UCLouvain

Institute of Mechanics, Materials and
Civil Engineering (iMMC)

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A penalization method for the Direct Numerical Simulation of low-Mach reacting gas-solid flows

B. Hardy, J. De Wilde, G. Winckelmans

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MaCKiE

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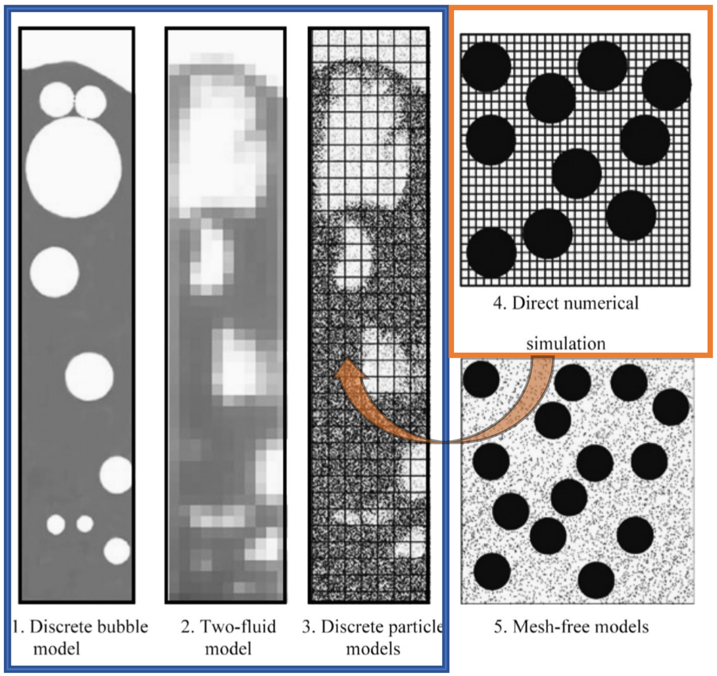
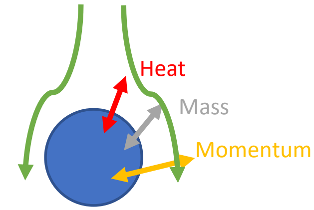
1. Motivation

- **Fluidized beds** : key technology for physical or chemical transformation (drying, coating, combustion, base chemicals production,…)
- Modeling strategies :



Reproduced from Deen et al, *"Review of direct numerical simulation of fluid–particle mass, momentum and heat transfer in dense gas–solid flow"*, Chem. Eng. Sc. , 2014

- **Large-scale** fluidized beds simulation:
  1-D model, TFM or CFD-DEM
  → need for closure laws



- **Direct Numerical Simulation** powerful tool to build new closure laws from fundamental conservation principles (mass, momentum, energy)
- Most DNS work based on
  - o incompressibility approximation
  - o 0-D description of the particle

2. The weakly compressible approximation

- Gas-solid reacting flows:
  - Heat release / consumption
  - Molecular weight changes ($A \rightarrow 2B, A + B \rightarrow C, \ldots$)
    - $\longrightarrow$ temperature and species concentration gradients in the vicinity of the particle surface
    - $\longrightarrow$ non-negligible **density fluctuations**
- Fully compressible Navier-Stokes equations: time step constraint fixed by the speed of sound $\longrightarrow$ **costly !**

  but…

- Most industrial flows occur at **low Mach**: $M = \frac{u}{c} \ll 1$
- **Weakly compressible formulation** of the N-S equations:
  - acoustic modes removed $\longrightarrow$ $\Delta t \simeq \Delta t_{incompressible}$
  - $p(\mathbf{x}, t) = p'(\mathbf{x}, t) + p_0(t)$
  - $p_0 = \frac{\rho R T}{\bar{W}}$: uniform thermodynamic pressure

Weakly compressible Navier-Stokes equations:

$$\frac{\partial(\rho \boldsymbol{u})}{\partial t} = -\nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) + \nabla \cdot \tau - \nabla p'$$

$$\frac{\partial T}{\partial t} = -(\boldsymbol{u} \cdot \nabla)T + \frac{1}{\rho c_p} \nabla \cdot (\kappa \nabla T) - \frac{dp_0}{dt} + \sum_{k=1}^{N_s} \dot{w}_k h_k$$

