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POOL CFD MODELLING: LESSONS FROM THE SESAME PROJECT

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ABSTRACT

The Computational Fluid-Dynamics (CFD) modelling of Heavy Liquid Metal (HLM) flows in pool configuration is investigated. We describe how the argument is treated within the SESAME project in its specific work package. The work package structure, based on a systematic approach of redundancy and diversification, is explained along with its motivation. The main achievements obtained and the main lessons learned are illustrated.

The paper focuses on the strong coupling between experimental activity and CFD simulation performed within the SESAME project. Two HLM fluids are contemplated: pure lead and Lead-Bismuth Eutectic. The objective is to make CFD a valid instrument in support to the design of safe and innovative Gen-IV nuclear plants.

Some effort has also been devoted to a highly challenging and innovative approach, the Proper Orthogonal Decomposition (POD) with Galerkin projection modelling, potentially able to cover some CFD applications at a much lower computational cost. To reach sufficient maturity, the method requires however input from sufficiently complex CFD simulations such as those produced in the present context.

Dedicated experimental campaigns on heavily instrumented facilities have been conceived with the specific objective to build a series of datasets suited for the calibration and CFD modelling validation. In pool configuration, the attention is focused on the balance between conductive and convective heat transfer phenomena, on transients representative of incidental scenarios and on the possible occurrence of solidification phenomena.

Four test sections have been selected for the dataset production: (i) the CIRCE facility from ENEA, (ii) the TALL-3D pool test section from KTH, (iii) the TALL-3D Solidification Test Section (STS) from KTH and (iv) the SESAME Stand facility from CVR. While CIRCE and TALL-3D were existing facilities, the STS and SESAME Stand facility have been conceived, built and operated within the project, heavily relying on the use of CFD support.

Care has been taken to ensure that almost all tasks were followed by at least two partners. We show on specific examples, how this strategy has allowed to uncover flaws and overcome pitfalls. We give an outlook on the work performed, the results achieved and remaining or new uncovered issues.

We conclude by opening to an upsized natural target application: the construction of the Gen-IV ALFRED CFD model and investigation on variants of its general circulation.

1. INTRODUCTION

In continuation from several European Projects from the 5th Framework Program (FP5) on, the SESAME project (2015-2019) supported the development of European liquid metal cooled nuclear reactors (Roelofs 2015, 2016). Within this project, a work package (WP) labelled "Pool Thermal-hydraulics" had the objective to qualify the CFD as a valid instrument for the design, control and analysis of the complex flow patterns of the primary system of liquid cooled reactors in pool configuration.

While the objective is clearly defined, the route to achieve it is quite lengthy and articulated. The CFD tool has not the goal to replace the system codes but is intended to complement them. Both tools occupy different regions of the space of investigation. CFD has to occupy its right place, whose extension is evolving in time due to the increase of available computational power and the progress of modelling.

The complexity of the physics, the geometry, the space and time scales involved is such that only RANS modelling will be considered with basically two equations turbulence models. We are well aware of the inherent limitations of such approach, at least partially compensated by the extensive use of experimental data.

To be validated, the CFD tool results must be compared with experimental data. Moreover, the experimental data must be produced so as to be usable for comparison with CFD. It is therefore important that the experimentalists get in due time some feedback on their results and take into account indications from the CFD results. In order to promote a common knowledge and understanding, both experiments and CFD have been pursued in parallel and in collaboration.

This paper will not look through the main technical achievement details or CFD modelling improvement. This is and will be treated elsewhere. Rather, it will give a general overview of the WP structure, organization and the rationales behind them. The conceptual objectives are then declined in a list of practical objectives, still taking into account a mitigation of potential risks. We shortly present the facility used and/or conceived during this work and which have conditioned all the numerical activity. Then we illustrate the process of interaction between partners with a list of issues that have been overcome thanks to this interaction.

2. WORK PACKAGE STRUCTURE

2.1. Redundancy and diversification

The WP is essentially built on a partially redundant and diversified structure. Redundancy improves the global safety of the project prosecution by maintaining the possibility to redirect consistently some constrained activity upon input failure. It promotes a high level of collaboration and exchange of know-how. It drastically reduces the probability of remaining stuck for a long time by some technical issue, simply by having access to other partners practice.

Redundancy regards:

- Experiments: two experiments per kind
- Data sets: two data-sets per kind
- Pre-test CFD models: performed by two partners for each experiment
- Post-test confront and CFD validation: performed by at least two partners
- Modeling extrapolation to nuclear reactors: performed by two partners.

Diversification regards:

- Experiments focus: consistency of the thermal-hydraulic loop vs. capture of solidification front
- Experiments size: from a few litters to several cubic meters
- Experiment facilities: both existing and new, or at least new test sections
- Carrier fluid: both lead and lead-bismuth eutectic (LBE)
- Software: commercial STARCCM+ and FLUENT or in-house PSI-BOIL
- Theoretical modeling consideration vs. effective model implementation, mainly with regards to solidification
- Development and testing of a new CFD approach, the Proper Orthogonal Decomposition Reduced Order Method (POD-ROM).

Diversification allows complementary information to be extracted from otherwise similar activities. No two partners produce the same results with the same means and each one brings a complementary added value. This brings positive emulation between partners rather than mere competition. It is also clear that using existing experimental facilities is safer and faster than conceiving, building and operating a brand new facility or a new test section.

2.2. Conceptual objectives

The global objective of the WP is to qualify CFD as a valid instrument for Gen-IV nuclear reactors design. In order to reach this goal, several intermediate objectives are pursued:

- Reach operability on relevant experimental facilities, sufficiently instrumented and operate successfully these facilities
- Generate consistent data bases
- Model the experimental facilities by means of CFD during the pre-design, design phase and experimental campaign definition
- Run successfully the CFD model, possibly giving useful input during the design phase
- Run the CFD model with the more similar possible operating conditions of the experimental campaign
- Manage to use the relevant experimental results from the databases for a comparison with the numerical results and analyze the possible discrepancies
- Improve the numerical model and/or reinterpret the experimental data
- Hopefully validate the numerical models
- Highlight remaining issues
- Consistently extrapolate the numerical models for real-size nuclear design

2.3. Practical objectives

Going from conceptual to practical, from the experimental point of view, the WP objectives become:

- Operate the CIRCE facility at ENEA to generate a database from a dedicated experimental campaign
- Operate the TALL-3D facility at KTH and extract from the database the relevant data of the 3D test section
- Conceive, build, instrument and operate a new facility, to be later named SESAME-Stand, at CVR, to investigate the solidification front propagation in a buoyancy driven pure lead pool. Generate a comprehensive database

- Conceive, build, instrument and operate a new or modified test section of TALL-3D, later called the Solidification Test Section (STS), to investigate the solidification front propagation and stability of Lead Bismuth Eutectic (LBE) under various forced flow conditions. Produce the related database

From the numerical point of view, the WP objectives become:

- Build the CFD model of the 3D test section of the TALL-3D facility and of CIRCE, developing know-how and getting technical confidence with all the relevant aspects of the simulations.
- Make numerical pre-tests, post-tests, confront and validation from experimental results.
- Support the conceptual, pre-design and design phase of SESAME-Stand and STS with preliminary (often simplified) simulations.
- Investigate the theoretical and technical issues relative to the incorporation of the solidification feature in a CFD simulation.
- Combine the new solidification features with the now consolidated thermal pool modeling to build and operate a CFD model representative of SESAME-Stand and STS experimental campaigns.
- Confront the experimental and the numerical results, focusing on the front position or propagation. Hopefully, validate the numerical model now upgraded with the solidification representation.

At it can be seen, there is a strong coupling between the experimental and the CFD activities. In Table 1 we describe this coupling on the experimental facility basis. It must be empathized that also the entire WP is coupled with other WPs and, in particular, the experimental part is coupled with numerical simulations of other types such as system-code and coupled CFD-system code simulations.

Table 1: Partners involved in relation to the experimental facilities.

Experimental Facility	Data base	CFD pre-tests	Post-test foreseen	Post-test effective
CIRCE	ENEA	CRS4-NRG	CRS4-NRG	CRS4-NRG
TALL-3D	KTH	KTH-CRS4	KTH-CRS4	KTH-CRS4
SESAME-Stand	CVR	CVR-CRS4	CVR-CRS4	CVR-CRS4-KTH
STS	-	KTH-CRS4	KTH-CRS4	-

3. RISK EVALUATION AND MITIGATION

3.1. Data base release

The four foreseen experiments are characterized by a quite different level of risk. The classical thermal pool investigations were considered very safe or quite safe.

The CIRCE experiment was considered as very safe because a similar experiment had already been conducted so that, in the worst case, data from the former experiment would have been used for the CFD modelling. And in fact such data have been used for the preliminary model setting during the initial pre-test-activity. The CFD modelling is quite demanding but CIRCE is conceptually a reduced scale mock-up of a MYRRHA like design which has already been successfully simulated. So, most of the technical difficulties have already been solved.

The TALL-3D experiment was considered as quite safe. The first two legs of the facility had been already largely operated. The third leg was already built and coupled to the rest of the facility but not yet tested. There was no backup solution for the data. The 3D test-section is quite more simple than CIRCE, so the CFD modelling was expected less difficult.

Instead, the solidification investigations were considered much more risky. Only PSI had a practical experience on freezing but its in-house code was 2D and restricted to very simple geometries. The effective possibility to implement solidification in commercial code for relatively complex geometries was totally unknown. From the experimental side, almost everything had to be invented from scratch. A critical point was to find convenient ways to track the solidification front.

With regards to the KTH solidification experiment. The initial idea was to use the existing 3D test section of TALL-3D or a variant of it and to use Ultrasound Doppler Velocity (UDV) sensors developed by HZDR and that should be adapted and customized for the solidification specificity. To ensure the compatibility of the test section with the UDV sensors, a strong collaboration between KTH and HZDR had to be established, with an efficient communication channel.

CVR was already operating a small Pb-Li loop, named MELILOO and the initial idea was to build up on this loop to adapt it for a solidification experiment. The entity of the modifications was initially unknown and was to be defined during the first part of the project. The carrier fluid was to be changed and the experiment was required to give complementary information with regards to the KTH one.

In fact, enforcing a valid balance between redundancy and diversification was the first challenge to bring contemporaneously for the definition of the two solidification experiments.

3.2. The POD-ROM modelling development

The POD-ROM approach to CFD, proposed by KIT, is in its very early stage of development and highly challenging. Its potential or expected results were therefore not required by other partner activities. Instead, it was free to progress, having at any time access to the available databases and to the pre-test and post-test simulations. This is in order to keep in mind the medium term objective which is to provide a fast alternative to CFD for nuclear applications requiring parametric studies with a large number of test cases.

4. THE EXPERIMENTAL FACILITIES

4.1. Time line

From the past experience, a common issue with regards to coupled experimental-numerical activity is that the experimental activity terminates too late and there is no time to compare the results or at best only time to acknowledge the discrepancies without possibilities to investigate and understand their origin. We definitively need to keep time to allow some understanding of the discrepancies, to improve the modelling and to check/validate the improvement. So, it was important that the experimental activity was scheduled as early as reasonably possible. More exactly, it is important that the first data are produced and shared as soon as possible.

We now present the experimental facilities involved in the WP together with the experimental campaign that were foreseen and possibly realized to produce the necessary data bases.

4.2. CIRCE

The facility is located in the Brasimone ENEA centre and is illustrated in Figure 1. It contains several tens of tons of LBE and the forced circulation is driven by Argon injection (gas-lift). In the context of this activity, its fuel pin simulator (FPS) has been used up to 750 kW, the heat exchanger is double wall bayonet type with helium gap and there is an Air DHR. The dedicated experimental campaign aimed at reaching forced flow high power steady states and at making transition to reduced power natural convection, reproducing the main features of a PLOF incident.

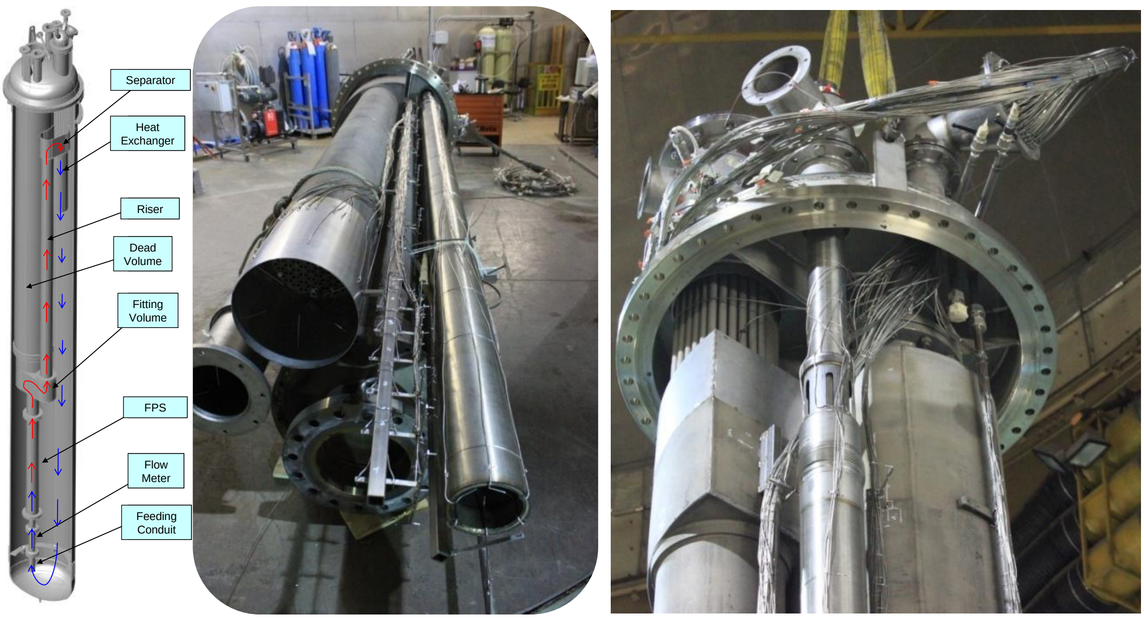

Figure 1: CIRCE facility from ENEA. Left, functional sketch. Components above the fitting volume (center) and at the top (right). Source: ENEA.

4.3. TALL-3D

The facility, 6.8 m high, is located at KTH and operated with LBE, see Figure 2. While initially composed of two legs, KTH has installed an additional hot leg with a 3D test section, introducing a 3D pool behaviour in the list of the phenomena which can be addressed in the facility. The experimental campaigns performed with the 3D pool test section investigate mixing phenomena and possible thermal stratification likely to appear also in pool-like lead-cooled reactors.

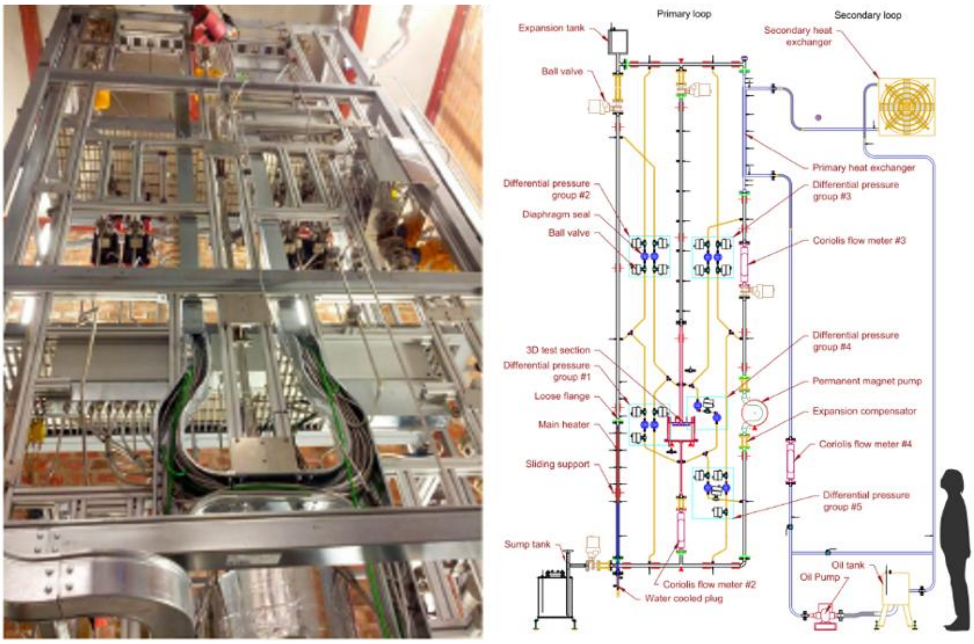

Figure 2: TALL-3D facility by KTH. Left, facility. Right, functional sketch. Source: KTH.

4.4. SESAME-Stand

The facility (Iannone 2017, Melichar 2019), shown in Figure 3, is operated with pure lead in natural convection. It has a mostly axial-symmetrical shape, with four heaters near the axis and cooled by an external controlled air flow. An internal obstacle separates the internal heating from the external cooling. The experimental campaigns aim at studying the appearance and evolution of a freezing front with different internal obstacles, at different power and air flow rate.

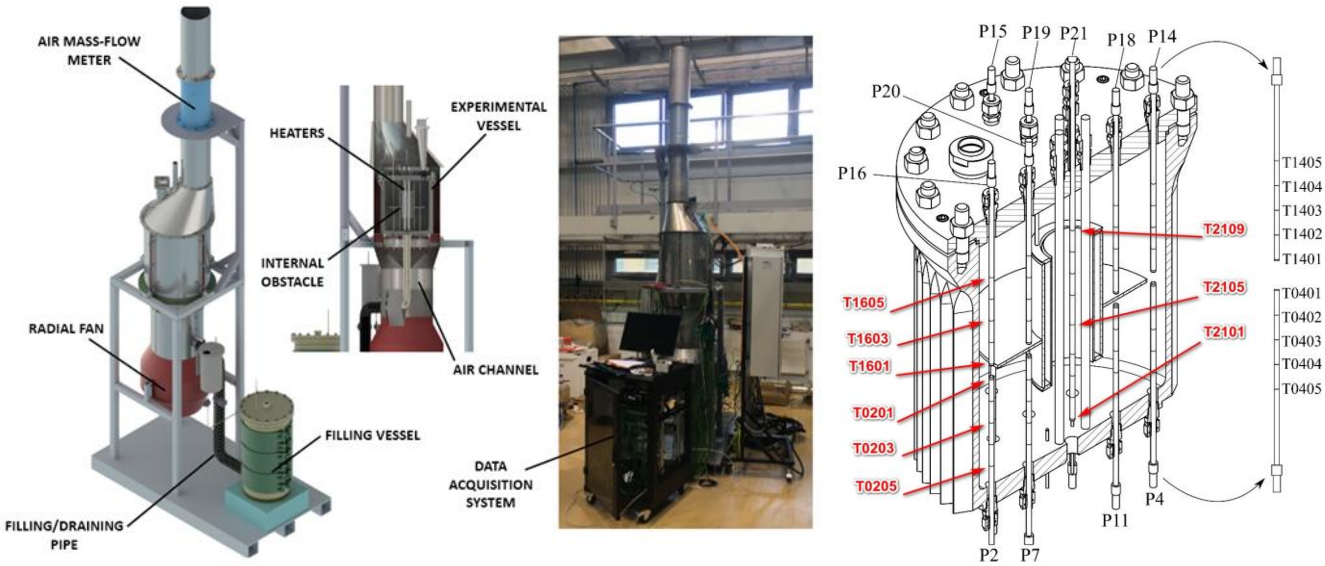

Figure 3: SESAME-Stand facility by CVR. Right, CAD design. Center, real facility. Right, main vessel design with TC positions. Source: CVR.

4.5. STS / HZDR-pool

The STS was designed to be installed in the hot leg of the TALL-3D facility of KTH (Jeltsov, 2018). It is a square box 20 cm large and 50 mm deep with decentred inlet and outlet. It was thought to be operated in turn with three different sets of instrumentation: (i) TCs for temperature measurement outside and inside the pool, (ii) FBGs for temperature measurement inside the pool and (iii) UDVs for measurement of the LBE flow velocity and location of the solidification front, as illustrated in Figure 4.

The design and manufacture of the UDV probes to be installed in the STS was to be performed by HZDR. Facing a number of open questions and issues concerning the solidification front measurement, HZDR decided to build its own instrumentation pool experimental facility, illustrated in Figure 5.

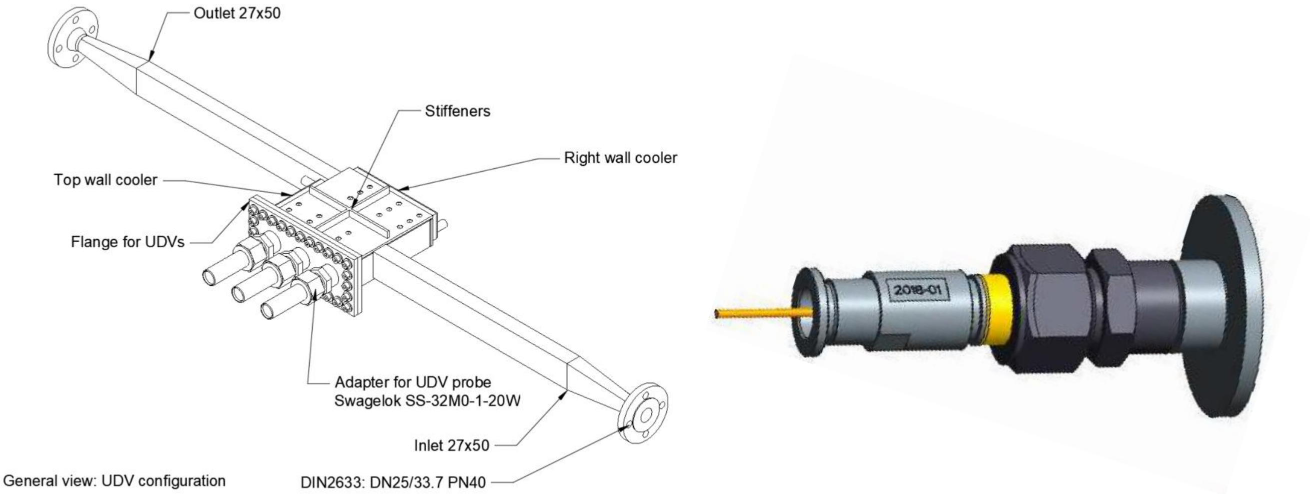

Figure 4: Left, final design of STS from KTH in configuration with UDVs from HZDR. Source: KTH. Right: UDV socket with installed transducer mounted at test section. Source: HZDR.

