# ADVANCED ATHLET MODEL FOR THE UPTF FACILITY S. Nikonov <sup>1</sup>, I. Pasichnyk <sup>2</sup> and K. Velkov <sup>2</sup>

<sup>1</sup> RRC "Kurchatov Institute", Russia <sup>2</sup> Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Germany

#### **Abstract**

The aim of the presented study is to determine the limits of application of the one dimentional system code ATHLET by describing in a pseudo 3D manner the thermohydraulic modelling of a reactor pressure vessel. For this purpose ATHLET simulation results are compared with available experimental data of the UPTF facility. Developed is a detailed ATHLET model based on a special preprocessor which is able to generate automatically a three dimensional nodalization of the facility. Based on this nodalization the preprocessor creates the necessary ATHLET input data set, including a description of the thermohydraulic objects and the connections between them. To take into account a spacial structure of interacting objects, advanced capabilities of ATHLET system code, namely cross connections in a system of parallel thermohydraulic channels are applied. Moreover in a new version of ATHLET several improvements are introduced: 1) an algorithm of the ATHLET Jacobian preconditioner is optimized; 2) a new direct sparse matrix solver based on the KLU algorithm of Tim Davis is implemented which gives a substantial acceleration of calculations for a large number of control volumes and makes feasible transient simulations with a detailed (ten thousands of control volumes) description of the investigated facility. The obtained comparisons have proved the advantages of the new modelling and applied computational algorithms and have confirmed the ability of the ATHLET code to describe in a pseudo 3D manner the thermohydraulic processes in a reactor pressure vessel.

#### Introduction

A development of an automated system of input data preparation for computer simulation tools aimed for numerical modelling of transients in complex thermodynamic systems (i.e. nuclear facilities with water moderator – VVER, PWR, BWR), such as, for example ATHLET, is caused by several reasons. Among them the main reason is an increase of the input data amount due to the desire to achieve more detailed description the parameter behaviour in the reactor volume. Especially relevant this task is for a coupled description of the thermodynamic and neutron-kinetic parameter distribution in reactor volume. The need to account for a coolant temperature and density feedbacks, when calculating with neutron-kinetic programs neutron fluxes in the active core of the reactor, demands higher requirements to the calculation of temperature and density fields both for a coolant and structural materials. Recently in several papers [1-6] describing coupled code system ATHLET/BIPR is shown a fundamental possibility of solving this problem for a case of coarse-grid partitioning model of the in-core space. In those cases to describe 3-dimensional distributions of thermohydraulic parameters the 1-dimensional system code ATHLET is used. ATHLET is able to account (with certain assumptions) for hydrodynamic coupling between parallel channels and for the neutron kinetic calculations the code BIPR8-KN is used.

Based on the experience with such 3-dimensional coarse grid partitioning, in which a coupling between control volumes in different directions of 3-dimensional space is described by a one-dimensional hydrodynamic code, a new methodology for creating design schemes of this kind is

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developed [7]. The main point of it is the software which automatically creates a three-dimensional description of all the necessary elements of the considered facility using such a degree of detail, which is based on the available documentation of the object, and which is necessary to solve the problem of facility modelling. It should be noted that a general approach in creating the initial data sets for different element types is rather difficult. This is due to the fact, that these elements can be quite different from each other and may represent different topological objects - rings, cylinders, ellipsoids of revolution, etc. and also derived from their crossing. In this regard, it is appeared to be more rational to use the object oriented approach, namely to assign every structure its class, the complexity of which depends on the complexity of the described structural unit. In this case, a set of input data for such preprocessor is simplified, and in some cases only general information for the group of elements is required from which group members can be constructed. This approach allows choosing a set of structures that describes an entire facility, which enables on the one hand, simpler approach to a creation of the input data block and, on the other hand, a very detailed description of every object. At this phase the main role is played by 3-dimensional analytic geometry, which determines the spatial coordinates of the chosen structure. The result of the program at this step is an ordered set of 3-dimensional coordinates, describing each item separately and the entire facility as a whole, and a set of characteristics of an object that can be used further for the automated preparation of an input data block for some thermal-hydraulic software, i.e. ATHLET. This block may include: the length of the object, elevation points, cross-sections of an object along the main flow, hydraulic diameter, a volume of an object, options for possible cross-connections in the transverse direction, etc. At the same time it is desirable to control the whole process of creation of 3-dimensional object with an available visualization tool

