Multifield CFD calculations of industrial geometries

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1

NEPTUNE_CFD CODE : BASE MODEL

- NEPTUNE_CFD is a three dimensional two-fluid code developed more especially for nuclear reactor applications.
- The code deals with compressible, unsteady, turbulent 3D twophase or multi-phase flow.
- The numerical approach is based on a finite volume co-located cell-centered approach.
- Equations of the two-phase flow model (so-called 6 equation model): mass, momentum and energy balance for both liquid and gas are solved.
- Turbulence for the liquid phase is modelled by a RSM (SSG)
- IATE + fragmentation, coalescence, condensation
- Forces exerted on bubbles : lift, drag, added mass and turbulent dispersion force.
- Wall transfer model for nucleate boiling



TWO-FLUID MODEL IN THE CODE NEPTUNE_CFD Ishii [1975]

Mass balance equation:

$$\partial_t(\alpha_k \rho_k) + \nabla (\alpha_k \rho_k \boldsymbol{u}_k) = \Gamma_k \text{ with } \sum_k \alpha_k = 1$$

Momentum balance equation:

$$\partial_t (\alpha_k \, \rho_k \boldsymbol{u}_k) + \nabla . \, (\alpha_k \, \rho_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = \nabla . \, \left(\alpha_k \, \mu_k \underline{S_k} \right) - \, \alpha_k \, \nabla P + \alpha_k \, \rho_k \boldsymbol{g} + \boldsymbol{F}^{spe}$$

Energy balance equation:

$$\partial_t (\alpha_k \, \rho_k H_k) + \nabla . \left(\alpha_k \, \rho_k H_k \boldsymbol{u}_k \right) = - \nabla . \left(\alpha_k \, Q_k \right) + \nabla . \left(\alpha_k \, \mu_k \underline{\underline{S}_k} \boldsymbol{u}_k \right) \\ + \alpha_k \, \partial_t P + \alpha_k \, \rho_k \boldsymbol{g} . \boldsymbol{u}_k + E_k^{Int}$$

[Ishii, M., 1975, Thermo-fluid dynamic, theory of two-phase, Eyrolles, University of Michigan]



Objectives:

Fluid-stavelopennemetion (PSI) PARENettorporforme movtake on the flow and step of the time internal or



Source: Orano Youtube

Two-phase flow patterns in tube bundles



Kanizawa & RIbatski IJMF (2016)





 Large bubbles, considered as too distorted to be accurately described by correlations, are simulated through an interface locating method.



> 1 billion of cells for the simulation of a whole reactor vessel containing small bubbles of 1mm



MODELLING STRATEGY: MULTIFIELD APPROACH



LIQUID / VAPOR INTERFACE

- Interface sharpening equation, Olsson and Kreiss [2005]:
 - To control the interface thickness



⁹

LIQUID / VAPOR INTERFACE

• Surface tension force, Brackbill et al. [1992]:

For deformable interfaces with a finite thickness

$$F_{CSF} = \alpha_k \, \sigma \kappa \nabla \alpha_k$$
 with $\kappa = - \nabla \cdot \left(\frac{\nabla \alpha_k}{||\nabla \alpha_k||} \right)$

Drag force law:

To couple the velocity of each field at the interface



[Brackbill, J.U. *et al.*, 1992, A continuum method for modeling surface tension, *J. Comput. Phys.*, Vol. 100, pp. 335-354]

LIQUID / VAPOR INTERFACE





VALIDATION ON ISOTHERMAL FLOWS





- Interfacial liquid / liquid flows:
 - Rayleigh-Taylor instability



Kelvin-Helmholtz instability





Multi-phenomena flows:

METERO experiment





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NEED OF THE INTERFACE LIQUID/VAPOR MODELS : CASE OF A RISING BUBBLE



STATIONARY BUBBLE

- 2D test case: square, 5 cm
- Mesh convergence study: 45², 64², 91², 128², 181², 256²
 and 512² cells
- Constant time step: 0,1 ms
- Physical properties:

	Density	Viscosity	Surface tension
Air	1,29 kg.m ⁻³	1,5.10 ⁻⁵ Pa.s	$0.00 \text{ M} \text{m}^{-1}$
Water	1000 kg.m ⁻³	1.10 ⁻³ Pa.s	0,08 N.M



