Numerical Simulation of Multidimensional Modes of Gaseous Detonation

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1 Introduction

Previously, a number of authors have performed theoretical studies devoted to formation and propagation of the two-dimensional cellular detonation in channels. But the flows with divergent detonation waves are of particular interest. These flows were investigated by R.I. Soloukhin in his brilliant experiments. Numerical simulation of cellular divergent detonation is a time-consuming problem by virtue of the necessity to perform high-resolution calculations in a vast spatial region for narrow chemical reaction zones. Three-dimensional cellular detonation is even more difficult to simulate and therefore it is poorly investigated.

2 Mathematical model and calculation method

For the description of a multicomponent gas mixture flows the system of Euler differential equations is used for 2D and 3D flows. The study is carried out numerically using the original software package in which the modified S.K. Godunov's method [1] for multi-block grids is implemented. This complex has a graphical user interface that allows to define and to modify the boundaries of the computational domain, to perform decomposition of the domain by curvilinear surfaces to hexahedral calculation blocks, define the multi-component mixtures, the initial and boundary conditions. Calculations can be performed both on the PC and on a supercomputer using code parallelization based on MPI. This paper presents the results of calculations performed on 1000-10000 CPU cores of the MSU supercomputer “Lomonosov” with computational meshes consisting of 0,1 to 10 billions of cells.

3 Cellular structure of divergent cylindrical detonation waves

Processes observed in experiments with the initiation and propagation of divergent detonation in a narrow gap between plates have been simulated. The detonation wave is formed in a tube adjoined at a right angle, and this gap passes therein through a circular hole. Due to the complexity of the flow region's geometry, the actual phenomenon is of a three-dimensional nature. But the flow inside the tube is close to one-dimensional, and the size of the interplate gap is sufficiently small. Therefore, transverse waves propagating in the direction normal to the plates are absent, and the two-dimensional divergent cellular detonation is realized within the gap. Fig. 1 shows for comparison (a) the experimental pattern and (b) the calculated pattern for wakes of triple points. One can see the good consistency of two-dimensional model for description of the process.

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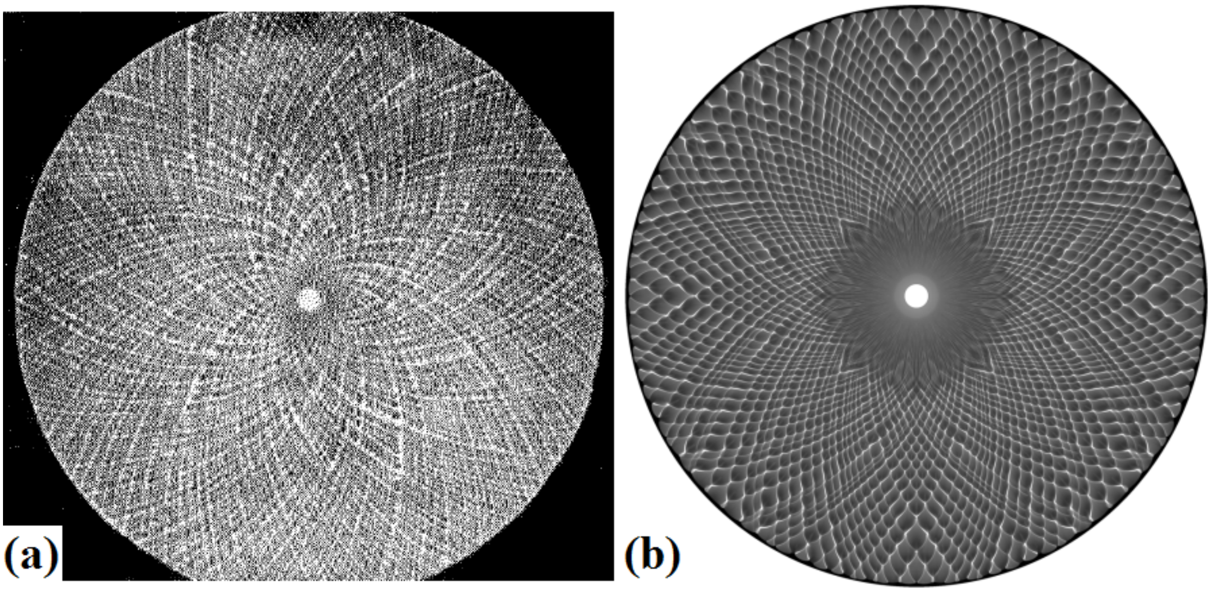