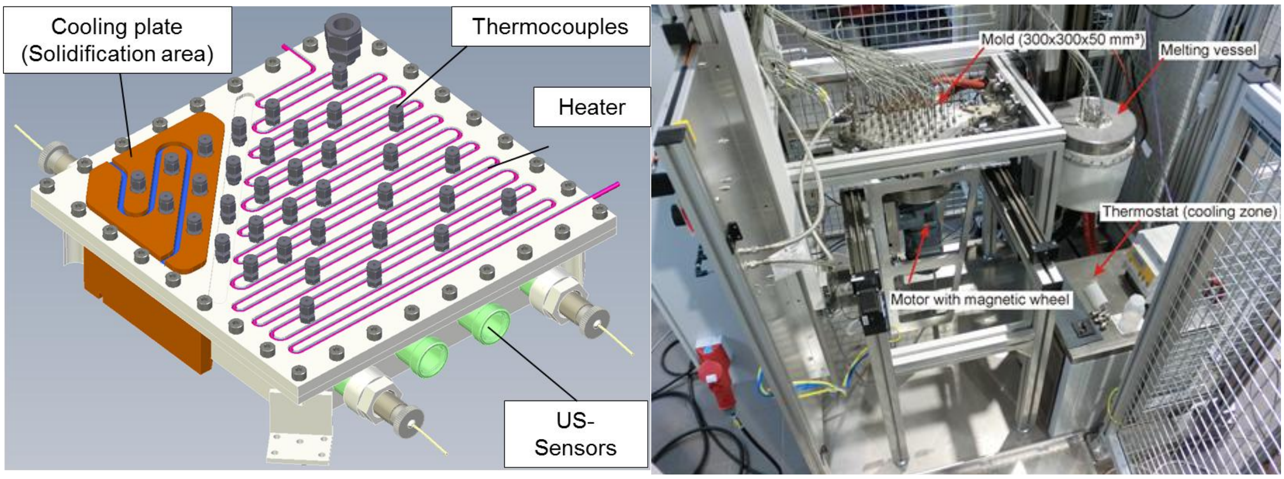

Figure 5: HZDR pool solidification facility for instrumentation testing. Left, pool design. Right, facility. Source: HZDR.

5. PITFALLS OVERCOME AND CROSS FEEDING

In this section, we give a few examples of problems solved or overcome thanks to an exchange of information or practice. As for many human activity, non-trivial CFD simulation is very demanding when practised in absolute for the first time. Knowing of the mere existence of successful similar simulations provides more confidence and in fact greatly speeds the construction process. It must be stressed that it is very easy to get stuck with modelling or CFD implementation on a particular issue while the solution or at least a sufficiently reasonable solution is, a fortiori, simple and/or obvious.

We illustrate with several examples the strong added value that a really collaborative behaviour brings.

5.1. The solid LBE thermal conductivity issue

From a bibliographic research performed by PSI to gather in one single working document the relevant physical properties of the main materials, it appears that there was no consistent data on the thermal conductivity of LBE. This is in relation with the observation that LBE is not stable in solid form and slowly separates in single components crystals in a process lasting several months.

So, how could we make a sound CFD model without this data? Other than PSI, only CRS4 and KTH are involved in the LBE solidification simulation. In fact, in the meantime, KTH had performed plenty of pre-design simulation. The partners asked how KTH did and where they got their data. There was no data, they simply took the value of liquid LBE at solidification temperature. In fact, this is more than sufficient and allows to start practising.

The thermal conductivity of solid LBE however still needs to be investigated.

5.2. Initial condition dependence of steady-state CIRCE model

The CIRCE facility is quite complex and it is good practice to start with cold flow steady-state. Then the model progressively incorporates thermal features. The first thermal feature is to implement in the energy equation a source term in the Fuel Pin Simulator, reproducing an experimental test case, and a sink term in the Heat Exchanger. Doing so, one partner noticed that the converged solution depended strongly on the initial condition and also on the solver parameters, such as the CFL number or the convergence tolerance. In fact, with adiabatic external boundaries and constant and opposite energy source terms, the system works at constant total energy content which is the initial one apart from the error introduced during the non-physical iterations towards the steady-state. Having a past experience with such closed systems, another partner had already been faced with this issue and had solved it by setting the sink term dependent on the LBE temperature in the HX. So, active collaboration has saved a lot of efforts because at this stage of the modelling it is very natural to enquire rather on meshing or convergence issues.

5.3. Small CIRCE improvement

The first CFD results from CRS4 on CIRCE where not satisfying. The real thermal stratification was not captured. At this time, it became clear that this thermal stratification was the result of a delicate balance between small intensity heat fluxes, mainly of conductive nature, or from small convected flows. So, several possible reasons have been investigated.

i. Some bypass flow could occur by droplet splashing from the flow separator, as shown in Figure 6 (left).
ii. The connection between the riser and the separator was not sealed allowing a possible small leakage.
iii. The opening made to insert the thermocouple wires on the FPS could lead to a separate local buoyancy driven flow (see Figure 6, center).
iv. There is a volume in the conveyor, close to the fuel simulator bundle exit where gas remains probably trapped during LBE filling (Figure 6, right). What happens in the long run to the gas cavity created is unknown. As a result, the thermal behaviour of this volume is also unknown.

Once these possible issues spotted, corrective actions have been taken when feasible at the first refurbishing of CIRCE: (i) the flow separator lateral wall has been extended upward, (ii) the riser top has been sealed to the flow separator and (iii) the holes have been mostly plugged, still allowing LBE to enter at filling but almost eliminating any associated local buoyant flow. Nothing was done on the forth item because there was no simple practical solution found.

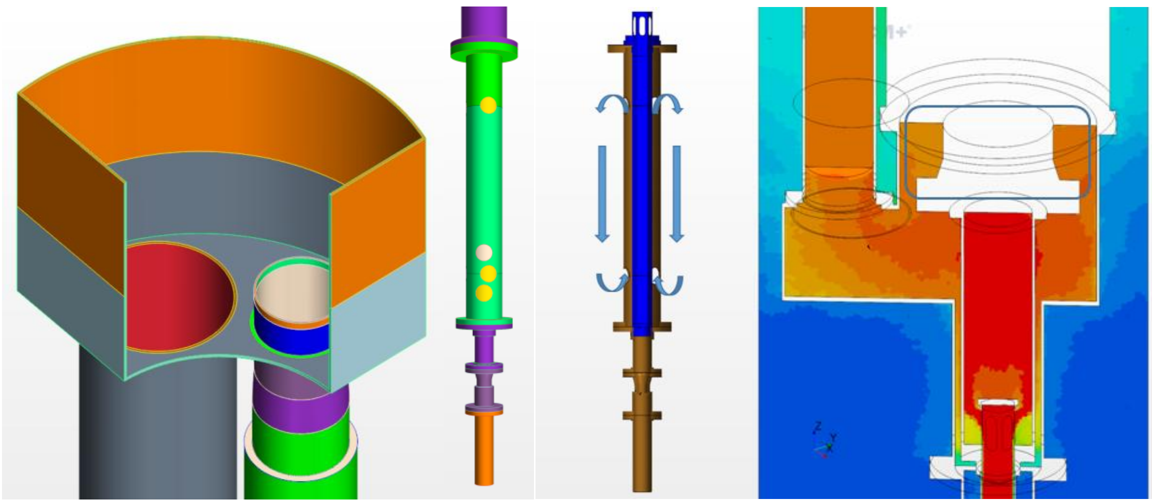

Figure 6: Illustration of small CIRCE improvement. Left, separator: in orange, added lateral wall. Centre, FPS lateral openings and possible buoyant recirculation pattern. Right: temperature in conveyor with indication of possible trapped gas region

5.4. STS water cooler

The STS from KTH has been designed with the support of many numerical simulations in parametric studies, see Figure 7. This allowed to came with a pre-final design. The design was then checked numerically by CRS4, and a flaw was discovered, not with the LBE vessel on which KTH focused its attention, but on the water cooler side. For heat balance measure and calculation, the temperature of the water must increase by more than 10K. This imposes restriction on the water flow rate. Simulation of the design showed a wall temperature up to 160 C and thus predicted an onset of boiling. We prefer prevent this to appear because it makes the simulations much more complex and questionable. Several attempts have been performed in parallel and in collaboration between KTH and CRS4 to remove the issue. Then KTH came out with an improved cooler design, checked again numerically by both organizations and avoiding boiling.

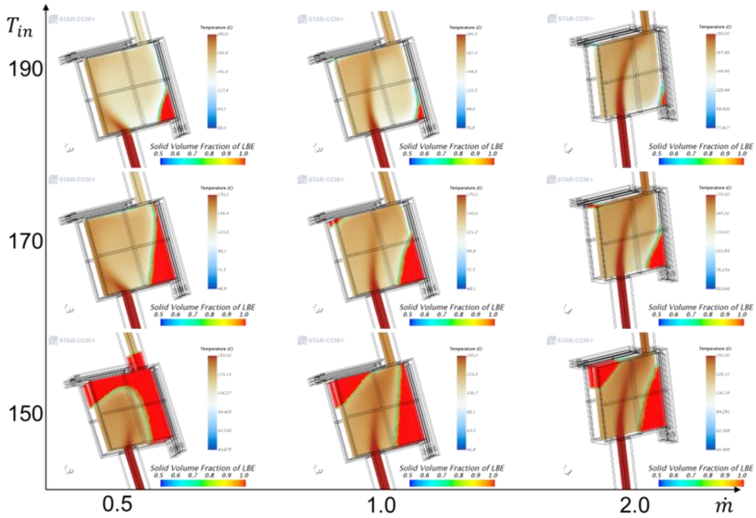

Figure 7: STS Pre-test parametric study performed by KTH: frozen fraction depending on inlet temperature and mass flow rate

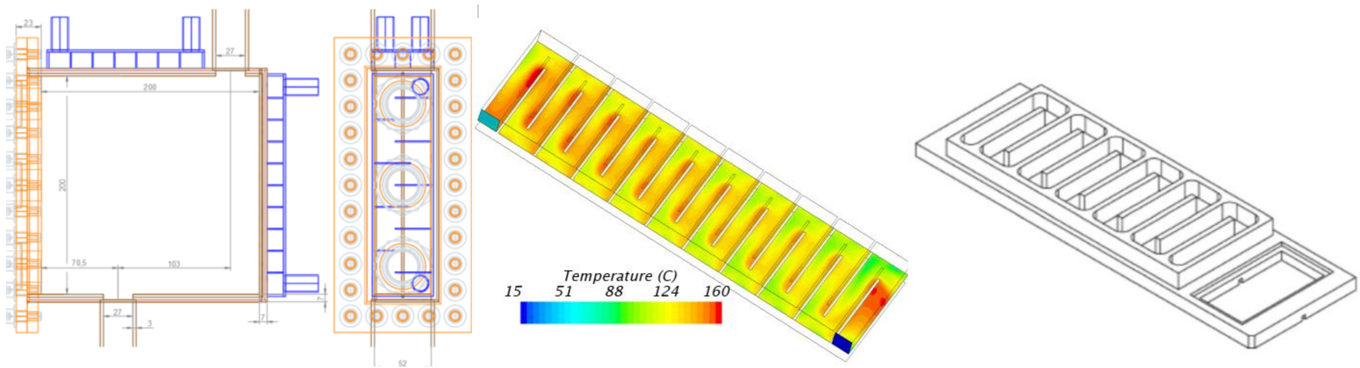

Figure 8: STS design with the water coolers leading to local boiling. Left, design. Centre, wall temperature. Right, improved design.

5.5. Spotted almost stagnant velocity field issue

The 3D-simulations of the SESAME-Stand pool performed by CRS4 tended to exhibit a very small intensity and stable strange spotted behaviour in the stagnant or very small velocity regions, as shown in Figure 9 (left). The reason was unknown, and it could even be a valid physical one. Note that CFD simulations are rarely performed with stagnant fluids, and if the main flow velocity is quite higher, the issue is not even noted because it is filtered by the colour bar scale. As the main flow was not perturbed, this issue was initially neglected. For the CVR freezing experiment, the velocities are quite low, at maximum about a few cm/s, and so the issue was clearly apparent.

Then CVR managed to define a test-case bringing numerically to partial freezing, and CRS4 tried to reproduce it. The time to reach a defined frozen volume was quite different in both cases. Moreover, we have been faced with technical issues:

- CVR had to use a structured mesh, an unstructured one leading to simulation crash.
- CRS4 was faced with occasional and non-averted simulation crash.

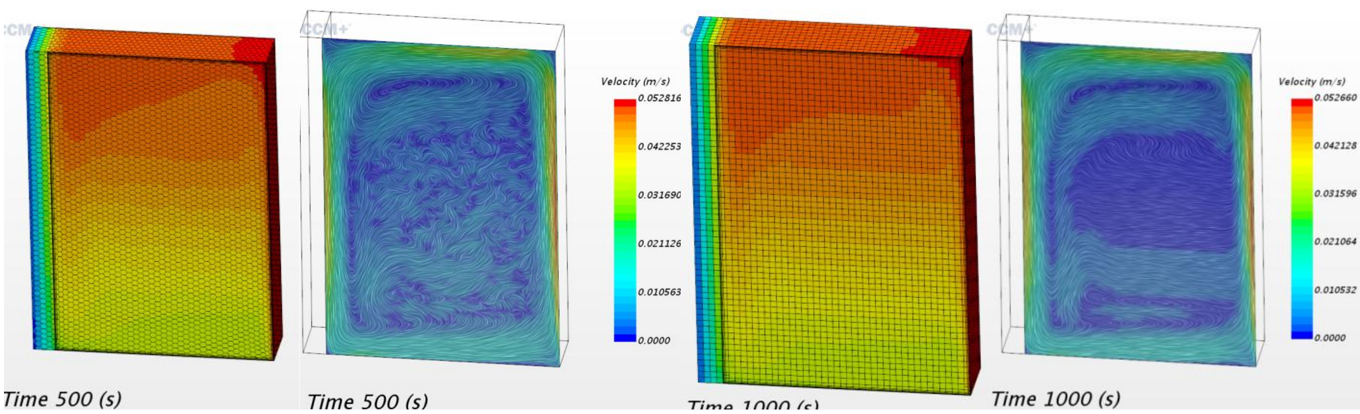

Figure 9: Buoyancy driven simplified test case. Temperature and flow with polyhedral mesh (left), with trimmed mesh (right)

Then the experimental results came and it was the time to reinvestigate the issue. Making a systematic analysis on a simplified (still 3D) case, we could exclude many causes: turbulence model, convergence parameters, turbulence, mesh size, CFL and a very undue sensitivity to the reference density. Taking inspiration from CVR experience, we used the Trimmed Cell mesher, which is the closer STAR-CCM+ mesh model to the structured mesh. Then, instantaneously, (almost) all problems disappeared and the flow became clean, as shown in Figure 9 (right). Moreover, it came out that freezing was now possible and safe with the default STAR-CCM+ main settings. This allowed to perform post-test with serenity and safely, refocusing the effort on the physics of the problem.

5.6. The thermal radiation issue

This issue spans over time and experimental facilities. It starts with the CIRCE modelling. In CIRCE, the thermal stratification is very sensitive to secondary flows and conjugate heat transfer. NRG noticed that there should be a consistent heat transfer through the gas gap of the riser insulation layer, and thus reduced the numerical gap to take this aspect in consideration, based on estimate of the various heat transfer contributions. The idea was expanded by CRS4 who noticed that in simple layers, the thermal radiation can be modelled with a temperature dependant thermal conductivity. It also implemented similar procedures for the “Dead volume” insulation gap and the free surface, thus improving the global modelling.

In a second time, experimental results of CVR from SESAME-Stand were produced and showed that the facility heat losses were much more intense than expected from the simulation and we should look for potential origin of these added losses. Then, observing that the air channel external border was much hotter than bare hand could stand (later measured at about 70°C), we could make an evaluation of the possible heat loss by radiation and it came out that is was responsible for about half the total heat losses. Thermal radiation thus plays an important role in the facility cooling and should definitively be taken in consideration in its modelling. In Figure 10, we show a representation of an experimental temperature profile at the onset of solidification. Then, in the centre, the numerical profile in the CVR model in absence of thermal radiation, with more than 200K above the experimental one, is shown. On the right, including the radiations, the numerical profile in the CRS4 model becomes much more similar and the difference of temperature falls below a few tens of degrees.

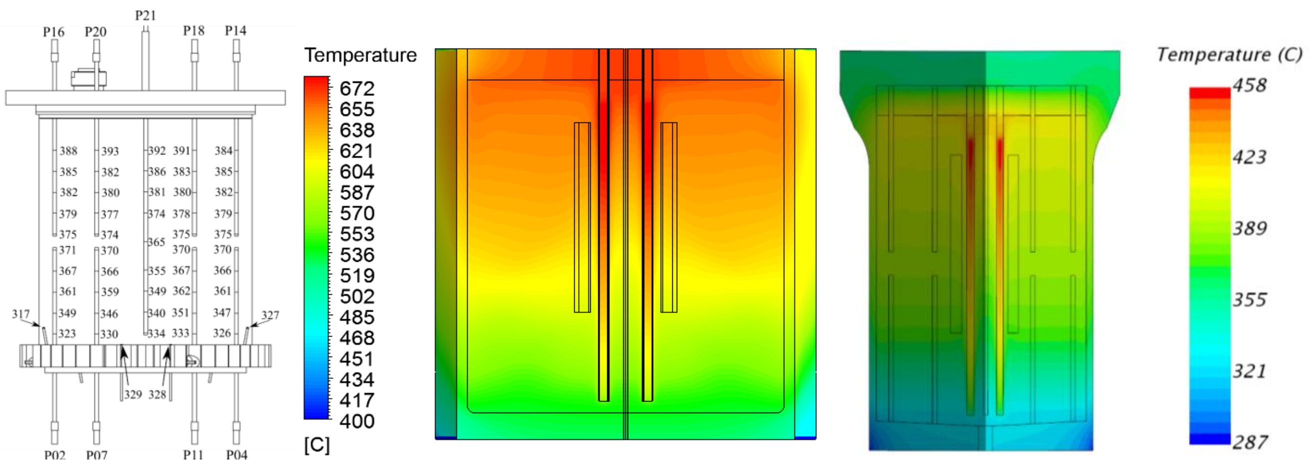

Figure 10: SESAME-stand from CVR. Experimental temperatures (left). Simulation without thermal radiation (center). Simulation with thermal radiation (right)

6. MAIN LESSONS AND RESULTS

6.1. Time line

The time line has proven to be very successful for the integration of experimental and numerical activities. Delays on experimental activity had small impact because the delays where staggered. The numerical activity could start with the modelling of the existing experimental facility for pre-test and design support for the facilities to be conceived and built. Then, when experimental results were available, comparison and validation could take place. So, the numerical activity could follow the development of the experimental one.

6.2. Experimental activity

Several strong technical issues on the facilities have been encountered during the project. Just to name a few, CVR had manufacturing delays and even a non-compliant main vessel that had to be re-worked, KTH damaged the heater of its 3D pool and ENEA had the CIRCE DHR plugged. All these issues could be absorbed by the time margin allocated, and that time margin has been fully consumed.

The redundant and diversification strategy has proven to be totally justified. While the possibility of failure has been considered, it was only on technical feasibility ground. The failure from KTH to build the STS was caused by internal administrative/political reasons and was really unexpected. However the backup strategy was independent of the cause and could save the solidification part of the project.

The calibration of the UDV sensors by HZDR for STS was much more problematic as expected, at the point that HZDR mounted its own dedicated freezing experiment. This experiment, not initially part of the project, has been at a later stage partially included and the experimental results will be made available to the consortium for possible later use, however too late to have its numerical counterpart within SESAME.

Being first of a kind, the elaboration of the freezing experiments has been much more demanding than expected. In our framework, controlling the heat losses usually means minimize them, so that the meaning of conservative assumptions was clear. Instead, we had to effectively control and monitor the heat losses.

6.3. Solidification modelling in LBE and Lead facilities

Solidification modelling is feasible at relatively high cost:

- FLUENT for SESAME-stand: only with structured mesh and increased relaxation factors
- STAR-CCM+ for SESAME-stand: only with Trimmed Cell Mesh
- STAR-CCM+ for STS: without particular issues

The flow in the STS facility is a forced one in a quasi 2D configuration while in SESAME-Stand it is buoyancy driven and tri-dimensional. Serious issues appeared only in this later case, which is unfortunately much closer to the foreseen final applications.

6.3.1. The "mushy zone" issue and the flow stop criteria

With regards to the solidification modelling in STAR-CCM+, a larger part is dedicated to the "mushy zone" modelling. The mushy zone is a region of transition, typically a few millimetres wide, across which solid dendrites develop to progressively occupy all the volume. Considering a sub-millimetre range homogenization, it is simulated by setting the viscosity as a strongly increasing function of the solid mass fraction, with several transition models available.

However, pure and eutectic substances do not develop any mushy zone and instead propagate a sharp transition front. Therefore, for the CVR experiment with pure lead, modelling a mushy zone would have been exclusively for numerical purpose, typically to smooth the transition in case the sharp interface brings stability or convergence issues.

The situation for the KTH experiment with LBE is slightly more articulated. Even with an initially perfect eutectic composition, the fluid could develop global or local deviations: global deviation in case of preferential oxidation and also additional local deviation in case of differential pressure forcing, in strongly rotating flows (by centrifugation) or in stagnant region by gravitational sedimentation. Simulations from PSI indicates the development of a mushy zone starting at about 1% deviation from the eutectic composition. However, some observation must be made:

- Possible impact of preferential oxidation, if ever, scales with the surface to volume ratio, which decreases with increasing facility size, making it largely irrelevant for full scale reactors.
- Local sedimentation (concentration gradient) has been observed but only in different contexts. No such sedimentation has ever been observed with LBE in the existing facilities.
- If ever, the mushy zone would be below the centimetre range while for the target full scale reactor, the mesh size remains above the centimetre so that an internal discretization of the mushy zone is at best irrelevant for our purpose.

When the concentration of dendrites is sufficiently high, the connectivity of the liquid phase may be interrupted. The high viscosity is no more sufficient and the flow must be stopped. This is done in STAR-CCM+ by setting a Flow Stop Flag, the concentration of solid phase at which the flow is completely stopped. In the case of mushy zone, this Flag must be set at a high concentration value. For our purpose, the situation is quite different.

The solidification modelling is conceived essentially for mixture of laminar flows in which the boundary layer is highly discretized so that the flow speed smoothly vanished close to the solid phase. Compatibility with turbulence is only formal, in fact the effective conductivity keeps the effect of the turbulent component at the time the flow has been stopped (this has been corrected by setting the turbulent Prandtl number as function of the Flow Stop Flag). We need to use this modelling for turbulent flows with no boundary layer (as the solidification front propagates inside the domain). So, while we must use the formalism available, we must change its meaning.

Considering a sharp interface, we have basically a one (large) cell layer with partial solidification, and a consistent flow speed tangent to the interface. Let us consider a case in which solid concentration is about 10%, and for this 10% the increased viscosity is not relevant to stop the flow. Then this solid fraction would be convected away by the flow, diffused by its turbulence and would therefore invade a large part of the fluid domain, which would be correct if solidification appeared by nucleation inside the fluid part. But this is not correct because the solidification grows from the interface.

The problem is that there is a lot of energy from the latent heat of fusion that is also erroneously convected away. To minimize this source of error, it is important to set the Flow Stop Flag at a very small value. In fact, we should use the minimum value which preserves the simulation stability. The error introduced becomes a geometrical error in which, from the flow path point of view, the solidification front is slightly ahead of its theoretical position by no more than a cell layer width. This strategy is thought to be globally minimizing, while not eliminating, the convected latent heat of melting issue using the available setting.

