Variational Multiscale Methods for Turbulent Reacting Flows

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Process intensification (PI)

PI is an approach to design more **innovative** and **efficient** processes to enhance mass and heat transfer without negatively affecting the environment.

- **Computational Fluid Dynamics** is useful for virtual design/optimization in PI.
- Most engineering applications encounter **turbulent flow**.
- Methods that help to understand existing phenomena and to **design new processes from scratch** are required.

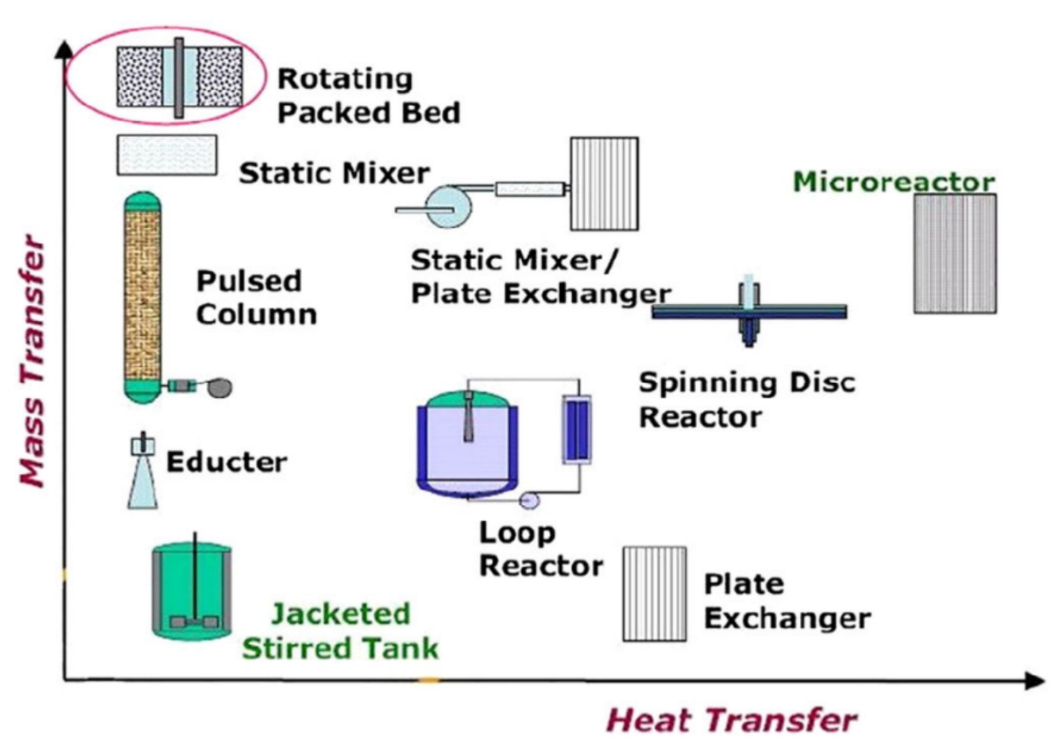

Figure 1: Process-intensifying equipment. Taken from [1].

Objectives

General objective: Develop and implement Variational Multiscale Methods (VMS) that are efficient and accurate to model turbulent reacting flows needed to achieve process intensification.

- **Implement** VMS for hydrodynamic problems.
- **Validate** the method and compare its precision to traditional stabilized approaches or explicit Large-Eddy simulations with benchmark turbulent flow problems.
- **Extend** those methods to support reacting flows that contain fast chemical reactions.
- **Assess** the efficiency of the method by simulating an intensified process.

