Review on Nuclear Thermal Propulsion Analysis of Fuel Element and Simulation Methods

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Abstract. This paper is mainly focused on reviewing different approaches for nuclear thermal propulsion analysis of fuel elements used for this matter. Mathematical models, simulation options and code generation that have been applied using computational tools such as OpenFOAM and other resources are considered. Additionally, experimental data from the Nuclear Engine for Rocket Vehicle Application (NERVA) is included in this paper. Nuclear thermal propulsion is known as one of the most important choice of propulsion technologies for coming manned missions to different interplanetary destinations. Systems based on Nuclear Thermal Propulsion (NTP) could improve vehicle returning and reduce missions risks. It can be done through travel time reduction and payload capacity improvement in comparison to for instance chemical propulsion systems. Nowadays developments of these systems are based on low enriched uranium fuels and this review work is focused on such fuel systems.

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1 Introduction

1.1 Fundamentals of Nuclear Propulsion

This type of rocket propulsion has some advantages and disadvantages. An important drawback is that the exhaust gasses are radioactive. On the other hand, the engine design is simple and can be started, stopped or restarted. This fact make these types of engines more suitable over other such as chemical rocket engines. Also, a nuclear rocket engine can produce bigger impulse and the energy resource to be able to start it is generated by itself. One of the first nuclear engines was developed during the ROVER program. Its initial basic concept was based on a graphite reactor loaded with highly-enriched uranium. In addition, hydrogen was used as propellant as well as coolant. Then, hydrogen was passed through fuel elements. This high temperature gas was discharged out of a nozzle creating thrust. Commonly, high performance is required for a high temperature gas. So, materials that can support long periods at these conditions are needed. As these kinds of propulsion engines started to evolve, fuel elements and nozzle configurations began to change as well. The program mentioned earlier was divided in four different sections, NERVA, KIWI, RIFT and PHOEBUS. The original idea of the NERVA project was to construct a 200000–250000 lb of thrust engine. Later, this NERVA reactor design changed the PHOEBUS model and other additional techniques were applied for testing purposes. Although at the beginning of the 70s this program was cancelled, it showed the benefits of the space technology advancements. The FE elements implemented in the 60s in different nuclear propulsion reactors such as the KIWI, PHOBEUS contained a graphite matrix. A set of coolant channels were coated with NbC or 2rC for carbon protection. Moreover, during those trials, mass losses were noted and this fact had an important effect on the neutronic features of the core reactor. At that time the development of novel fuel elements that could operate at high temperatures was started [6,12,19,23,30].

Nomenclature

NTP Abbreviations

NERVA Nuclear Engine for Rocket Vehicle Application
LEU low-enriched uranium
NTP Nuclear Thermal Propulsion
NRX Nuclear Rocket Experiment
HEU High-enriched uranium
LEU low-enriched uranium

OpenFOAM Symbols

k Turbulent Kinetic Energy
P Fluid Pressure
U Fluid Speed
T Temperature
ρ Density
ϵ Turbulent Dissipation

So, Nuclear thermal propulsion (NTP) is one of the most suitable technologies taken into inconsideration for space agencies such as NASA for long term or deep missions to space. It looks like the main source of energy is fission to be able to heat a fluid, particularly hydrogen which allows to get very high temperatures. Also, it permits to obtain a larger specific impulse (Isp) compared to chemical rockets. It is well known that most relevant performance variables of a rocket engine are Isp, thrust, and thrust to weight ratio. It is important to point out the importance of the temperature of gas that enters a nozzle in which the higher the temperature the higher Isp. The trust of the type of system is primarily driven by the pressure of the chamber, expansion nozzle and nozzle mass flow. Some studies state that common thrust and Isp values can vary from 10–100 klbf and 800–1000 s. One of the biggest programs for the development of NTP systems was the Nuclear Engine for Rocket Vehicle Applications (NERVA). During this program many technical information and experimental data were generated. Approximately, 20 reactor models were designed, manufactured, and tested. All NERVA designs are based on highly enriched uranium (HEU) fuel systems. The majority of these nuclear rockets designed under this program utilized graphite based, extruded hexagonal fuel elements in which nineteen coolant channels were included. Although many significant advancements were achieved during the NERVA program, there is a lot of research and development required to meet the future objectives of space agencies as NASA. It is important to note that the biggest challenge would be to change to low-enriched uranium (LEU) fuel systems. The initial research projects related to NTP systems were mainly experimental with different engines tested pointed earlier (Kiwi, Phoebus, Pewee, NERVA NRX). In the Phoebus case, its design was then modified by NERVA NRX series and other techniques were applied to carry out the first flight system to evaluate. The NERVA NRX-A6 was certainly the last uranium-

fueled reactor that was tested. This program was cancelled because a lack of funding from government [5,7,16,26–28,35].