To achieve stability in the calculations, for such system code as ATHLET, the ratio of the control volumes of neighbour elements can not be larger as 2-3. In the current version of the preprocessor, all control volumes are created automatically, the actual control of control volumes length makes a user via input file of the preprocessor, which is taken into account during the process of automatic creation of the mesh.

At the next step an input data set, based on the results of modelling of facility objects, is automatically prepared. Control keys are inserted into the original input data set, which define section mark-up needed for the insertion of created data blocks. Mainly these sections for the ATHLET input file are given by the following control words (CW):

- PARAMETERS,
- TOPOLOGY,
- OBJECT,
- BORTRANS,
- REDEFINE,
- HEATCOND,
- ROD,
- GCSM.

Geometric properties of the objects are used partially or totally for the creation of input data sets. All data for all objects are saved into files labelled by corresponding CW's, which later are inserted into a main input data block. During this step all information which is previously located between the CW's is to be fully replaced. It is possible to replace only blocks of some special type of information for a particular CW. It is again desirable to control an automatic process of object creation with a visualization tool.

The presented approach is used in the current paper to study a specified transient in the UPTF facility [8]. At first the procedure to create the ATHLET input data set is described and in Section first results of the simulation are presented.

## 1. ATHLET input for UPTF facility

The objective of the UPTF tests is the full-scale experimental investigation of three-dimensional single and two-phase flow behaviour in the primary system of a PWR during ECC-relevant phases of a loss-of-coolant accident. The test program consists of integral tests for simulation of overall primary system behaviour and separate-effect tests for the in-depth analysis of thermal hydraulic processes in the subareas upper plenum, upper core tie plate, downcomer of the reactor pressure vessel (RPV) and primary system loops connected to the RPV.

The UPTF is a full-scale simulation of the primary system of a 1300 MWe pressurized water reactor nuclear power plant designed by Siemens, KWU Group. It contains all major components with the exception of the nuclear core, active pumps and real steam generators. The thermal hydraulic behaviour of the core is simulated with the controlled injection of steam and water. One of the four primary loops is used for modelling pipe breaks and is divided into hot and cold broken loop legs, both of which terminate in the containment simulator. A LOCA is simulated by opening the respective break valves. The ECC injection modes available in the UPTF allow the necessary experiments to be performed for the varying ECC concepts of German and US/Japanese PWR plants. Detailed description of the facility can be found in [8]

In preparing the data to the preprocessing program several assumptions that affect the description inside the RPV are made. In the lower volume of the facility that simulates the space of the lower plenum of the RPV, lower part of coolant injection devices into fuel assembly (FA) dummies is not modelled (in the real reactor, they are not available). Instead the porous approximation model is used which preserves the original volume according to the data given in [9]. Injection devices geometry is used to calculate local hydraulic resistance in in two mutually orthogonal directions: a flow along the vertical axis of the facility and a cross-flow, which determines the mixing of the coolant. In modelling the active zone the upper part of the injection device is also not considered. Instead a shortened model of the core is replaced by the real model with the elongation of fuel assemblies to the real value and the relocation of the upper core support plate at the level of its position in an RPV. The volume of the active core corresponds to the one given in [9].

During the modelling of the RPV internals, excluding inlet/outlet nozzles of the coolant tubes and control rods guiding tubes, the three main geometry types are identified:

- 1) Geometry characterizing a regular structure (Type 1) rectangular grid, formed by the FA's in the active zone. This is a system of parallel channels extending from the bottom of RPV up to the RPV cover. Each of these channels may have its own internal structure, which defines thermohydraulic properties of the channel, i.e. inlet and outlet part of FA, heat generating part of FA with spacers, guiding tubes for instrumentation, etc. At the same time the form of the channels grid during modelling remains constant.
- 2) To the second type (Type 2) belong elements, which are bounded on the one side by the system of parallel channels with rectangular grid, and on the other side by the vessel wall of the facility. An example of such structure may be elements forming lower plenum boundary or regions at the outlet nozzles.