Methodology

We discretize the *incompressible Navier-Stokes* equations and the *advection-diffusion-reaction* equation:

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\,\boldsymbol{u} = -\nabla p^{*} + \nabla \cdot \boldsymbol{\tau} + \boldsymbol{f}$$

$$\frac{\partial C_i}{\partial t} + \boldsymbol{\nabla} \cdot (C_i \boldsymbol{u}) = D_i \boldsymbol{\nabla}^2 C_i + S$$

$\boldsymbol{u}$: velocity	C_i: concentration of i
p: pressure	D_i: diffusivity of i
$\boldsymbol{\tau}$: deviatoric stress	$\boldsymbol{f}, S$: source terms

1. Achieve an efficient implementation of VMS using the **Finite Element** open-source software Lethe (`https://github.com/lethe-cfd/lethe`) and a **matrix-free approach**.

2. Develop and implement **benchmarks** for both complex turbulent flow and turbulent reacting flows (e.g. periodic hills).

3. Couple the hydrodynamic part with the reaction part of the code.

4. Set up and simulate a **process-intensified equipment**, such as a static mixer.

Scientific contribution and impact

Short-term:
numerical method able to simulate concrete problems involving turbulent reacting flows at an affordable cost.

Mid-term:
method that will help to design innovative and sustainable processes from scratch.

Long-term:
method useful for product development in other areas (e.g. aerospace engineering).

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Preliminary results: the periodic hills case

Complex **turbulent flow benchmark**:

- Flow separation from a curved surface
- Unsteady shear layer
- Recirculation
- Attached and detached boundary layers

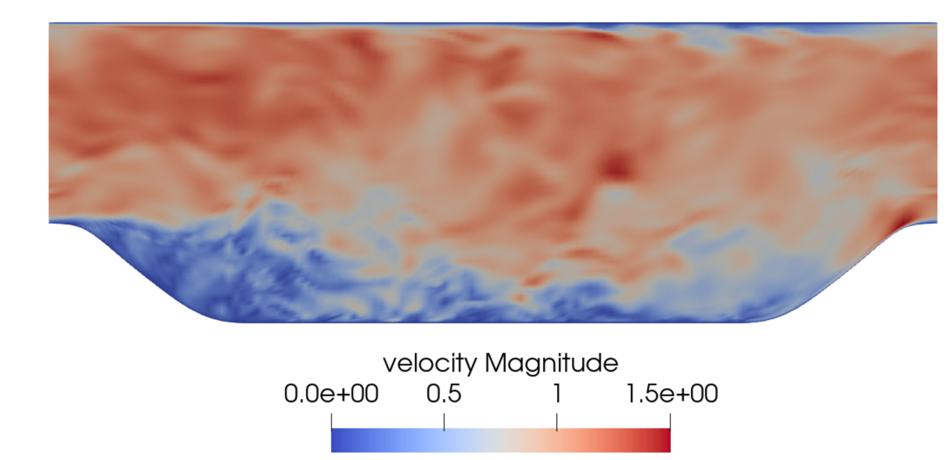

Figure 2: Snapshot of the flow over periodic hills.

We simulate the flow over periodic hills for Re = 5600 using a stabilized FEM formulation with linear elements:

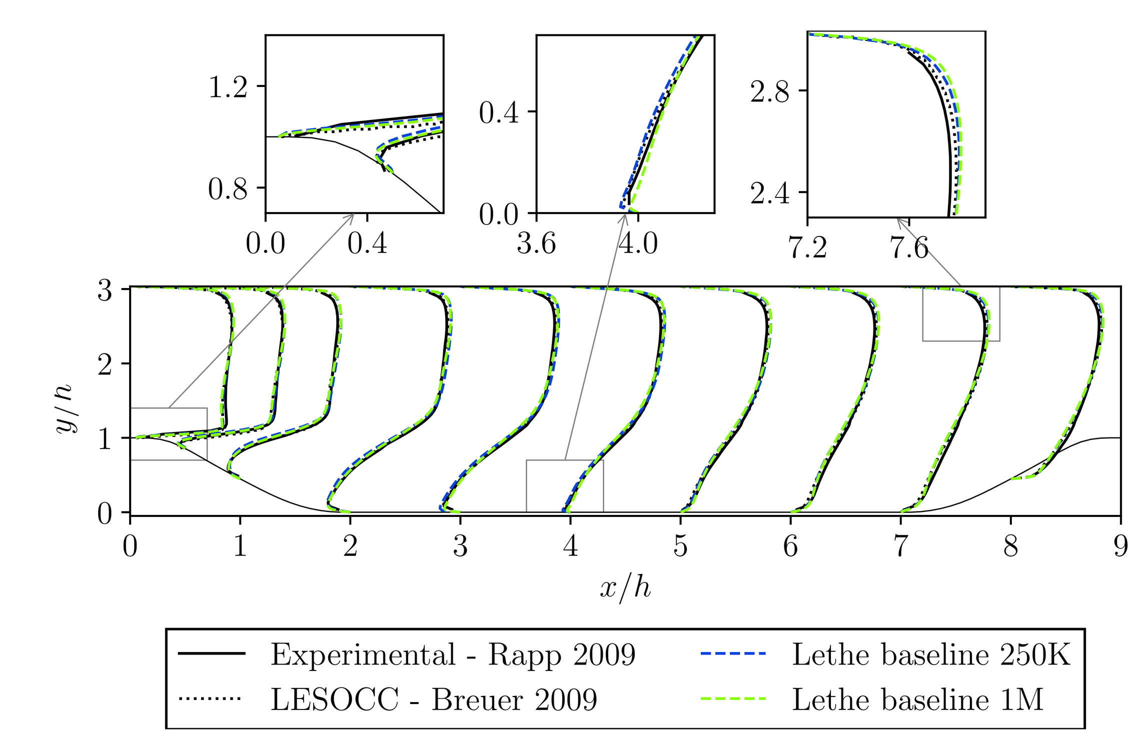

Figure 3: Average velocity in the x direction throughout the geometry.