- Circularity: $C = \frac{2\pi R}{L}$
- Laplace equation in 2D: $P_{in} P_{out} = \frac{\sigma}{R}$
- Capillary number: $Ca = \frac{\mu_{cl}U_{cg}}{\sigma}$, $U_{cg} = \frac{\sum_{\alpha_{cg}>1.10^{-3}} \alpha_{cg}\rho_{cg}U_{cg}}{\sum_{\alpha_{cg}>1.10^{-3}} \alpha_{cg}\rho_{cg}}$ and $U_{cg}^{Int} = \frac{\sum_{\alpha_{cl}\alpha_{cg}>0.1} \alpha_{cg}\rho_{cg}U_{cg}}{\sum_{\alpha_{cl}\alpha_{cg}>0.1} \alpha_{cg}\rho_{cg}}$

STATIONARY BUBBLE



METERO EXPERIMENT (CEA)

- M. Bottin, J.P. Berlandis, E. Hervieu, M. Lance, M. Marchand, O.C. Öztürk, G. Serre, "Experimental investigation of a developing two-phase bubbly flow in horizontal pipe".
- This experiment has been developed in the frame of the NEPTUNE project, jointly developed by CEA, EDF, AREVA and IRSN.



- The test section, 5.40 m long, has an inner diameter D = 0.1 m
- air injection tubes have been set to ensure uniform bubble injection in the inlet section.
- Inlet : water (0–5 m/s)+ air bubble (0–0.7 m/s).
- \rightarrow provide a flow pattern map.

METERO: FLOW PATTERN MAP FOR X/D = 40

Calculations : Jg is fixed and JI increases



Transition from slug to stratified flow (TSS)

transition from plug to slug flow (TPS)

transition from buoyant bubble flow to stratified bubble flow (TBBSB) transition from stratified bubbles regime to plug (TSBP)



STRATIFIED BUBBLES FLOW REGIME: HIGH VALUE OF LIQUID MASS FLOWRATE 600 000 cells

Dx ~ 0.8 mm

JL = 4.42 m/s; **JG = 0.1273 m/s is fixed**

JL = 4.55 m/s; JG = 0.094 m/s





Bubble velocity at 40D (stratified bubbly flow).

Void fraction at 40D (stratified bubbly flow).



PLUG FLOW REGIME: MEDIUM VALUE OF LIQUID MASS FLOWRATE

JL = 2.12 m/s; JG = 0.1273 m/s JL =

JL = 2.4 m/s; JG = 0.03m/s





Figure 9c: Bubble velocity at 40D (plug flow).

Figure 9d: Void fraction at 40D (plug flow).

SLUG FLOW REGIME : LOW VALUE OF LIQUID MASS FLOWRATE

JL = 1.06 m/s; JG = 0.1273 m/s

JL = 0.53 m/s; JG = 0.062 m/s





Bubble velocity at 40D (slug flow).

Void fraction at 40D (slug flow).



Stephane Mimouni, *CFD calculations of flow pattern maps and LES of multiphase flows*, Nuclear Eng and Des.



Zoom sur la vibration des tubes GV

Validation of the two-phase numerical model MAXI2 Experiment Freon/Freon

Time: 0.050000 s



Water freon two-phase flow

VISCACHE Experiment

MAXI : 3 FIELDS → QUITE ENCOURAGING



DNB : INDUSTRIAL CONTEXT

In nucleate boiling, heat flux increases and reaches a maximum value with increasing wall temperature.

ightarrow severe damage or meltdown of the surface.

A vapour film isolates the fuel from the water: the fuel heats up sharply and suddenly





NEW PHASE CHANGE TERM

• Zero thickness interface (W.m⁻²): $q_l^S = \lambda_l \nabla T_l \cdot n$: accross the liquid-vapor interface

• Non-zero thickness interface (W.m⁻³):
$$\lim_{h \to 0} \left(\int_{V^{Int}} q_l^V(x) dx^3 \right) = \int_{A^{Int}} q_l^S(x^{Int}) dA$$

