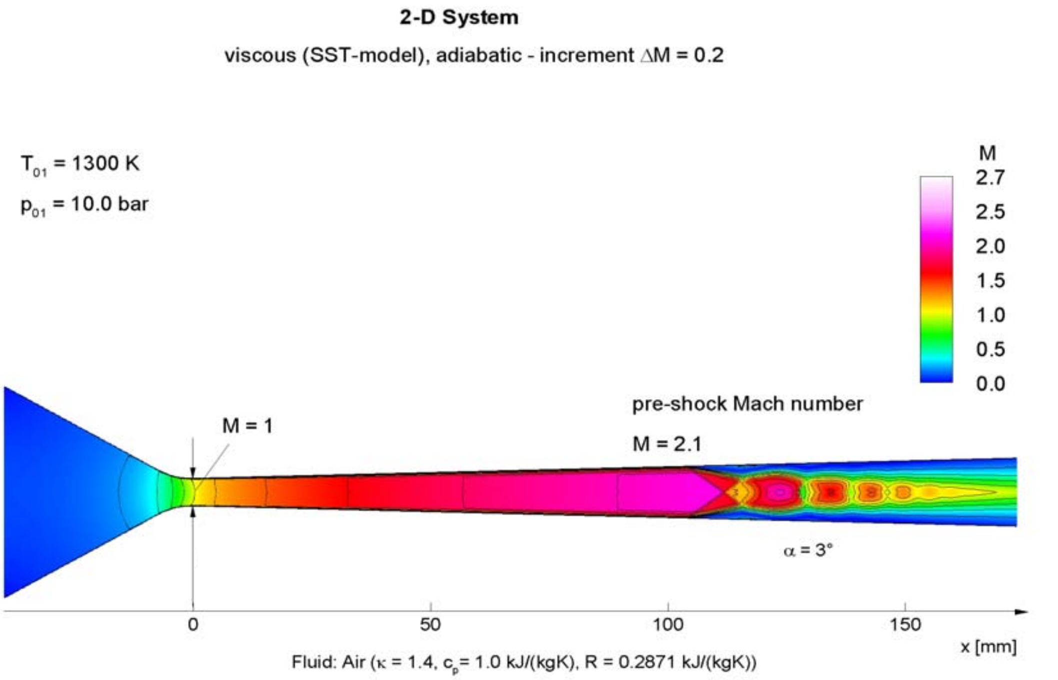

Fig. 4: The viscous case with a shock train

A closer look at the shock system (Fig. 5) shows that a boundary layer separation caused by the pressure gradient, leads to two oblique shocks which form an aerodynamic nozzle in interaction with the boundary layer [4]. Because of that the main flow accelerates and decelerates several times until a subsonic speed is reached.

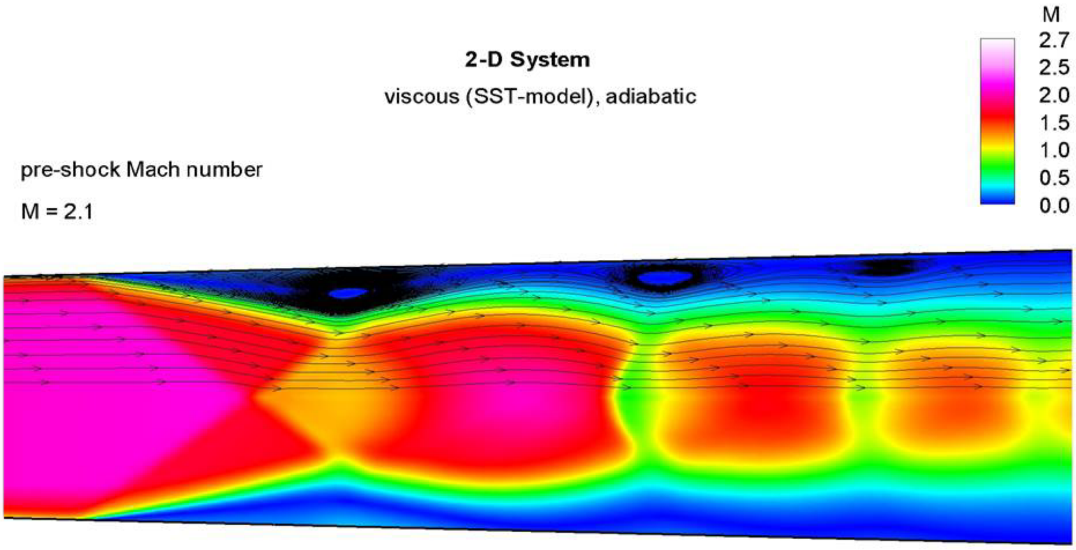

Fig. 5: Shock train or “pseudo-shock system”

Along each streamline the precursor experiences different temperatures and velocities. Thereby, the reaction rate in the subsonic downstream part of the reactor differs and also the time for coagulation. Both facts have direct influence on the particle size. To reach the favoured narrow size distribution an optimisation is required.