3) The third type (Type 3) contains elements located between two cylindrical surfaces, i.e. a downcomer.

Figure 1 shows the left low corner of the RPV cross section at the level of the lower support grid. All three types of elements are presented with their numeration scheme, their edges and faces.

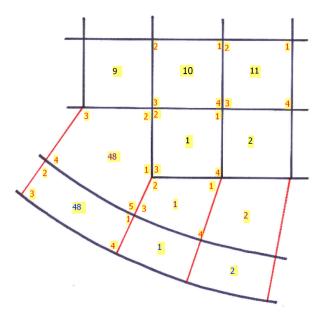


Figure 1 A general grid structure used to create objects. 10 – FA number, 48 – number of boundary element, 48 – number of element between two cylindrical surfaces, 1 – edge number.

An enumeration of the elements of the regular grid, formed by FA's and extending from the bottom to the top of the RPV, starts from the left FA of the lower row and goes to the right. An enumeration of the edges of this structure starts from right upper corner and goes further counter clockwise. i-th element face is placed between i-th and (i + 1)-th edges.

A construction of a boundary element is performed as follows. Through any two outer edges of any FA rays are carried out that connect these edges to centre of coordinate (this is a projection of edges on the plane and all constructions are performed in the plane). Then the rays are extended to intersect with the circle defining the outer boundary (inner boundary – FA faces lying between the selected edges) of the boundary element. Hence, one boundary element may be connected with several FA's or with one FA one or two faces. An enumeration of boundary elements can start from any selected element and goes counter clockwise. Figure 1 explains that boundary element "1" starts from the first FA and connected only with the first FA. The boundary element "48" is connected to "1" and "8" FA's. The creation of the elements of third type as well as the enumeration of edges and faces of second and third element types is also shown on Figure 1. The entire structure basically goes through the whole RPV from the bottom to the top. The outer elements geometry does not change, only its internal structure changes. Type 2 and Type 3 elements geometry can be changed according to the changes of the outer boundary elements diameters. But their relative position remains the same.

With regard to the construction of nozzle elements, their formation, on the one hand predetermined by the partition of the downcomer (or of the upper plenum) on the elements over a circle and is related to the formation of boundary elements. On the other hand, a nozzle partitioning in the vertical direction determines a nozzle elements grid as well as makes the grid partitioning for nozzles inlet and outlet.

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As a result of the pre-processor work at the first step the geometric 3-dimensional objects as well as a file with input data for the visualisation package are created, which enables a 3-dimensional graphical representation of the facility as a whole or of its complex cross section. Further the preprocessor forms files, which contain ready-to-use information for the following sections of an ATHLET input file:

- PARAMETERS,
- TOPOLOGY,
- OBJECT,
- BORTRANS,
- REDEFINE.

It should be noted that in describing the topology of objects, determining their relationship with each other, for parallel channels with a free boundary the interaction in the transverse direction on all faces of objects are taken into account. At the same time for each of the already formed ATHLET objects a graphical file is created.

Any changes in the real geometry of one of the facility structures or a modified detalization in a description of a group of similar objects (i.e. to make a partition for downcomer smaller or, conversely, larger in the tangential direction) requires a substantial change in an ATHLET input data. On the contrary, the current approach requires only small changes in the preprocessor input file, which specify a new system of boundary elements creation, how many they are and how they are connected to FA's. New objects together with a new topological scheme related to the required are automatically created. It is clear, that it affects not only a downcomer but also elements of the lower plenum, nozzles and etc. An overhead can be estimated as several minutes to change input data for the preprocessor and a few seconds of preprocessor work to obtain a ready ATHLET input data set. Without a preprocessor this work is very tedious and requires a lot more time. Hence, the new approach enables to carry out investigations of model sensitivity and build a most suitable scheme for each particular case.

