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► **To cite this version:**

G. Billo, Michel Belliard. Numerical modeling of an in-vessel flow limiter using an Immersed Boundary Approach. 44ème Congrès National d'Analyse Numérique (CANUM), May 2018, Cap d'Agde, France. cea-02400165

**HAL Id: cea-02400165**

**<https://cea.hal.science/cea-02400165>**

Submitted on 21 Feb 2020

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# Numerical modeling of an in-vessel flow limiter using an Immersed Boundary Approach

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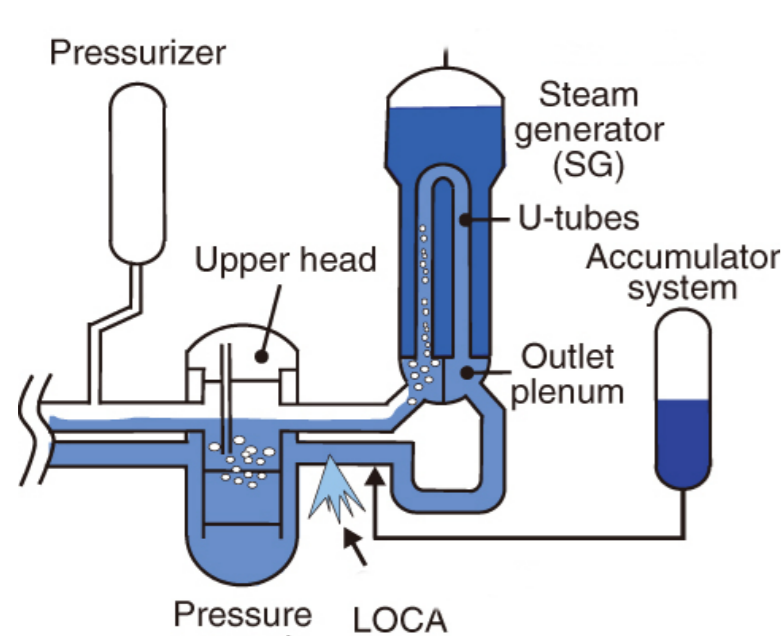
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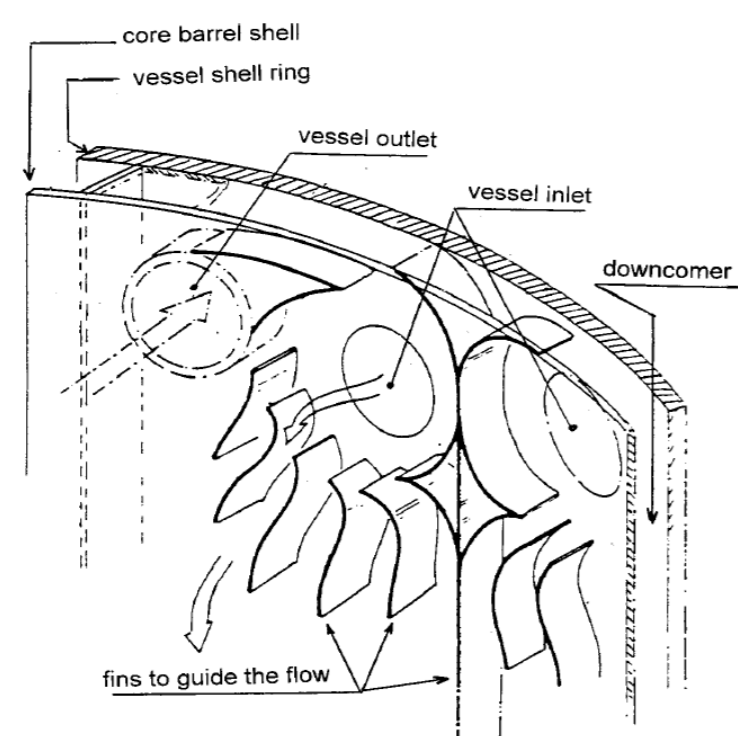
## 1. Context

- In-vessel retention of water in case of large-break Loss Of Coolant Accident (LOCA) in Advanced PWR (Generation III) [1]

LOCA in Pressurized Water Reactor



In-vessel flow limiter [2]



- Characteristics of the flow
  - Two-phase flow
  - Compressibility
  - Low Mach number
    - ↪ compressible Homogeneous Equilibrium Model (HEM)
    - ↪ fractional-step method (projection scheme)
- Numerical optimization of the flow limiter
  - Maximizing the Pressure drop
  - Big amount of simulations - fast computations
    - ↪ Fictitious Domain approach
- PhD project started in 2017