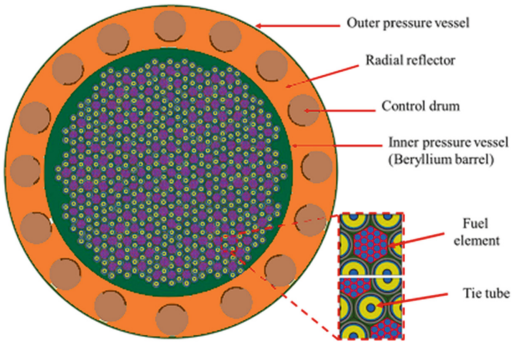

Fig. 1. NERVA configuration core, from [45]

However, these reactor programs could show that they are feasible with a high efficiency for the advancement of technologies for space propulsion. Highly-enriched uranium (HEU) was used in early NTP system designs which is not currently recommended regarding security and governing matters. Nowadays, designs are focused on high-efficiency engines based on low enriched uranium fuel (LEU). To be able to accomplish high specific impulse as well as thrust to weight values, these recent LEU developments would need geometry changes and length and configuration of the core. These adjustments might bring some doubts related to some parameters relations such as heat transfer that were studied within the NERVA program. Several specific Reynolds numbers were set for the large data obtained. However, it may not be totally used in recently developed designs. Likewise, the doubts mentioned earlier could be reduced by setting new experimental works that are expensive and are not available yet [45]. Hence, it is necessary to complete these costly experiments by using modeling and computational tools for simulation. Some of the research works covered in this review employed for instance Finite Volume Methods (FVMs) that seems to be a very suitable numerical method for NTP modeling. Also, these approaches have been used for many years for thermal hydraulic analysis based upon code generation [16,20].

For instance, the KLAXON code was one the first computational models utilized for NTP studies. Despite this, this methodology relied on just a 1D model. Then, another work implemented a 3D numerical method for simulations of a NERVA-type engine through a computational fluid dynamics code known as UNIC. In this simulation a CHT (Conjugate Heat Transfer) solver was applied [8]. This research proved that there is an important capacity of modeling a NTP through Finite Volume Methods. A very well - known computational source is OpenFOAM. It is a open-source finite volume method code to resolve problems

regarding chemical reactions, turbulence, and heat transfer phenomena. In addition, OpenFOAM is used for many nuclear usages. A very significant option is GeN-Foam which is a OpenFOAM based solver. It can execute different simulations for cores of reactors [13,14]. This review work is focused on OpenFOAM applications in which CHT approaches are used. The simulations conditions established are similar to the preliminary experimental tasks. The NRX-A6 trial reports provide initial data and results of measurements that were taken for OpenFOAM validation. In this current review, a detailed description of geometry configuration, thermal analysis and other variables is given. This simulation and analysis method can be a source solution to assist other codes such as THERMO [38]. Moreover, OpenFOAM and THERMO results are compared.