To control a creation of 3-dimensional objects a graphical package written in FORTRAN with OpenGL library is used [10]. Figure 2 shows general and top view of the UPTF facility. The structure of the main elements of object creation is clearly seen. On Figure 3 relative positions of objects are presented and Figure 4 gives a view of some primitive objects used in the modelling.

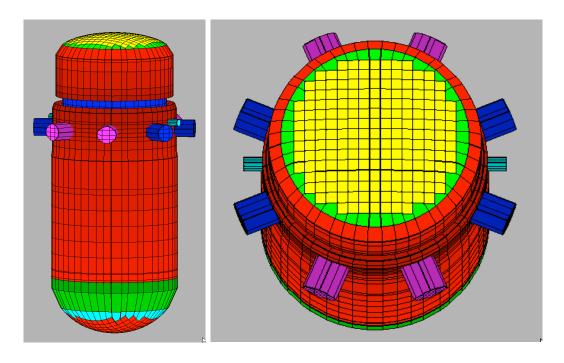
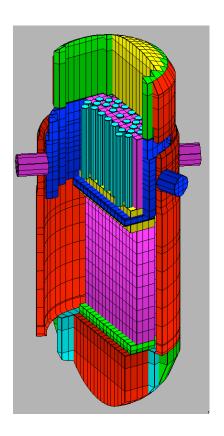


Figure 2 General view and top view of UPTF facility



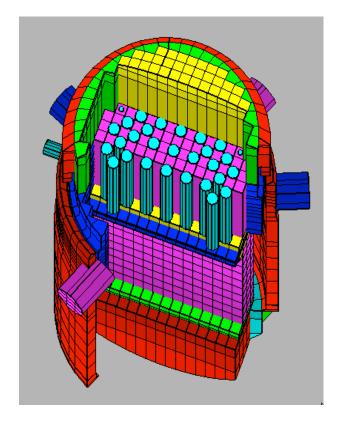
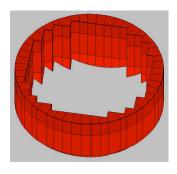
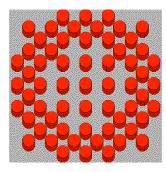


Figure 3 Complex intersections from different angles





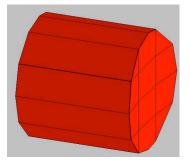


Figure 4 Objects used in the modelling of UPTF facility. From left to right: Lower Plenum Boundary Elements, Upper Plenum Shielding Tubes, Inlet Nozzle

### 2. UPTF-TRAM Test C3

To test the new scheme the C3-13A experiment is taken. The UPTF-TRAM Test C3 was carried out to investigate the mixing of low borated condensate with the highly-borated ambient water during reflux condenser mode of operation following a "Small Break Loss of Coolant Accident" (SB-LOCA). In the experiment C3-13A at some initial point (temperature of system 74°C, pressure in the RPV outlet 1.435 MPa) the hot water from JNG system ("Notkühleinspeisesystem", Emergency Cooling System) is injected into all cold legs and cold water from NKW system ("Notkühlwasser", Emergency Cooling Water) is injected into cold leg 2. Drainage goes through hot leg 4, other legs are disconnected from the system. The water mixture (comprising ECC water and hot water)

flowing into the RPV downcomer from cold leg 2 forms a cold water plume. In the upper part of the downcomer the water is thermally layered outside the plume and there is a significant temperature difference between this water and the cold water plume. The intensive mixing of the cold water with the surrounding hot water results in an azimuthally uniform temperature profile without a plume present at and lower than 3300 mm below the lower edge of the cold leg, and a relatively uniform temperature throughout the entire height. Figure 5 and Figure 6 show initial boundary conditions for mass flow, temperature and pressure of the coolant. On Figure 7 the location of detectors is presented.