Fig 1. Traces of triple points besides the diverging cylindrical detonation wave. The results of the experiment (a) and calculation (b)

4 Cellular detonation in three-dimensional channels

Three-dimensional cellular detonation in semi-closed channels with fixed square, rectangular, circular and elliptical cross sections has been obtained. Formation of cellular structure was spontaneous due to one-dimensional initial distribution of gas-dynamic parameters in channels. The length of the channels was equal to 1 m, the rectangular cross-section was $H_x \times H_y$ with H_x and H_y from 1 to 20 mm, the elliptic cross-section had semi-axes a and b in range from 0.5 to 10 mm. In the case of rectangular cross-section a Cartesian grid with constant pitch was used. For elliptic channels a special mesh was constructed, similar to O-grid and not condensing to the axis of symmetry. Linear size of computational cells in all cases did not exceed 0.1 mm.

In all cases the detonation of a stoichiometric propane-air mixture at rest under normal conditions (1 bar, 20 °C) was studied. It was considered that the channel has a flat closed end, near which in the zone of 3 cm width initiation of detonation occurs due to instantaneous uniform electric discharge. By the statement of the problem the flow initially is one-dimensional, the parameters of which depend only on the longitudinal coordinate *z*. But because of the instability and the rounding errors at machine precision one-dimensional detonation wave is transformed to cellular at some distance. This spontaneous transition was observed in calculations for all channels, which had large enough at least one linear dimension of the cross section, allowing the propagation of transverse waves. The local maximum pressure map constructed inside the channel during the calculation formed a numerical three-dimensional soot foil diagram similar to those in simulations of two-dimensional cellular detonation.

To verify the calculation scheme and software complex as a whole a limiting transition $H_x \rightarrow 0$ for the case of rectangular cross-section was carried out. In this case H_y was fixed equal to 20 mm. Calculations have shown that transition to a regular two-dimensional cellular detonation is realized. Thus, when H_x=1 mm numerical soot foil diagram on one of the surfaces of three-dimensional channel in the *yz* plane practically did not differ from that obtained in the two-dimensional calculation. However, in the case H_x=1 mm at some distance from the place of origin of the cellular detonation there is a small dependence of gasdynamic parameters on the coordinate *z*, within a range of 0 to 1 mm. In the case of H_x=2 mm, H_y=10 mm numerical soot foil diagram on one of the wider sides of the three-dimensional channel is highly diffuse, and in the *z*-direction there is a significant change in the parameters.

For channels that are significantly different from the flat two-dimensional, principally three-dimensional cellular structure of detonation was obtained with transverse waves propagating in the plane of the section. The shape of the traces on the surface of the channel is different from the rhomboid, but reminds periodically structure, although quite “chaotic”. Fig. 2, for example, illustrates the soot foil diagram on the surface of the channel of square section with H_x=H_y=10 mm obtained in numerical simulation.