## 2. Computational Fluid Dynamics

### 2.1 Governing equations

- First modeling : One-phase, no energy balance
  - ↪ compressible Navier-Stokes equations

$$\begin{cases} \rho [\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}] - \nabla \cdot \bar{\sigma} + \nabla p = \rho \mathbf{g} \\ \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \end{cases}$$

with  $\rho$  the fluid density,  $\mathbf{u}$  the fluid velocity,  $p$  the pressure,  $\bar{\sigma}$  the viscous stress tensor and  $\mathbf{g}$  the gravity vector

↪ weak compressibility model for low mach

$$\partial_t \rho \simeq \partial_p \rho \partial_t p \simeq c^{-2} \partial_t p \quad (1)$$

with  $c$  the speed of sound in the fluid

↪ gravity is neglected

- Future modeling :
  - Add an energy balance equations
  - Adapt the weak compressibility model

$$\partial_t \rho \simeq \partial_p \rho \partial_t p + \partial_h \rho \partial_t h$$

with  $h$  the enthalpy

- Extend to two-phase flow with HEM

### 2.2 Fractional-step method [3]

- Semi-discrete governing equations
- Time-splitting of the momentum balance equation :

$$\begin{cases} \delta t^{-1} (\rho^{n+1} \mathbf{u}^* - \rho^n \mathbf{u}^n) + \Theta(\rho^{n+1}, \mathbf{u}^n, \mathbf{u}^*, \bar{\sigma}^*) + \nabla p^n = 0 \\ \delta t^{-1} \rho^{n+1} (\mathbf{u}^{n+1} - \mathbf{u}^*) + \nabla \phi^{n+1} = 0 \end{cases} \quad (2)$$

where  $n \in \mathbb{N}$  in superscript corresponds to the time index,  $\delta t$  is the time step,  $\phi^{n+1} = p^{n+1} - p^n$ ,  $\mathbf{u}^*$  and  $\bar{\sigma}^*$  are respectively the predicted velocity and stress tensor  $\Theta(\rho^{n+1}, \mathbf{u}^n, \mathbf{u}^*, \bar{\sigma}^*) = \rho^{n+1} [(\mathbf{u}^n \cdot \nabla) \mathbf{u}^*] - \nabla \cdot \bar{\sigma}^*$  represents the inertia and viscous terms

- Using the weak compressibility model (1) and the mass balance :

$$\begin{cases} \delta t^{-1} (\rho^{n+1} \mathbf{u}^* - \rho^n \mathbf{u}^n) + \Theta(\rho^{n+1}, \mathbf{u}^n, \mathbf{u}^*, \bar{\sigma}^*) + \nabla p^n = 0 \\ (c \delta t)^{-2} \phi^{n+1} + \Delta \phi^{n+1} = \delta t^{-1} \nabla \cdot (\rho^{n+1} \mathbf{u}^*) \\ \mathbf{u}^{n+1} = \mathbf{u}^* - \delta t (\rho^{n+1})^{-1} \nabla \phi^{n+1} \end{cases}$$

- Prediction ↪ predicted velocity calculation
- Projection ↪ pressure corrector calculation
- Correction ↪ velocity correction

## 3. Immersed obstacles modeling

### 3.1 Motivation and principle

- Thin no-penetration obstacles
- Need of fast computation
  - ↪ Fictitious Domain approach [4]
- Limit the added degree of freedom
- Take into account the obstacle implicitly
  - ↪ Immersed Boundary Method (IBM) [5]
  - ↪ Penalized Direct Forcing (PDF) [6, 7]
- Dirichlet Boundary Conditions at the obstacle
  - Taken into account via a forcing term in the momentum balance

### 3.2 Adaption to projection scheme

- Forcing term splitted over prediction and projection [8, 9, 10]

$$\begin{aligned} \mathbf{f}_P^{n+1} &:= \frac{\chi}{\eta \delta t} (\rho_i^{n+1} \mathbf{u}_i^{n+1} - \rho^{n+1} \mathbf{u}^*) \\ \mathbf{f}_C^{n+1} &:= \frac{\chi}{\eta \delta t} \rho^{n+1} (\mathbf{u}^* - \mathbf{u}^{n+1}) \end{aligned}$$

with  $\mathbf{f}_P^{n+1}$  and  $\mathbf{f}_C^{n+1}$  respectively the forcing term related to the prediction and projection equations,  $\rho_i^{n+1}$  and  $\mathbf{u}_i^{n+1}$  respectively the imposed density and velocity at the obstacle,  $\chi$  the characteristic function of the solid domain and  $0 < \eta \ll 1$  the penalization parameter

