



FROM RESEARCH TO INDUSTRY

THERMAL SUB-GRID BOUNDARY LAYER MODELLING AROUND BUBBLES AT MODERATE REYNOLDS AND PRANDTL NUMBERS

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Upscaling approach for two-phase flows in the field of energy



Upscaling approach for boiling investigation

Simulations at three scales:

- Local or DNS : Reference data ⇒ Too costly
- Intermediate: Modelling of strong fluctuations and variations of temperature:
 - ⇒ Thermal boundary layer modelling
- Averaged (RANS Euler-Euler): Macroscopic closures
 - ⇒ Interfacial heat transfers for non-resolved interfaces



Interfacial heat and mass transfer (Nub) predictions challenges





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Need: A liquid-vapour heat transfer model in bubble swarms

• Heat transfer exchange coefficient (Nusselt number Nu_b) which determines **condensation/evaporation** rate at the interface:

$$Nu_{b} \propto \int_{\Gamma} \nabla T \cdot \boldsymbol{n}_{\Gamma}|_{\Gamma} dS$$
$$Nu_{b} = f\left(\boldsymbol{Re}_{b}, \boldsymbol{Pr}_{l} = \frac{\alpha_{l}}{\nu_{l}}, \boldsymbol{\mu}_{v}/\boldsymbol{\mu}_{l}, \boldsymbol{\alpha} = \frac{\Omega_{v}}{\Omega_{l}}, \boldsymbol{Ja} = \frac{\rho_{l}Cp_{l}\Delta T}{\rho_{v}\mathcal{L}^{vap}}\right) \quad (1)$$

Problem: Capture the strong variations $Nu_b \propto |\nabla T \cdot \boldsymbol{n}_{\Gamma}|_{\Gamma}$ is costly

Thermal boundary layer thickness $\delta << D_b$ \downarrow Separation of scales \downarrow Local refinements

Solution: A DNS thermal boundary layer coupling (conceptualisation)

- Keep the **explicit tracking** of the interface (Front-Tracking).
- Enhance the prediction of strong variations on a finite thickness.
- Reduce the computational cost





From available methods to a novel approach

LRS methodology

DNS simulations and post-processing tool

A priori implementation and results

Conclusions and prospects



Available approaches

RADIAL/NORMAL **TEMPERATURE** VARIATIONS ARE EXPECTED TO BE HIGH ↓ INVESTIGATE A UNI-DIRECTIONAL REFINEMENT APPROACH

Uni-directional refinement approaches

- (1) Fit an analytical form of solution (Quasi-Static Correction, **QSC**).
 - ⇒ Inspired by of Bothe and Fleckenstein 2013; Weiner and Bothe 2017.
 - (⇒ Grosso *et al.*, 2023, in writing.)
- (2) Laminar Radial Sub-resolution (LRS).
 - \Rightarrow Current presentation !



Inspiration: Thin/turbulent Boundary Layer Equation (TBLE)



It consists in a **LES-RANS** coupling to solve for near wall turbulence and transfers:

(1) Turbulence on flat plates, channels (Benarafa et al. 2006).

(2) Heat transfer on flat plates, channels by Chatelain 2004.

(3) Turbulence on complex geometries (turbines...) coupled to an Immersed Boundary Method of Bizid 2017.

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LRS methodology

Toward a laminar radial sub-resolution (LRS)



Principles of LRS (Laminar Radial Sub-resolution)

- Solve for each phase temperature **separately**.
- Resolve a unidirectional problem in the osculating spherical basis for each interface portion (Front-Tracking).





LRS methodology

Governing equations in the osculating sphere frame of reference



Hypotheses

- Interface attached frame of reference $u_r \leftarrow u_r |u_r|_{\Gamma}$.
- Temporal term neglected $\partial_t = 0$ *i.e.* **quasi-static** approach.
- No azimuthal variations: $\frac{\partial^n \Theta}{\partial \phi^n} = 0, u_{\phi} = 0.$

Radial advection-diffusion equation in spherical coordinates (2D-axi)







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DNS simulations and local post-processing tool

Simulation setup: Steady rising bubble (3D)

Dimensionless numbers

$$\boldsymbol{Ar^*} = \left(gD_b\frac{\rho_l - \rho_v}{\rho_l}\right)^{1/2}\frac{D_b}{\nu_l}; \boldsymbol{Pr_l} = \frac{\alpha_l}{\nu_l}; \boldsymbol{Re_b} = \frac{U_{term}D_b}{\nu_l}; \boldsymbol{Ja} = \frac{\rho_l C p_l \Delta P}{\rho_v \mathcal{L}^{vap}}$$

Numerical setup

Hypotheses:

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- No phase change $Ja \rightarrow 0$.
- $T_{\Gamma} = T^{sat}$.
- Outflow boundary conditions $\nabla T \cdot \boldsymbol{n}_{\Omega} = 0.$
- Bubble is kept spherical.

