Wave dynamics in counter-current gas-liquid flows for distillation process applications

G. Lavalle[a], Y. Li[b], S. Mergui[b], N. Grenier[a], G. Dietze[b]

[a]LIMSI, CNRS, Univ. Paris-Sud, Univ. Paris-Saclay, Orsay, France
[b]FAST, CNRS, Univ. Paris-Sud, Univ. Paris-Saclay, Orsay, France

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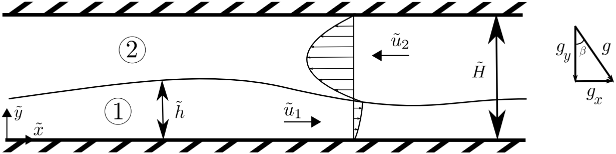
General frame

Gas-liquid flow in confined channels: non-linear interfacial waves development

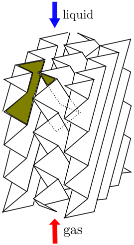


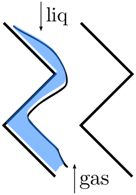
ANR project “wavyFILM” among FAST, LIMSI and Air Liquide: harnessing waves on liquid films to optimize distillation processes

Main issue

- heat and mass transfer in thin films under counter-current gas is crucial in chemical applications, e.g. absorption of CO_2 in packed towers and distillation [Valluri *et al.*, *Chem. Eng. Sci.* 2005]
- measurements of heat and mass transfer in packed towers are laborious
- CFD is decisive for full flow analysis and support industrial design

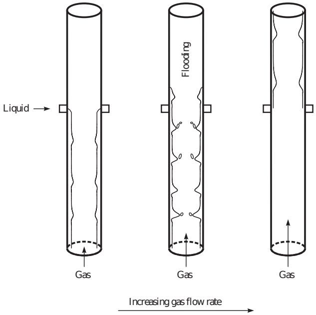
Waves intensify heat and mass transfers because increase the interfacial gas-liquid area [McCready & Hanratty, *AIChE* 1965]

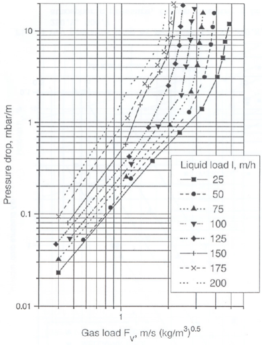




Flooding

The liquid fills the entire column: drop of performances because the gas is obstructed [Spiegel & Meier - *IChemE 1992*]





Objective: intensify heat and mass transfer while avoiding flooding

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DassFlow solver: brief

- DassFlow is our DNS flow solver developed by LIMSI and IMT/INSA Toulouse: open-source, 2D, unstructured mesh
- parallelized with MPI while keeping high performances (tested up to 600 cores on French supercomputers: $\simeq 1.1\mu s/dt/cell$)
- Formulation: two-fluid model (one velocity and one pressure in each point)
    - no advection or reconstruct the interface (the interface is captured by the scheme through the volume fraction) $\longrightarrow$ easy implementation
    - diffuse interface model $\longrightarrow$ interface diffusion: low diffusive numerical schemes are necessary
- Method: compressible model
    - easier implementation and general use
    - ill conditioned for low Mach flows $\longrightarrow$ low-Mach scheme is necessary
- Schemes: finite volume, second-order numerical schemes
- Feature: surface tension, non-isothermal, 3D (ongoing)

Two-fluid model

Index 1 and 2 for liquid and gas phases

One velocity $\mathbf{u}$ and one mixture pressure p in each point:

$$\begin{aligned} \partial_t \tilde{\rho}_1 + \nabla \cdot (\tilde{\rho}_1 \mathbf{u}) = 0 \ , \qquad & \tilde{\rho}_1 = \alpha_1 \rho_1 \\ \partial_t \tilde{\rho}_2 + \nabla \cdot (\tilde{\rho}_2 \mathbf{u}) = 0 \ , \qquad & \tilde{\rho}_2 = \alpha_2 \rho_2 \end{aligned}$$

$$\partial_t [(\tilde{\rho}_1 + \tilde{\rho}_2)\mathbf{u}] + \nabla \cdot [(\tilde{\rho}_1 + \tilde{\rho}_2)\mathbf{u} \otimes \mathbf{u} + p\mathbf{I}] = \nabla \cdot (\tau_v + \tau_c) + (\tilde{\rho}_1 + \tilde{\rho}_2)\mathbf{g}$$

Relation between p and $\tilde{\rho}$ to close the set of equations:

$$p_1 = p_0 + c_1^2(\tilde{\rho}_1/\alpha_1 - \rho_0)$$
$$p_2 = p_0 + c_2^2(\tilde{\rho}_2/\alpha_2 - \rho_0)$$
$$\alpha_1 + \alpha_2 = 1$$