6.4. Validation of the CFD turbulence models

From the comparison between the experimental and numerical data, it has not been possible to make an evaluation of the discrepancies brought by the turbulence model. The main reason is that there is an unexpected large uncertainty related to the measures and the boundary conditions. It is also not simple to understand what can be compared.

The experimental tests were usually carried out in two phases, at least during their conception:

- Bring the system in a well-defined steady-state
- Induce a transient by modifying some controlling parameter such as the heat source or the pumping worth.

Depending on the transient scenario, a new useful steady state could or could not be reached. The simulation first objective is therefore to reproduce at best the steady-state and eventually proceed with the transient. It was in some way considered quite certain that a reasonably steady state could be reached and reproduced. This is not really the case. Here are the three main reasons:

- The CIRCE-ICE tests never reached steady state. For example, the pool temperature probes show a behaviour than seems to converge to some asymptotic value. But when the test is pursued, this asymptotic value turns out to be a local maximum and then the value changes monotonically for several hours with a seemingly asymptotic non-zero slope. Moreover, there are non-negligible variations at all time scale available of important data such as the heating power or the mass flow rate. Some data are missing, not allowing to investigate the global thermal balance. This is because the power of the heat-exchanger is unknown as well as the power extracted from the dead volume, this latter strongly influenced by the unknown fluid condition (entrapped gas of LBE) just below.
- The global heat balance of the TALL-3D test section is inconsistent, typically of the order of 10%, when considering the official properties of the insulation material. A possible explanation could have been heat losses through the thermo-couple wires, but a conservative estimation both theoretical and numerical has shown that this cannot be the main cause of discrepancy. Another explanation involving a mass flow rate error has been deeply investigated both by KTH and CRS4 and resulted to be globally inconsistent. A defect of some insulation material remains for now the more plausible possibility, but without knowing witch one, where and to what extent. Note that due to the large difference of temperature inside and outside the facility, the energy unbalance cannot be explained by a defect of the turbulence modelling.
- The cooling in SESAME-stand is also largely controlled by thermal radiation heat losses. But the intensity shape and ratio between the lateral, bottom and top radiation losses is both unknown and quite difficult to estimate and simulate reasonably. In any case, any attempt to do it is faced with uncontrollable errors, forbidding any fine tuning conclusion on the turbulence and solidification models.

6.5. POD-ROM modelling

As any innovative methodology, the POD-ROM modelling was supposed to provide great results at very little cost. As any innovative technology put in practice, things are somewhat more articulated. However, the development performed during the project have led to the following consideration:

- The methodology has confirmed its potential.
- It is technically more complex than expected requiring not only an energy like minimisation but also a minimisation of the gradients associated. Otherwise, the method revealed to be unstable.
- It can currently deal only with laminar thermal flows. Minimum maturity requires inclusion of turbulence and of conjugate heat transfer.
- The method is indicated where 3D information is relevant, thus precluding system codes, and where a huge number of parametric test cases must be simulated, making CFD too expensive.

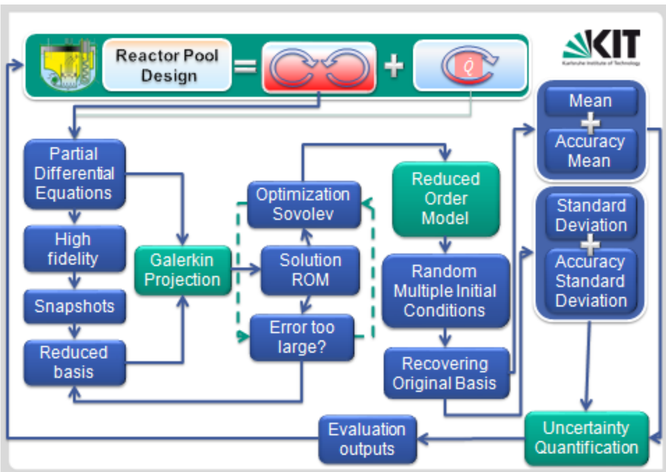

Figure 11: Conceptual sketch and contextualization of the POD-Galerkin approach. Source: KIT-IKET.

The name of the modelling method has been changed from POD-ROM to POD-Galerkin. Its flow-chart and contextualization is shown in Figure 11. As benchmark, the method has been applied with success to a Reyleigh-Benard convection flow between two plates at different temperature, having an analytical solution. The first velocity and temperature mods are shown in Figure 12.

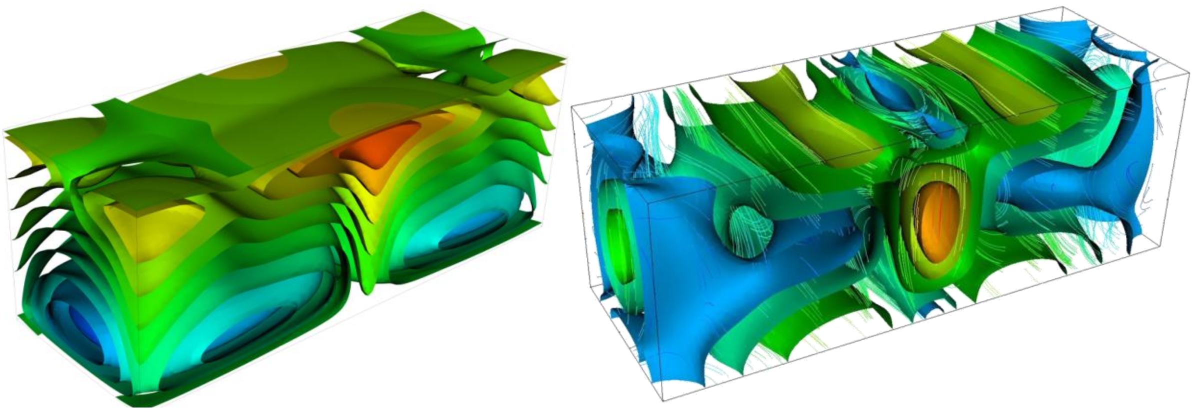

Figure 12: Reyleigh-Benard convection POD-Galerkin simulation. Left, first temperature mod. Right, first velocity mod. Source: KIT-IKET.

7. EXTRAPOLATION TO ALFRED

We must keep in mind that our target is to qualify CFD to support the design of Gen-IV nuclear plants. The experimental and numerical activities performed on the facilities are needed to explore and validate different aspects of the modelling. It is interesting to make an attempt to combine the acquired know-how to support the design of one of the most promising Gen-IV demonstrator. This attempt has been quite successful and is the result of a process involving redundancy and diversification that we illustrate now.

For the CIRCE modelling, CRS4, rich from its experience with MYRRHA entire primary loop model (Moreau, 2013 2014, Buckingham, 2015), made a quite precise and articulated geometrical model, while the physical modelling was essentially the same as in MYRRHA. Instead, for budgetary reasons, NRG (Zwijsen, 2018) opted for an quite simplified geometrical model, making use of a CAD model created by UniPi, allowing thus to focus on the physical modelling, confronted for the first time. See Figure 13 for the illustration of all models.

Taking input one from the other, while switching to the ALFRED modelling, NRG developed a more detailed geometrical model, including the structural parts with their width (see Figure 14). In the meantime, CRS4, build an oversimplified ALFRED geometrical model with baffles in lieu of structures (see Figure 15). From one side, NRG had already gained confidence with the physical modelling and could now focus on secondary flow features that only a robust geometrical model can provide, having as reference the CIRCE model from CRS4 and a quite detailed design from the LEADER project (Janssens, 2013). From the other side, CRS4 simplified its ALFRED geometry to ease some degree of parameterization. This was in order to investigate swiftly several options based on a more recent ANSALDO concept supported by an only very simplified preliminary design. The decision was taken having observed that the main flow features could already be captured with the CIRCE design from NRG.

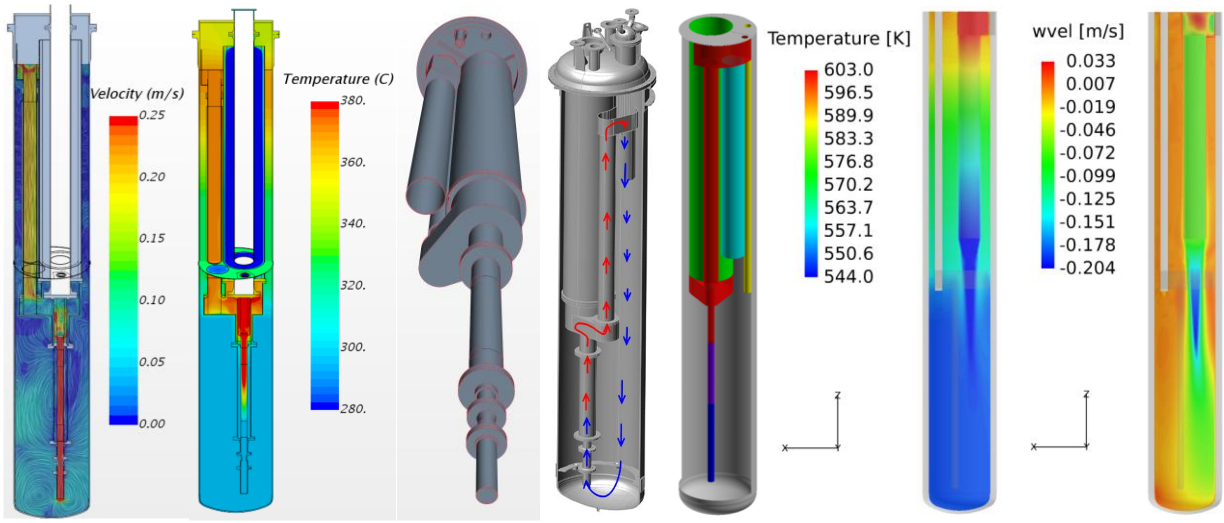

Figure 13: CIRCE representation. Centre, CAD from ENEA. Left, detailed CFD by CRS4. Right, simplified CFD by NRG.

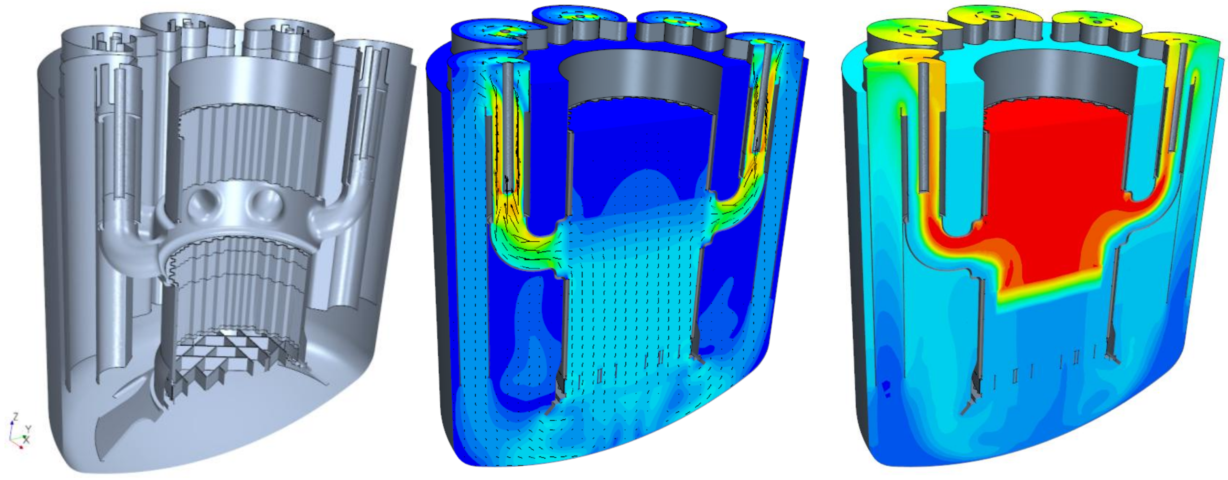

Figure 14: ALFRED according to LEADER project. Geometry (left).Velocity field (center). Temperature (right). Source: NRG.

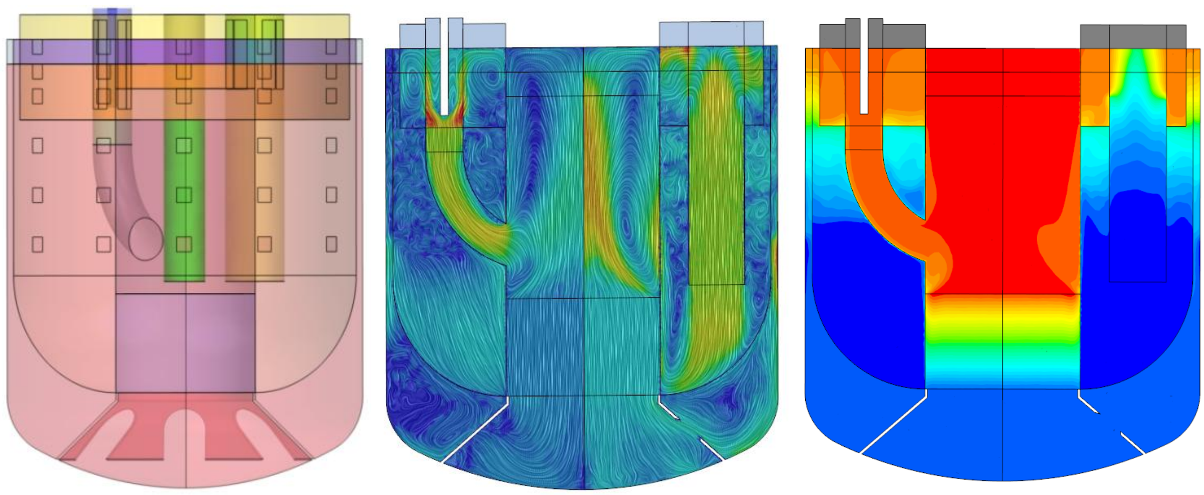

Figure 15: ALFRED according to Ansaldo design. Geometrical structure (left). Velocity field (center). Temperature (right)

8. CONCLUDING WORDS

Most of the objectives of this collaborative work have been achieved. In particular, experimentalists have learned to take input from pre-test simulations and CFD analysts have learned to provide useful information. Data bases have been produced and successfully used for comparison. With regards to the CFD validation, we definitively need to reformulate the objective. Up to now, CFD has proven to give a representation of the experiment that is complementary to the experimental measures. It gives far from perfect results, but results that are sufficiently good to pinpoint possible flaws in the experiment such as inconsistencies or insufficient information. For various reasons, the numerical results are often initially not satisfying. However, this is considered to bring important advantages since the search for the causes is the process that has brought to an essential improvement of the understanding. Basic turbulence modeling is still considered sufficient because it has not yet become the main source of errors. By increasing the complexity of the experiments, we increase the difficulty of the completeness needed to characterize them. This is however considered an ongoing improvement process.

Finally, it is now possible to investigate Gen-IV reactors with CFD on a much more solid basis and with much more confidence.

ACKNOWLEDGMENT

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NOMENCLATURE

Abbreviation and acronym

ALFRED	Advanced Lead Fast Cooled European Demonstrator
CAD	Computer-Aided Design
CFD	Computational Fluid Dynamics
CFL	Courant-Frierichs-Lewy
CIRCE	Circulation Eutettico
D	dimensional
DHR	Decay Heat Removal
FP	Framework Program
FPS	Fuel Pin Simulator
Gen-IV	Generation IV
HLM	Heavy Liquid Metal
LBE	Lead-Bismuth Eutectic
MYRRHA	Multi-purpose hYbrid Research Reactor for High-tech Applications
PLOF	Protected Loss Of Flow
POD- ROM	Proper Orthogonal Decomposition- Reduced Order Model
RANS	Reynolds Averaged Navier-Stokes
SESAME	Thermal hydraulics Simulations and Experiments for the Safety Assessment of Metal cooled reactors
STS	Solidification Test Section
VoF	Volume of Fluid
WP	Work Package

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CAPTIONS

1. Figure 1: CIRCE facility from ENEA. Left, functional sketch. Components above the fitting volume (center) and at the top (right). Source: ENEA.

2. Figure 2: TALL-3D facility by KTH. Left, facility. Right, functional sketch. Source: KTH.

3. Figure 3: SESAME-Stand facility by CVR. Right, CAD design. Center, real facility. Right, main vessel design with TC positions. Source: CVR.

4. Figure 4: Left, final design of STS from KTH in configuration with UDVs from HZDR. Source: KTH. Right: UDV socket with installed transducer mounted at test section. Source: HZDR.

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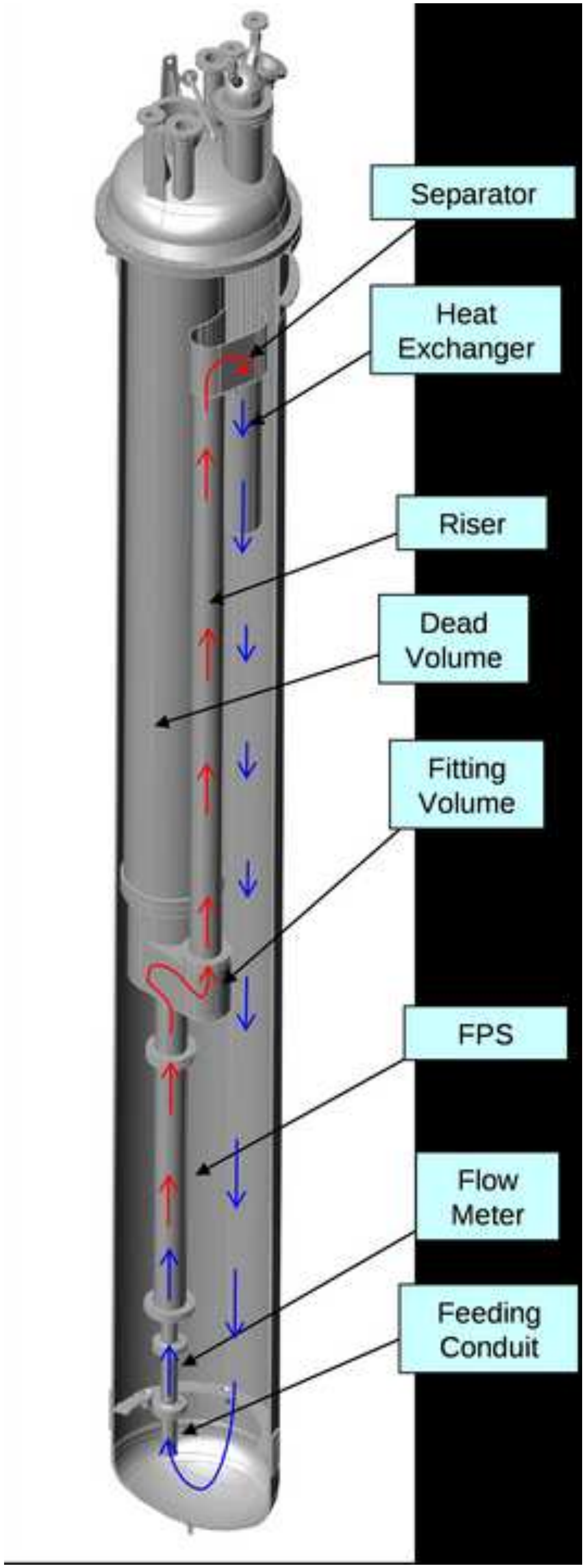

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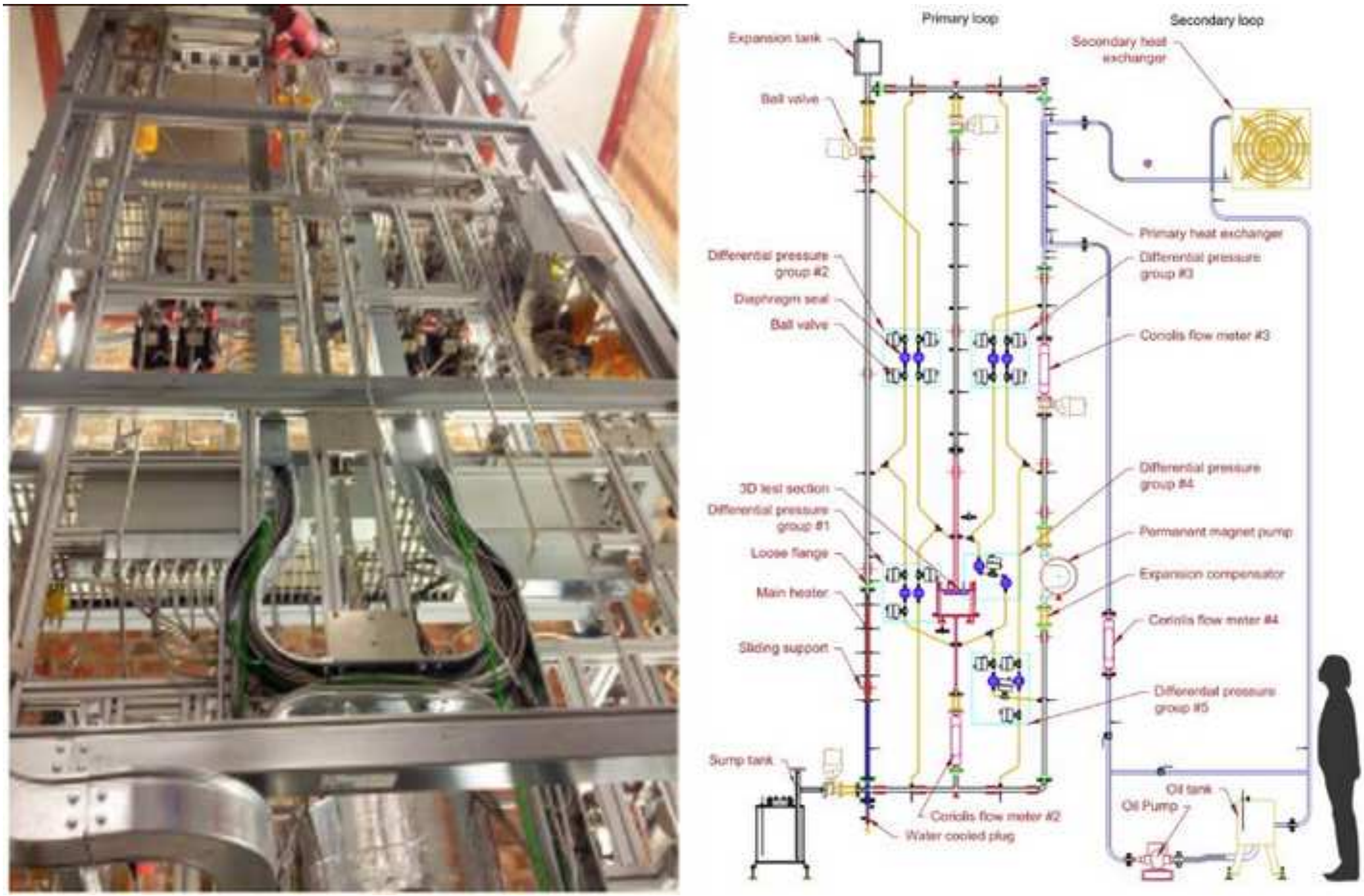