2 Nuclear Thermal Core Description

At the beginning of the 1960s, there used to be a lack of information regarding the properties and manufacturing techniques of materials used for NRE core (zirconium, uranium carbides, and zirconium hydride). However, a well-known fact is that a fuel based on UC-ZrC and UC-NbC with nearly can supply the hydrogen heating until 3.000 K. Hence, later studies found that the right progress is the consideration of materials with heating melting points such s uranium, zirconium and monocarbide. A typical nuclear core is made of fuel elements with cooling channels in which a high pressure fluid (hydrogen) flows. Normally, fuel elements (FE) are hexagonal-shaped with a composite matrix (U, ZrC). During previous research works, coolant channels were coated with ZrC in order to avoid reactions of the carbon contained in the matrix with the hydrogen. On the other hand, a Nuclear Reactor Engine (NTR) has turbopumps that are in charge of pressurizing the hydrogen and other components such as the nuclear reactor and nozzle. Also, the fuel core has tie tubes that are responsible of getting additional thermal energy to drive the pumps. In addition, high temperatures are reached by the fluid as it passes across the cooling channels and then increases in the converging-diverging nozzle. Core temperatures can get up to 2500 K which is very close to the maximum temperature of the hydrogen. Regarding pressure, a common usual NTR core can be about 3 MPa. However, some experimental devices are able to run at even higher pressures. A summary of operating conditions for a typical NTR NERVA engine is given. A schematic is displayed in Fig. 2. Within the experiments carried out during the NERVA program, the one known as the NRX-A6 trial is certainly the best documented. The NRX-A6 core has different clusters that contain six fuel elements. These are around an unfueled element in the center. Thermocouples are located in the unfueled elements. An important matter to point is the fact that to design a high performance NTR engine will need a good comprehension of these tricky processes as well as core material developments that are able to support high temperatures and flow rates of hydrogen [2,3,11,22,29,33,43].

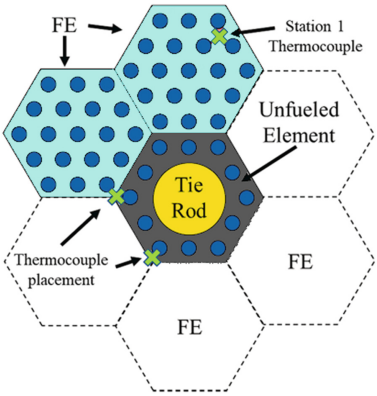

Fig. 2. Cluster of fuel elements for NERVA, from [45]

3 Mathematical Model Simulation Methods and Codes

Recently, OpenFOAM's CHT (Conjugate Heat Transfer) is the method employed as heat transfer model for graphite-based fuel elements. Also, the results obtained are compared to experimental data given by the NRX-A6 technical reports. In addition, a wide array of numerical methods have been developed. Some of them are still being developed because of several functioning limitations [8,21, 31,41]. For nuclear reactor analysis, an implementation of multiphysics coupling approaches are mainly involved. The neutronics/thermal (N/TH) is the most used and is being extensively-researched. The coupling solutions for the neutron transport equation solution can be divided into tight and loose. Tight is related to new computations code and loose are solved individually or decoupled. Coupling is achieved when information is exchanged by the boundary condition between them. Also loose coupling is also classified as internal and external coupling [4,15,24,37]. OpenFOAM (Open Field Operation And Manipulation) is a open free source C++ toolbox. OpenFOAM is based on a large library that provides several core functionalities such as discretization of partial differential equations, meshing, linear equations solutions, turbulence models and others. The users can develop resources to solve differential equations as well as new boundary conditions. This computational tool also offers solvers for specific problems, tools for meshing and pre and post-processing procedures. OpenFOAM mostly runs in parallel. In order to run an application, an OpenFOAM case should be set up. A case is just a directory that contains all the required files to be able to run a particular case. In Fig. 1 the basic structure of a case is shown. Each folder has a specific task. The *constant* directory has the mesh in the *polyMesh* subdirectory and the configuration files contain physical properties. In the *system* directory all the information about the solution process is found. It has mostly the following files:

– *controlDict*

– *fvSchemes*
– *fvSolution*

The first one defines control parameters to run a case. It includes solver, starting/ending times and time steps. The *fvSchemes* is employed to choose a discretization scheme. *fvSolution* manages the linear equation solvers and algorithms of solution. In addition, the directories of time have single data for all fields such as pressure p or velocity $\boldsymbol{U}$. Initial conditions are commonly established in the *0* time directory.

3.1 Semi-Implicit Method for Pressure Linked Equations (SIMPLE)

SIMPLE algorithm is a extensively iterative strategy for solution of the Navier-Stokes equations. It is basically a estimation-and-adjustment approach to calculate pressure. It begins by assuming a pressure field $p*$. It is then changed in the iteration procedure with pressure modifications p'. Hence, the field of pressure can be got from:

$$p = p* + p' \tag{1}$$

Some similar corrections are done to velocities as follows:

$$u = u* + u' \tag{2}$$

$$v = v* + v' \tag{3}$$

$$w = w* + w' \tag{4}$$

The velocity changes are computed from the pressure adjustments by taking a velocity change formula. This is obtained from the discretized equation of momentum in which some terms are omitted. There are two steps to perform when this algorithm is applied. The first one is the solutions of momentum equations for the new "starred" velocities. If the pressure field is not adjusted, the velocity field will not fulfill the equation of continuity. The main goal of the SIMPLE algorithm is to fix the pressure field in the iteration process in such a way that the velocity field can closely meet the equation of continuity. To be able to do so, the changes of pressure have to be done in some way. So, to accomplish this, a pressure change equation is acquired from the equation of continuity with some modifications. In the second step, these pressure adjustments equation is solved and a new pressure field is computed (Eq. 1). After that, the velocity fields are updated by using velocity changes formulas. The last step is to find the solution of other differential equations for other variables such as temperature, turbulence. New iterations are needed until convergence is got and no additional pressure adjustments are required [17,18,34,36,46].

3.2 Conjugate Heat Transfer (CHT) Model

The Conjugated heat transfer method is when there are two or more thermal subdomains which are connected. Likewise, heat transfer differential equations

are solved. These equations are linked by conjugate conditions on the interfaces of the subdomain. This condition is normally about requiring temperature continuity and heat flow. It is important to specify that in subdomains of solid kind, the heat equation is the only one that is solved. However, in fluid subdomain cases the equations, the Navier-Stokes equations and the energy equation have to be resolved. A couple of numerical approaches are considered within this methodology. One of them is to find the solution of the equations in all subdomains. The other one is utilize iterations to solve the differential equations in the subdomains individually. Boundary conditions are set for the subdomains and these are updated after a subdomain is solved. Iterations continue until solutions for all subdomains converge [10,27,39,42]. The OpenFOAM CHT solver taken indicated as *chtMultiRegionSimpleFoam* is a steady-state solver that can model turbulence of compressible flows by using the SIMPLE algorithm. Since this solver has a multiregion skill, it is used to mesh each region or subdomain. Hence, the recent studies have employed this option to be able to model for instance the heat transfer or fluid mechanics of the propellant and subdomains of solid fuel. Also, an interface for boundary conditions called *turbulentTemperatureCoupledBaffleMixed* is used by the CHT solver to combine fluid and solid regions. The following are the governing equations:

$$\lambda_1 \nabla_\perp T_1 = \lambda_2 \nabla_\perp T_2 \tag{5}$$

where λ denotes the thermal conductivity and T is the interface temperature. The suffixes 1 and 2 are the domains placed at the boundary of the interface. $\nabla_\perp$ is the gradient operator. Then, the heat flow q_s can be determined as follows:

$$q_s \approx \frac{T_s - T_i}{\nabla_i} \lambda_i(T_s) \tag{6}$$

where $\lambda_i(T_s), T_s, T_i)$ and ∇_i are the thermal conductivity, temperature of the interface, temperature of the first cell and the normal distance from the domain ($i = 1$ or 2). Additionally, the surface temperature is computed as follows:

$$T_s = \frac{\frac{\lambda_1}{\nabla_1} T_1 + \frac{\lambda_2}{\nabla_2} T_2}{\frac{\lambda_1}{\nabla_1} + \frac{\lambda_2}{\nabla_2}} \tag{7}$$

where the values of thermal conductivity λ_1 and λ_2 are calculated in both domains (1 and 2) considering thermodynamic properties combined with the model of turbulence. The following is a short description of the CHT solver:

Read fluid fields and solid fields;
while t < tMax **do**
  for all all fluid regions **do**
    Solve the equation of momentum;
    Solve the equation of energy and update thermophysical characteristics;
    Solve the equation of pressure and adjust velocities;
    Solve the equations of turbulence;

end for
for all solid regions **do**
Solve the equation of energy and update thermophysical characteristics;;
end for
t++;
end while

Firstly, a reading of all fields is done for all regions. After, the differential equations are solved at each time interval for all fluid regions and solid regions. The solution procedure begins by collecting initial fields and resolving equation of momentum for velocities. Then, the energy equation is solved and the thermophysical attributes are updated based upon the new temperature and pressure field of the former time step. Besides, the pressure equation should be solved and velocities are corrected in order to meet the equation of continuity equation by employing the recent field of pressure. Finally, the turbulence equations are computed for a fluid region the turbulence viscosity is updated. Regarding solid regions, just the energy equation is solved. The several regions are joined by boundary conditions. Once a equation is solved, the respective region boundary conditions are upgraded.