- The projection scheme (section 2.2) must be adapted
  - Forcing terms added in (2)
  - Taking the divergence of the projection equation
    - ! \ Derivative of discontinuous function  $\chi$  comes out
    - ↪ Jump term appears (distribution theory)
- Neglecting the jump term, the projection scheme becomes :

$$\begin{aligned} \delta t^{-1} (\rho^{n+1} \mathbf{u}^* - \rho^n \mathbf{u}^n) + \Theta(\rho^{n+1}, \mathbf{u}^n, \mathbf{u}^*, \bar{\sigma}^*) + \nabla p^n &= \mathbf{f}_P^{n+1} \\ (c \delta t)^{-2} \phi^{n+1} + \eta (\eta + \chi)^{-1} \Delta \phi^{n+1} &= \delta t^{-1} \nabla \cdot (\rho^{n+1} \mathbf{u}^*) \\ \mathbf{u}^{n+1} &= \mathbf{u}^* - \delta t (\rho^{n+1})^{-1} \nabla \phi^{n+1} \end{aligned}$$

## 4. Spatial discretization

- PDF originally proposed for Finite Difference [6, 7]
- ↪ Adaption to a Finite Element formulation [1]

### 4.1 Finite Element formulation

- Code used for the first modeling : TRUST/GENEPI+
  - Hexahedral elements
  - velocity interpolated with  $\mathbb{Q}_1$  functions and pressure with  $\mathbb{Q}_0$
  - ! \ Unstable pair of elements
- Trick of TRUST/GENEPI+ to avoid or limit instabilities :
  1. Write the Weak form of system (2)
  2. Integrate by parts the term involving  $\nabla \phi^{n+1}$
  3. Write the Finite Element formulation
  4. Lump and invert of the mass matrix in the projection step
  5. Use the discrete divergence and mass balance to recover an equation only on  $\phi^{n+1}$
- The matrices obtained for an element  $\Omega_e$  are the following :
  - Lumped mass matrix :

$$M_{ii}^e = \rho_e \int_{\Omega_e} \varphi_i$$

- Gradient-divergence matrix :

$$B_{aj}^e = \int_{\Omega_e} \partial_{x_a} \varphi_j$$

- Advective matrix :

$$N_{ij}^e = \sum_{a=1}^3 \left( u_{ae} \int_{\Omega_e} \partial_{x_a} \varphi_j \varphi_i \right)$$

- Advective matrix :

$$D_{ij}^e = \sum_{a=1}^3 \left( \int_{\Omega_e} \partial_{x_a} \varphi_j \partial_{x_a} \varphi_i \right)$$

with  $\varphi_i$  the  $\mathbb{Q}_1$  basis function associated to the node  $i$  of the mesh and  $u_{ae}$  the component of the velocity in direction  $x_a$  approximated at the centroid of element  $e$

### 4.2 Generalised Finite Element Method (GFEM)

- For future modeling, an extension to GFEM is considered
- Principle : enrich the finite element basis with other functions
  - eXtended Finite Element Method (XFEM) : enrichment with heavyside (discontinuous functions)
  - Multiscale Finite Element Method (MsFEM) : enrichment with function representative of subgrid phenomena
- Interest for the modeling of the flow limiter
  - XFEM : capability to model infinitely thin obstacles with discontinuous basis functions
  - MsFEM : capability to model turbulence by enrich the finite element basis with wall laws

## 5. Turbulence modeling

### 5.1 One-phase flow

- Many existing models for turbulence
  - Direct Numerical Simulation (DNS)
    - ↪ no more physical models added
  - Large Eddy Simulation (LES)
    - ↪ subgrid models are needed
  - [Unsteady] Reynolds Averaged Navier-Stokes ([U]RANS)
    - ↪ closure laws or models are needed
  - Detached Eddy Simulation (DES)
    - ↪ hybrid RANS/LES triggered by mesh size
- Due to the need of fast computation :
  - DNS and LES are too expensive in terms of mesh size
    - ↪ ruled out for the aimed application
  - RANS (or URANS) seems more affordable
    - ↪ can involve scalar modeling of the turbulence (i.e. can avoid solving new transport equations for turbulent quantities)
    - ↪ Spalart-Allmaras model without wall distance discussed
- Wall laws play a very important role
  - Usual meshing size condition will not be respected at the walls
    - ↪ use of walls laws to model boundary layers correctly
  - The idea is to take into account those wall laws with the GFEM
    - ↪ enrich FEM basis with wall laws (section 4.2)

### 5.2 Two-phase flow

- Still an open question, many phenomena are brought up
  - Unstabilities at the interface between the two phases
  - definition of wall laws for a two-phase mixture
- ↪ modeling difficulties, models are at the research stage
- Due to the deadlines of the PhD project
  - ↪ two-phase turbulence will probably not be tackled

## 6. Conclusions and perspectives

- First modeling (currently in development)
  - One-Phase Navier-Stokes with weak compressibility model
  - Projection scheme
  - Penalized Direct Forcing for massive obstacles
  - FEM formulation
- Second modeling = first modeling +
  - + Add energy balance and adapt the weak compressibility model
  - + Adapt the modeling to infinitely thin obstacles with GFEM
- Third modeling = second modeling +
  - + Modeling of turbulence : [U]RANS + wall laws with GFEM
- Perspectives
  - Extend the modeling to two-phase mixture (HEM)

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