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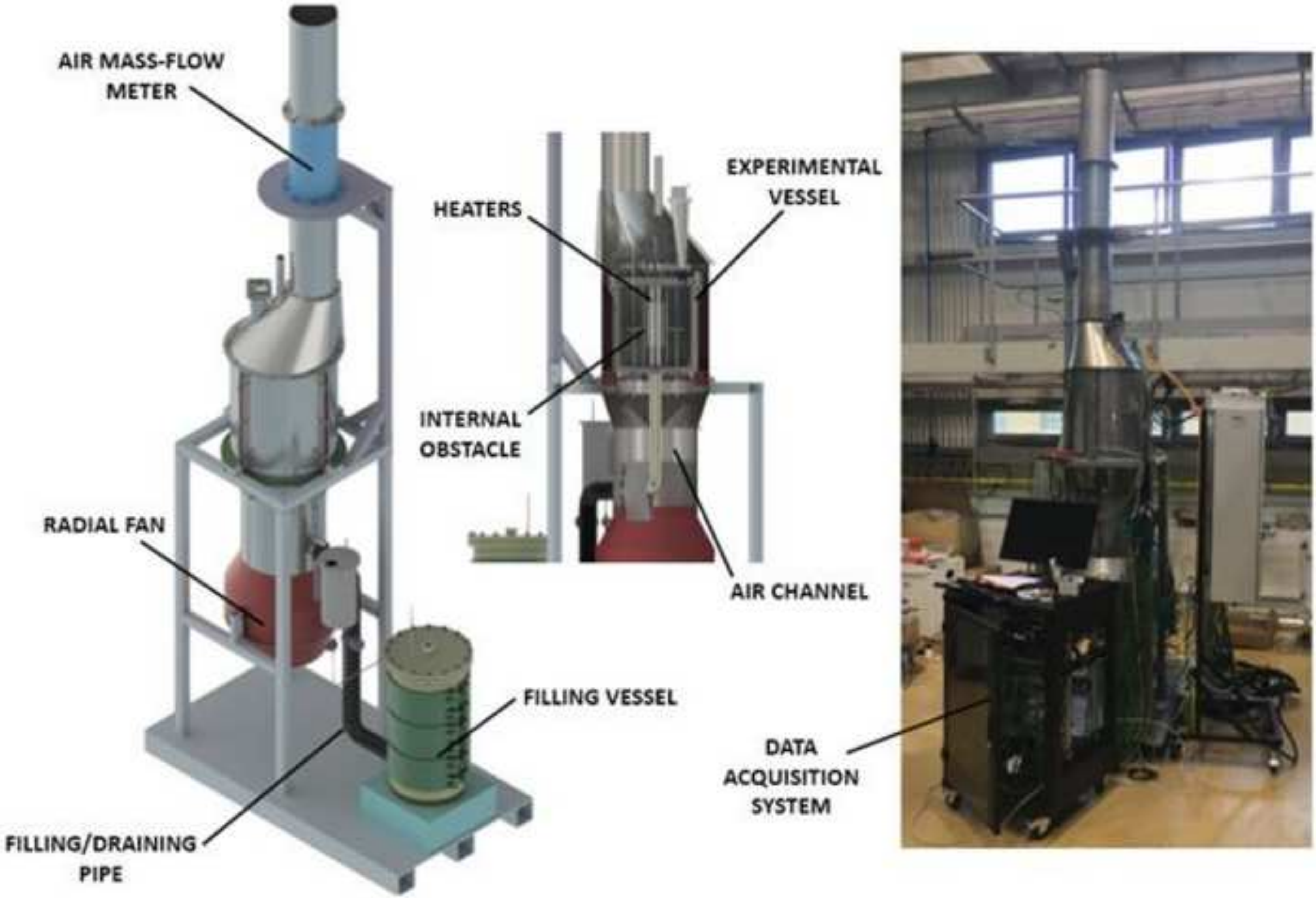

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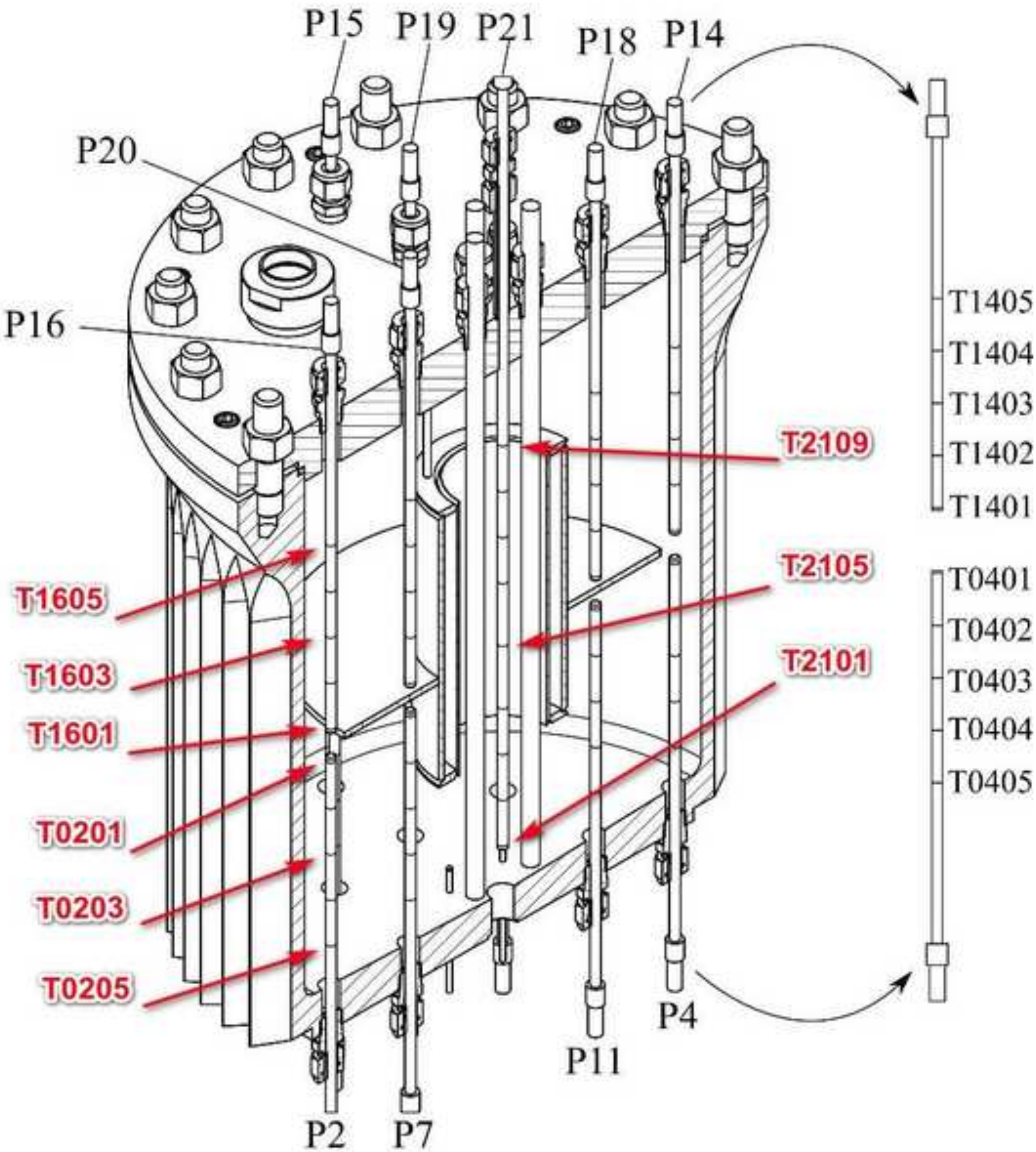

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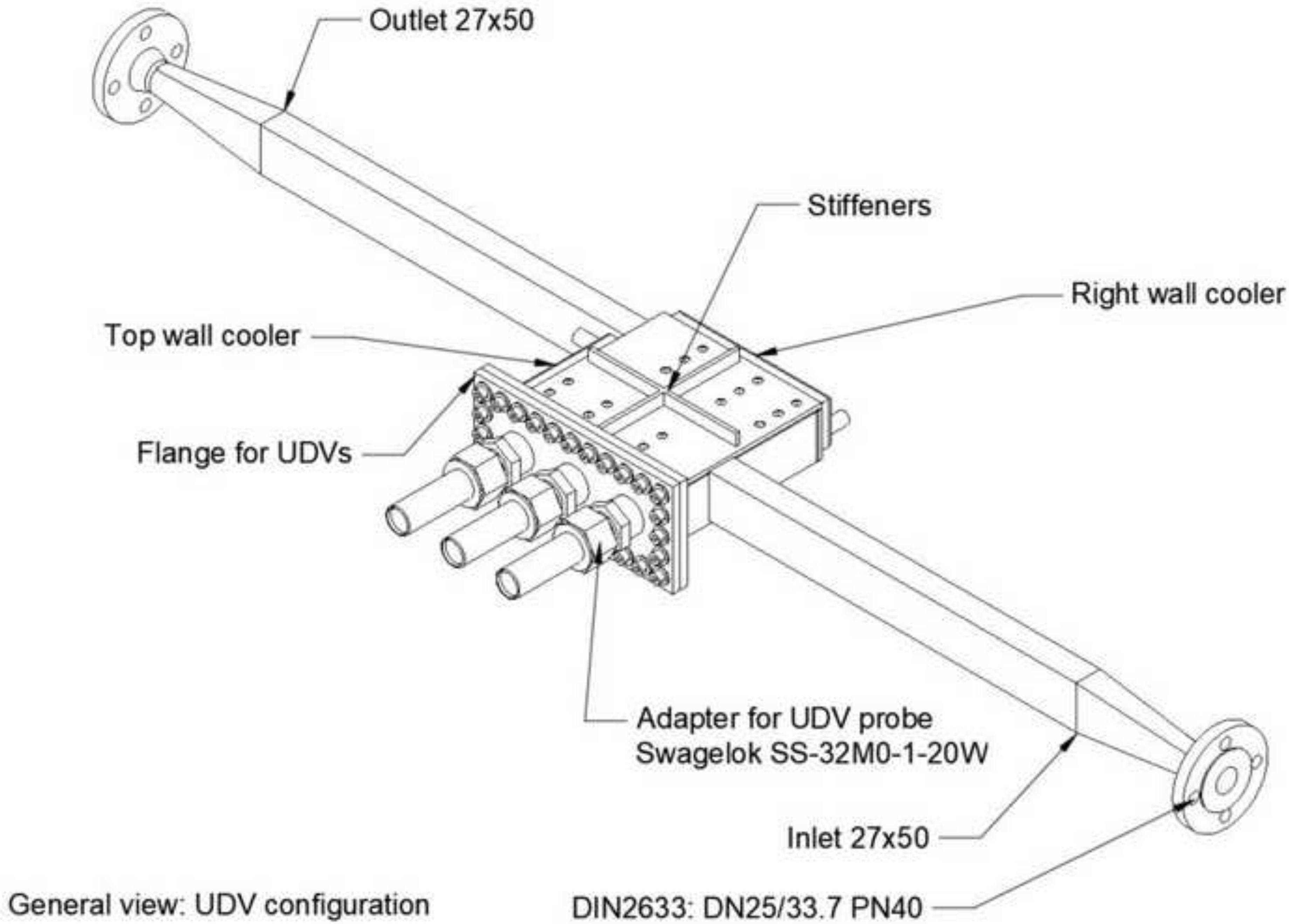

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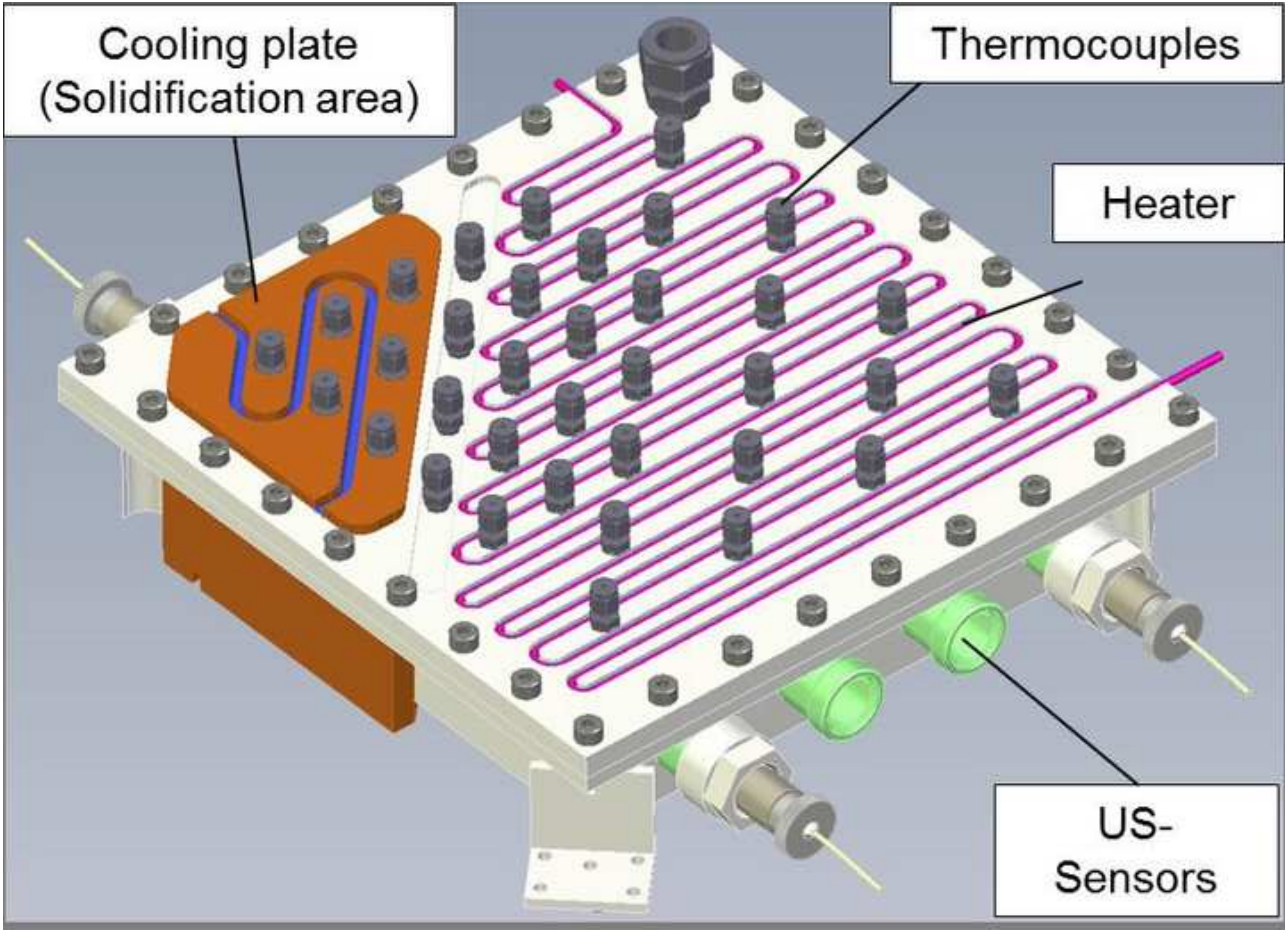

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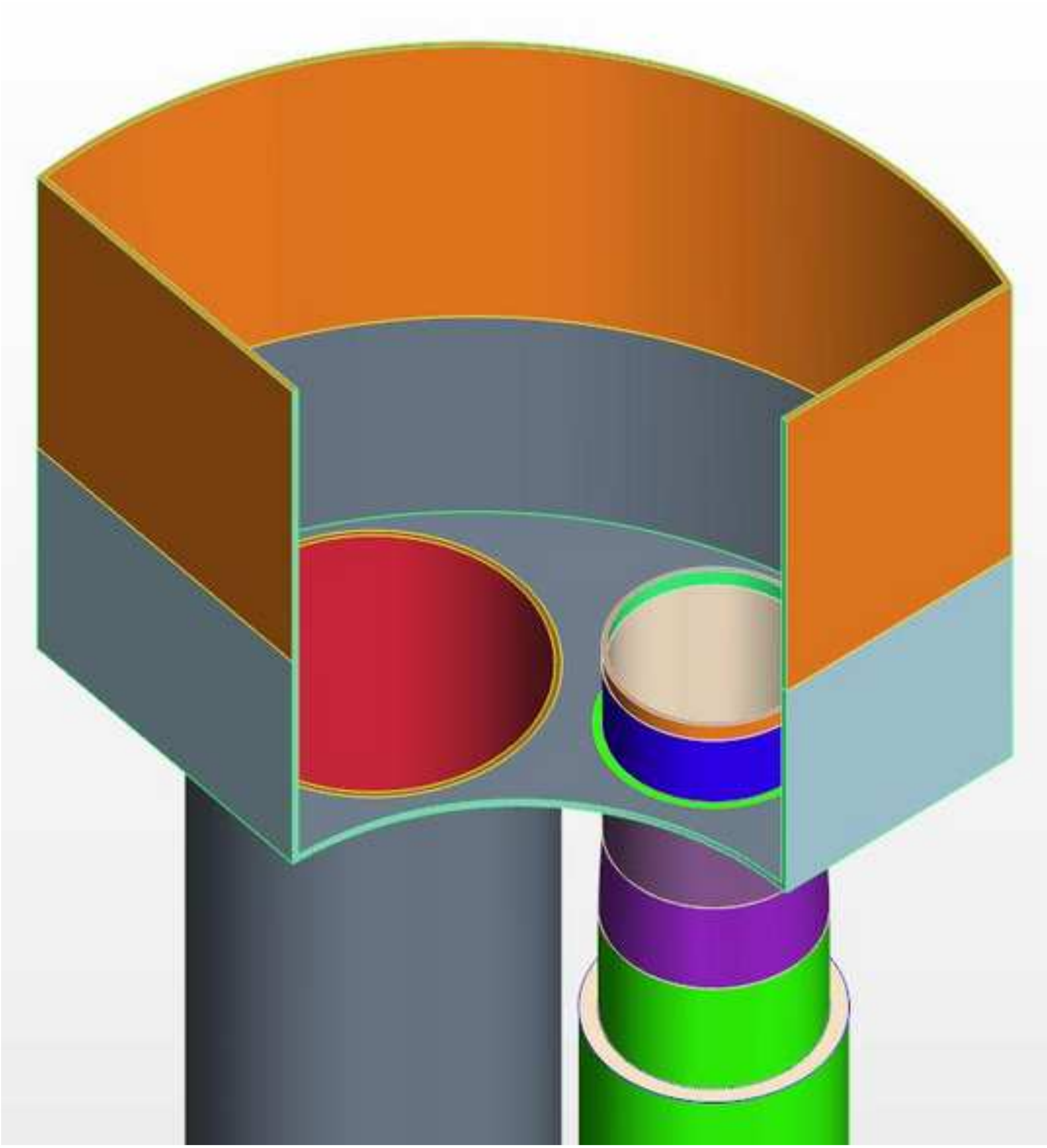

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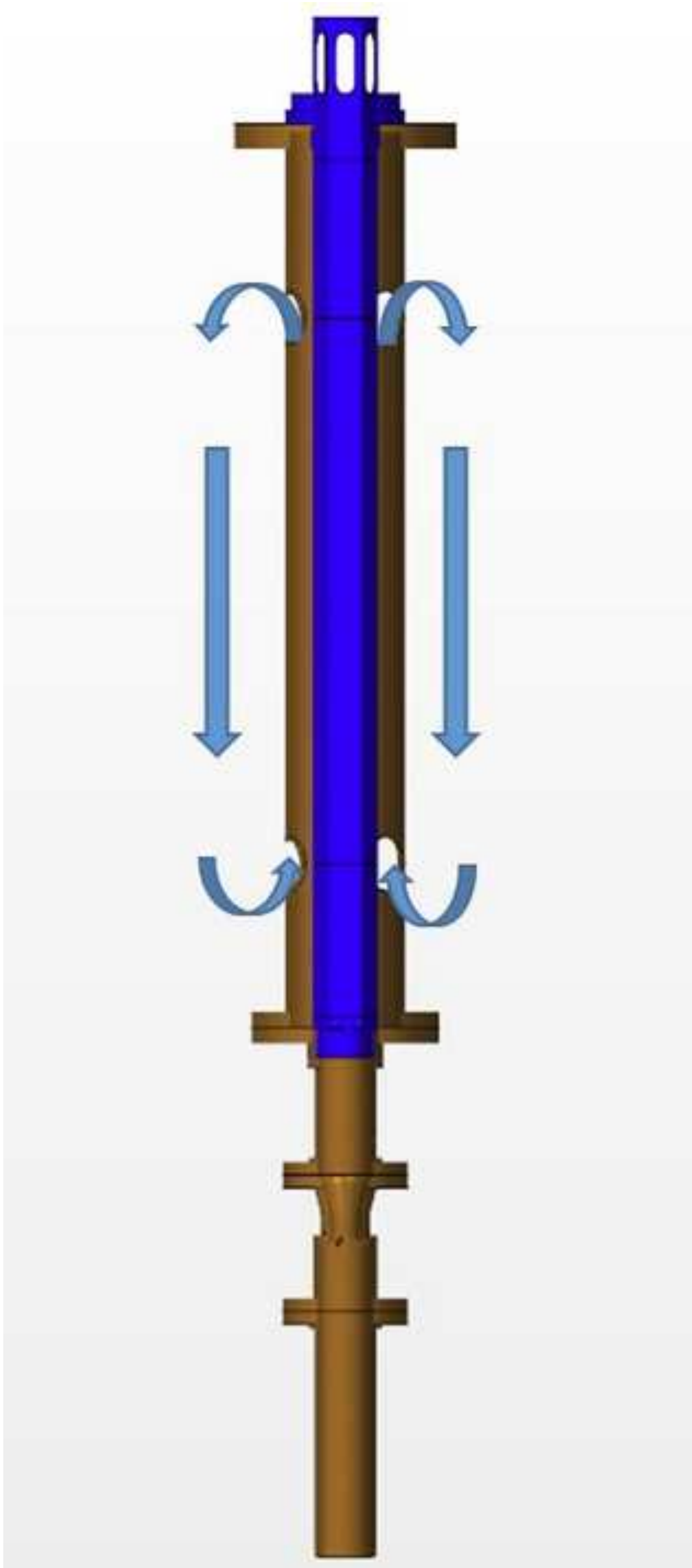