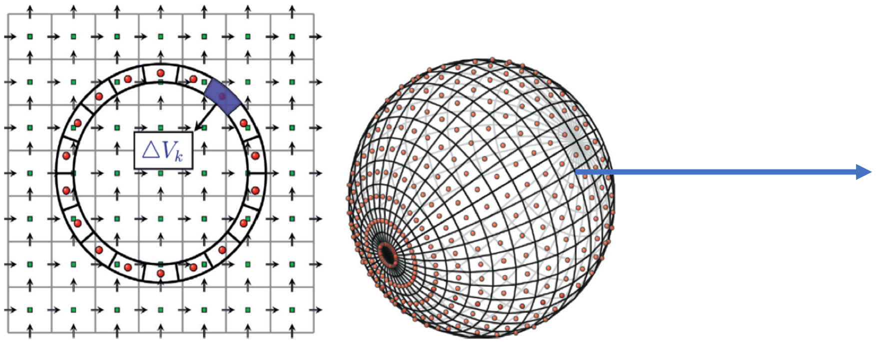
= 0 if open domain ($p_0 = p_{atm}$)

$$\frac{\partial Y_k}{\partial t} = -\,(\boldsymbol{u} \cdot \nabla)Y_k + \frac{1}{\rho} \nabla \cdot \left(\frac{\rho D}{\overline{W}} \nabla (Y_k\, \overline{W}) \right) - \dot{w}_k$$

Density is updated from the equation of state: $\rho = \frac{p_O \overline{W}}{RT}$

3. The penalization method

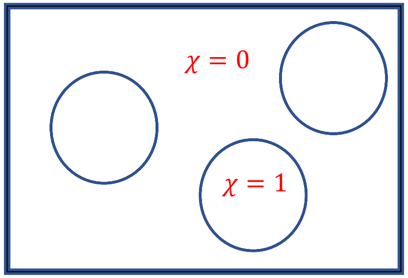
- Classical *Immersed Boundary Method* :



Reproduced from : H. Tavassoli, S. H. L. Kriebitzsch, M. A. van der Hoef, E. A. J. F. Peters, and J. A. M. Kuipers, "Direct numerical simulation of particulate flow with heat transfer," *Int. J. Multiph. Flow*, vol. 57, pp. 29–37, Dec. 2013.

Lagrangian tracking of surface points used to impact the presence of the solid phase on the flow fields

- *Penalization method* : the solid phase is tracked with a **mask** function, χ



- Solid phase = porous media with **vanishing permeability** η

- Classical Navier-Stokes equations are penalized with **additional source terms** to enforce the desired surface boundary condition

What kind of boundary condition ?

- **Dirichlet** : $\phi = \phi_s$

  e.g. $\boldsymbol{u} = \boldsymbol{u_s}, T = T_s, Y_k = Y_{ks}$

$$\frac{\partial \phi}{\partial t} = RHS \; - \boldsymbol{\chi} \frac{(\boldsymbol{\phi} - \boldsymbol{\phi_s})}{\boldsymbol{\eta}}$$

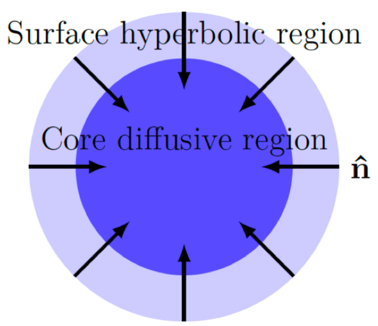
  η controls the accuracy: the smaller, the more accuracte
  implicit treatment is trival $\longrightarrow$ η as small as we want !

- **Neumann-Robin** : $\alpha\phi + \beta \frac{\partial \phi}{\partial n} = f$

  $\frac{\partial T}{\partial n} = 0$: no heat flux
  $Da\, Y_k + d_p \frac{\partial Y_k}{\partial n} = 0$: surface reaction ; $Da = \frac{k d_p}{D_f}$: Damköhler number

$$\frac{\partial \phi}{\partial t} = (\mathbf{1} - \boldsymbol{\chi}) RHS \; - \boldsymbol{\chi} \frac{\left(\boldsymbol{a\phi} + \boldsymbol{b}\, \boldsymbol{n_i} \frac{\boldsymbol{\partial \phi}}{\boldsymbol{\partial x_i}} - \boldsymbol{f}\right)}{\tilde{\boldsymbol{\eta}}}$$

  The source term is no longer local $\longrightarrow$ **explicit** treatment
  $\longrightarrow$ stronger constraint on the time-step