Physical parameters range of study:

- $Ar^* \in \{10; 50\}$
- $Pr_l \in \{1; \ 2.5; \ 5\}$
- $D_b/\Delta \in [12, \ 96]$
- Domains sizes: $\{[3, 3, 4]; [4, 4, 6]\} \times D_b$



Rising bubble at $Ar^* = 50$, $Pr_l = 1$ ($Re_b \approx 62.5$).



DNS simulations and local post-processing tool

Interpolate the fields on probes and re-compute advection-diffusion terms





Post-process quantities on probes

$$\theta_{VISU}$$
 BOTTOM (1) EQUATOR (2) TOP (3)
[-90, 90] ° -90° 0° 90°

DNS simulations and local post-processing tool

Local temperature profiles and normal derivative: T and $\nabla T \cdot \widetilde{e_r} = \frac{\partial T}{\partial r}$





(a) Temperature $(D_b/\Delta = 64, \text{ Fine})$

(b) Radial temperature gradient $\frac{\partial T}{\partial r}$

- \Rightarrow Strong variations observed at the bubble's top and equator regions.
- \Rightarrow Misprediction of the normal temperature gradient (Top and Equator regions): 30% relative error at $D_b/\Delta = 16$.

DNS simulations and local post-processing tool PROMES CLA Hierarchy of terms: convective and diffusive terms Highlighting the importance of tangential convective terms (1)(2) Convective term (K.s-1) Diffusive term (K.s⁻¹) -25-75 -50 -25 θ (°) Tangential convective term $\left|\frac{u_{\theta}}{\partial t}\right|^{2T}$ Spherical convective term $\left|u_r \frac{\partial T}{\partial r} + \frac{u_{\theta}}{\partial r} \frac{\partial T}{\partial r}\right|$ Tangential diffusive term $\left|\alpha_l \Delta T - \frac{\alpha_l}{2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r}\right)\right|$ Total diffusive term $|\alpha_l \Delta T|$ Normal convective term $|u_r \frac{\partial T}{\partial r}|$ fotal convective term $|u \cdot \nabla T|$ Normal diffusive term $\left|\frac{\alpha_{t}}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial T}{\partial r}\right)\right|$

(a) Convective terms (Fine)

(b) Diffusive terms (Fine)

THREE DISTINCT REGIONS:

- \Rightarrow Radial convection dominates in (1) and (3).
- \Rightarrow Tangential convective term gains importance in (2) (especially if Pr_l increases).
- \Rightarrow Radial diffusion dominates in (2) and (3).





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Tangential terms effects on the sub-resolution







(a) $\frac{1}{r} \frac{\partial T}{\partial \theta}$, $D_b / \Delta = 16$

(b) $\frac{1}{r} \frac{\partial T}{\partial \theta}$, $D_b/\Delta = 64$





Interfacial temperature gradient enhancements $\left.
abla T \cdot oldsymbol{n}_{\Gamma}
ight|_{\Gamma}$







(a) Case A $C^{\theta}_{\text{coarse}}$ only

(b) Case B $C_{\text{coarse}}^{\theta}$ and $D_{\text{coarse}}^{\theta}$

		Case A	Case B	
/1) 0	ottom	Gradient	Coarse gradient value	
		underestimated	almost retrieved	
(2) Equator		Values underestimated		
		for $-5 < \theta < 25^{\circ}$		
(3)	Тор	Overall enhancement for $\theta > 25^{\circ}$		



Method's dispersion and global Nu_b convergence: $\nabla T \cdot \mathbf{n}_{\Gamma}|_{\Gamma} \sin{(\theta)}$



(a) Case **B** $C^{\theta}_{\text{coarse}}$ and $D^{\theta}_{\text{coarse}}$



(b)	Cas	e C
C_{fine}^{θ}	and	D_{fine}^{θ}

		Case B	Case C	
(1) Bottom (2) Equator		Low dispersion	Beduce dispersion	
		Dispersion is significant	Integral value underestimated	
(3)	Тор	Precise and accurate prediction		