Brackbill's methodology:



$$\int_{A^{Int}} q_l^S(x^{Int}) dA = \int_{V^{Int}} q_l^S(x) \delta(\mathbf{n}(x^{Int}).(x - x^{Int})) dx^3$$

$$= \int_{V^{Int}} \lambda_l \nabla T_l \cdot \mathbf{n}(x) \, \delta(\mathbf{n}(x^{Int}).(x - x^{Int})) dx^3$$

$$\lim_{h \to 0} \nabla c(x) = \mathbf{n}(x) \, \delta(\mathbf{n}(x^{Int}).(x - x^{Int})) [c]$$

$$\int_{A^{Int}} q_l^S(x^{Int}) dA = \lim_{h \to 0} \left(\int_{V^{Int}} \lambda_l \nabla T_l \cdot \frac{\nabla c(x)}{[c]} dx^3 \right)$$

$$q_l^V(x) = \lambda_l \nabla T_l \cdot \frac{\nabla c(x)}{[c]}$$

Extension to the two-fluid model: $q_{k}^{V} = \alpha_{k}\lambda_{k} \nabla T_{k} \cdot \nabla \alpha_{k} : implemented in the CFD code$

[Brackbill, J.U., *et al.*, 1992, A continuum method for modeling surface tension, *J. Comput. Phy.*, Vol. 100, pp. 335-354]

PHASE CHANGE FOR THE CONTINUOUS PHASES





Phase change



- New phase change model for large interfaces change
 - Brackbill's methodology
- Validation on various academic test cases:
 - Convergence studies
 - Pressure conditions occurring in nuclear power plants
- Industrial application (OK not shown here):
 - Non-isothermal turbulent two-phase flow
 - Industrial geometry
- Some issues remain :
 - Results sensitive to the time step and mesh refinement → calibration on verification test cases.
 - \rightarrow Improve the numerical robustness of the mass and energy source terms !!

INTERFACE LOCATING METHODS \rightarrow LES



EQUATION FILTERING

- LES filter G: $\overline{\varphi}(x,t) = G \circ \varphi = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} G(x-y,t-t')\varphi(y,t') \, dy \, dt'$
- Filtered mass balance equation:

$$\rho_k \partial_t \overline{\alpha_k} + \rho_k \nabla . \left(\overline{\alpha_k} \ \overline{u_k} \right) + \tau_{interf} = 0$$

Filtered momentum balance equation:



$$\rho_{k}\partial_{t}(\overline{\alpha_{k}}\ \overline{u_{k}}) + \tau_{time} + \rho_{k}\nabla.(\overline{\alpha_{k}}\ \overline{u_{k}}\otimes\overline{u_{k}}) + \tau_{conv} = \mu_{k}\nabla.(\overline{\alpha_{k}}\ \overline{\underline{S_{k}}}) + \tau_{diff}$$
$$-\overline{\alpha_{k}}\nabla\overline{P} - \tau_{pressure}$$
$$+ \overline{\alpha_{k}}\rho_{k}g + \widehat{F_{CSF}} + \tau_{superf} + \overline{F_{Drag}} + \tau_{drag}$$

[Vincent, S., Tavares, M., Fleau, S. *et al.*, 2016, *A priori* filtering and LES modeling of turbulent two-phase flows Application to phase separation, *Comput. Fluids*]



SUBGRID TERMS

• Filtered curvature: $\hat{\kappa} = -\nabla \cdot \left(\frac{\nabla \overline{\alpha_k}}{||\nabla \overline{\alpha_k}||} \right)$

Subgrid terms	Expression
$ au_{interf}$	$ \rho_k \left(\nabla . \left(\overline{\alpha_k \boldsymbol{u}_k} \right) - \nabla . \left(\overline{\alpha_k} \overline{\boldsymbol{u}_k} \right) \right) $
$ au_{time}$	$\rho_k \big(\partial_t (\overline{\alpha_k \boldsymbol{u}_k}) - \partial_t (\overline{\alpha_k \boldsymbol{u}_k}) \big)$
$ au_{conv}$	$\rho_k\left(\nabla . \left(\overline{\alpha_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k}\right) - \nabla . \left(\overline{\alpha_k \boldsymbol{u}_k} \otimes \overline{\boldsymbol{u}_k}\right)\right)$
$ au_{diff}$	$\mu_k\left(\nabla.\left(\overline{\alpha_k\underline{\underline{S}_k}}\right) - \nabla.\left(\overline{\alpha_k\underline{\underline{S}_k}}\right)\right)$
$ au_{pressure}$	$\overline{\alpha_k \nabla P} - \overline{\alpha_k} \nabla \overline{P}$
$ au_{superf}$	$\sigma(\overline{\alpha_k \kappa \nabla \alpha_k} - \overline{\alpha_k} \hat{\kappa} \nabla \overline{\alpha_k})$