3.3 Generalized Nuclear Foam - GeN-Foam

For many years, simulation of nuclear reactor transient behaviour has been dependant on coupling of diverse codes for diffusion of neutron and thermal hydraulics (1D). In addition, recent research works on nuclear reactors analysis have used different codes that are focused on porous medium. One of these approaches is the GeN-Foam which can be applied to fuel elements as well as core of nuclear reactors. An advantage that can be pointed is the capacity to handle the porous medium equations are returned to the regular Navier-Stokes equations. Furthermore, another benefit is the possibility to be used with unstructured mesh configurations. It also has a wide range of applications and different mesh details (coarse or fine). Likewise, the possibility to solve different physics variables is included as well [14,36]. This solver contains four main sub-solvers elements: thermal-hydraulics, thermalmechanics, neutronics and a 1D sub-solver which tests temperatures in fuel. All of them use an unstructured mesh that is an importance difference compared to other codes which just operate with structured meshes. All sub-solvers have the capacity of parallel computing. For equations discretization issues, a finite-volume method is implemented and the algebraic equations obtained are resolved by applying OpenFOAM linear iterative solvers.

3.4 Thermal Hydraulics Equations

One of the main objectives of GeN-Foam option is to study the complete core of a nuclear reactor. It has been seen that a standard turbulence modeling such

as RANS (Reynolds averaged Navier-Stokes) has a high computational cost. So, an alternative is to deal with these kind of arrangements as porous media. The resulting equations of mass, momentum and energy in this type of media are:

$$\frac{\partial \gamma \rho}{\partial t} + \nabla \cdot (\gamma \rho \mathbf{u}) = 0 \tag{8}$$

$$\frac{\partial \gamma \rho \mathbf{u}}{\partial t} + \nabla \cdot (\gamma \rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot (\mu_T \nabla \mathbf{u}) - \nabla \gamma p + p_i \nabla \gamma + \gamma \mathbf{F_g} + \gamma \mathbf{F_{ss}} \tag{9}$$

$$\frac{\partial \gamma \rho \mathbf{e}}{\partial t} + \nabla .(\mathbf{u} \gamma (\rho e + p)) = \nabla \cdot (\gamma k_T \nabla T) + \gamma \mathbf{F_{ss}} \cdot \mathbf{u} + \gamma \dot{Q}_{ss} \tag{10}$$

where $\mathbf{F_{ss}}$ represents the drag force on the fluid carried out by the sub-scales layouts. $\dot{Q}_{ss}$ is the volumetric heat transferred during the interaction of the fluid and the sub-scale layout.

3.5 Thermal Mechanics Equations

It is a solver provided by OpenFOAM commonly known as *solidDisplacementFoam*. It is used to check core structure deformations due to induced temperatures. The following displacement equation D_f is solved:

$$\mathbf{v}_f \cdot \nabla \cdot D_f = \alpha (T - T_r ef) \tag{11}$$

where $\mathbf{v}_f$ is axial direction and α is an expansion coefficient [9,32,40,44,47].

3.5.1 Turbulence Model The most common model taken for turbulence flow modeling and simulation is the $k - \epsilon$ one. It can work with different Reynolds numbers. The last research studies have used high R_e values. This model is very suitable when flow paths do not have curvatures or are all straight. An important issue is that eddy viscosity is considered as scalar. Nevertheless, this assumption may be true just for regions in which the fluid is completely developed. On the contrary, when near walls is not certainly valid. Therefore, some additional analysis is needed for near-wall when the $k - \epsilon$ approach is applied. To be able to deal with these possible concerns some additional OpenFOAM functions are also taken into consideration (*epsilonWallFunction* and *kqRWallFunction*) [1].

3.5.2 OpenFOAM Mesh Structure The OpenFOAM mesh type used for fuel elements modeling is hybrid. It is made of hexahedron and tetrahedron cells (structured and unstructured). The structured mesh is placed close to the solid-fluid region (Fig. 3). On the other hand, the unstructured one is employed in the other domains (coolant and solid). Regarding quality of the mesh, finite volume methods (FVM) normally require high - quality meshes. These can be structured or non- structured. A non-orthogonality approach can be used to correct issues that may generate inaccurate solutions [25,31,45].