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Overall gain in precision



Nusselt number relative error (%)

$Ar^* Pr$	Coarse $\frac{D_b}{\Delta}$	Fine $\frac{D_b}{\Delta}$	$\left(\frac{\Delta_{\mathrm{fine}}}{\Delta_{\mathrm{coarse}}} ight)^3$	Reference error (%)	$C_{\text{coarse}}^{ heta}, D_{\text{coarse}}^{ heta}$ Error (%)	$C_{ ext{fine}}^{ heta}, D_{ ext{fine}}^{ heta}$ Error (%)
1.0	16	64	64	16.06	8.67	3.61
50 2.5	22	90	68.5	19.46	8.61	1.53
5.0	22	90	68.5	31.78	12.29	0.73

 \Rightarrow Enhancements using coarse (raw) source terms.

 \Rightarrow Tangential terms need a careful treatment.







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Conclusions

- A priori assessment is promising at steady state.
- Tangential terms are too significant to be neglected!
- Error reduces drastically 16-32 \rightarrow 8.7-12.3% using raw CFD mesh quantities (Velocity u_r , u_{θ} , tangential terms $C^{\theta}_{\text{coarse}}$, $D^{\theta}_{\text{coarse}}$).

Achieved with 64 times less cells than the fine mesh.

• Extra-modelling of the tangential terms ($C^{\theta}_{\text{fine}}, D^{\theta}_{\text{fine}}$) could lead to higher enhancements.

<5% relative error on Nu_b .

 Method is suitable for any interface tracking methods (FT-IBM, Level-Set) / interface capturing methods (VoF)

Prospects

- Two way coupling and *a posteriori* assessment.
- 3D multi-bubbles column at moderate Peclet numbers ($Pe_b = Re_bPr_l \leq 400$).





THANK YOU FOR YOUR ATTENTION !

KEYWORDS:

- Two-phase flow
- Ghost-fluid
- DNS-Front-Tracking
- Heat transfer
- Boundary-Layer modelling
- Sub-resolution approach



French Alternative Energies and Atomic Energy Commission - www.cea.fr

PROMES - www.promes.cnrs.fr



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Continous one-fluid approach



Mass, momentum and energy conservation in conservative form

The continuous local and instantaneous system of equations used to describe two-phase flows with phase is given by:

$$abla \cdot \boldsymbol{u} = -\dot{m}_v \left(\frac{1}{\rho_v} - \frac{1}{\rho_l} \right) \delta_{\Gamma}$$
(3a)

$$\partial_t(\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) \\ = \nabla \cdot (p\boldsymbol{I} + \mathcal{D}_{\boldsymbol{u}}) + \rho \boldsymbol{g} + \kappa \sigma \boldsymbol{n}_v \delta_{\Gamma}$$
(3b)

$$\frac{\partial_t (\rho C_p T) + \nabla \cdot (\rho C_p u T)}{-\nabla \cdot (\lambda \nabla T) + \dot{m} \ \delta_{\tau} C^{vap}} \tag{2c}$$

$$= \nabla \cdot (\lambda \nabla T) + \dot{m}_v \delta_\Gamma \mathcal{L}^{vap}$$
(3c)

$$\partial_t \chi_v + \boldsymbol{u}_{\Gamma} \cdot \nabla \chi_v = 0 \tag{3d}$$

$$T_{\Gamma} = T^{sat} = \text{const} \tag{3e}$$

$$\boldsymbol{u}_{\Gamma} = \boldsymbol{u}_l - \frac{\dot{m}_v}{\rho_l} \boldsymbol{n}_v \tag{3f}$$

$$\dot{m}_v = \rho_v (\boldsymbol{u}_v - \boldsymbol{u}_\Gamma) \cdot \boldsymbol{n}_\Gamma$$
(3g)

It remains true in the sense of the distribution (Dirac δ "function"). The discontinuity is embedded in the discretised field.