+ τ_{drag}

✓ New subgrid terms: $\tau_{pressure}$ and τ_{drag} ✓ LES filter: 7 subgrid terms



PHASE INVERSION BENCHMARK Vincent et al. [2008]



	Density	Viscosity
Oil	900 kg.m ⁻³	0,1 Pa.s
Water	1000 kg.m ⁻³	0,001 Pa.s

Time = 0.00 s128³ cells 256³ cells 512³ cells Mesh Time step 0,8 ms 0,2 ms 0,05 ms Cores 144 1152 1152 Duration 2 months 7 hours 47 hours

 Results consistent with DNS obtained with onefluid models: Vincent, Tavares, Fleau et al. [2016]

[Vincent, S., Tavares, M., Fleau, S. *et al.*, 2016, *A priori* filtering and LES modeling of turbulent two-phase flows Application to phase separation, *accepted in Comput. Fluids*]

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TURBULENCE MODELS COMPARISON



[Vincent, S., Tavares, M., Fleau, S. *et al.*, 2016, *A priori* filtering and LES modeling of turbulent two-phase flows Application to phase separation, *accepted in Comput. Fluids*]



CONCLUSIONS – LARGE EDDY SIMULATION

Equation filtering:

- Ist time for a two-fluid model applied to large interfaces
- New Specific subgrid terms
- Turbulence models:
 - Limited modeling errors with structural models especially ADM
- ADM implementation:
 - Exploratory results encouraging
 - Multiple implementation choices that have to be deeply investigated



Time and space order should be increased numerical scheme \rightarrow diffusion \rightarrow interacts LES filter ? numerical effects vs turbulence modelling ?



CONCLUSION

- Large interface model needs its own closure laws : a surface tension model, a drag force law necessary to couple the velocity of the two continuous fields at the interface + interface sharpening equation in order to control the interface thickness.
- validation of the multifield approach : Verification cases, Validation cases, Integral validation cases
- Sensitivity to mesh refinement
- LES vs Rans for large interfaces
- Phase changes : dispersed gas phase and continuous gas phase → SFR ... DNB, Steam Generator, ...
- Dynamics of capillary bridges in a crack (capillarity, wetting effects)
- HPC : Recently steam generator 1.5 Billion cells in two-phase flow !!
- Meet the requirements for industrial needs BUT:
- Pb of Spurious currents should be addressed
- LES calculations for large interfaces in industrial applications
 Seprementions for large flow
- Transition regimes flow

Background

During the course of hypothetical accidents in a PWR which lead to large mass and energy releases into the containment (Steam Line Break, Loss of Coolant Accident, etc.), spray systems are used in the containment in order to limit overpressure, to enhance the gas mixing in case of the presence of hydrogen and to drive down the fission products. Thus, spray modeling and wall condensation play an important part in thermal-hydraulic containment codes.



WETTING, CAPILLARITY AND DYNAMIC OF THE TRIPLE LINE

Enceinte sous pression : quel débit de vapeur à travers les fissures du béton?





CAPILLARITY EFFECTS



Surface tension force:
$$F_{CSF} = \alpha_k \sigma \kappa \nabla \alpha_k$$
 with $\kappa = -\nabla \cdot \left(\frac{\nabla \alpha_k}{||\nabla \alpha_k||} \right)$

In order to compute more precisely the interface curvature, we diffuse the interface: $\sqrt{\nabla}$



WETTING EFFECTS



WETTING ANGLE : CALIBRATION OF THE MODEL



DYNAMICS OF CAPILLARY BRIDGES

Dynamics of a capillary bridge accross a narrowing in a crack





Débordement de barrage: <u>3 champs</u> (liquide et gaz continus, gouttes dispersées)



SAUT DE L'ANGE: 22,5M DE CELLULES







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SAUT DE L'ANGE

Premiers calculs: position du jet, vitesse.

Fragmentation du jet : turbulence, ...

Maillage ~ 5mm , 1 mm \rightarrow trop grossier?

Calculer d'autres essais