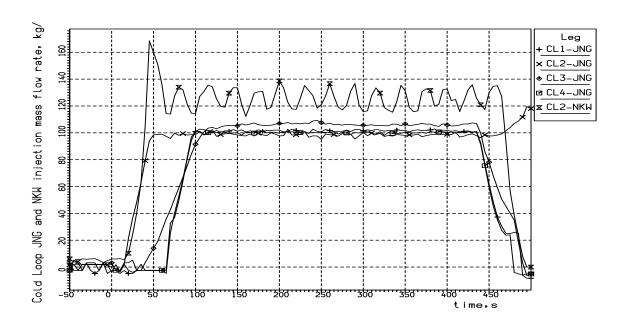
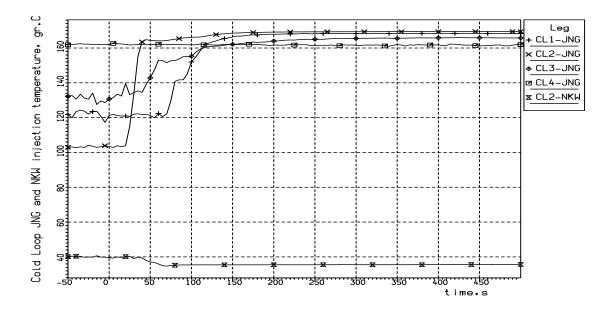


Figure 5 Cold water injection (experiment)



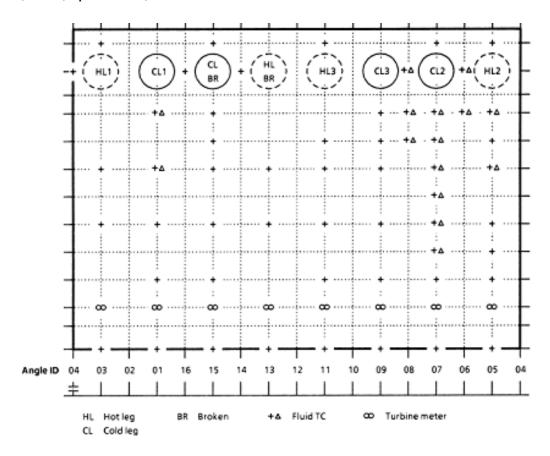


Figure 7 The location of measuring instrumentation for temperature and coolant velocity

#### 3. Results

The total ATHLET model of UPTF facility contains 4089 objects, 13205 control volumes and 15604 connections (junctions). The total time of the transient is 500 sec. Calculations are performed using a new version of ATHLET with an optimized matrix solver [11]. The simulation of the C3-13A experiment is performed on Intel Xeon CPU L5420 2.5 GHz architecture and the CPU time is given in Table 1

Table 1

# **CPU Timing**

# of time steps	1043
Total CPU time	12969 sec
Martix optimization	~36% of total CPU time
Transient CPU time	~64% of total CPU time

On Figure 8 to Figure 11 the comparison of experimental and calculated data for temperature and velocity distribution are presented. The axial levels correspond to nodes where thermocouples and turbine meters are located (see Figure 7). AngleId = 7 corresponds to region of maximal mass flow (along the axis of cold leg 2); AngleId = 15 corresponds to the region of maximal distance from cold leg 2, and AngleId = 11 is taken as an intermediate value between AngleId = 7 and AngleId = 15. One

clearly sees that there are some quite strong discrepancies in the initial state for some axial levels. This is due to nonuniform temperature distribution in the facility in a steady state. According to the description of the experiment the initial temperature distribution must be uniform, but in reality, this is not observed. Apparently, the required steady state has not been reached in reality before the start of the transient. To take into account this nonuniformity, it is planned to use interpolated values of measured temperatures directly in the simulation. Qualitatively, the experimentally measured temperature distribution is described fairly well for all nodes of the experimental grid. At first glance quantitative differences are due to the uncertainties of the initial state and, to a greater extent, due to the uncertainty in the bypass mass flow between the downcomer and the upper plenum in the region of hot leg nozzles. The reliable information about the cross section area of the bypass and he mass flow through it is not available. Several calculations are performed attempting to estimate indirectly this value. Based on estimations given in [8] two limiting cases for minimal and maximal bypass are considered. It appears that the effect of the bypass is quite substantial which is clearly seen from Figure 8 to Figure 11. Similar to the temperature distribution, the velocity distribution (see Figure 11) shows a strong dependence on the bypass value. Since at AngleId=7 an intensive mixing of the cold water with the surrounding hot water takes place, the current model can predict only the trend value of the flow velocity.