4 Numerical simulation and comparison with experiment

Prior to the realisation of the pilot facility, experiments with inert gas at low temperatures were performed to validate the simulations. The measured and the simulated static pressure distribution along the sidewall is shown in Fig. 6.

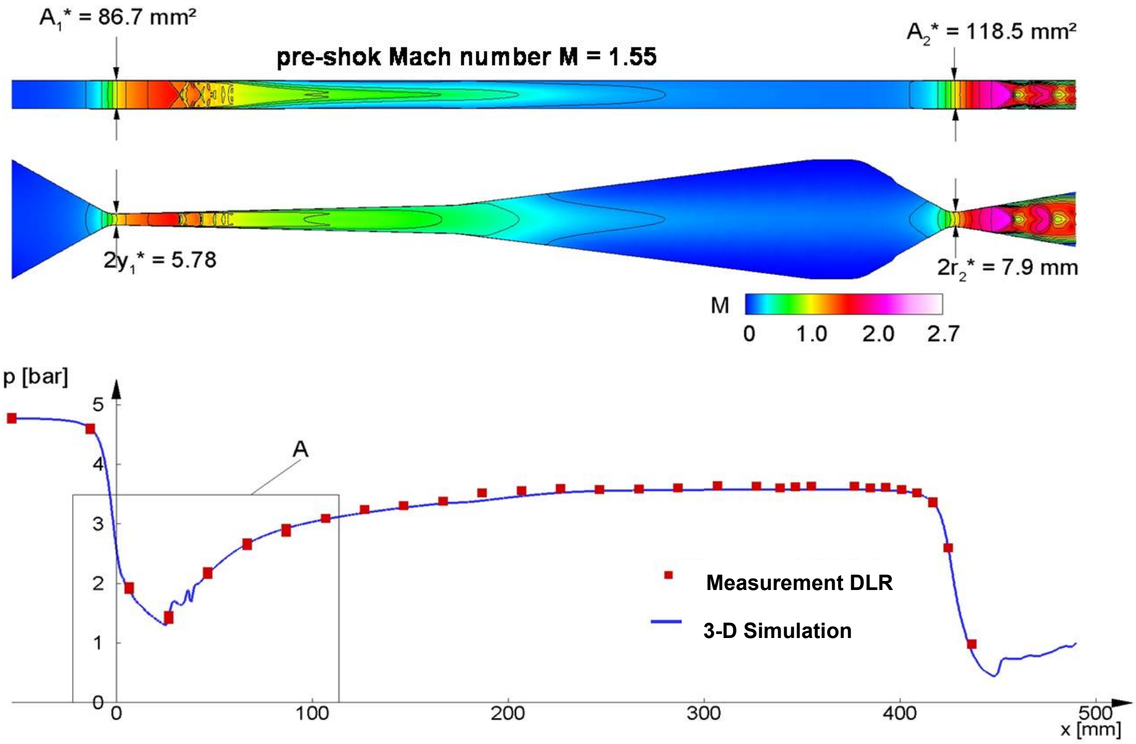

Fig. 6: Mach number distribution – top,
Static pressure distribution along the axis – bottom

A more sensitive possibility to validate the numerical results is the exact shock position, which can be displayed by a Schlieren picture (Fig. 7).