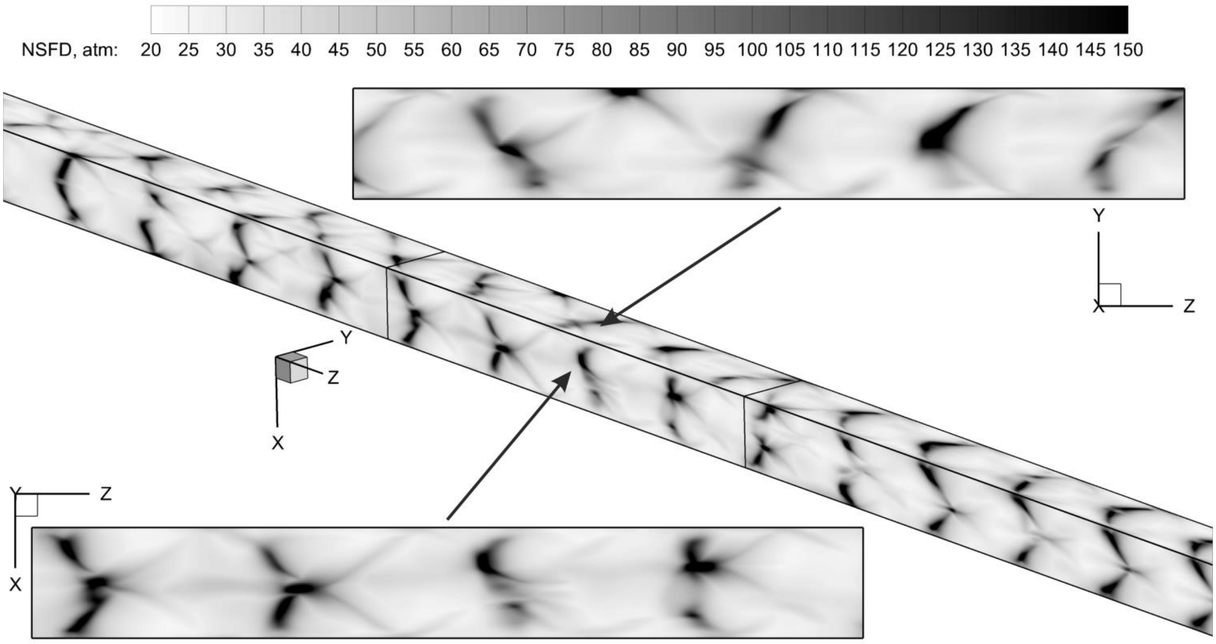

Fig. 2. Numerical soot foil diagram on the surface of the channel of square section H_x=H_y=10 mm

In this case the surface of the leading shock has several kinks that move along the front as it propagates and the structure of the flow behind the front is quite complex. In particular, the combustion front of complex shape is observed behind the head detonation wave front, covering some unburned “drops” of propane-air mixture (Fig. 3).

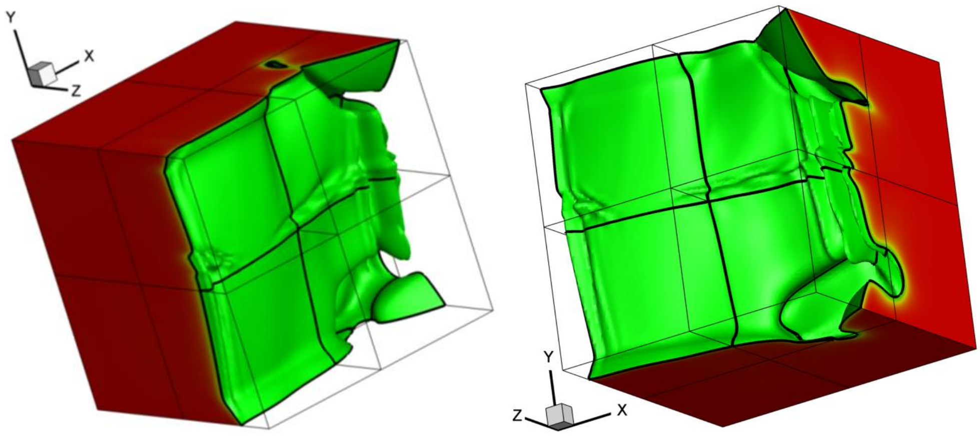

Fig. 3. The area where the concentration of water is higher than 50% of the maximum

Fig. 4 illustrates the emergence of a three-dimensional cellular detonation in a circular channel. In this case, the trace picture appears as on the side of the channel, and on plane surfaces parallel to its axis.

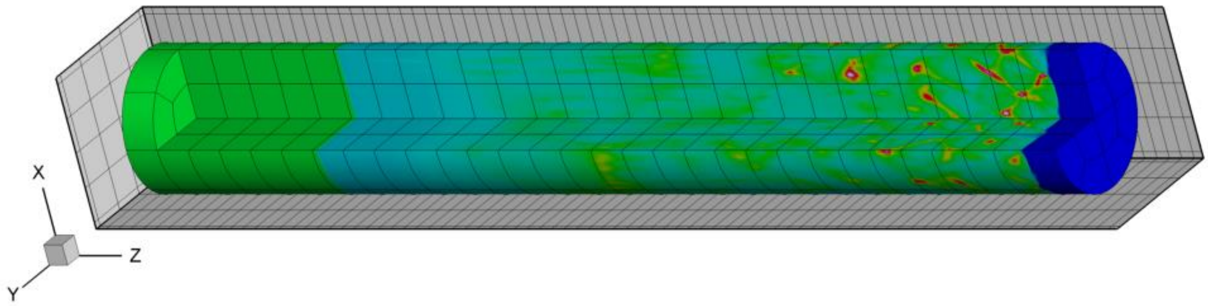

Fig. 4. The emergence of three-dimensional cellular detonation in the channel of circular section

Cross-sectional dimensions determine the approximate number of transverse waves that can be observed during the propagation of detonation. In addition, in locations of breakpoints of the channel surface or at points of minimum curvature a stronger cumulation of transverse waves is observed. It can be seen in sections of three-dimensional soot foil diagram (Fig. 5).