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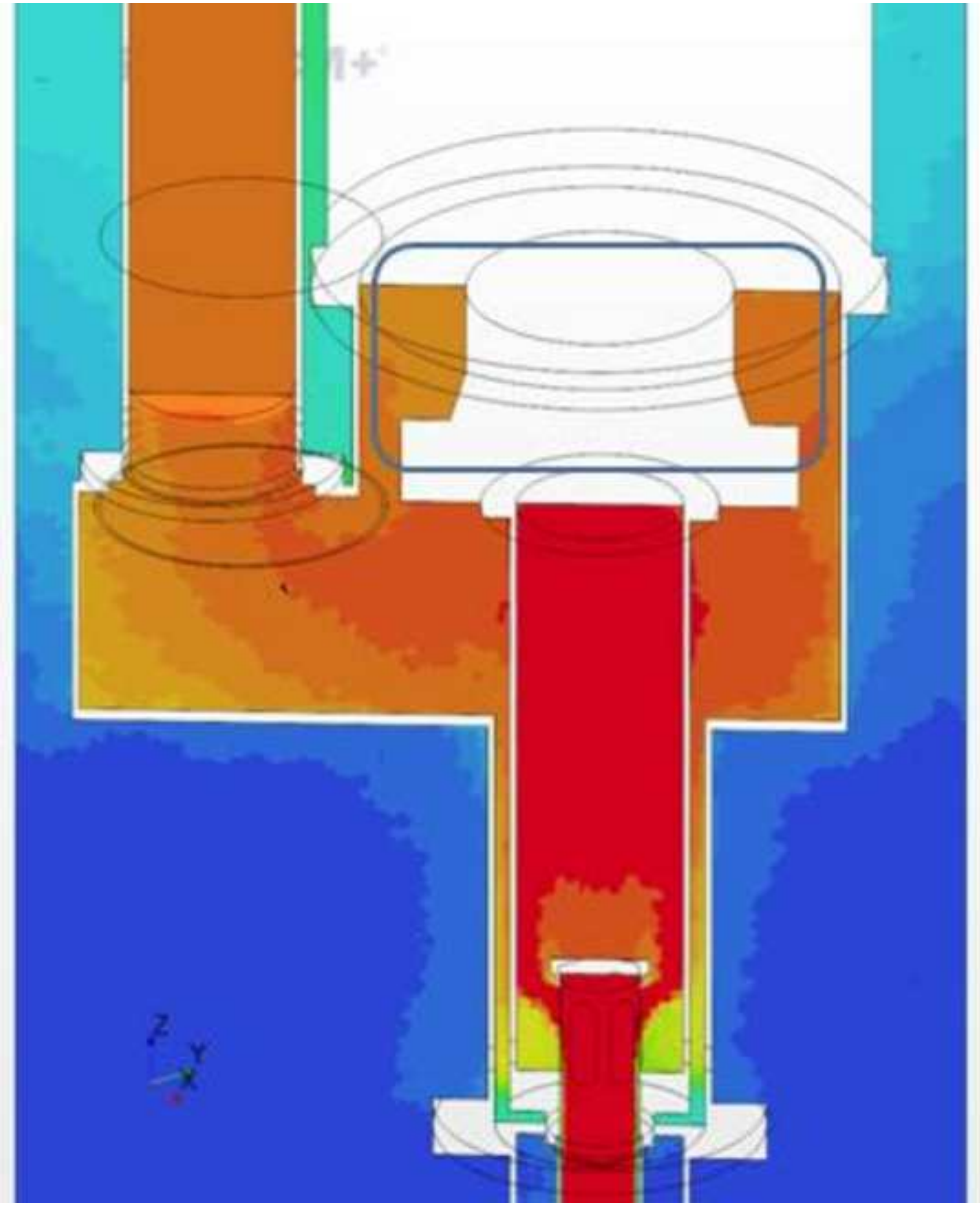

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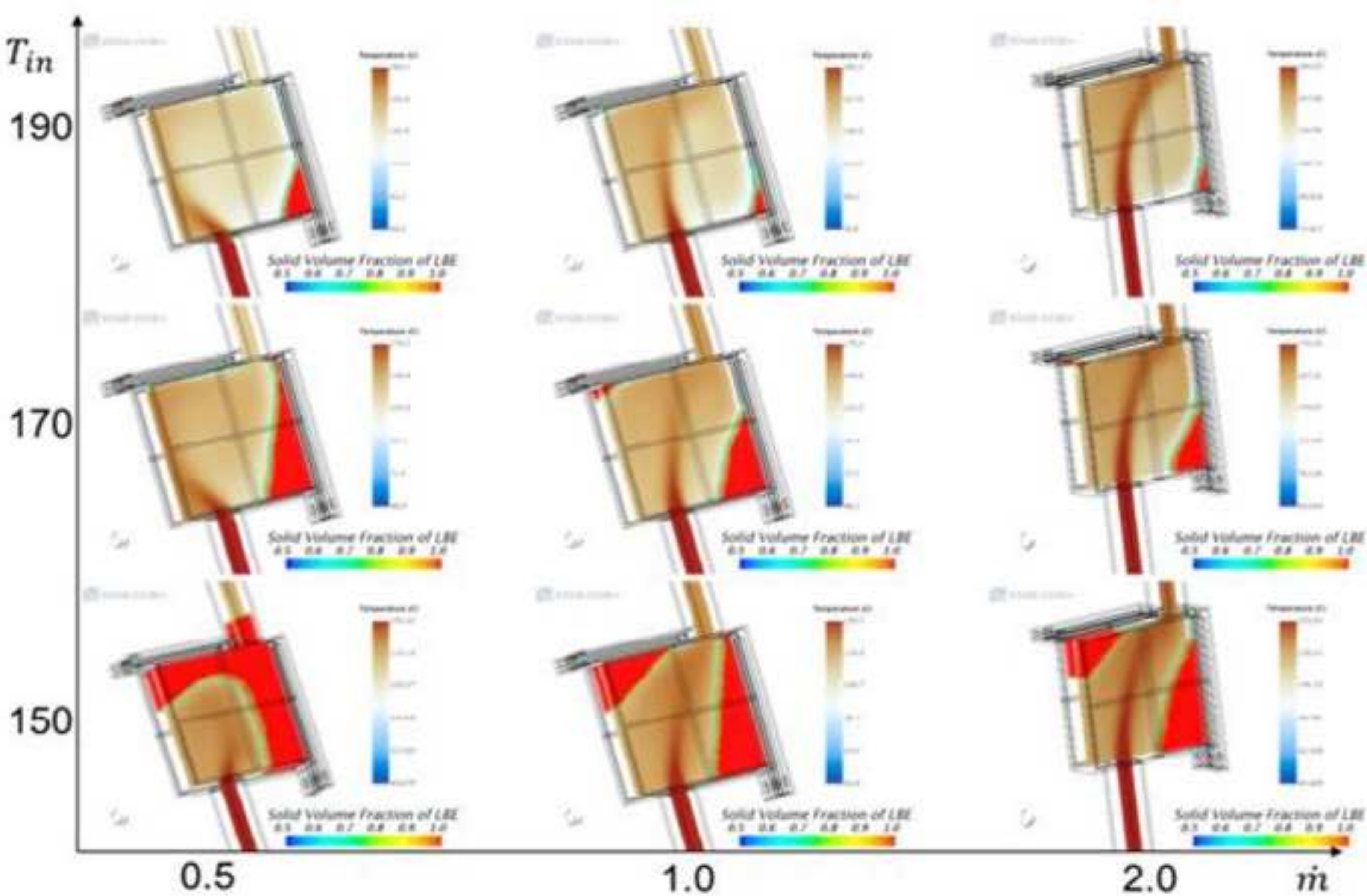

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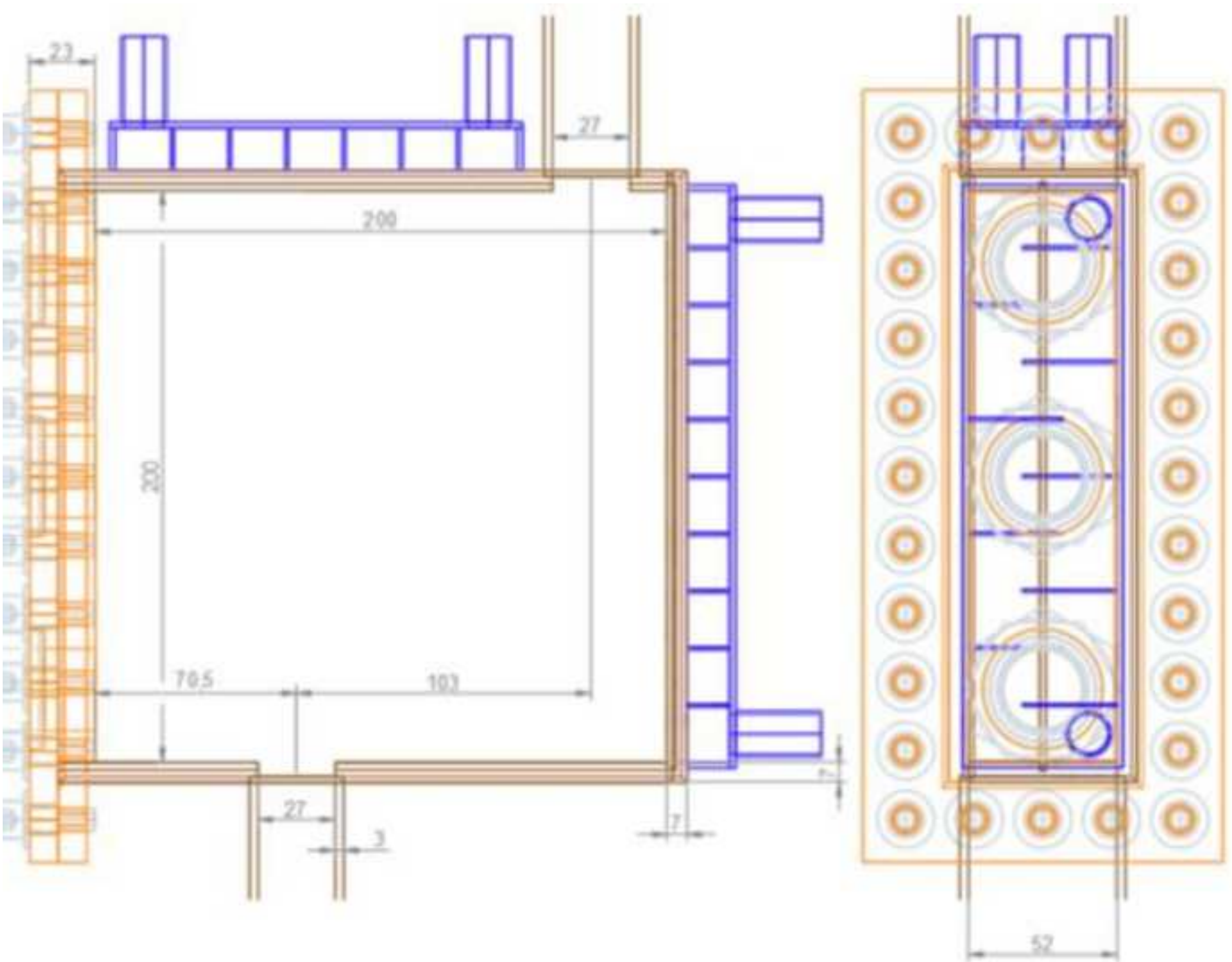

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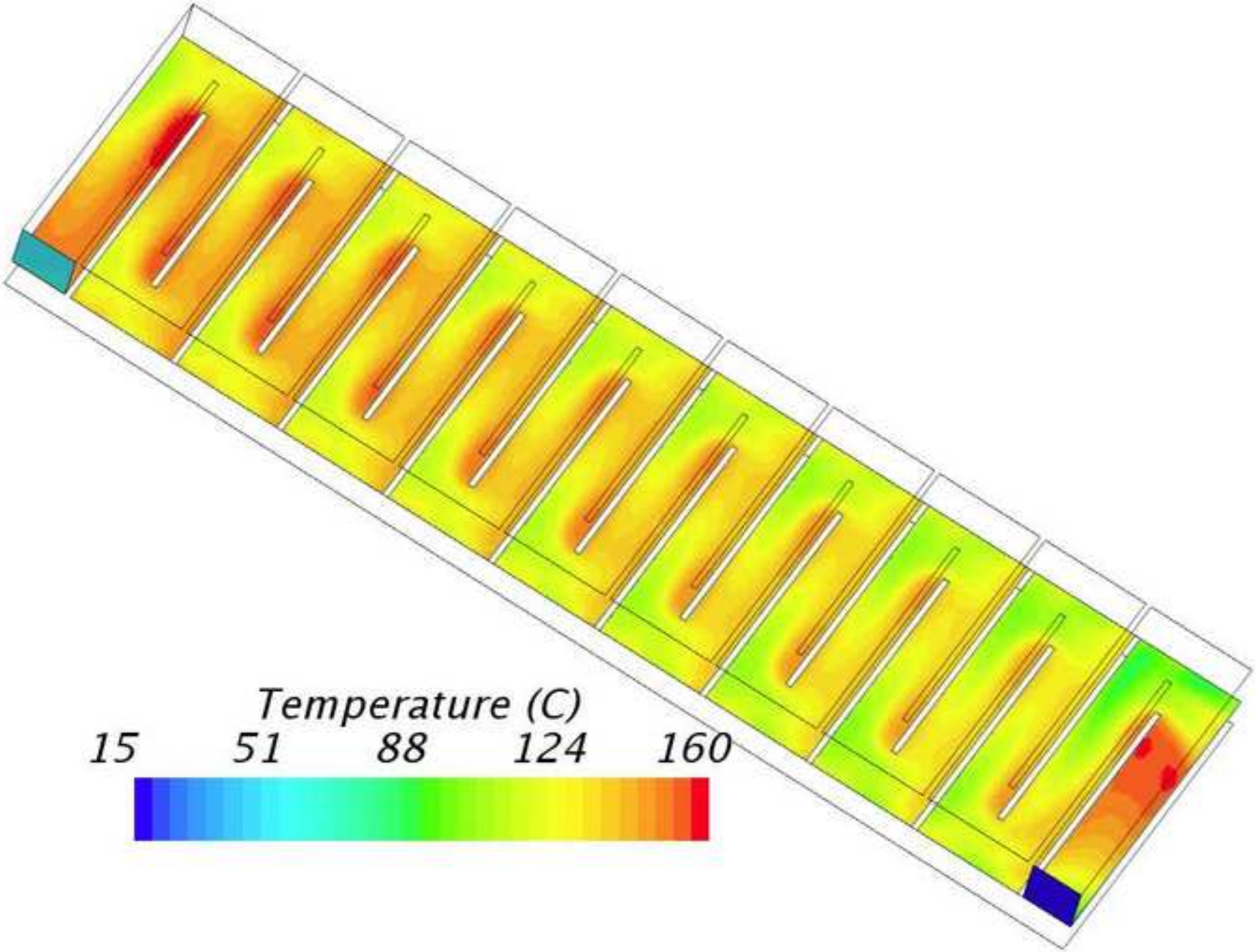

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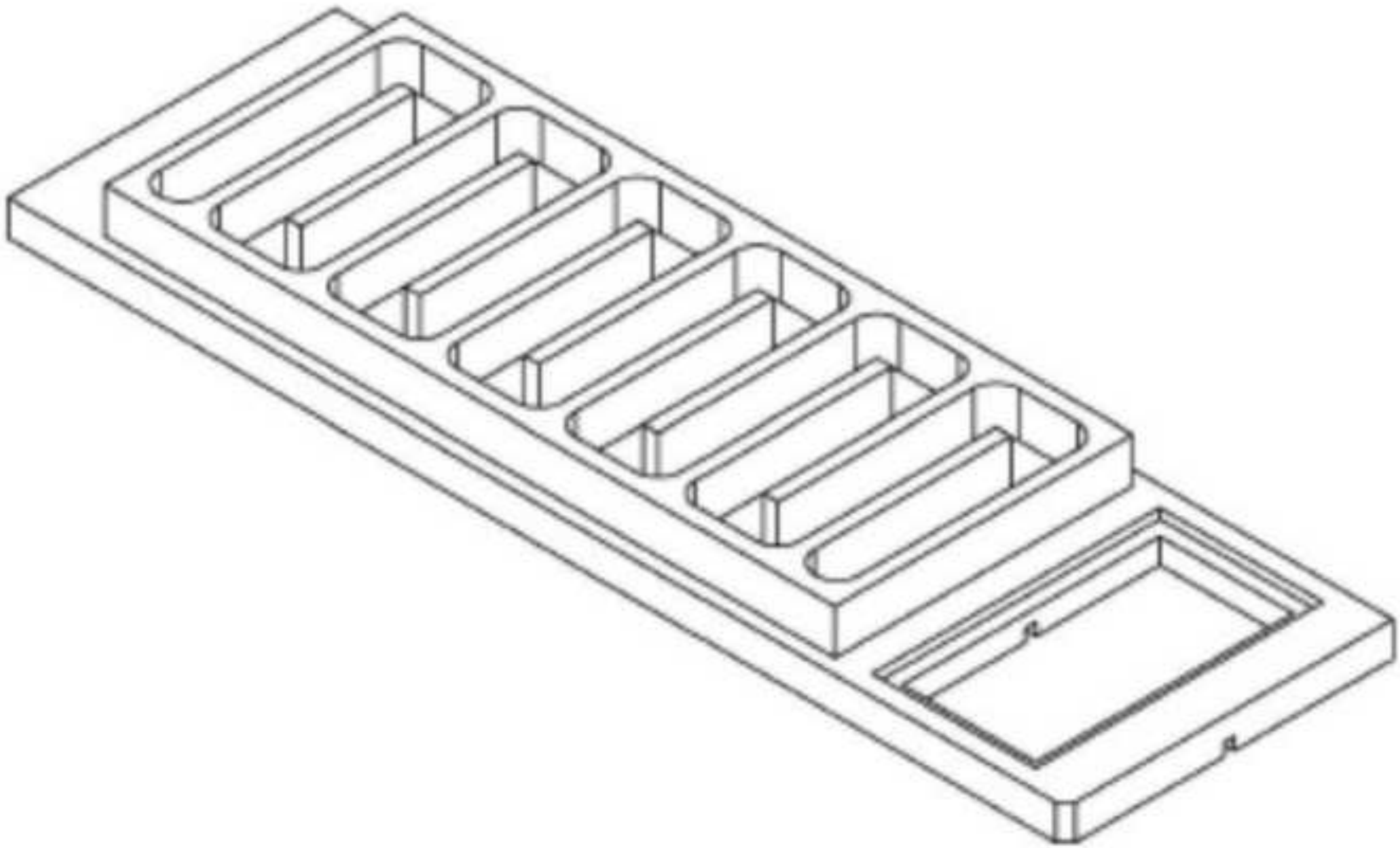

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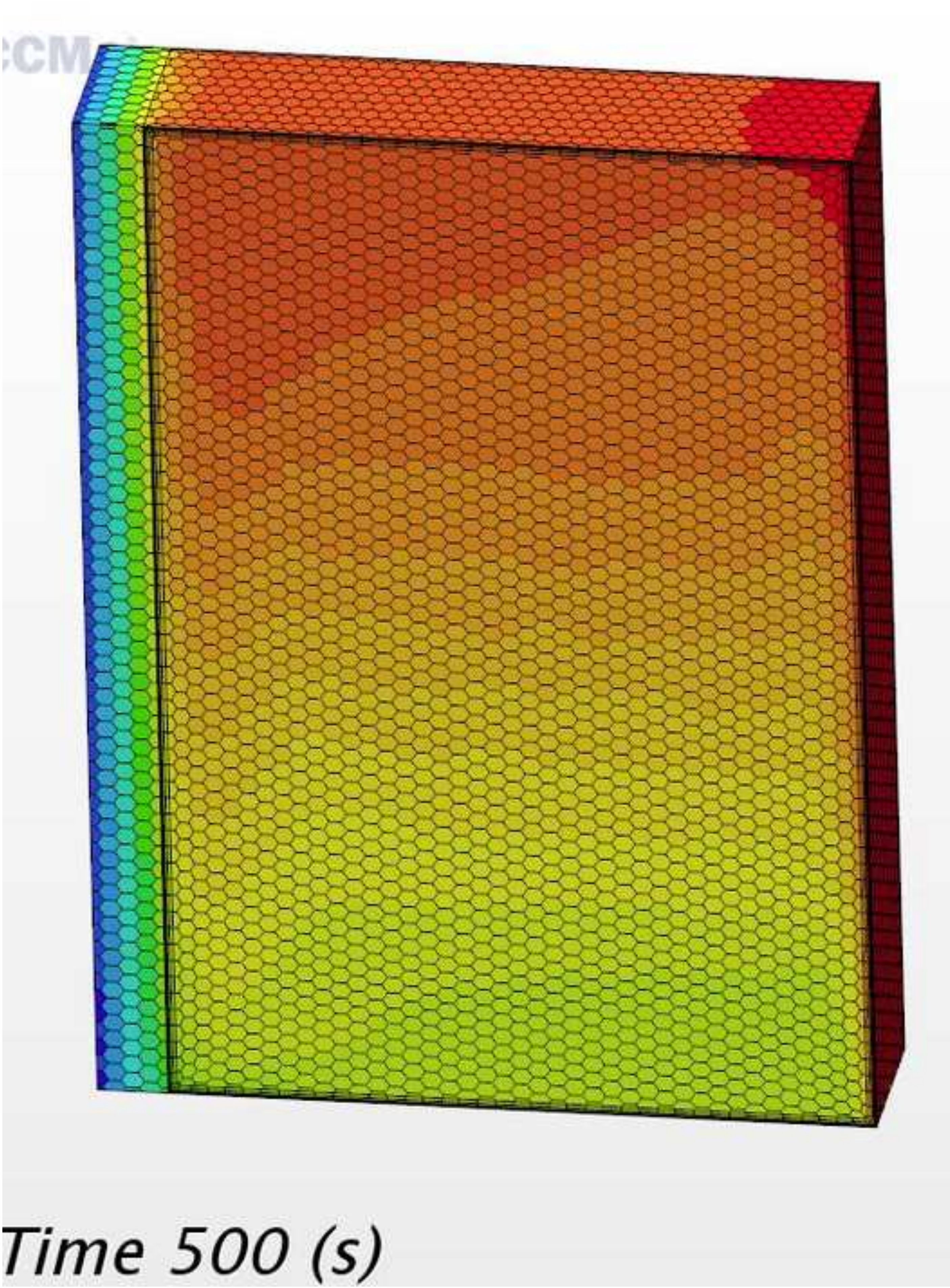