TrioCFD solver details and discretisation



Discretisation: Marker and cells/Staggered grid



Curvature calculation: differential approach of Mathieu 2003

$$\kappa = -\frac{\boldsymbol{n}_{\Gamma}^{S} \cdot \boldsymbol{n}_{\Gamma}^{V}}{\boldsymbol{n}_{\Gamma}^{V} \cdot \boldsymbol{n}_{\Gamma}^{V}} = -\frac{\frac{\partial S}{\partial x} \frac{\partial V}{\partial x} + \frac{\partial S}{\partial y} \frac{\partial V}{\partial y}}{\left(\frac{\partial V}{\partial x}\right)^{2} + \left(\frac{\partial V}{\partial y}\right)^{2}}$$
(4)

$$dV = \left(\frac{\partial V}{\partial x}, \ \frac{\partial V}{\partial y}\right) \cdot (dx, \ dy) = \boldsymbol{n}_{\Gamma}^{V} \cdot d\boldsymbol{x}_{i}$$
(5a)

$$dS = \left(\frac{\partial S}{\partial x}, \ \frac{\partial S}{\partial y}\right) \cdot (dx, \ dy) = \boldsymbol{n}_{\Gamma}^{S} \cdot d\boldsymbol{x}_{i}$$
(5b)



Inhouse Ghost-Fluid Method (GFM) (i)



Sub-grid diffusion model and spreading procedure



- Compute normal vectors *n*, distance function *d*, curvature *κ*.
- Second order evaluation of gradient at ř = R + d_i/2.
- Sub-grid model to evaluate the gradient at the interface.

$$\Delta_{sph}T \approx \kappa \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} = 0 \qquad (6)$$

• Extend temperature with same analytical expression.



(b) Spreading procedure. Stored values are initially in pure cells.

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Inhouse Ghost-Fluid Method (GFM) (iu)



Differences with the literature

Literature:

- Aslam's *n*th order extrapolation (Aslam 2004)
 - \Rightarrow Extrapolate each derivative iteratively on a pseudo-time step τ .
 - \Rightarrow Starting from $\frac{\partial^n T}{\partial r^n}$ and ending with zero order derivative *i.e.* T.
- Implicit diffusion
 - ⇒ Impose the saturation temperature $T_{\Gamma} = T^{sat}$ in the diffusion matrix taking into account the interface position (Gibou, Fedkiw, et al. 2002; Gibou, Chen, et al. 2007; Tanguy et al. 2014).

TrioCFD methods:

- Extended field T^{ext} verifying $T_{\Gamma} = T^{sat}$.
- Updated temperature field T^{n+1} does not ensure saturation temperature condition.
- Explicit diffusion.



Appendix B: LRS details

A posteriori coupling with the resolved field (details)



Coupling with the resolved field

- Eulerian (A) ⇒ Boundary layer (B)
 - ⇒ Local temperature value(s) (Fitting, B.Cs).
- (B) Boundary layer ⇒ Eulerian (A)
 - $\Rightarrow \text{ Interfacial temperature} \\ \text{gradient correction} \\ \nabla T \cdot \boldsymbol{n}_{\Gamma}|_{\Gamma}.$
 - $\Rightarrow \text{ Temperature and fluxes} \\ \text{correction on faces } f: \\ T_f, \nabla T \cdot \boldsymbol{n}_{\Gamma}|_f.$





Appendix C: LRS details

Boundary layer enhancement techniques (details)



Various numerical approaches to enhance predictions of strong variations



- (a) Particle-attached mesh in polar coordinates (2D) from Vreman 2016
- (b) Adaptive Mesh Refinement from Popinet 2014; Zhao, Zhang, and Ni 2021
- (c) VoF to single-phase simulation framework developed by Weiner 2020
- (d) Analytical profile fitted on the first mesh average concentration value: quasi-static approach of Weiner and Bothe 2017
- (e) Unsteady boundary layer tracking approach Aboulhasanzadeh et al. 2012

Appendix D: DNS results

Temperature error field at $Ar^* = 50$, $Pr_l = 1$. ($Re_b = 62.5$)

Temperature error distribution



 $\times 10^{-3}$ $\times 10^{-3}$ 5.00 5.00 4.50 4 4.50 4.00 4.00 3 -3.50 🛱 3.50 🛱 $2 \cdot$ - 3.00 สี 3.00 គ Z-axis (m) Z-axis (m) - 2.50 2.50 0 - 2.00 2.00 -1- 1.50 - 1.50 🚊 -2-2- 1.00 1.00 -30.50 - 0.50 -30.00 0.00 -2 -20 2 0 2 $\times 10^{-3}$ $\times 10^{-3}$ X-axis (m) Y-axis (m) (a) $D_b / \Delta = 16$ **(b)** $D_b / \Delta = 64$

Error is less than 5% on average. The error made at the interface is not propagating significantly through the domain. It reinforces our trust in an *a priori* methodology.