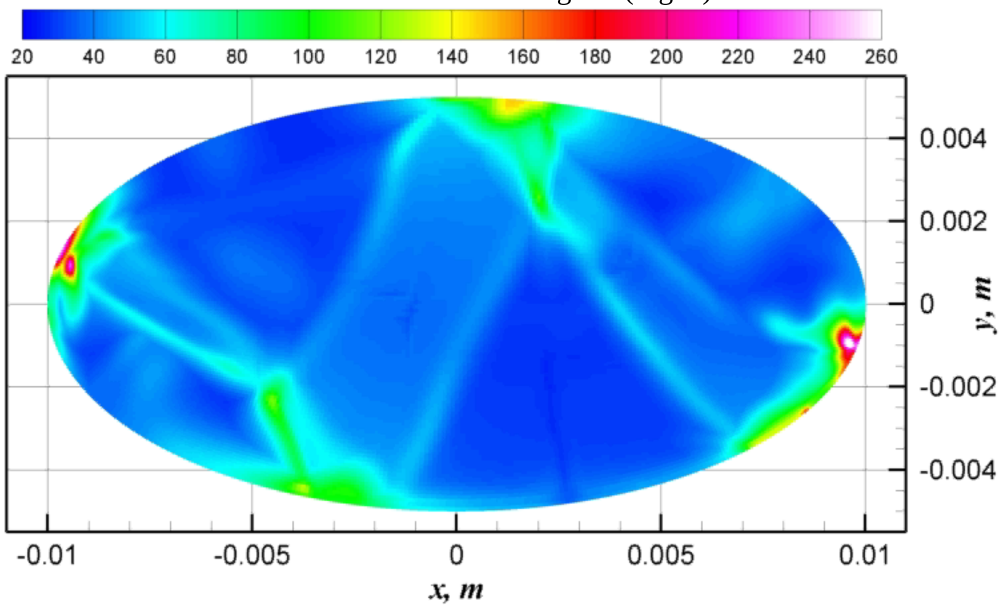

Fig. 5. Slice z=0.5 m of three-dimensional soot foil diagram obtained for the elliptic channel with a=1 mm, b=0.5 mm

In all cases, the three-dimensional structure of a cellular detonation occurs for sufficient length of the cross-section in two coordinates. At the same time, the propagating transverse waves can have any direction perpendicular to the direction normal to the front. As a result, the structure of the waves and trace pattern are irregular, sometimes chaotic.

5 Spinning detonation in three-dimensional channels

Decrease of both transverse dimensions of the channel leads to disappearance of 3D cellular detonation. If the width of the channel is less than the critical one, transverse waves are weak and the detonation is almost one-dimensional. If the width of the channel is greater than mentioned critical value but is quite small for large amount of transverse waves, some symmetrization may occur. For circular channel it leads to spinning detonation, which was obtained in calculations without any external impact, with strongly 1D initial distribution, and due to instability of 1D flow. Fig. 6 shows traces of triple points (soot foil diagram) on the surface of circular channel with diameter 6 mm. The left part of the figure illustrates the initial phase – irregular and undeveloped spinning detonation at the distance 22 cm. The right part corresponds to developed and stationary spinning detonation in the same calculation at the distance 75 cm. The soot foil diagram on the last figure has been constructed for the moment when the head front is in the field of view, so this figure also shows the values of pressure behind the head front on the surface of the channel.