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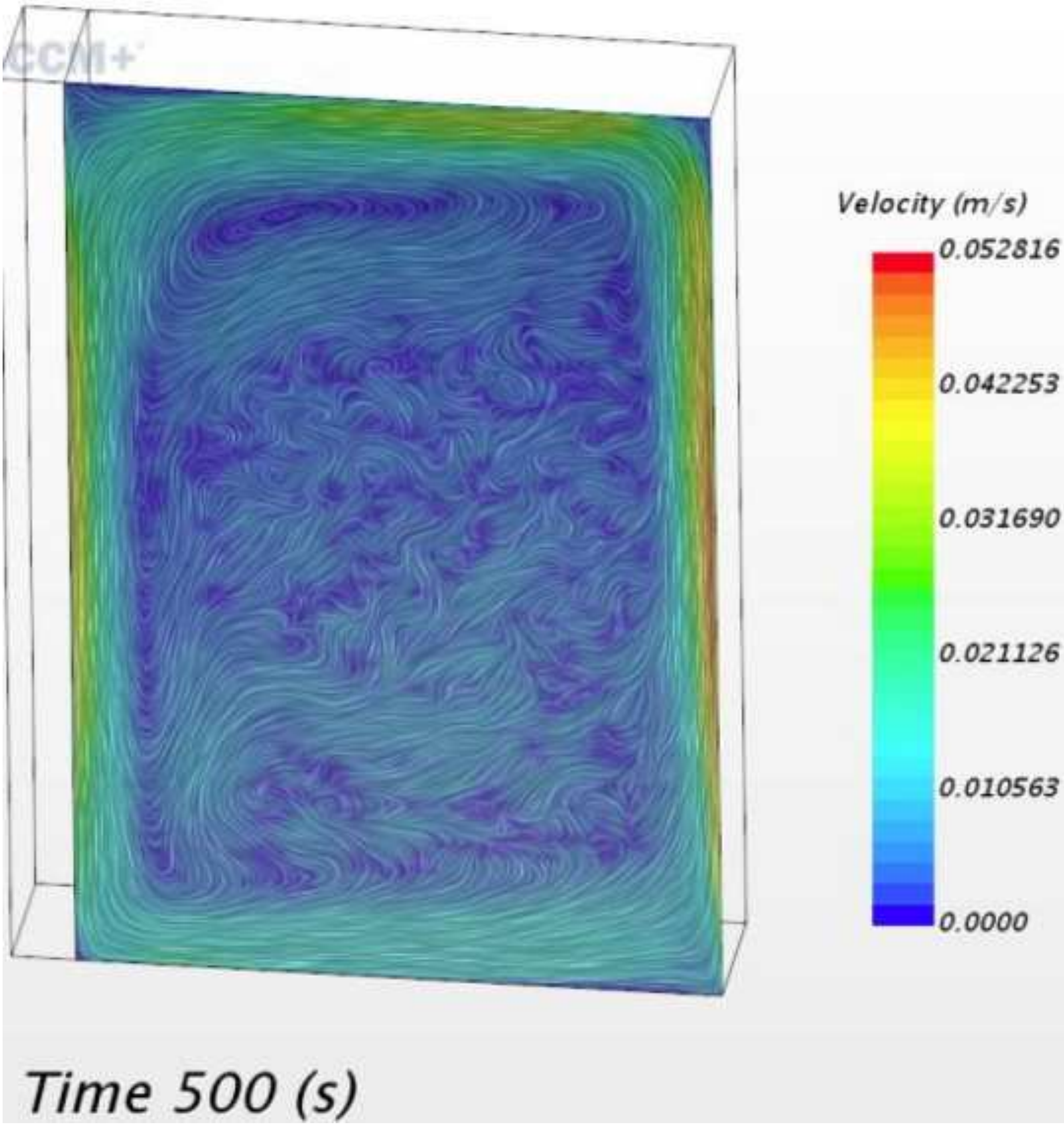

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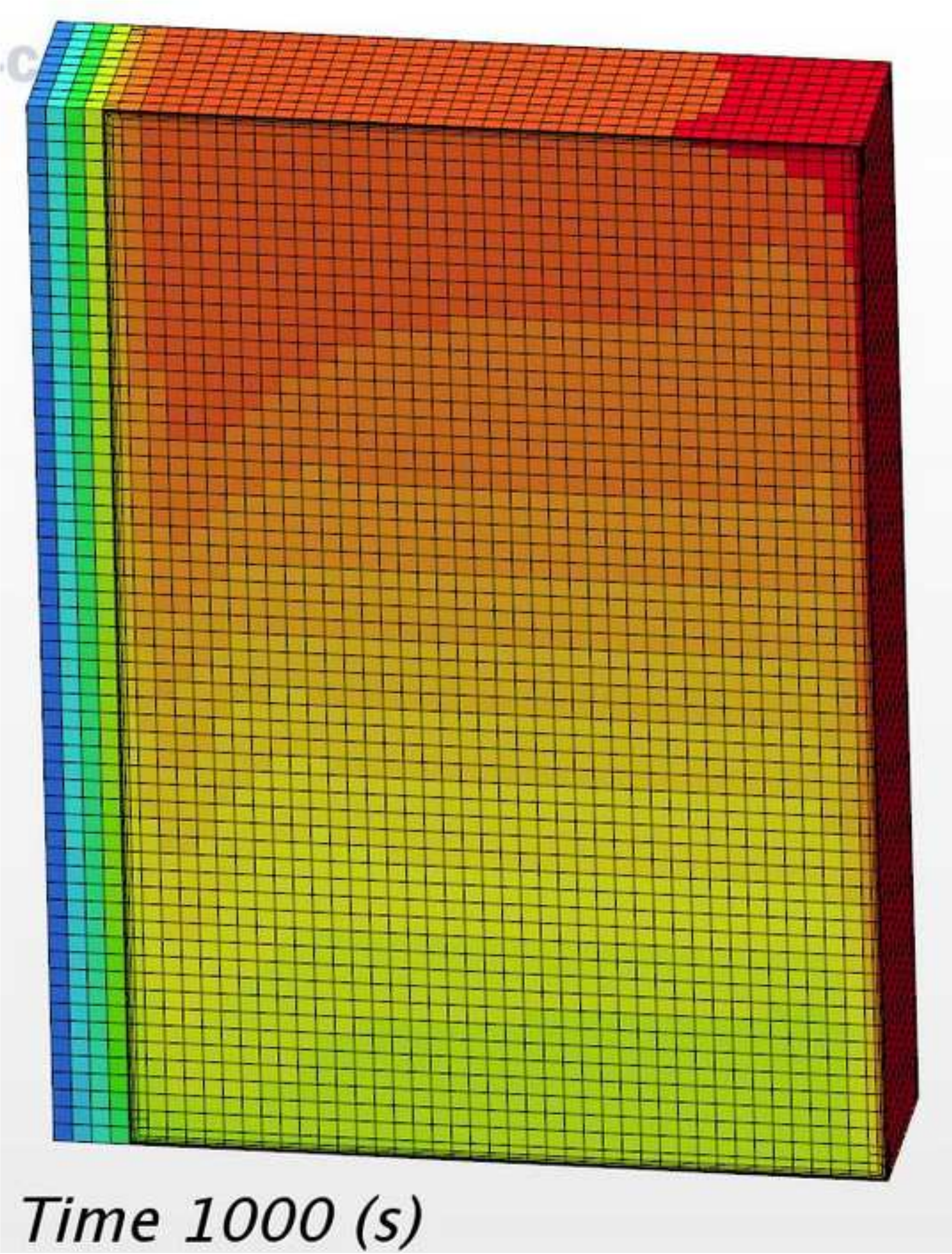

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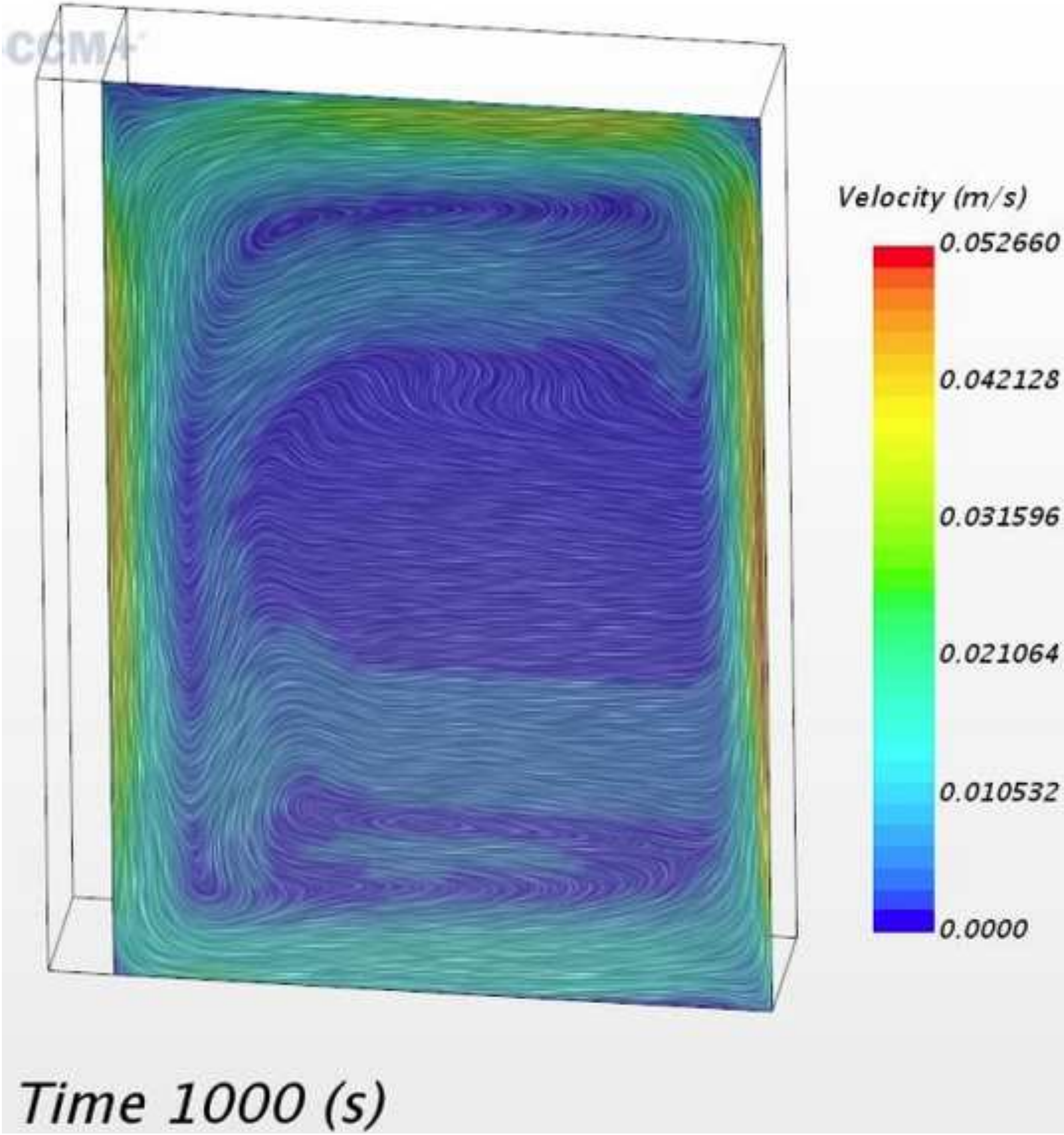

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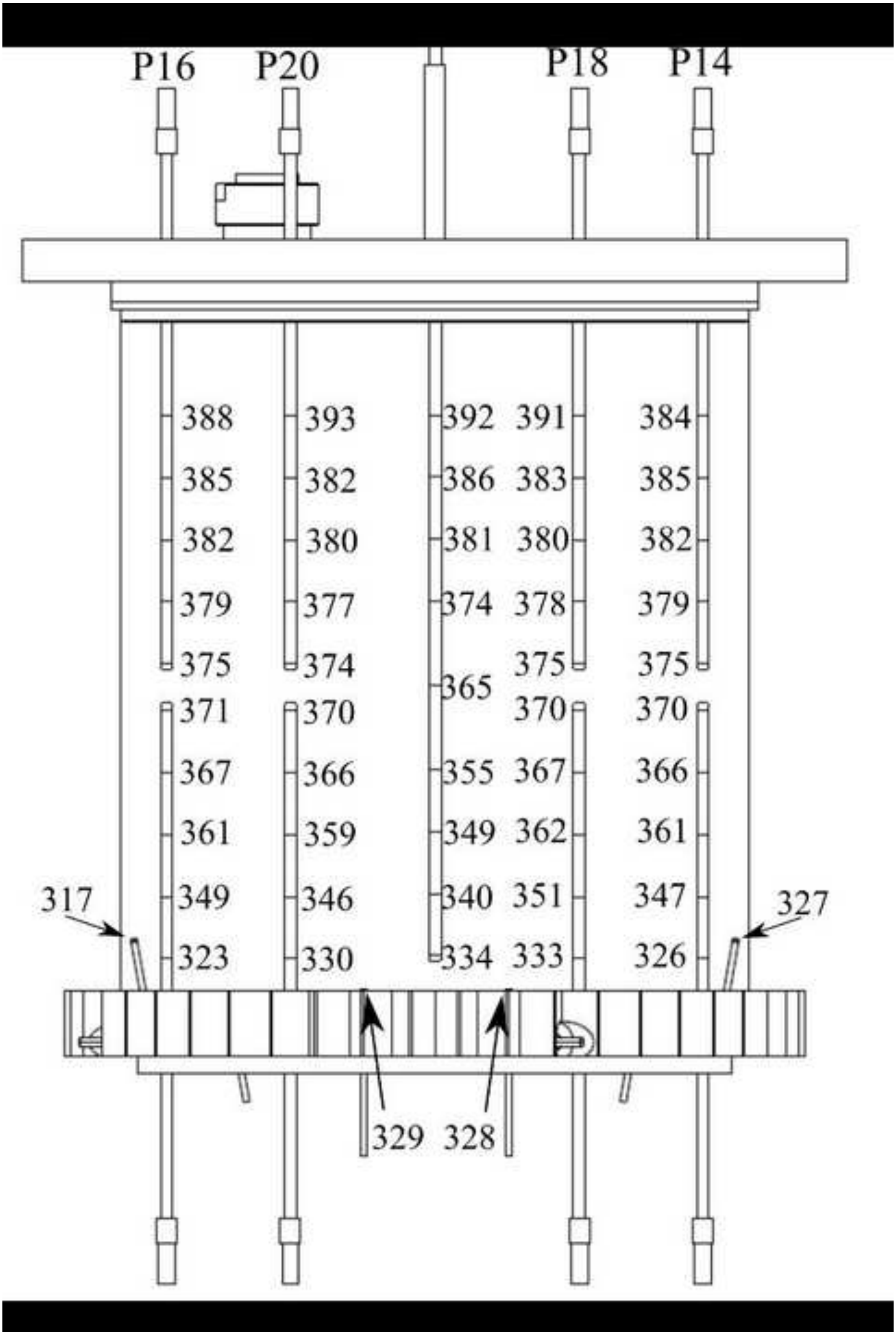

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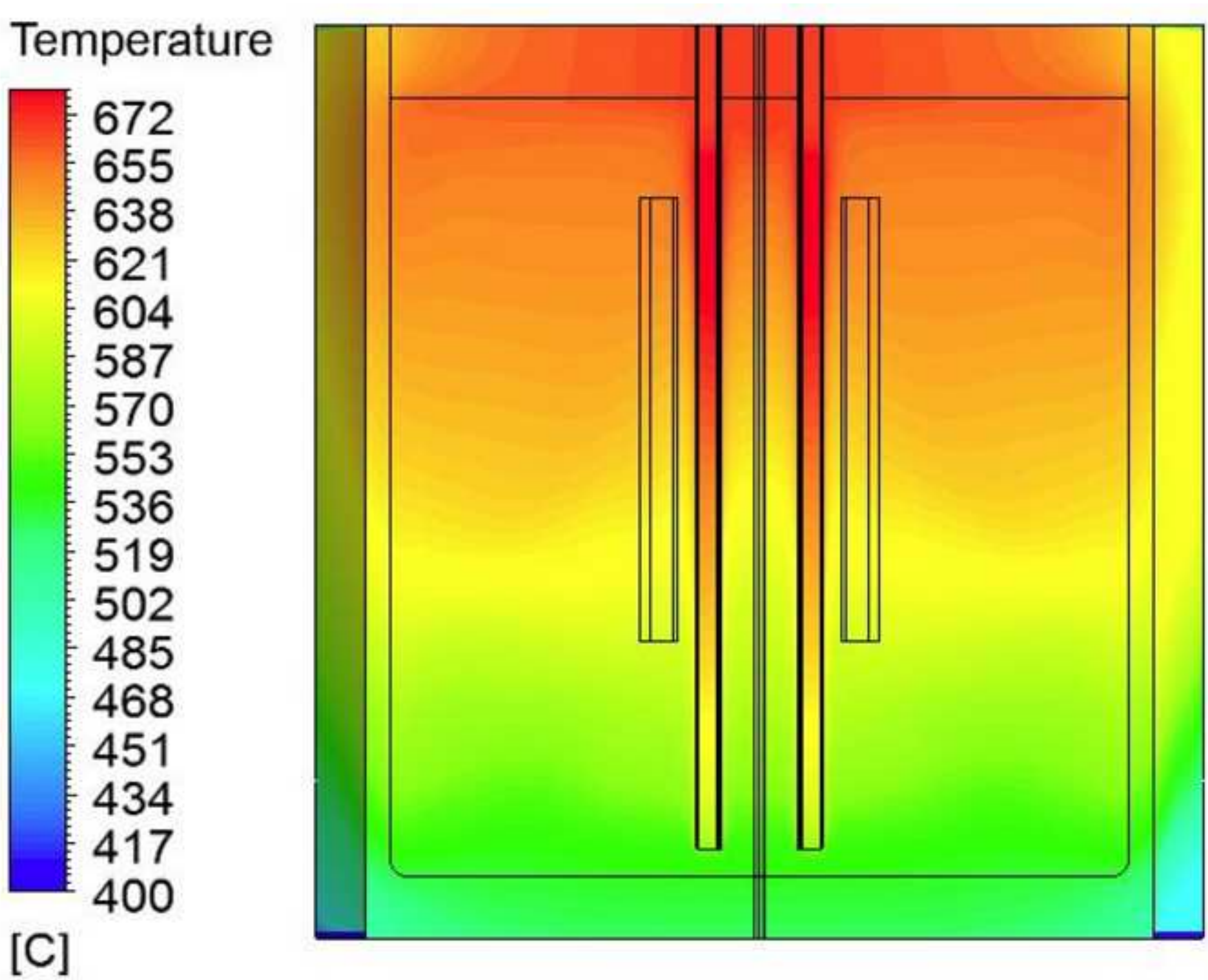

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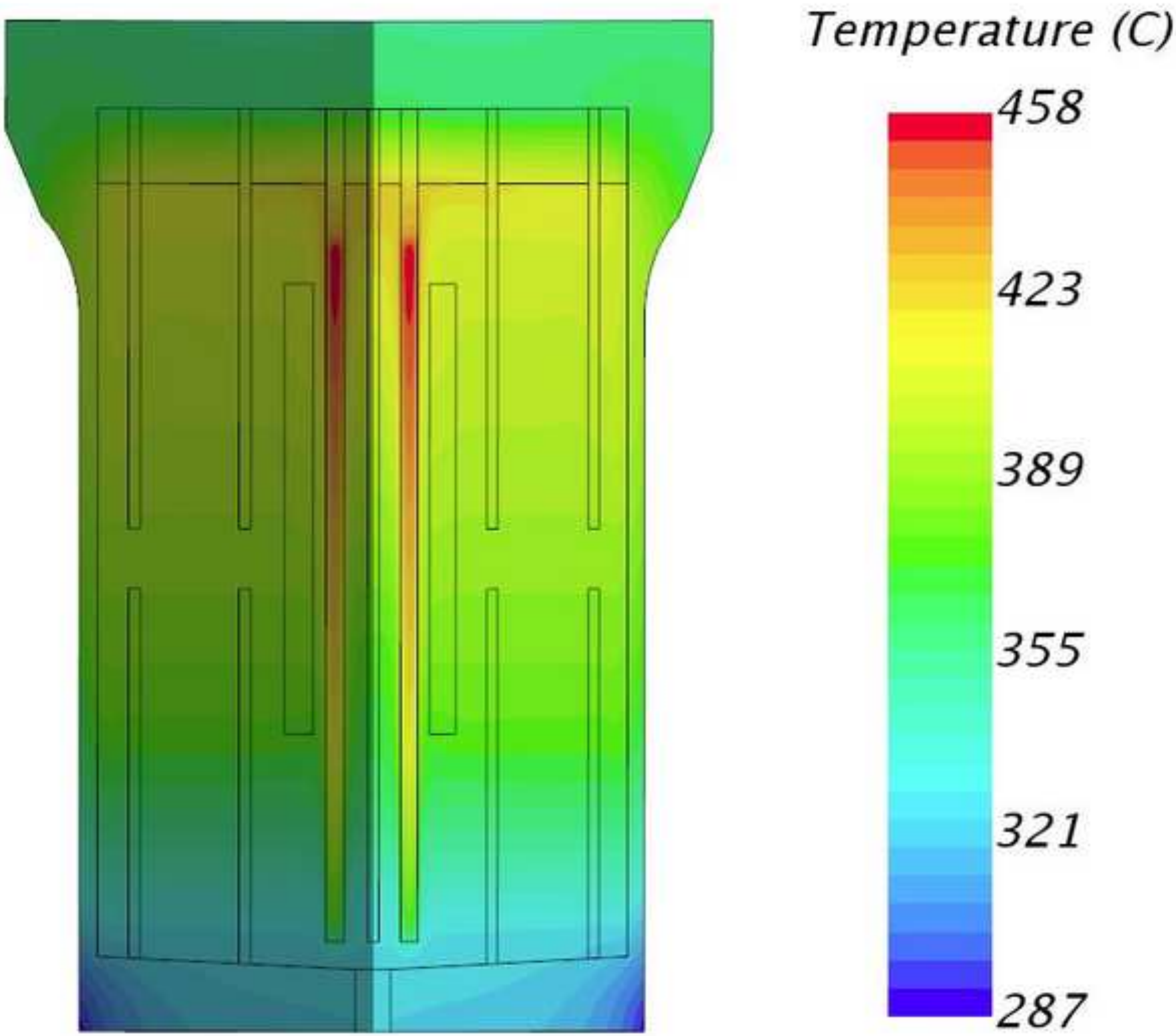

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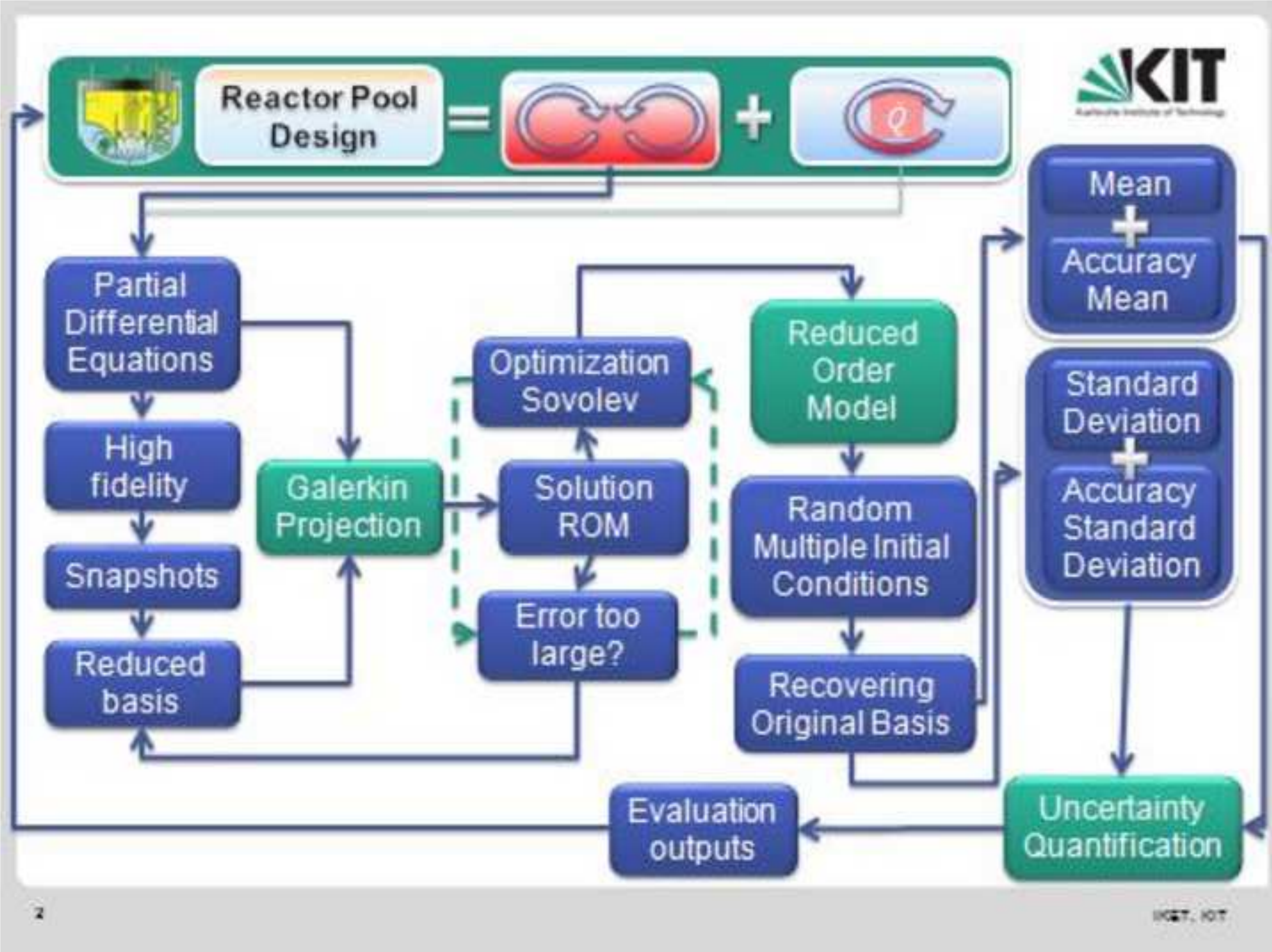