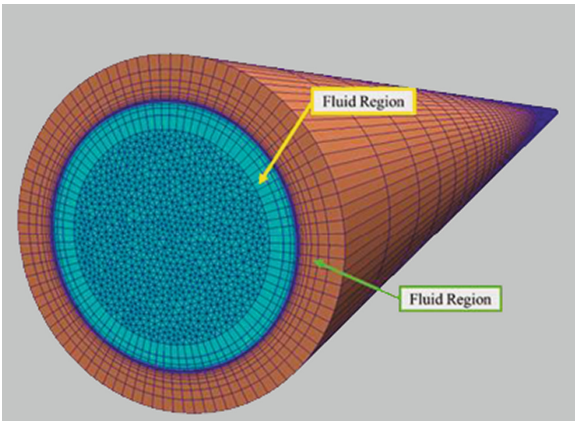

Fig. 3. OpenFOAM geometry for validation, from [45]

4 Summary

There is a wide range of methods that can be implemented for nuclear reactor analysis. For instance, some of them involve either neutronics or thermal-hydraulics coupling and even some deterministic models. Therefore, different solution methods for the neutron transport equations can be used. It seems that the THERMO technique is no totally reliable when applied to new designs. It may have some limitations for thermal hydraulic computations. On the contrary, OpenFOAM shows much better results since it does not depend on heat transfer interactions as the CHT solver is applied. A simple comparison between OpenFOAM and THERMO is done for validation work purposes by using data mapping of the outcomes got from [45] after post-processing (Figs. 5 and 6). Regarding the experimental tasks realized in the same study (Fig. 4), an analysis is performed between some experimental data and OpenFOAM. THERMO results are not included in this data mapping approach. Some good approximations are seen particularly in the exit temperature of the propellant. In this case is noted that THERMO can not provide a reasonable temperature approximation. In the axial mean temperature a right correspondence is observed. In [18] another important comparison is analysed among three distinctive coupling methodologies (OpenFOAM, RMC and Monte Carlo). In addition, other variables that may get an important variation are the fuel temperature, fuel distribution over the core within the reactor, deformation of the core due to change in temperature and power change. A new solver named thermalMechanicsFoam is employed to solve thermal expansion and heat conduction analysis in the core. On the other hand, RCM is applied for simulation of reactor core and its neutron transport features. The RCM and OpenFOAM strategies provide results which are very adequate with no significant differences and accurate for coupling computations. Other

solving approaches such as Monte Carlo and 3D Thermal Hidraulic codes (3D TH) are even more precise nowadays. However, more research and validations studies would be required since there are still some computational restrictions and troubles with code improvements. Likewise, Picard and JFNK methods also need more research to be able to validate their performance and accuracy. Currently, most numerical simulation works apply the Picard system for coupling due to its higher reliability. Despite this, it has some low computational capability. Some additional methods have been added to be able to upgrade the low computational issue. For multiphysics coupling simulations the main solution method that could be considered in the near future is the JFKN approach. This solving option offers a high-efficiency performance. An interesting novel model based on OpenFOAM in which 1D, 2D or 3D domains are not really necessary to solve the governing equations. Hence, it is important to notice some advantages for the residuals of the pressure equation and iterations for several applications of interest. For future work this code development will be added to the GeN-Foam system for validation and examination.