#### 4. Conclusion

First results of simulation of UPTF facility, using new detailed nodalization scheme together with optimized ATHLET matrix solver, are shown. In this paper, it was not intended to investigate the process in detail. The main task was to work out a method for constructing a 3D nodalization scheme of ATHLET system code and its subsequent validation on a 3D experimental thermohydraulic data. In the future the sensitivity of the model to various changes in the initial and boundary conditions will be analysed. It is also expected to add, using the preprocessor, the model of turbulent exchange in a system of parallel channels for a downcomer region. Currently ATHLET is able to calculate only convective cross flows in the system of coupled parallel channels.

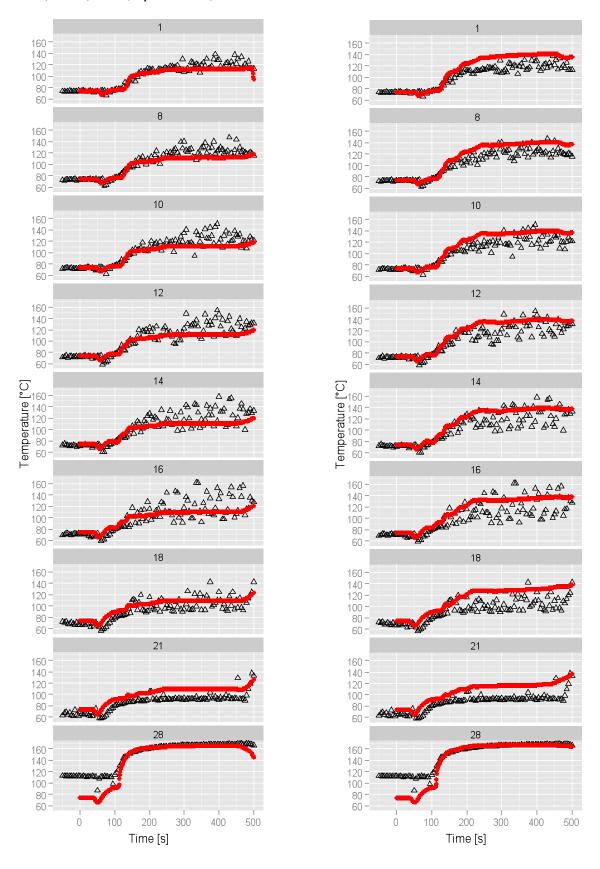


Figure 8 Temperature distribution for AngleId = 07 and for several axial levels. Left – maximal, right – minimal bypass correspondingly. Red line – simulation, triangles – measurement.

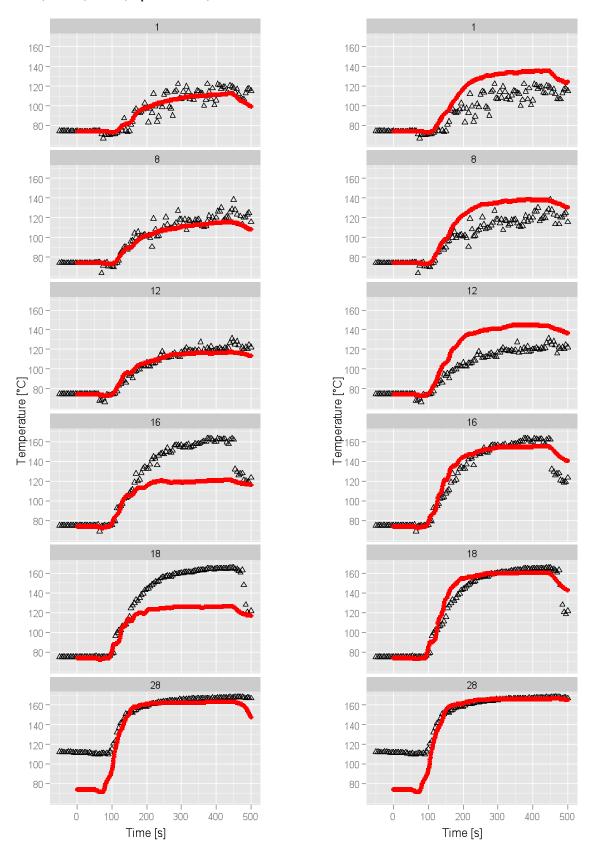


Figure 9 Temperature distribution for AngleId = 11 and for several axial levels. Left – maximal, right – minimal bypass correspondingly. Red line – simulation, triangles – measurement.