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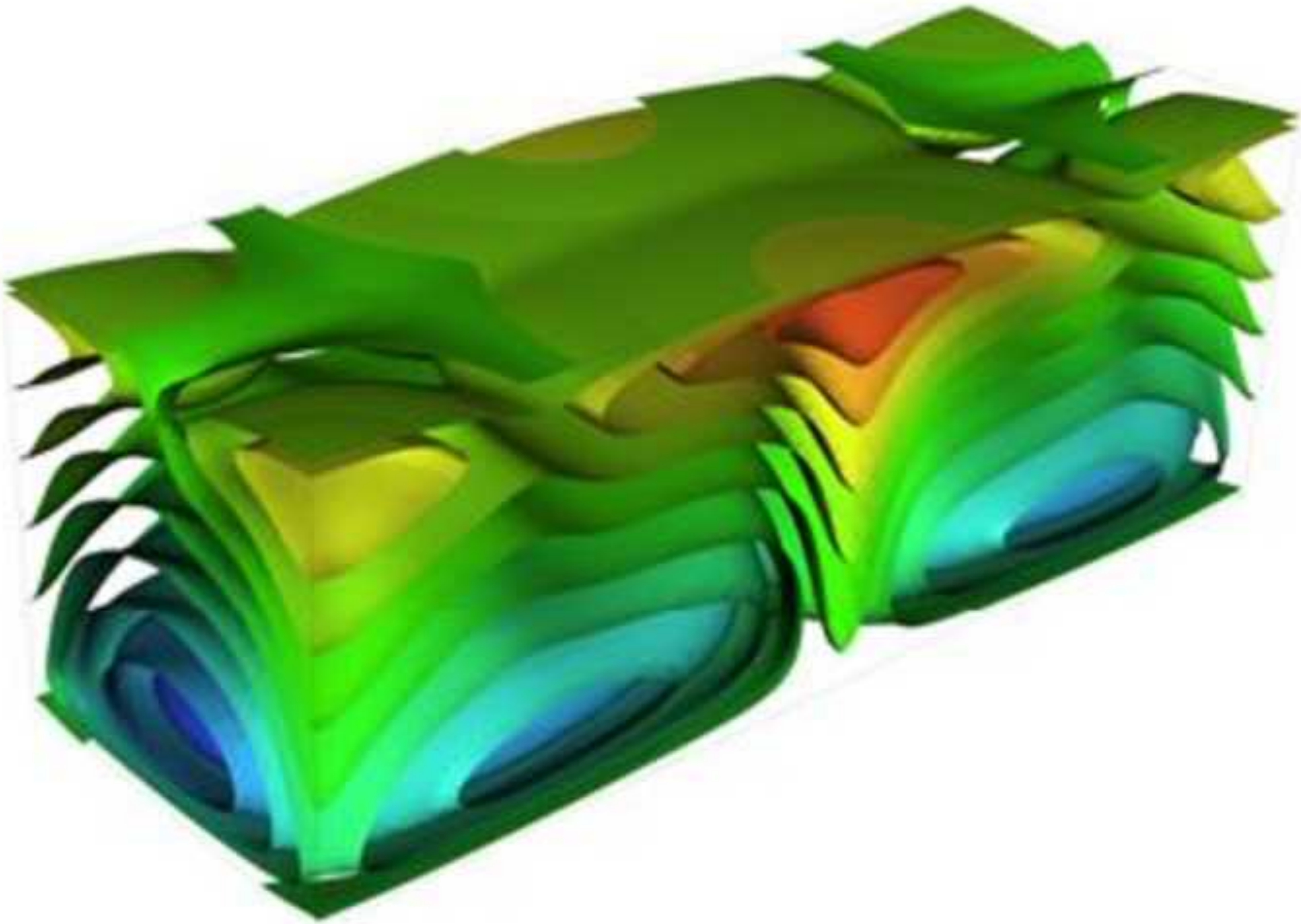

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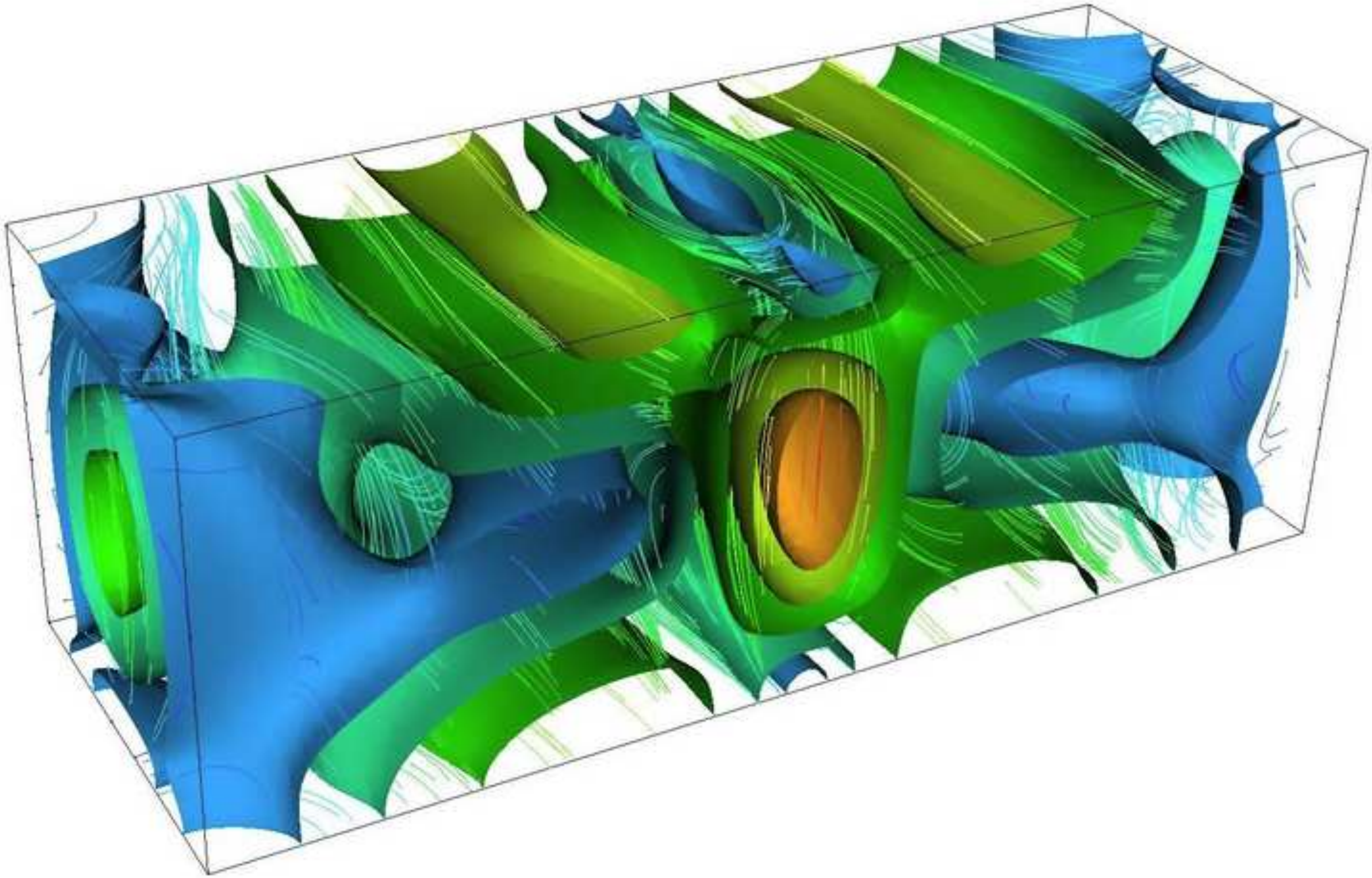

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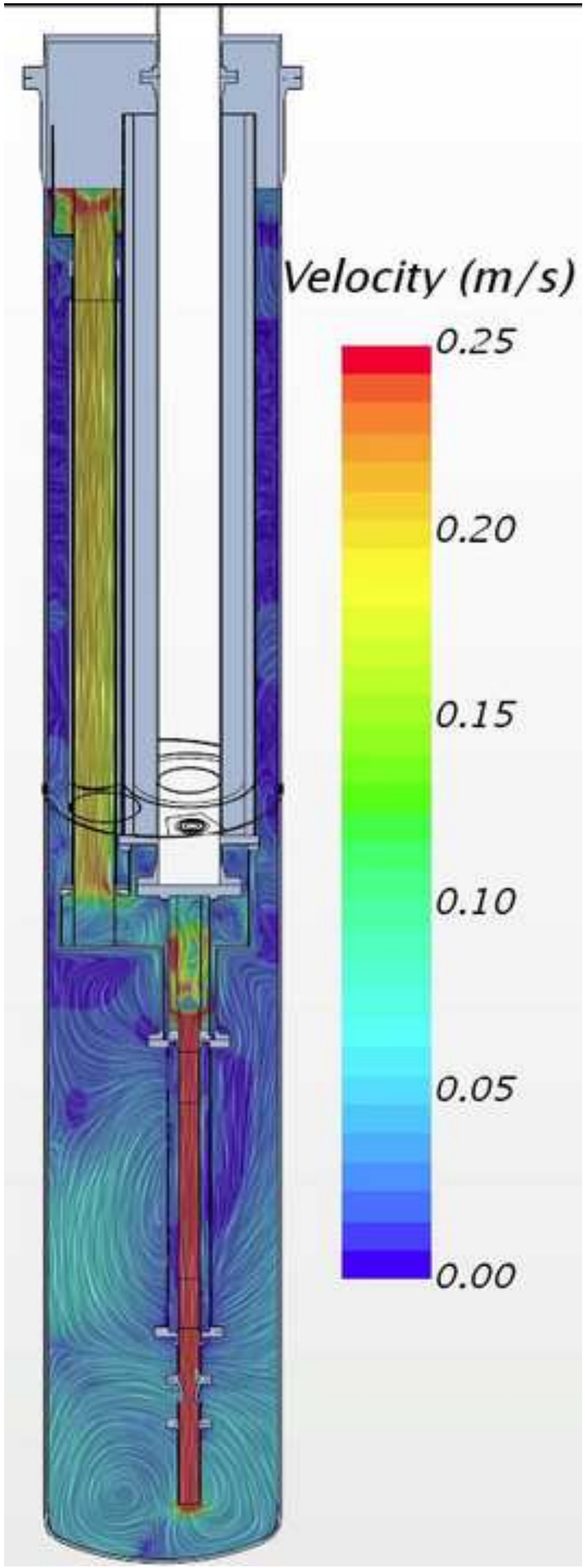

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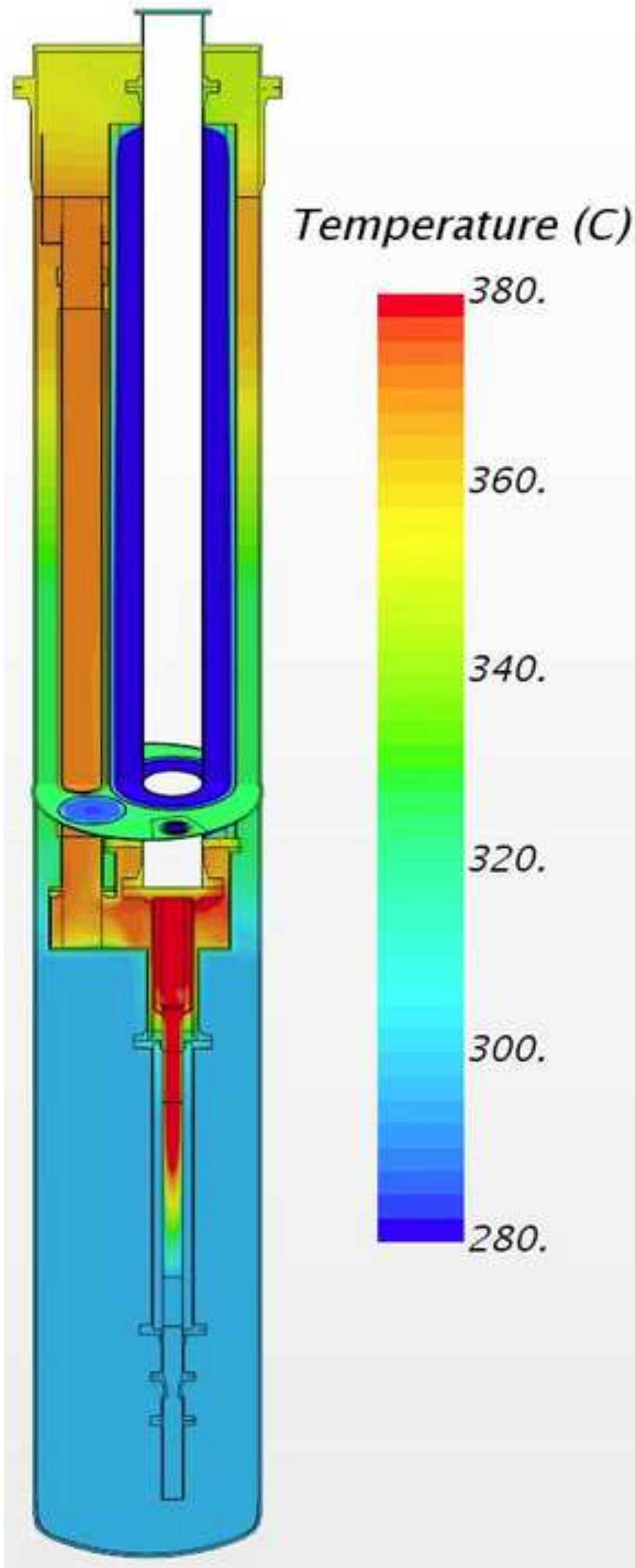

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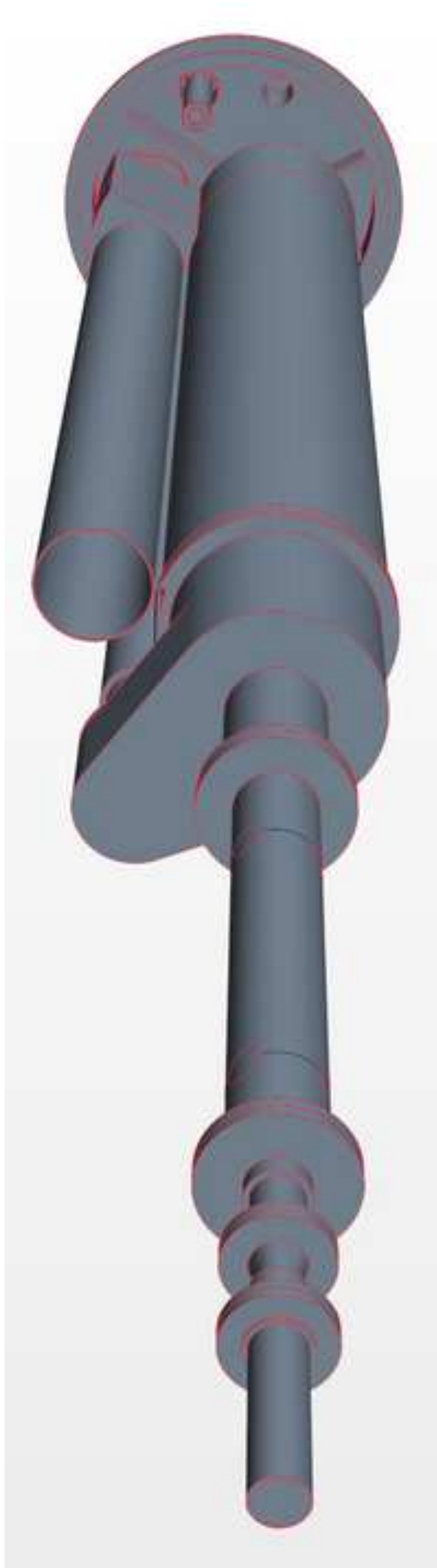

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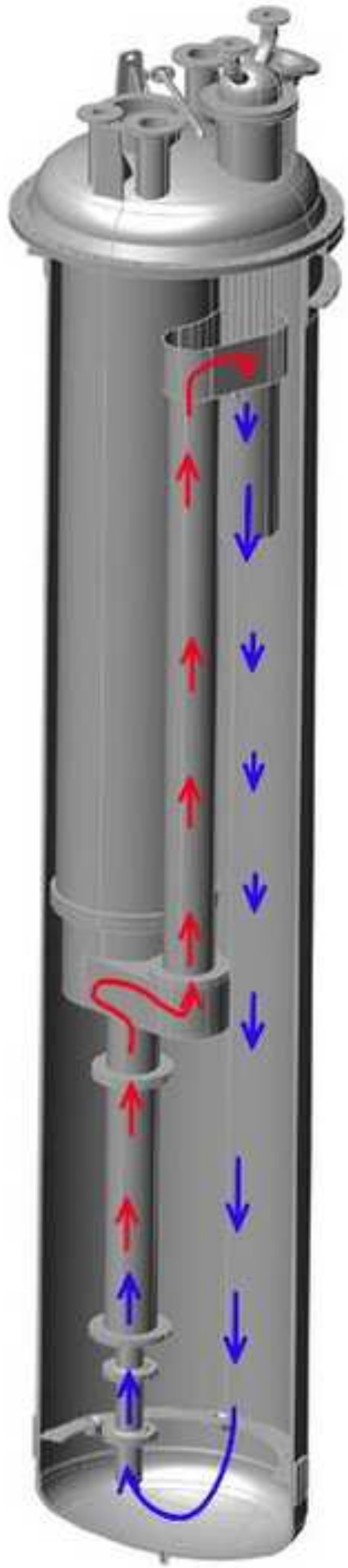

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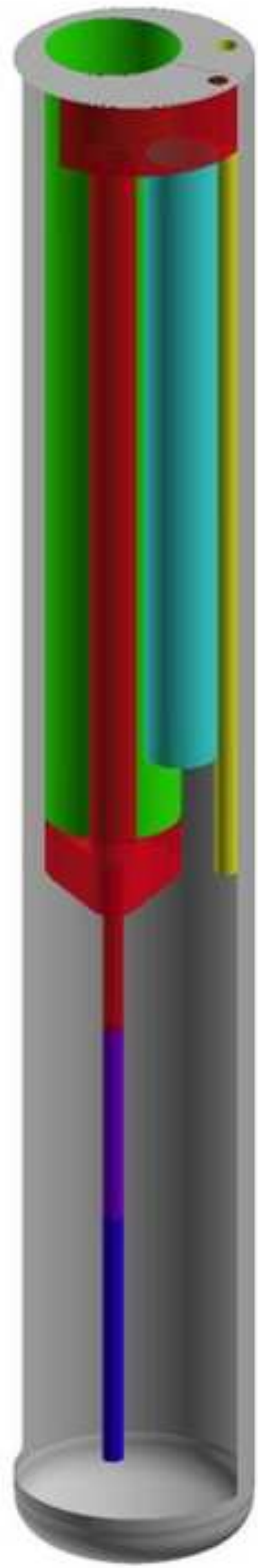

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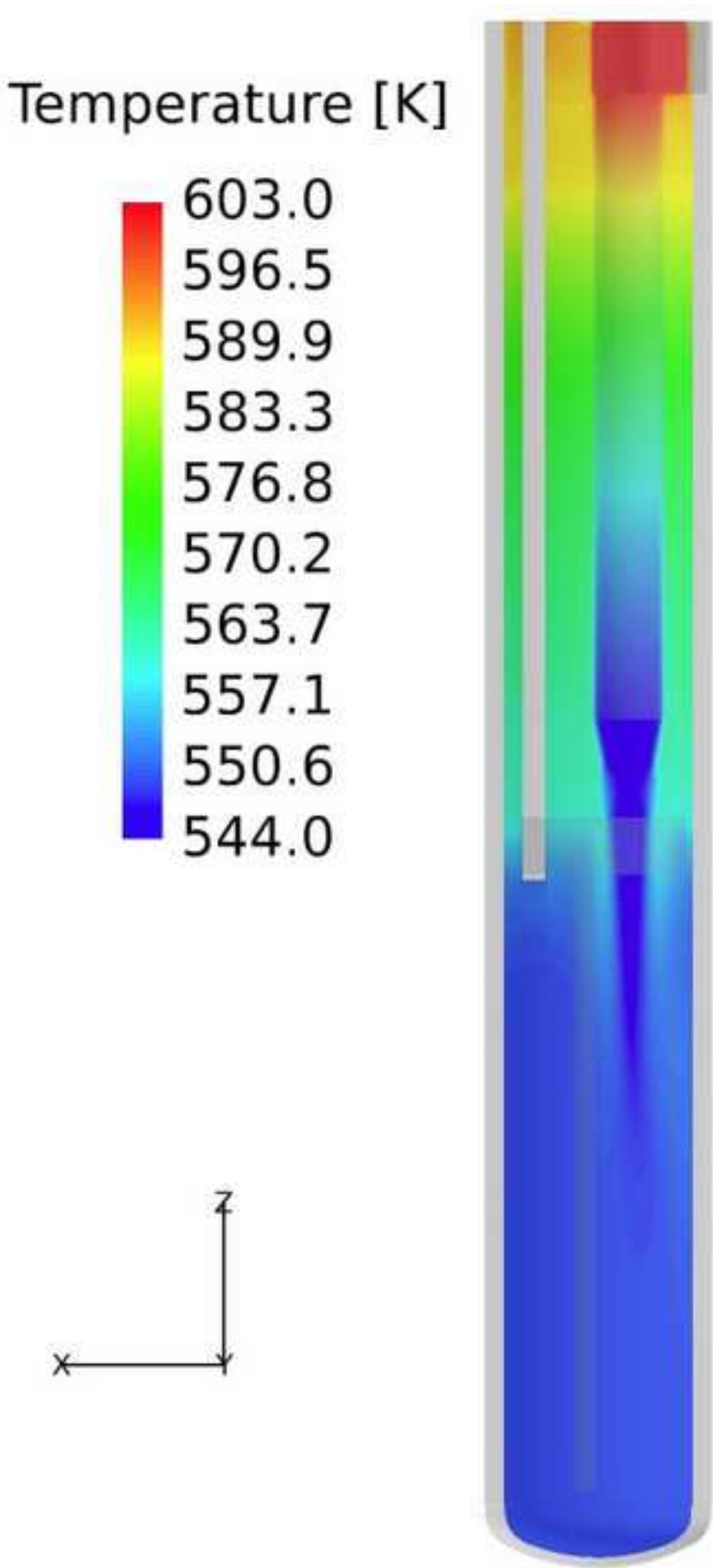

