Numerical methodology for the analysis of Molten Salts natural circulation systems

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Introduction
Context of the work

- This study is focused in the cases in which the system response is driven by natural convection.

- This narrows its range of applications to states of the plant in which the main source of power is the decay heat, and to the associated systems. In our case for example the draining tanks.

- There is a decrease on the degree of coupling of the different physics, allowing to concentrate the efforts in thermal-hydraulic aspects.
Natural convection and instability

- The system dynamic state is determined by the balance of various phenomena like thermal expansion, temperature gradients, viscous forces.
- For a given set of conditions, the state of the system could become unstable and susceptible to perturbations, leading to an undesired dynamic.
- In the case of a molten salt additional specific phenomena like internal heat generation and radiative heat transfer have to be considered.
Objectives of the work - Main activities

- The development of a numerical methodology capable of performing a thorough description of the system.
- The selection of a base case for the numerical implementation of the methodology.
- The application of the developed methodology in the design of a natural circulation experiment.
- The experimental campaign that will allow to study the performance of the methodology.
Description of the Methodology
Methodology capabilities

Conceived for the evaluation of possible configurations for the design of safety systems, requiring:

- A description of the system through a CFD simulation for selected configurations.
- To identify transitions between the different states within a given range of parameters (study of bifurcation phenomena).
- To characterize the dynamic states in terms of stability.
- A stage of computational cost reduction due to the large of cases to consider, through the use of Reduced Order Methods.
Suitable configuration

Extended description of the system
- Behavior in a range of parameters
- Detection of bifurcation phenomena
- Transition between dynamic states

Basic description of the system
- Capture different phenomena
- Dynamic behavior of the system

Stability Analysis
- Evaluation of dynamic states
- Restrict range of applicability

Select a possible configuration
- Only general constraints
Description of the base solution

- The resolution of the thermal-hydraulic problem is based in the open source library OpenFOAM 6, which uses the finite volume method (FVM) approach.
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- Due to the relatively low velocity of the fluid and the absence of high temperature gradients the flow can be considered as incompressible. Boussinesq approximation for buoyant flows is applied.

\[ \rho(T) = \rho_{ref}[1 - \beta(T - T_{ref})] \]
\[ \nabla \cdot U = 0 \]
Stability analysis of the solution

● For the stability analysis a tool based on linear stability analysis is used, working with small perturbations around a base solution.

\[ U(x, y, z, t) = U_0(x, y, z) + \delta U(x, y, z, t) \quad \text{with} \quad |\delta U| \ll |U_0| \]

\[ p^*(x, y, z, t) = p_0^*(x, y, z) + \delta p^*(x, y, z, t) \quad \text{with} \quad |\delta p^*| \ll |p_0^*| \]

\[ T(x, y, z, t) = T_0(x, y, z) + \delta T(x, y, z, t) \quad \text{with} \quad |\delta T| \ll |T_0| \]
Stability analysis of the solution

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\[
\nabla \cdot \delta U = 0
\]

\[
\frac{\partial \delta U}{\partial t} + (U_0 \cdot \nabla)\delta U + (\delta U \cdot \nabla)U_0 + \nabla \delta \rho^* - \nabla \cdot [\nu D(\delta U)] + \beta g \delta T = 0
\]

\[
\frac{\partial \delta T}{\partial t} + (U_0 \cdot \nabla)\delta T - (\delta U \cdot \nabla)T_0 - \nabla \cdot (\alpha \nabla \delta T) = 0
\]
Stability analysis of the solution

- For the stability analysis a tool based on linear stability analysis is used, working with small perturbations around a base solution.

- Additionally, the perturbations are considered to have a wavelike form and the linear problem is reduced to an eigenvalue problem (EVP).

- Implemented as a coupled routine between OpenFOAM and MATLAB.
Reduction of computational cost

- Reduced Order Models are used in different stages of the process to decrease the computational cost.
- For the stability analysis, to reduce the cost of solving the EVP, this is solved with a time-stepping approach combined with the Dynamic Mode Decomposition (DMD) method.
- The resulting eigenvalues give information about the stability of the system.
Reduction of computational cost

- The main problem continues to be the large amount of cases to be considered in a design stage.
- The method used for this purpose is called POD-FV-ROM and has been developed at the Department of Energy - PoliMi.
- Extracts information about the dynamics of the system from full order simulations to obtain results for a different set of parameters.
Reduction of computational cost

\[ u(x, t) \quad \longrightarrow \quad u_r(x, t) = \sum_{i=1}^{N_r} a_i(t) \varphi_i(x) \]
Reduction of computational cost

\[ u(x, t) \rightarrow \mathbf{u}_r(x, t) = \sum_{i=1}^{N_r} a_i(t) \varphi_i(x) \]
Reduction of computational cost