Viscous stress: $\tau_v = -2/3\mu\nabla \cdot \mathbf{u}\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$
Capillary tensor (CSS formulation): $\tau_c = \sigma\left(\mathbf{I} - \frac{\nabla\cdot\alpha\otimes\nabla\cdot\alpha}{|\alpha|^2}\right)|\alpha|$

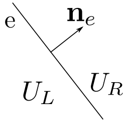
Discretization

Low-Mach scheme

Finite volume: $Q^{n+1} = Q^n - \frac{\Delta t}{\mathcal{V}} \sum_e F_e^n l_e + \Delta t S^n$

Numerical flux at cell edges: $F_e = v_e^+ U_L + v_e^- U_R + p_e \mathbf{n}_e$ with

1. $p_e = 1/2(p_R + p_L)$ centered scheme [Dellacherie *JCP2010*]
2. $v_e = 1/2(\mathbf{u}_L + \mathbf{u}_R) - \gamma_e(p_R - p_L)$ ($\gamma_e > 0$ stabilizes the scheme)



Based on a semi-implicit low-Mach scheme [Grenier et al. *JCP2013*, Lavalle et al. *JCP2015*]:

- implicit continuity equation (via Newton method)
  - CFL condition not computed with sound speed
- explicit momentum balance equation

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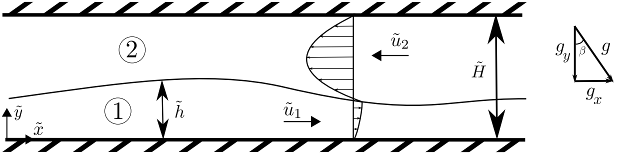
Validation of DassFlow solver

Fluids: DMSO and air



Validation of linear waves vs. Orr-Sommerfeld theory and of non-linear waves vs. experiments (Dietze et al. *JFM2009*, Kofman et al. *IJMF2017*)

1. vertical falling film in aerostatic gas atmosphere
2. vertical and inclined falling film with counter-current laminar gas flow

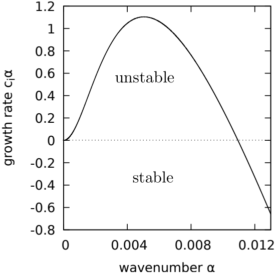
After validation, the aim is to analyse extremely-confined film-gas flows, with interfacial heat transfer

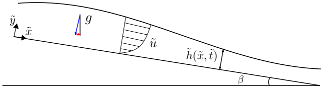
A note on thin-film linear instability

Liquid film in passive gas

Kapitza instability

- de-stabilizing mechanism: inertia
- stabilizing mechanisms: surface tension, viscosity, gravity



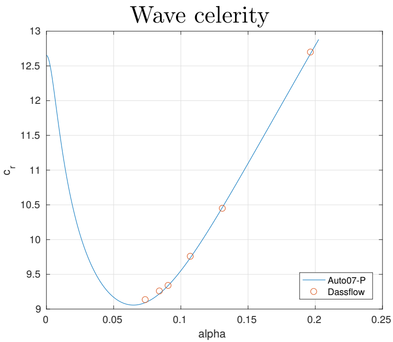


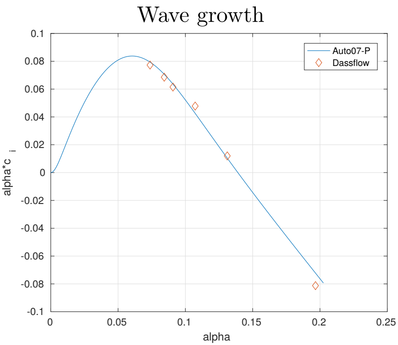
Benjamin, *JFM 1957*
Yih, *PoF 1963*

Linear stability (aerostatic gas)

Comparison against Orr-Sommerfeld theory

Vertical falling film at $Re_L = 15$ in aerostatic gas atmosphere: a small sinuisoidal disturbance is applied at the free surface ⟶ celerity and growth of linear waves is computed


Wave celerity

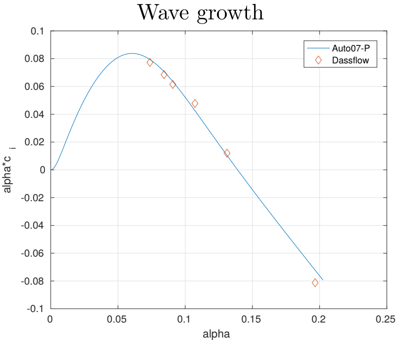

Wave growth

Linear stability (aerostatic gas)

Comparison against Orr-Sommerfeld theory

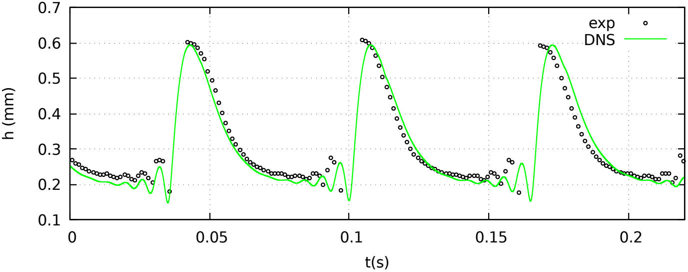
Vertical falling film at $Re_L = 15$ in aerostatic gas atmosphere: a small sinuisoidal disturbance is applied at the free surface $\longrightarrow$ celerity and growth of linear waves is computed