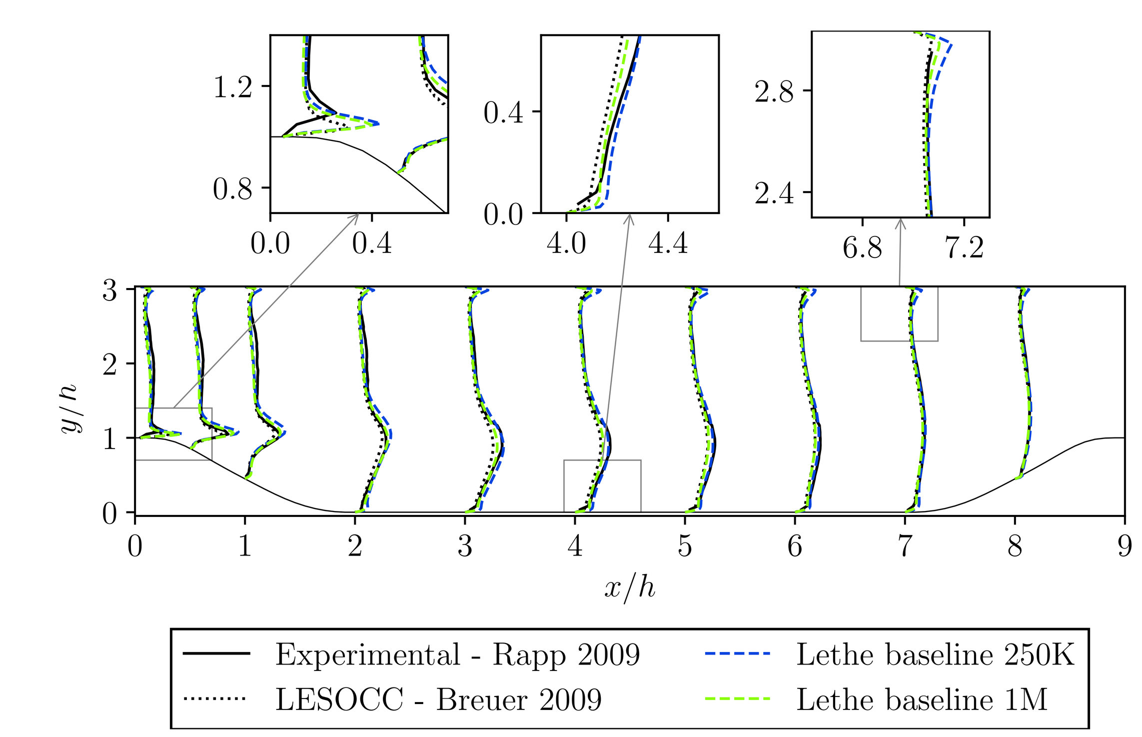

Figure 4: Reynolds normal stress in the x direction throughout the geometry.

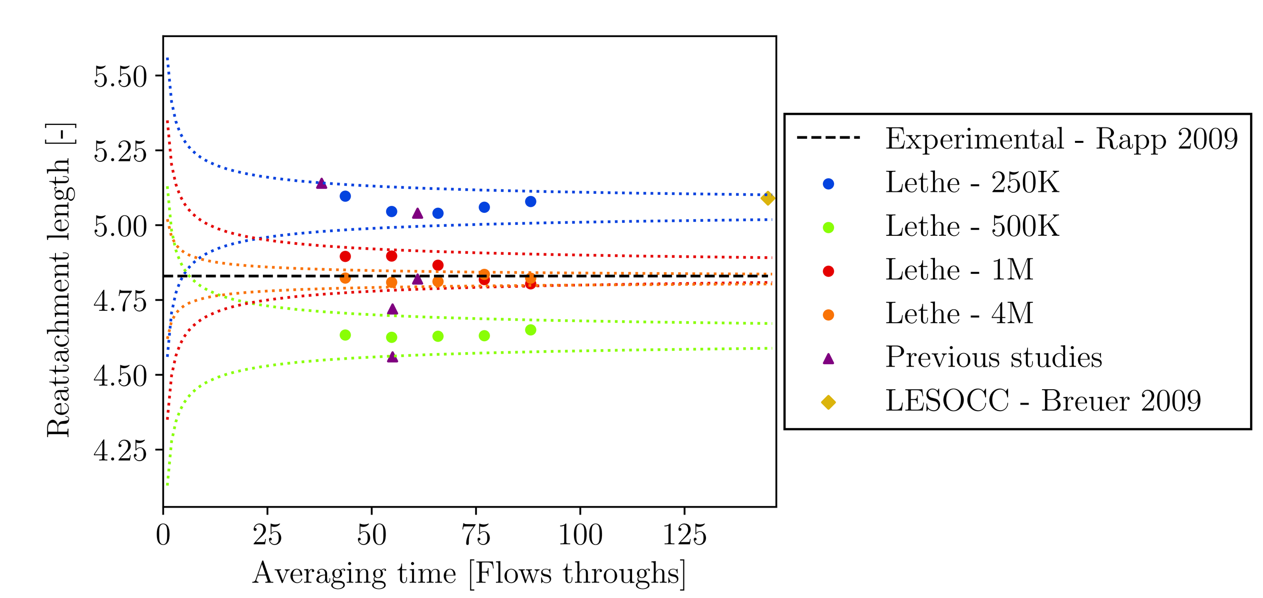

Figure 5: Reattachment point extracted at different averaging times for different mesh resolutions.

- Very **good agreement** for both average velocity and Reynolds normal stress in the x direction using **coarser meshes** than the ones used in previous studies.
- **Reattachment point** converges towards experimental value as the mesh is refined.

References

[1] D. C. Boffito and D. Fernandez Rivas, "Process intensification connects scales and disciplines towards sustainability," *The Canadian Journal of Chemical Engineering*, vol. 98, pp. 2489–2506, 2020.