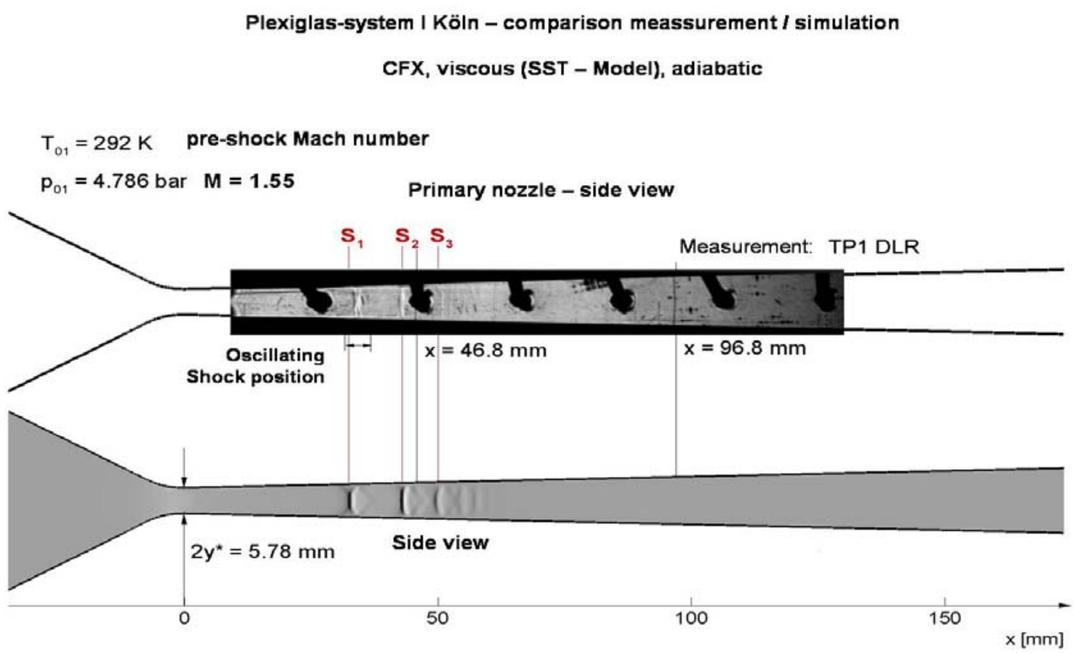

Fig. 7: Experimental-/ numerical Schlieren picture

5 Optimisation of the shock system

Due to the positive pressure gradient across the shock the boundary layer in the smooth channel thickens and thereby effectively forms a convex wall contour. By superimposing a negative pressure gradient this effect can be minimized. We apply active suction, which provides an expansion upstream of the shock and decreases the boundary layer thickness. The result is depicted in Fig. 8, where a straight shock is formed in the centre of the channel even though there is a separation region subsequent to the shock position.

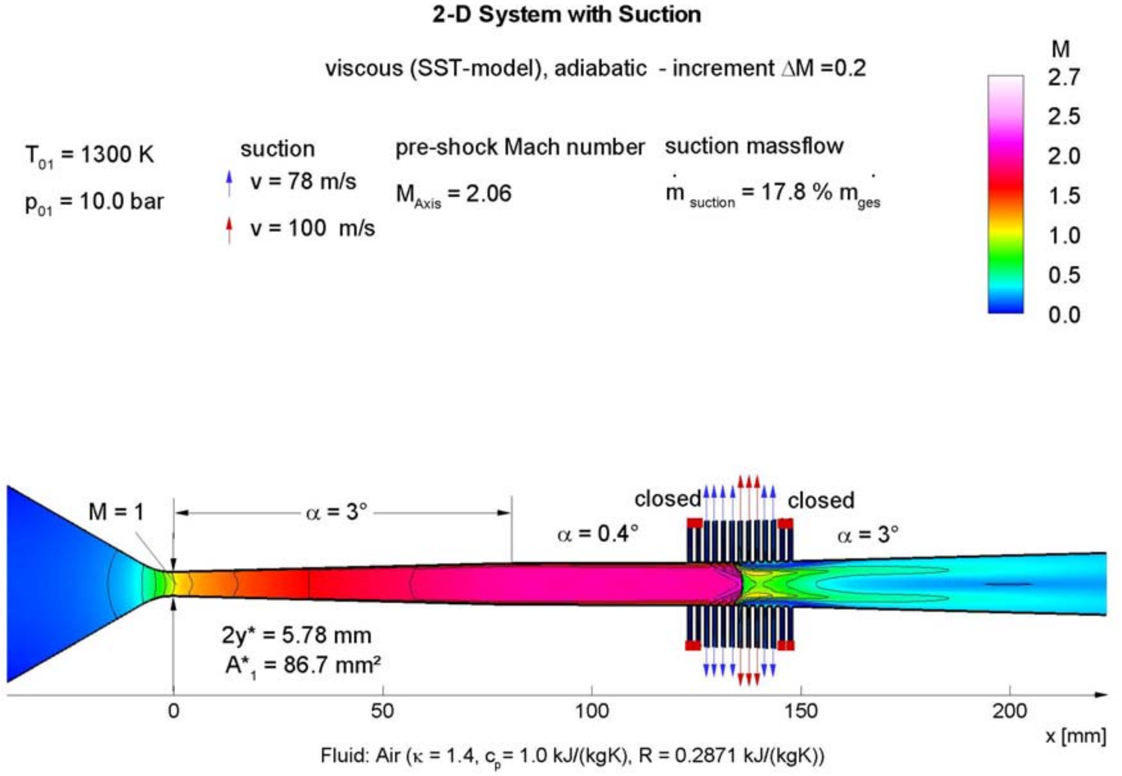

Fig. 8: Active suction slots with defined velocity

Suction in the environment of the nano-particle reactor is difficult to implement, because of the high temperatures and the presence of the precursor. Therefore, a passive control technique is applied to achieve similar results without active suction. We alter the wall curvature in order to create an expansion fan that interacts with the shock (Fig. 9). The pre-compression is compensated at the core of the flow domain and a normal shock is formed. The temperature distribution along the axis in Fig. 9 shows the comparison with/without the concave wall contour modification. Due to this modification a stronger shock is created in the channel core and thereby the maximum static post-shock temperature is increased by 15%. The higher static post shock temperature leads to a faster ignition of the precursor, which is necessary to ensure the formation of a narrow particle size distribution.