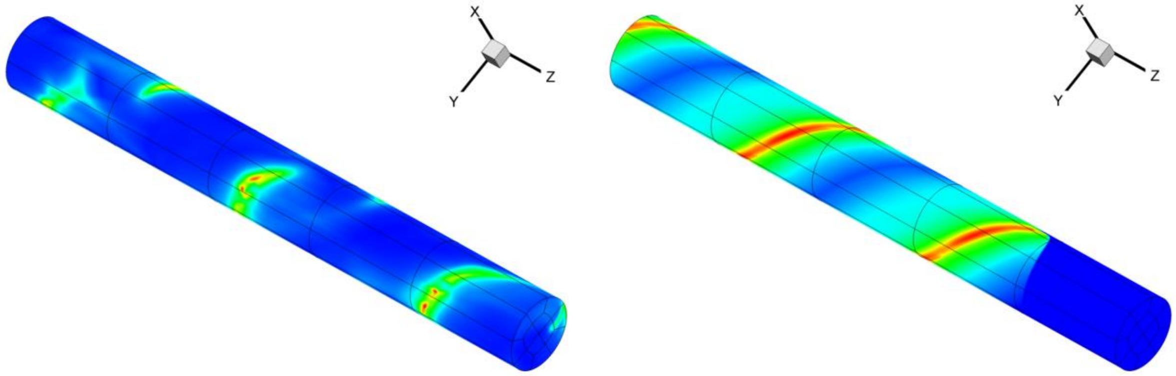

Fig. 6. Formation of three-dimensional spinning detonation in the channel of circular section

The process of spontaneous formation of developed spin detonation obtained in calculations raised the necessity of studying the stability of spin detonation to various perturbations. For this reason, the calculations for the transition of spin detonation from 6-mm diameter channel to the channel of larger or smaller diameter D through a short section of conical shape. Calculations have shown that there is a range of values of D such that the spin detonation maintains or recovers. Fig. 7 is presented to compare 3D views of different channels fragments with numerical soot foil diagrams upon spin detonation exiting the 6-mm channel and entering channels with diameters 4, 5, 8 and 10 mm. To analyze the patterns of flow that emerge in calculations, also the sweeps of lateral channel surface coated with soot foil diagrams were visualized (Fig. 8). They clearly demonstrate the traces left by transverse waves on the surface of the channel and the stages of spin detonation formation. Developed spin detonation can be identified by periodically repeating oblique stripes.

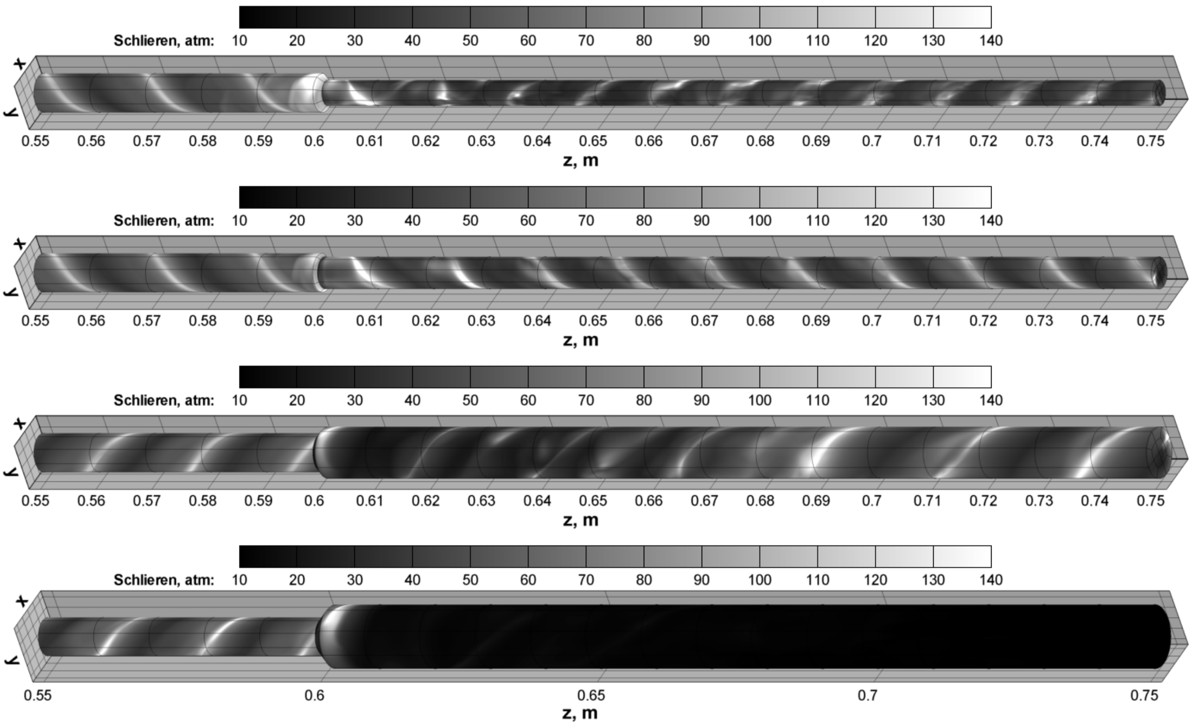

Fig. 7. Channels' fragments with numerical soot foil diagrams upon spin detonation exiting the channel of 6-mm diameter and entering channels with diameters 4, 5, 8 and 10 mm