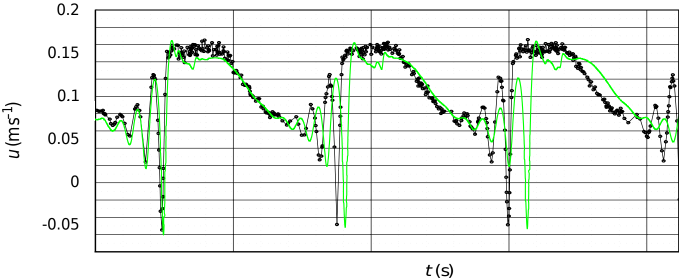
Why no points on the left of the most unstable wavelength? With periodic domains, this means to impose a wavelength larger than the most unstable, thus the instability will follow the shorter, i.e. the most unstable.



Non-linear waves (aerostatic gas)

Comparison against Dietze's experimental data ($\beta = 90^o, Re_L = 15$)

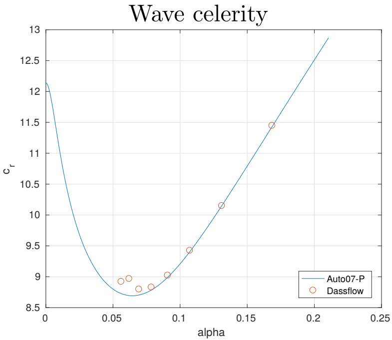




Linear stability (counter-current gas)

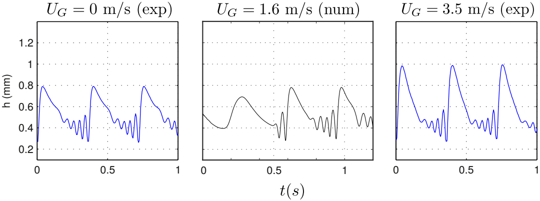
Comparison against Orr-Sommerfeld theory

Vertical falling film at $Re_L = 15$ with counter-current gas at $Re_G = 120$: a small sinuisoidal disturbance is applied at the free surface ⟶ celerity and growth of linear waves is computed

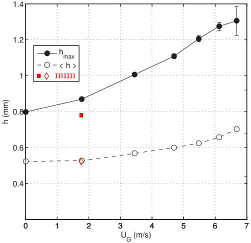


Non-linear waves (counter-current gas)

Comparison vs. Kofman's exp. data ($\beta = 5^o, Re_L = 45$, $Re_G = 1900$)



$U_G = 0$ m/s (exp) $U_G = 1.6$ m/s (num) $U_G = 3.5$ m/s (exp)



Comments: this run lasted for 135h on 576 cores (2 millions elements) on Myria (CRIANN supercomputer) with $\simeq 1.1\mu s/dt/dx/proc$. Still ongoing: 10% discrepancy on h_{max} so far.

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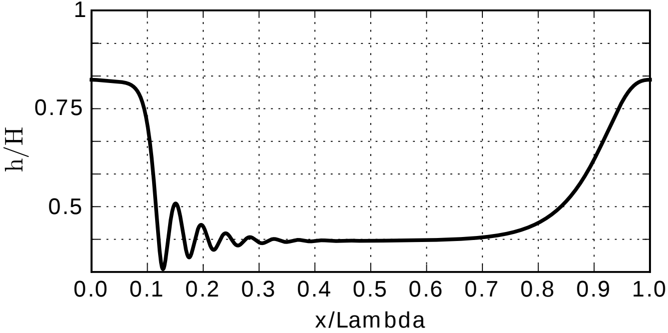
Next step on wave dynamics

Wave flattening in strongly confined channels

Use Dassflow to investigate gas-liquid dynamics in very strong confinement $\longrightarrow$ small gap between wave crest and top wall: saturated non-linear waves might flatten.



Result obtained through second-order low-dimensional film model (Dietze & Ruyer-Quil *JFM2013*).

Conclusions and perspectives

Results:

- validation of DassFlow:
    - celerity and growth of linear waves in good agreement with Orr-Sommerfeld results
    - non-linear wave profiles in good agreement with experiments of thin films with and without counter-current laminar gas

Future tasks:

- validation of the heat transfer numerical module of DassFlow against experiments performed at FAST
- optimization of flooding regimes in confined film-gas flows (find optimum regime to intensify heat transfer avoiding flooding)

`gianluca.lavalle@limsi.fr`
`https://sites.google.com/site/gianlucalavalle/`
`https://wavyfilm.limsi.fr`