Full Order Simulation
(OpenFOAM)

\[ u(x, t) \]

\[ u_r(x, t) = \sum_{i=1}^{N_r} a_i(t) \varphi_i(x) \]

Reduced Basis
Reduction of computational cost

Full Order Simulation (OpenFOAM)

\[ u(x, t) \]

\[ \mathbf{u}_r(x, t) = \sum_{i=1}^{N_r} a_i(t) \varphi_i(x) \]

Reduced Basis
Reduction of computational cost

Full Order Simulation (OpenFOAM)

\[ u(x, t) \]

\[ u_r(x, t) = \sum_{i=1}^{N_r} a_i(t) \varphi_i(x) \]

Reduced Basis
Reduction of computational cost

Full Order Model
(OpenFOAM)

\[ \begin{align*}
\{ u_t + (u \cdot \nabla)u - \nu \Delta u + \nabla p &= 0 \\
\nabla \cdot u &= 0
\end{align*} \]

Reduced Order Model
(Python)

\[ \frac{d a_j(t)}{dt} = v \sum_{i=1}^{N_r} B_{ji} a_i(t) - \sum_{k=1}^{N_r} \sum_{i=1}^{N_r} C_{jki} a_k(t) a_i(t) \]

\[ j = 1, \ldots, N_r \]
Reduction of computational cost

Full Order Model
(OpenFOAM)

PDE system
(N-S equations)

Reduced Order Model
(Python)

ODE system
(Temporal coefficients)

Field reconstruction

\[ u_r(x, t) = \sum_{i=1}^{N_r} a_i(t) \varphi_i(x) \]
Select a possible configuration

Basic description of the system
- Computational Fluid Dynamics simulations with OpenFOAM

Stability Analysis
- OpenFOAM implementation for linearized system.
- MATLAB implementation for EVP (DMD).

Evaluation of the proposed configuration

Extended description of the system
- ROM implemented in Python based in FOM OpenFOAM results
Preliminary Results
Selection of the base case

- The literature is reviewed in search for a natural convection phenomenon that adjust to our constraints:
  - A simple geometry and a laminar regime.
  - Several dynamic states.
  - Availability of data.
- The Rayleigh-Bénard convection is found as the best candidate for this first stage.
Verification of implementation

- The performance of the different implementations have been assessed against a benchmark of a differentially heated cavity.

- Similar complexity than our base case: 2D laminar natural circulation case.

- The obtained results show good agreement with the literature values, for each of the different stages.
Results of the base case

- Rectangular 2D cavity, simulations were carried out for a range of geometric (A) and physical parameters (Ra).

\[ A = \frac{H}{W} \]

\[ Ra = GrPr = \frac{g\beta \Delta T L^3 Pr}{v^2} \]
Results of the base case

- Different dynamic states were found, for a different number of circulation cells. Both steady-state and oscillatory dynamics were encountered.
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- Different dynamic states were found, for a different number of circulation cells. Both steady-state and oscillatory dynamics were encountered.
A bifurcation diagram can be constructed for the studied range, where it can be appreciated the degree of complexity arising for a simple case.
Results of Stability Analysis

\[ 5.0 \cdot 10^4 < Ra < 1.2 \cdot 10^5 \rightarrow 1 \text{ cell steady} \]
Conclusions and further development
Conclusions

● The different steps of the methodology were implemented and successfully tested against literature results.

● The use of a simple case shows the possibility of a complex dynamic arising of the system, highlighting the need for a tool that is able to assess effectively a large amount of possible configurations.
Upcoming tasks

- Increase the complexity of the implementation with the addition of turbulence modeling, compressible cases.
- Extend the application of the stability analysis to oscillatory cases.
- Investigate of ROM for the detection of bifurcation points.
- Application of the developed methodology for the design of an optimal configuration for a experimental campaign.
Thank you for your attention
Implementation of POD-FV-ROM

- Selection of the spatial modes using POD-Galerkin projection (OpenFOAM).
- Construction of the ROM matrices from the obtained modes (OpenFOAM).
- Resolution of the ROM equation and obtention of the time coefficients (Python).
- Reconstruction of the fields and comparison with full order results (OpenFOAM).
Results of POD-FV-ROM