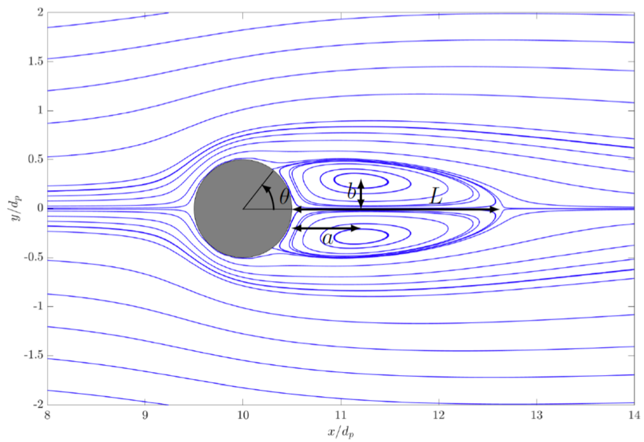


Characteristics propagate the boundary condition inwards
$\longrightarrow$ propagation is stopped before the core region to avoid crossing of characteristics

4. Results

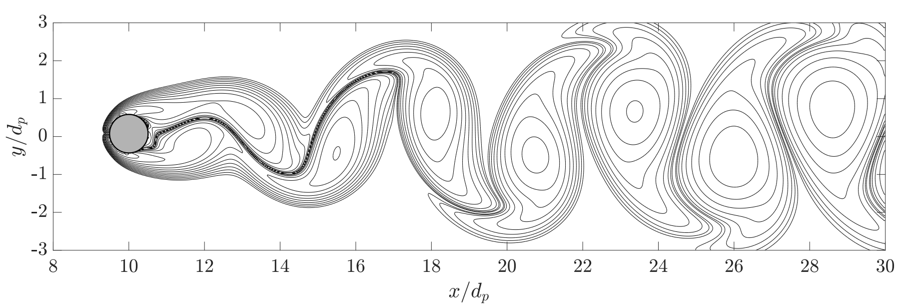
A. Validation (non-reactive case)

- $Re_p = 40$

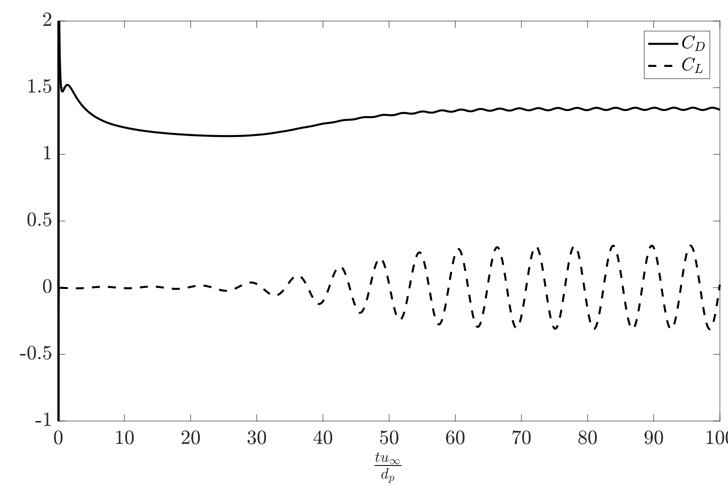


Study	C_D	$\frac{a}{d_p}$	$\frac{b}{d_p}$	$\frac{L}{d_p}$	θ
Present	1.57	0.73	0.57	2.15	53.1°
Bigay et al. [27]	1.57	0.70	0.59	2.22	50.3°
Canuto & Taira [28]	1.54	0.72	0.59	2.24	53.8°
Linnick & Fasel [29]	1.52	0.72	0.60	2.28	53.6°
Denis & Chang [30]	1.52	–	–	2.35	53.8°
Tritton* [25]	1.59	–	–	–	–
Bouard & Countanceau* [26]	–	0.76	0.59	2.13	53.8°