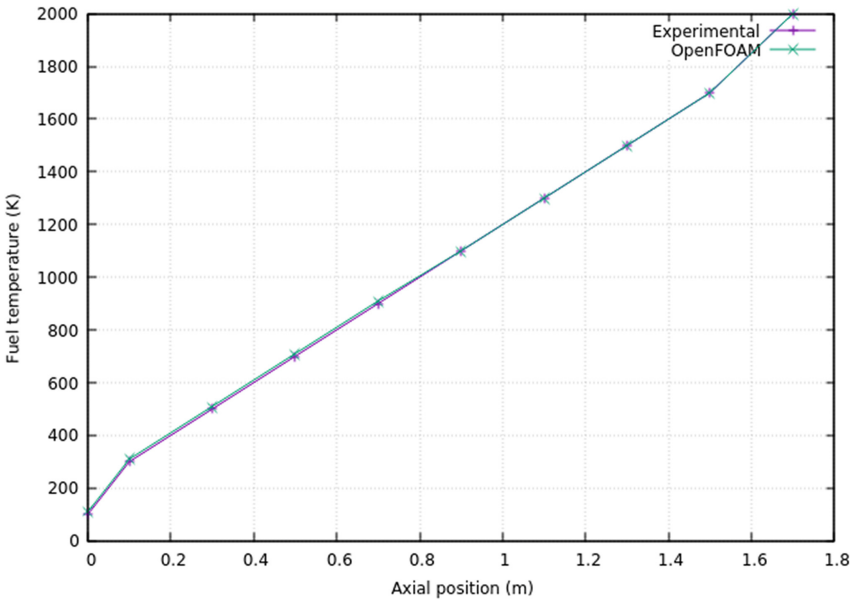

Fig. 4. Numerical and experimental comparison, from [45]

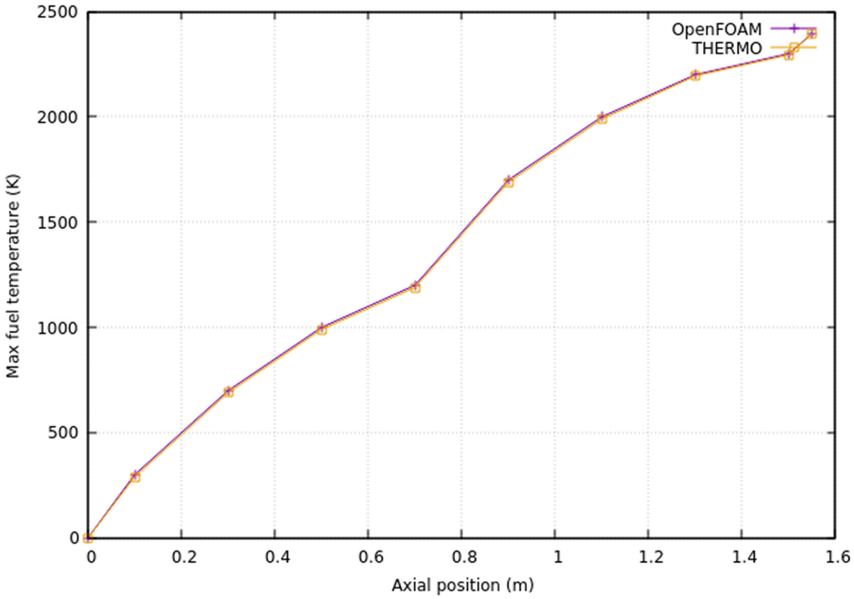

Fig. 5. Code comparison/Fuel maximum temperature), from [45]

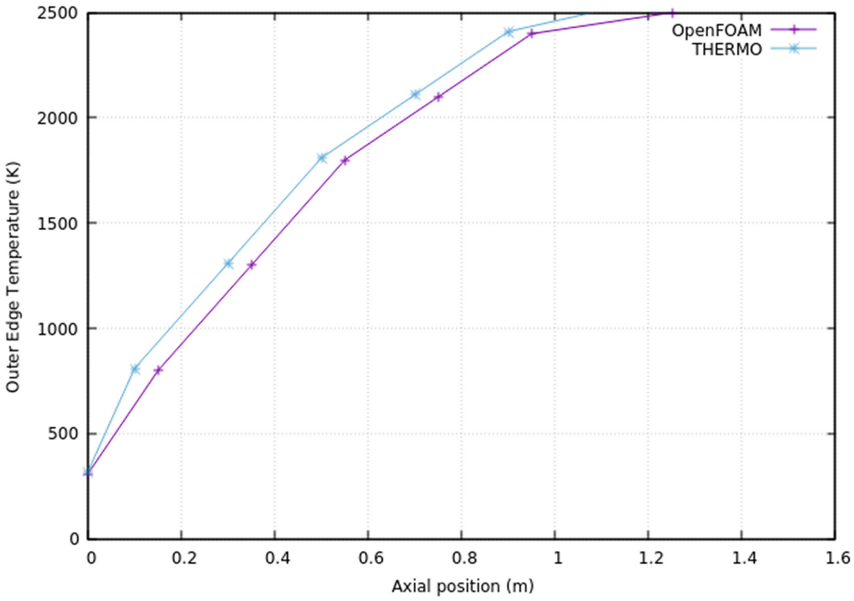

Fig. 6. Code comparison (Fuel outer edge temperature), from [45]

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