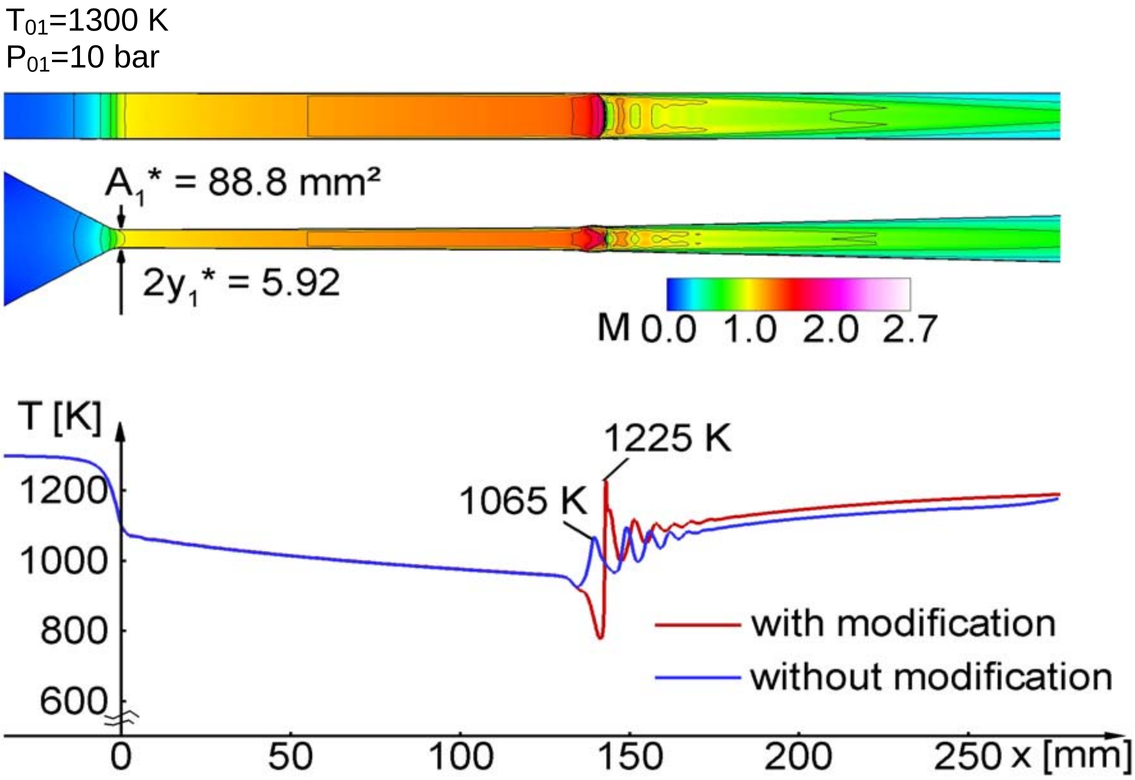

Fig. 9: Temperature distribution with/without concave contour modification

6 Conclusion

The instantaneous ignition by a well-defined sudden temperature rise across a shock and the aerodynamic quenching with a supersonic nozzle enables a new way of nano-particle production and quality. Therefore, a profound knowledge of aerodynamic effects and chemical reactions is needed. With this requirements, validated simulations can be the basis for further cost effective development and improvement. The non-homogeneous temperature rise because of the shock boundary layer interaction could be prevented by active and passive control techniques. But the construction and control of the active suction slots under the given conditions is not cost effective feasible. Simulations showed, that a modified concave wall contour has a similar, slightly weaker effect on the flow, but it is easy to implement into an existing nozzle.

References

[1] Schild, A., Gutsch, A., Mühlenweg, H., Pratsinis, S.E., „Simulation of nanoparticle production in premixed aerosol flow reactors by interfacing fluid mechanics and particle dynamics", J. Nanoparticles Res. 1, 305-315, (1999)

[2] Grzona, A. et al., "Gas-phase Synthesis of Non-agglomerated Nanoparticles by fast Gasdynamic heating and Cooling", ISSW26 2007 - 26th International Symposium on Shock Waves, Göttingen, Germany, (2007)

[3] Al-Hasan, N., Schnerr, G.H., "Aerodynamic optimization of Laval nozzle flow with shocks: Numerical investigation of active/passive shock control via expansion fans", Proceedings in Applied Mathematics and Mechanics (2008)

[4] Matsuo, K., Miyazato, Y., Kim, H.D., "Shock train and pseudo-shock phenomena in internal gas flows", Progress in Aerospace Science 35, 33-100, (1999).