- $Re_p = 100$

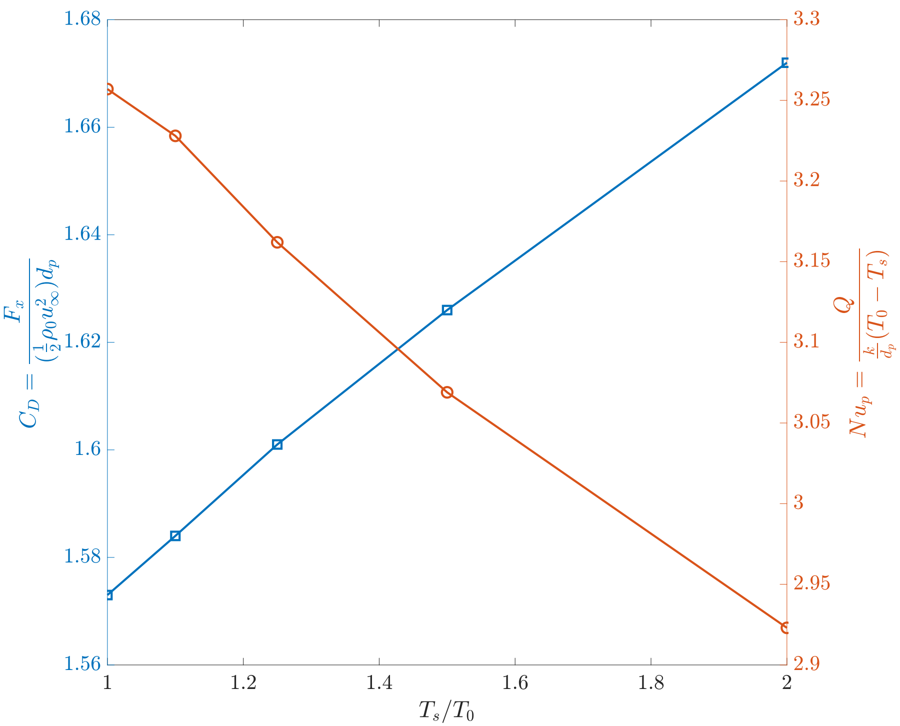


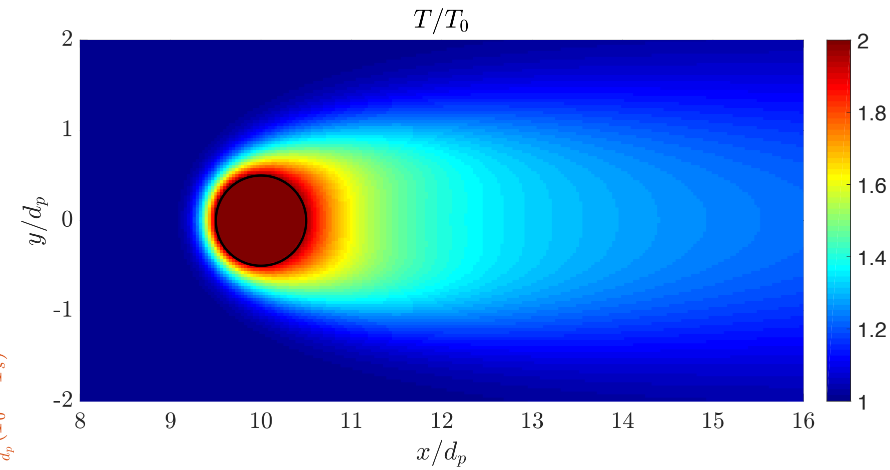
Study	$\overline{C_D}$	St
Present	1.34	0.170
Canuto & Taira [28]	1.34	0.167
Mittal et al. [31]	1.35	0.165
Apte et al. [32]	1.36	0.165

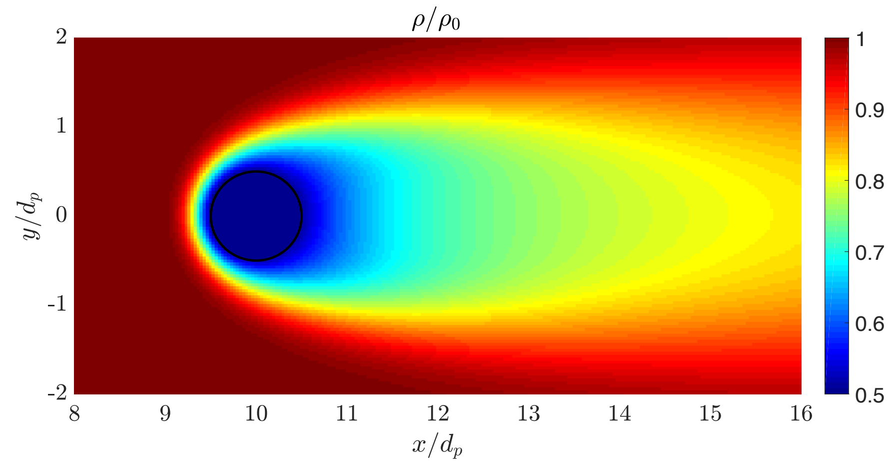


B. Impact of compressibility on C_D, Nu

- Set of numerical simulations with increasing values for the solid-phase temperature T_s
- $\uparrow$ of the drag and $\downarrow$ of the heat transfer coefficient when $\frac{T_s}{T_0}$ $\uparrow$