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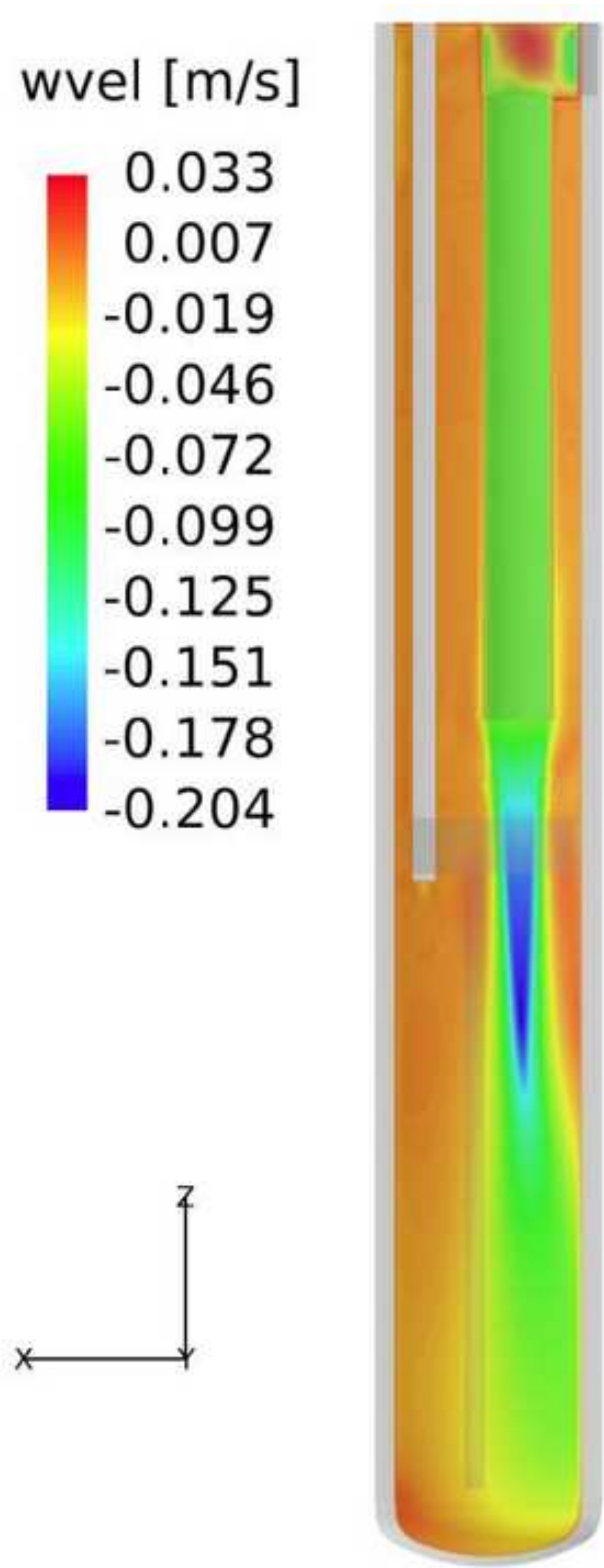

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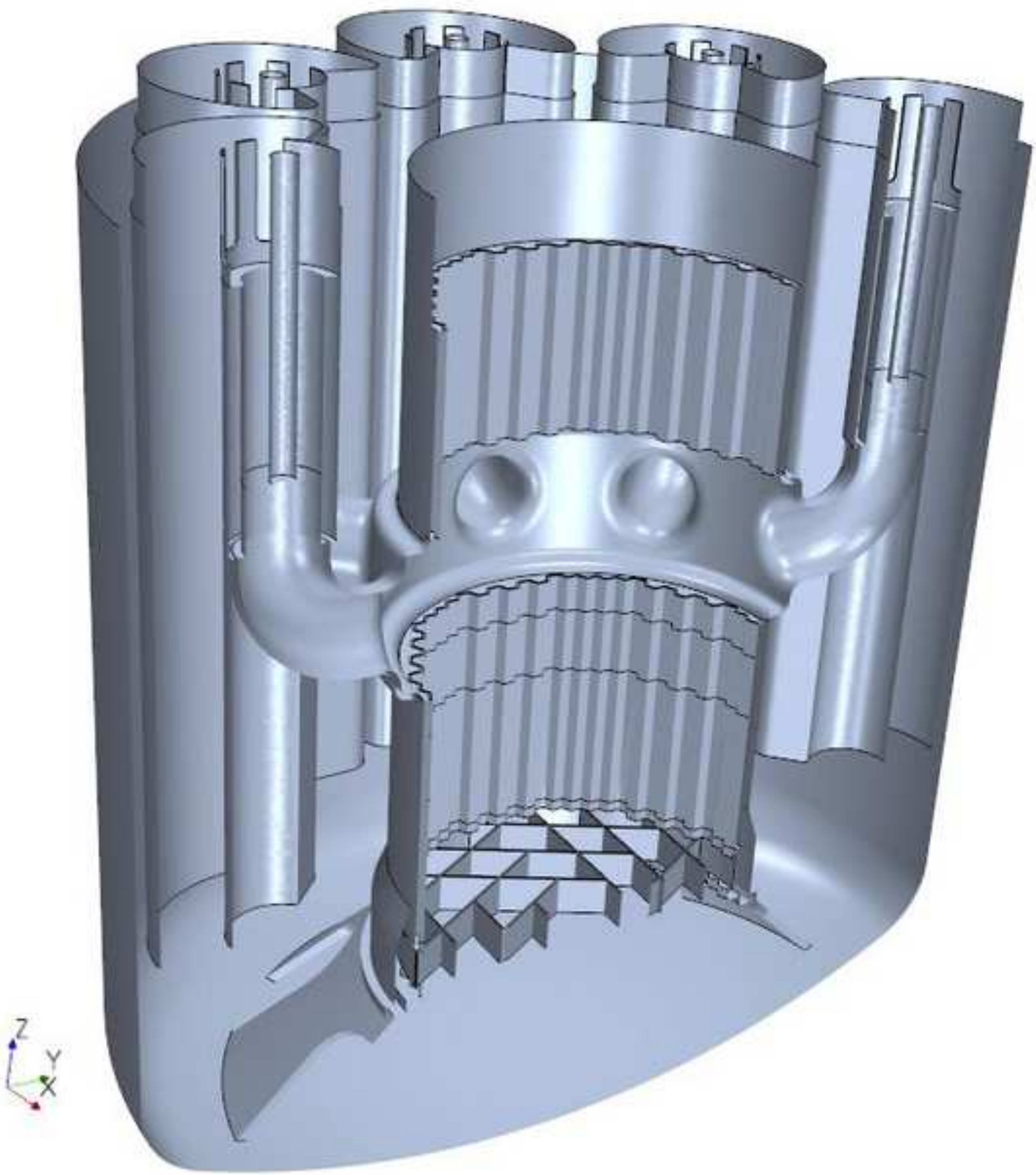

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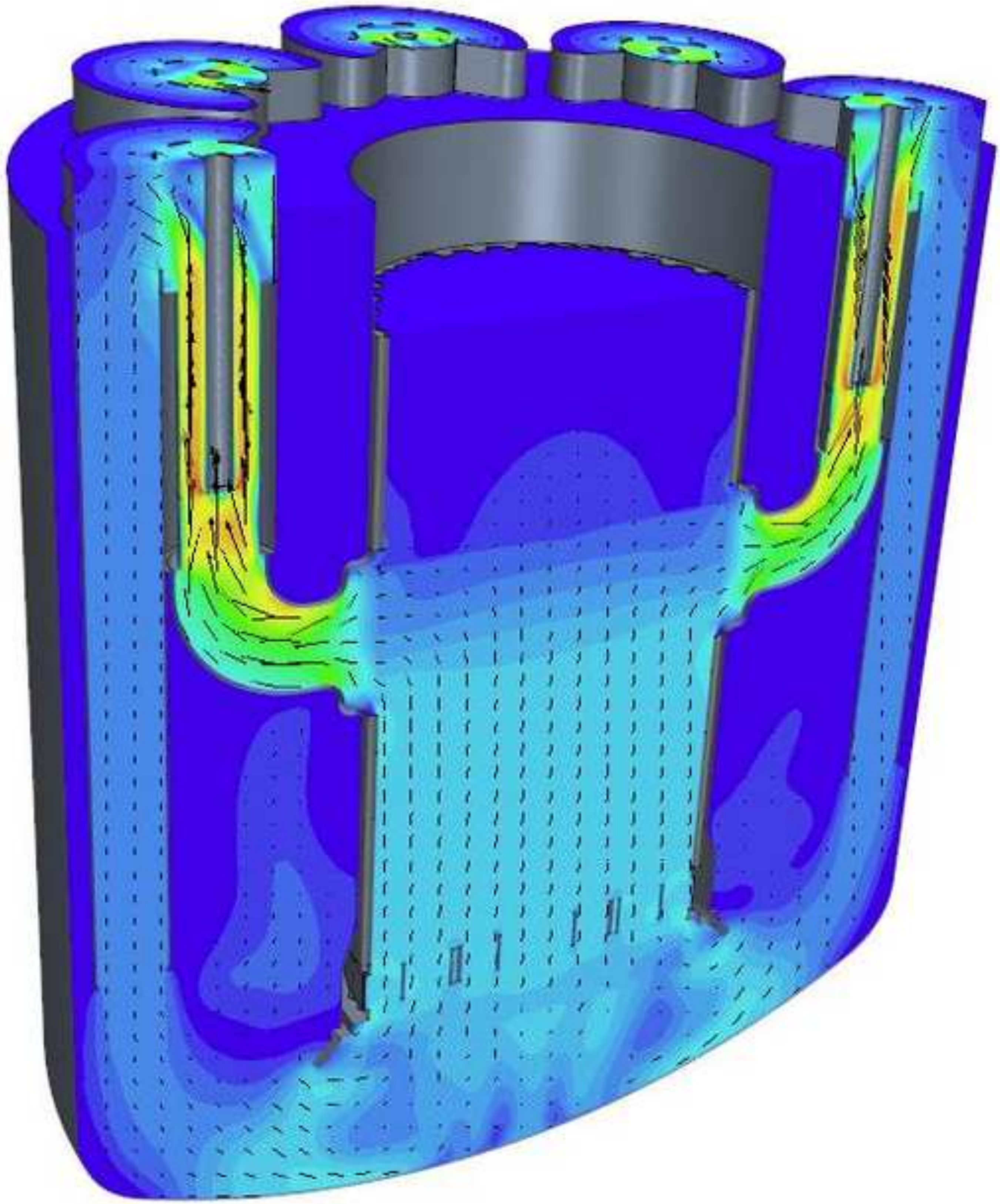

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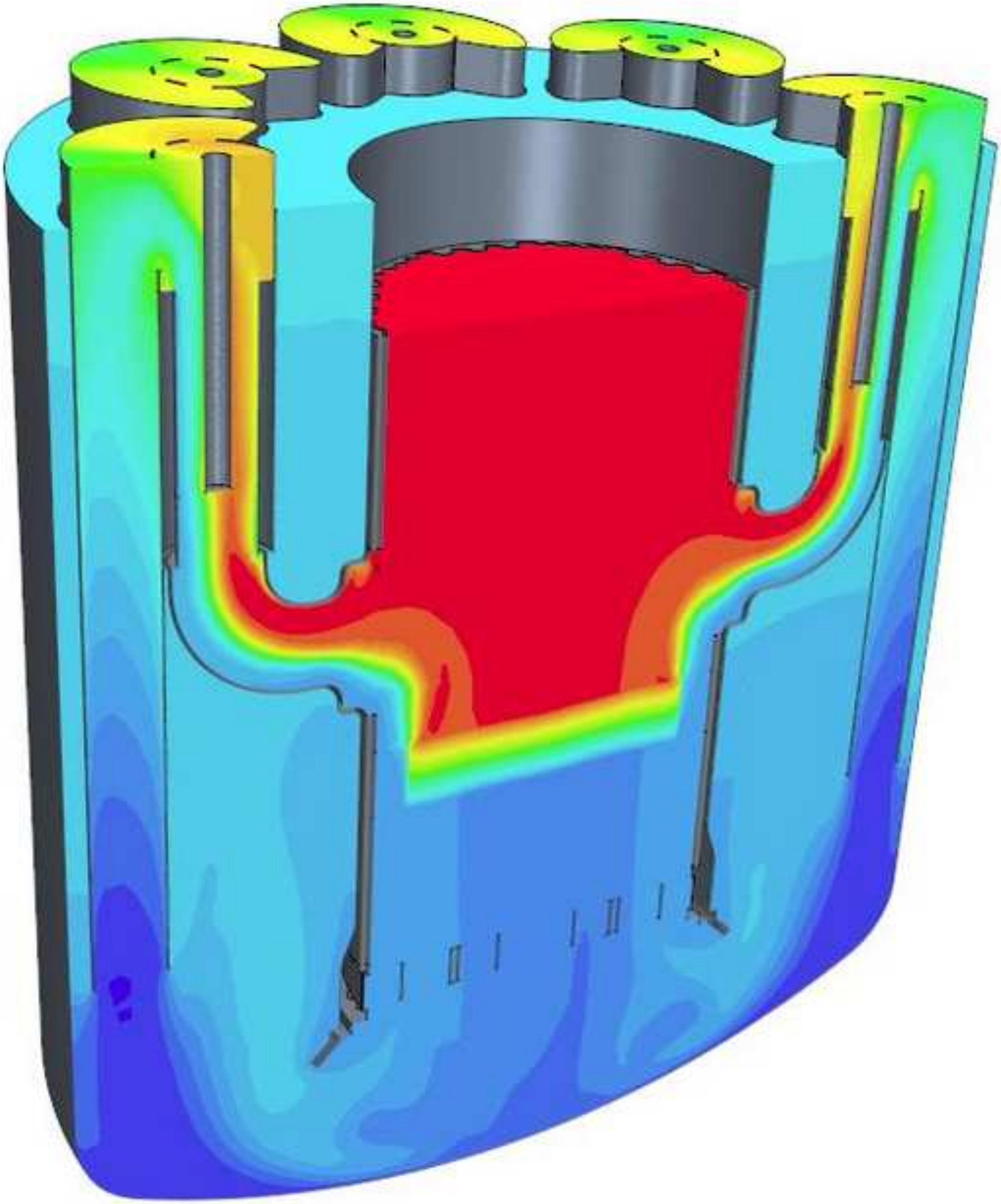

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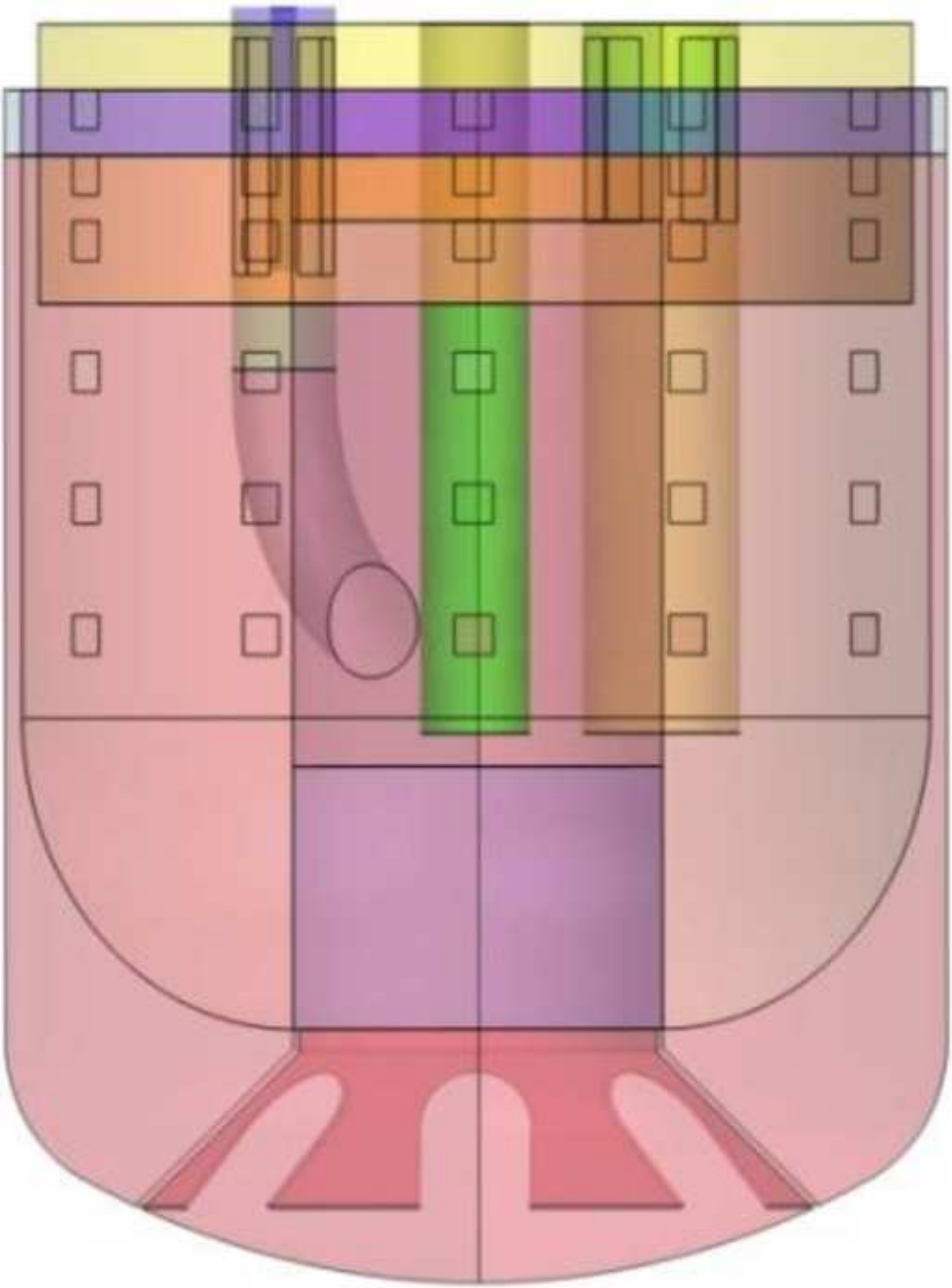

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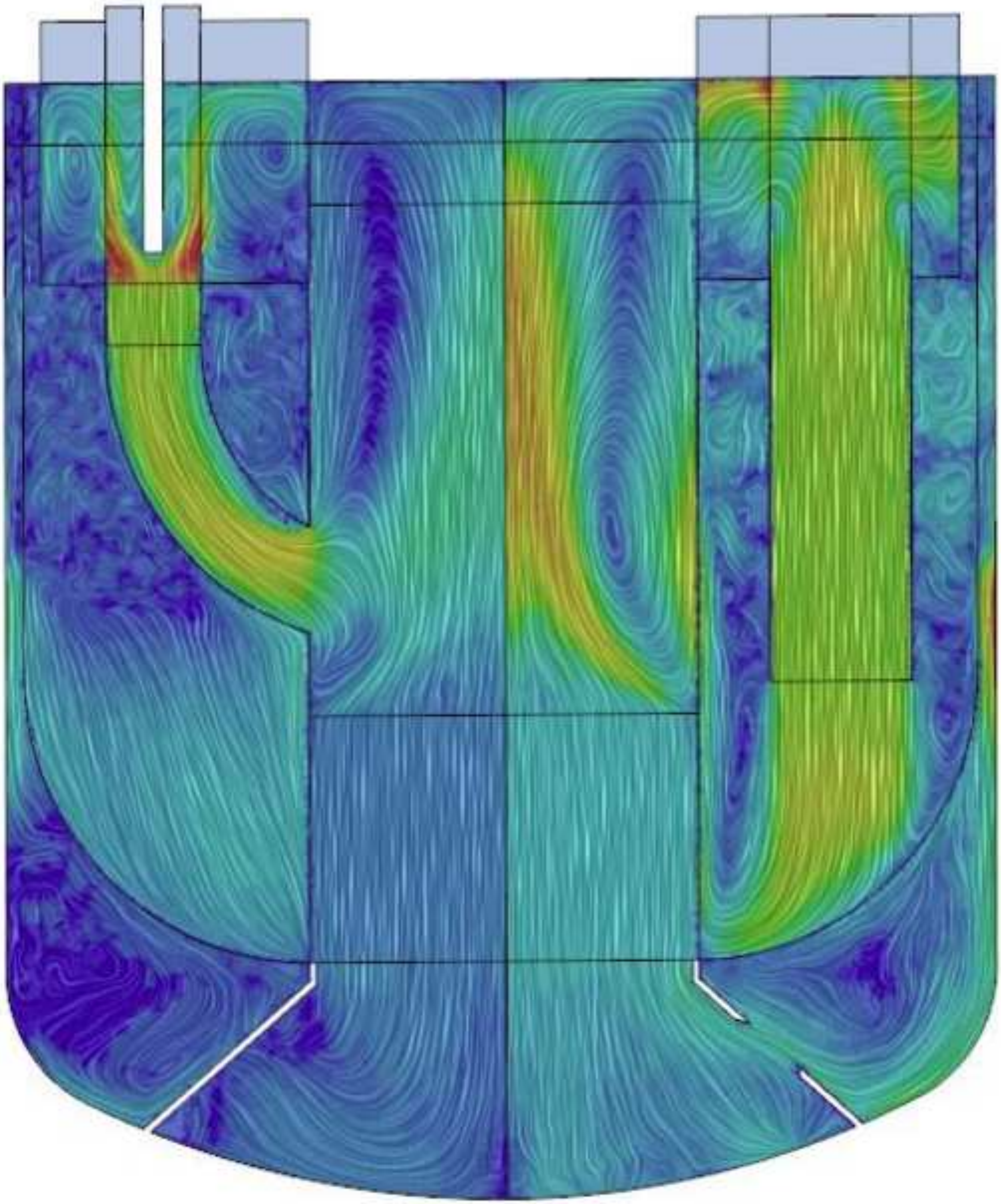

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