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Appendix D: DNS results

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Overall Nusselt number grid convergence ($Ar^* = 10, Ar^* = 50$)





Nusselt number values for increasing spatial resolution D_b/Δ

(a) $Ar^* = 10, Re_b \approx 3.6$

(b) $Ar^* = 50, Re_b \approx 62.5$

(a) Nusselt number converges rapidly to the reference solution, (b) Nusselt number prediction depends clearly on the Prandtl number. Correlations Eq.(29a) from Feng and Michaelides 2001 Increase in liquid Prandtl number $Pr_l = \frac{\alpha_l}{\nu_l}$:

- \Rightarrow Thermal boundary layer gets thiner
- \Rightarrow Spatial resolution requirements increases linearly i.e. $Pr_l\times 2 \to \Delta_{x,y,z}\times 2 \to N_{cells}\times 8$

Appendix D: DNS results

Local velocity field profiles: $u_r(r)$, $u_{\theta}(r)$, $u_{\phi}(r) = 0$





(a) Radial velocity u_r

(b) Tangential velocity u_{θ}

- $\Rightarrow u_r$ profiles are **linear** in the radial direction.
- $\Rightarrow u_r$ is cancelling approximately at the interface for numerical reasons. (viscosity calculation favouring one of the two phases and offset "virtually" the point of zero velocity)
- $\Rightarrow u_{\theta}$ profiles are **non-linear** in the radial direction.

Appendix D: DNS results

Tangential temperature derivative $\nabla T \cdot \widetilde{e_{\theta}} = \frac{1}{r} \frac{\partial T}{\partial \theta}$





(a) $D_b / \Delta = 16$

(b) $D_b/\Delta = 64$

- \Rightarrow Post-processed tangential derivative term is very **noisy** for $D_b/\Delta = 16$.
- \Rightarrow Not well captured even if less significant !
- \Rightarrow Zero tangential n^{th} order derivatives imposed implicitly by $T_{\Gamma} = T^{sat}$.
- \Rightarrow **Modelling** this term could be interesting.

Appendix E: Additionnal results

Predicted temperature profiles in the interface vicinity $\nabla T \cdot \boldsymbol{e}_r(r)$





(a) Case A - $C_{\text{coarse}}^{\theta}$



(c) Case F - C_{fine}^{θ} , D_{fine}^{θ}

		Case A	Case B	Case F		
(1)	2	Wrong sign of	Gradient error reduced	Coherent with coarse		
		$ \nabla T \cdot \boldsymbol{n}_{\Gamma} _{end}$	at the bottom	and fine solutions		
(2) "	Not a clear o	oar onhancomont	Enhancements close to the interface			
		Not a clear enhancement		Discrepancies observed at the probes'end		
(3)	<i>2</i>	Clear enhancement over the probe length				





Regularised profiles

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Levich-Ruckenstein regularised profiles employed by Legendre, Borée, and Magnaudet 1998:

$$\frac{\nabla T \cdot \boldsymbol{n}_{\Gamma}(\theta)}{\nabla T \cdot \boldsymbol{n}_{\Gamma}|_{\theta=\pi/2}} = \frac{\sqrt{a}\cos^{2}\left(\frac{\pi/2-\theta}{2}\right)}{\sqrt{(a-1)+\cos\left(\pi/2-\theta\right)}} + b; \qquad a^{th} = 2; \ b^{th} = 0$$
(7)

Nusselt number formula ($r = R_b$)

$$Nu_{b} = D_{b}R_{b}^{2}/\Delta T \int_{S_{\Gamma}} \underbrace{\nabla T \cdot \boldsymbol{n}_{\Gamma}|_{\Gamma}\sin\left(\theta\right)}_{\text{Integrand}} d\theta d\phi \tag{8}$$

Where ϕ varies between 0 and 2π and θ between 0 and π .



Perspectives and questions

- Operators straddling the interface should be adapted:
 - \Rightarrow Split the two phases' resolution (Forget about Ghost Fluid Methods?).
- Applicability to condensing bubbles:
 - \Rightarrow Effets of the velocity jump \dot{m}_v , $Ja \neq 0$?
 - \Rightarrow Same treatment for the velocity ?
- A multi-bubbles column configuration aimed in the thesis:
 - ⇒ Quasi-Static approach still relevant ?
 - \Rightarrow Will thermal boundary layers **perturbations** are fast ?

WILL DISCONTINUOUS NUMERICAL TREATMENTS OF QUANTITIES OVERCOME DIFFUSE METHODS ?