C. Infinitely fast reaction

- In the case of a very fast reaction $A \rightarrow B$, the **surface is free of reactant:** $Y_{A,s} = 0, Y_{B,s} = 1.$

  All the mass flux transferred from the fluid has reacted (no accumulation) :

$$\dot{m}_{A,f\rightarrow s} = R_A$$

- The heating rate induced by the reaction is obtained as

$$Q_r = \sum_{k=1}^{N_S} R_k h_k$$

- Mass balance over the whole particle (infinitely fast solid heat conduction approximation)

$$m_s c_{ps} \dot{T}_s = Q_r + Q_{f\rightarrow s}$$

  → update T_s at next time: **new Dirichlet BC**

- Practical feature of the penalization method : interfacial fluxes can be estimated from **volume integration:**

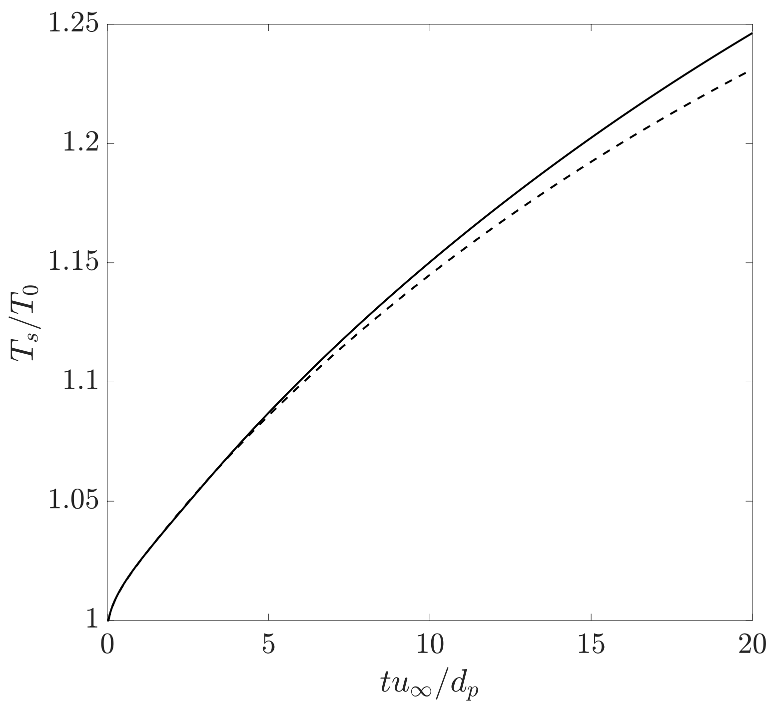
  e.g.

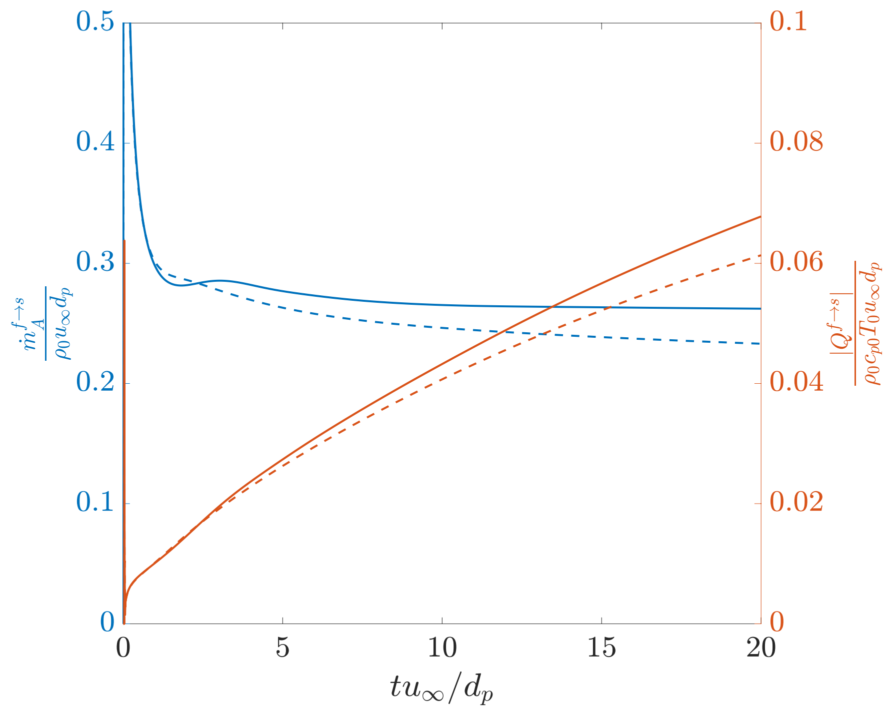
$$\dot{m}_{A,f\rightarrow s} = \int_{V_S} \chi\rho \frac{(Y_A - Y_{A,s})}{\eta}\, dV$$