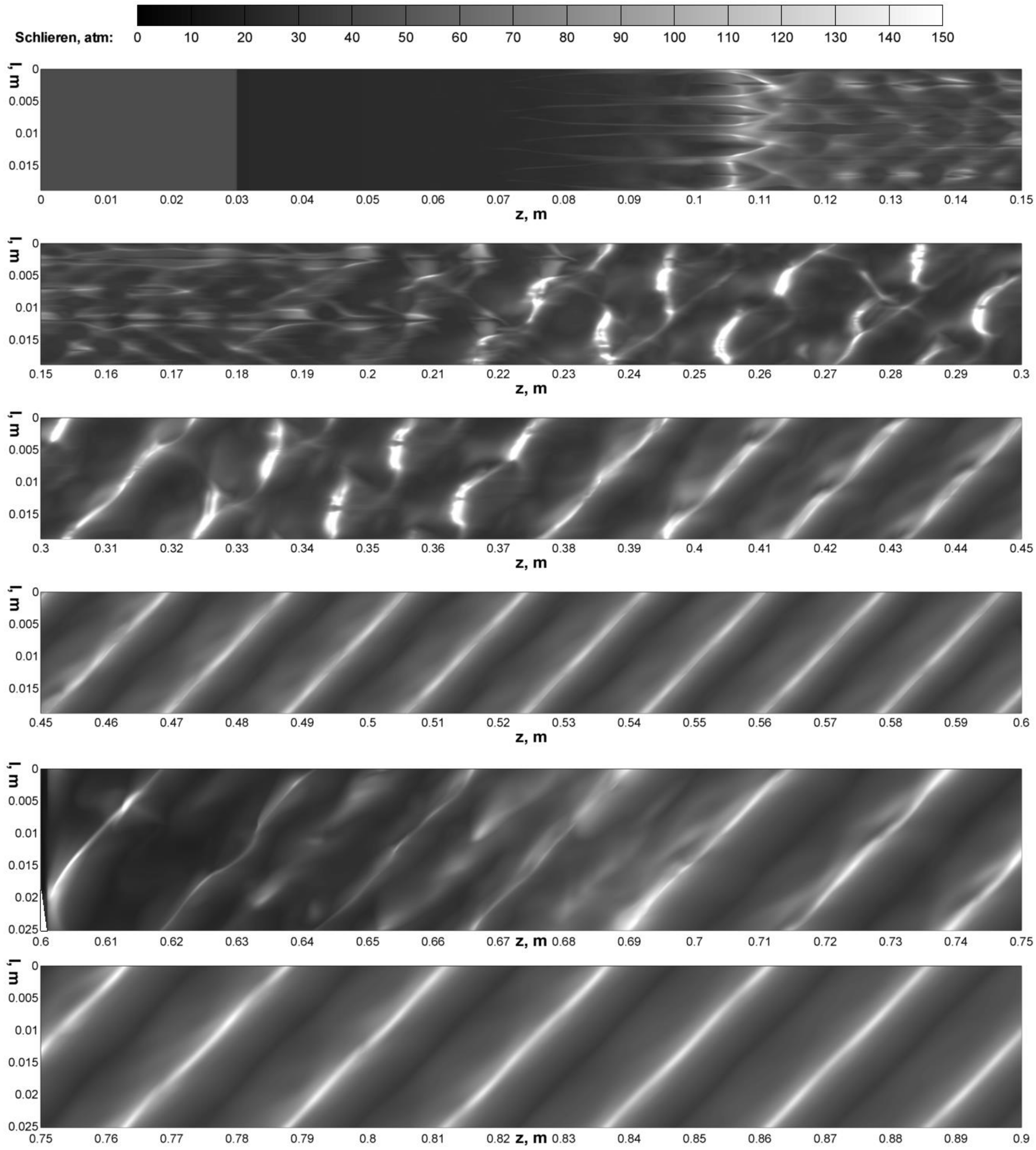

Fig. 8. Sweep of lateral surface with numerical soot foil diagram for the channel widened from 6 to 8 mm

6 Acknowledgements

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