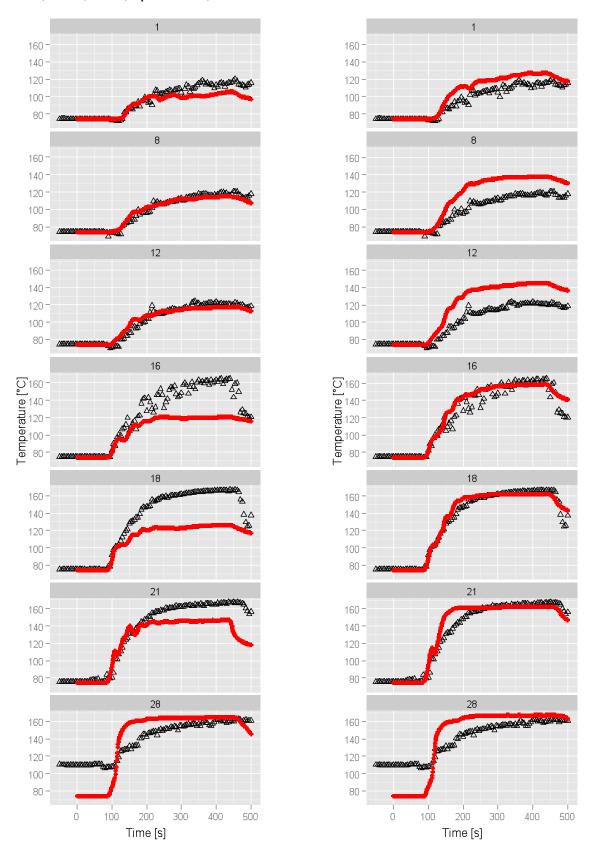


Figure 10 Temperature distribution for AngleId = 15 and for several axial levels. Left – maximal, right – minimal bypass correspondingly. Red line – simulation, triangles – measurement.

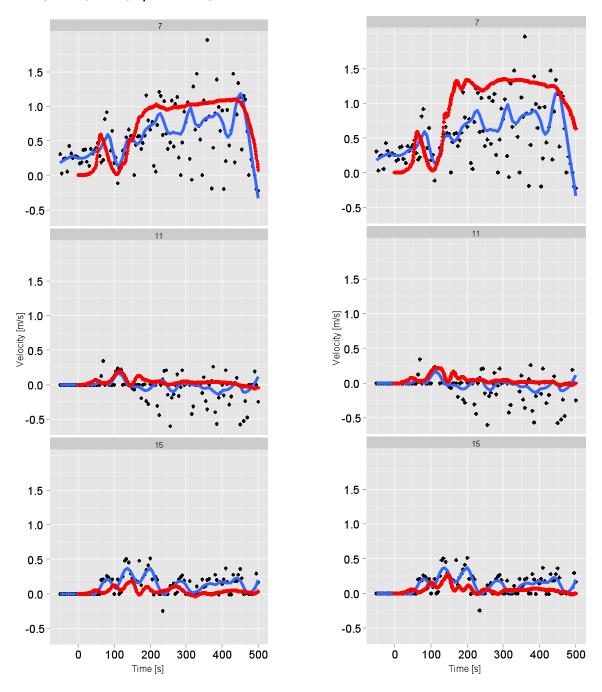


Figure 11 Velocity for AngleId's = 07, 11 and 15. Left – maximal, right – minimal bypass correspondingly. Red curve – simulation, triangles – measurement, blue curve – local polynomial regression fitting (loess) of measurement data with span=0.15.

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