$$Q_{f\rightarrow s} = \dot{T}_s \int_{V_S} \rho c_p dV + \int_{V_S} \chi\rho c_p \frac{(T - T_s)}{\eta} dV$$

C. Infinitely fast reaction

- Comparison of the the solid phase temperature increase between the incompressible (solid line) and the weakly compressible (dashed line) case
- Reduced mass transfer induced by the temperature increase (density decrease)
  → reduced heat release in the solid phase
  → slower increase of T_s





D. Finite-rate surface reaction

- Using the Neumann-Robin implementation of the penalization method, we can treat **finite-rate** surface reactions

  e.g. first order irreversible reaction $A \rightarrow B$ or $A \rightarrow 2B$

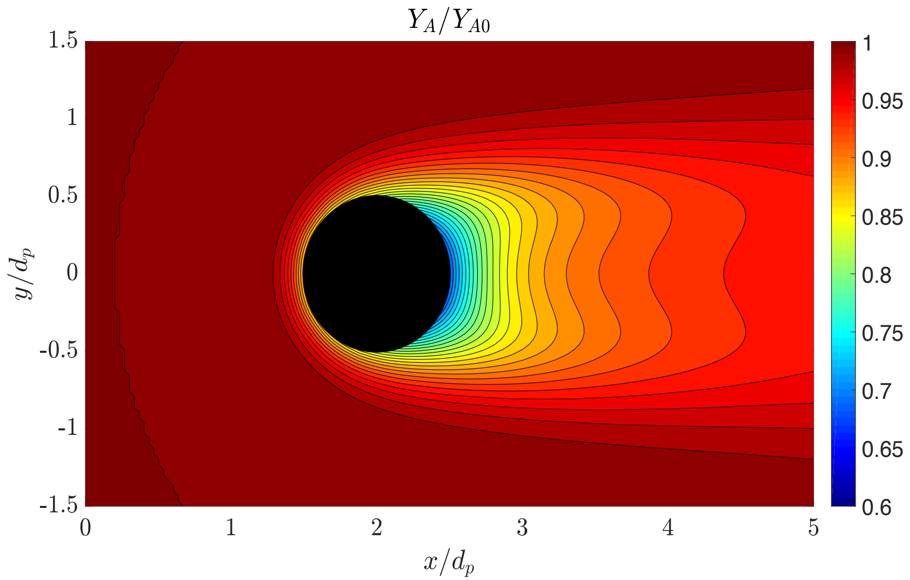
- Balance between the diffusive flux and the consumption rate of reactant A:

$$-\rho D \frac{\partial Y_A}{\partial n} = k \rho Y_A$$

  corresponds to a Robin-type BC:

$$Da Y_A + d_p \frac{\partial Y_A}{\partial n} = 0$$

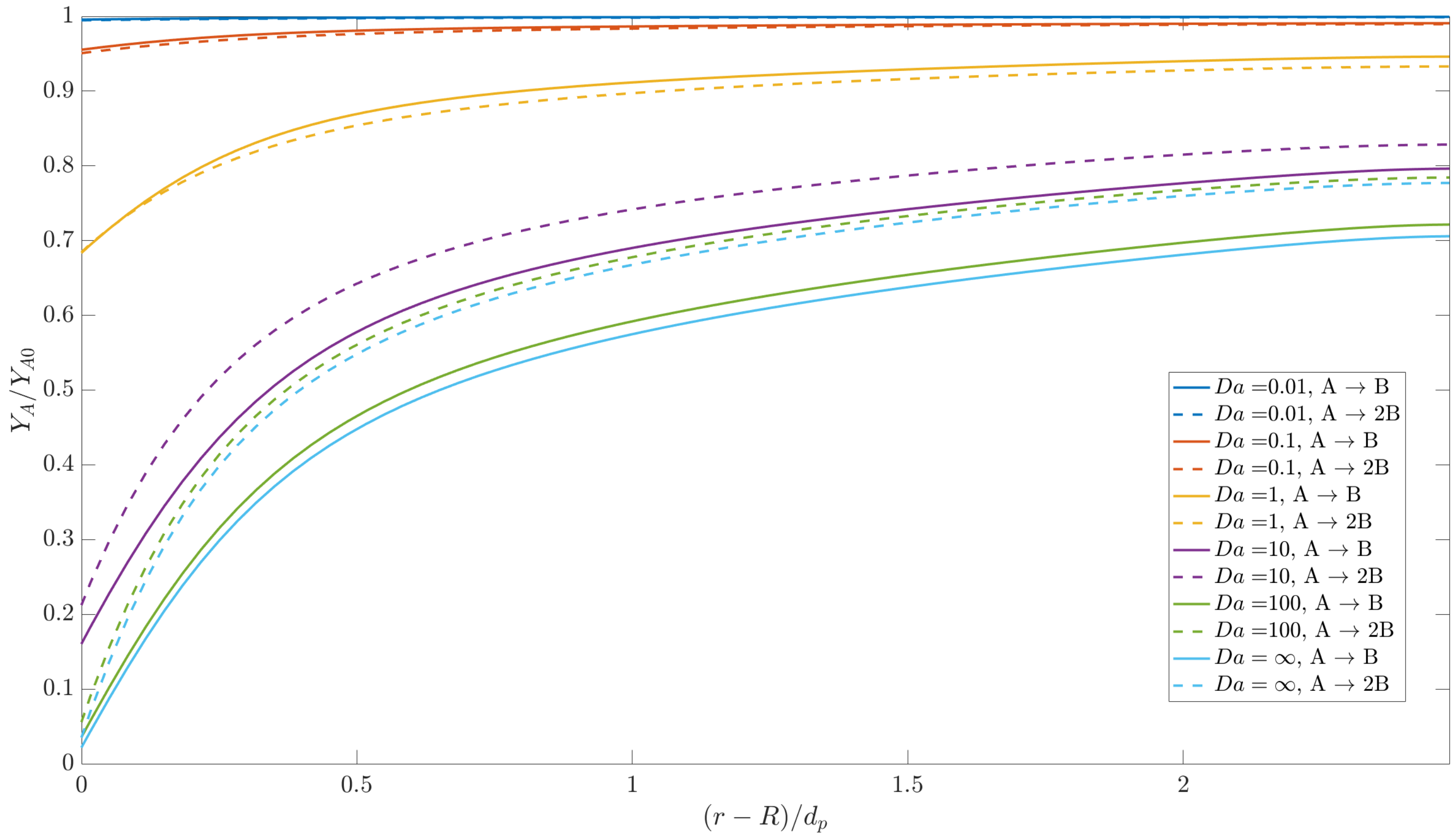
- Mass fraction field: $Re_p = 40, Sc = 0.7, Da = 1$



D. Finite-rate surface reaction

Impact of expansion ($A \rightarrow 2B$) on conversion ?

At higher Damköhler number, i.e. when diffusion becomes rate-limiting, volume expansion decreases the reactant conversion



5. Conclusion and outlook

- Original combination of the weakly compressible approximation and the penalization method

- Easy-to-implement method with computational cost similar to the fully incompressible case

- Application to a large range of situations in reaction engineering
    - Dirichlet BC : fixed temperature, composition (infinitely fast reaction)
    - Neumann-Robin BC : finite-rate surface reaction

- In each case, the impact of density changes induced by temperature and composition fluctuations is assessed

What's next ?

- 3-D implementation in in-house 4th order code (in progress)
- DNS of a small-scale fluidized bed (up to 10^3 particles)
- Extraction of transfer laws for feeding large-scale models

Acknowledgements

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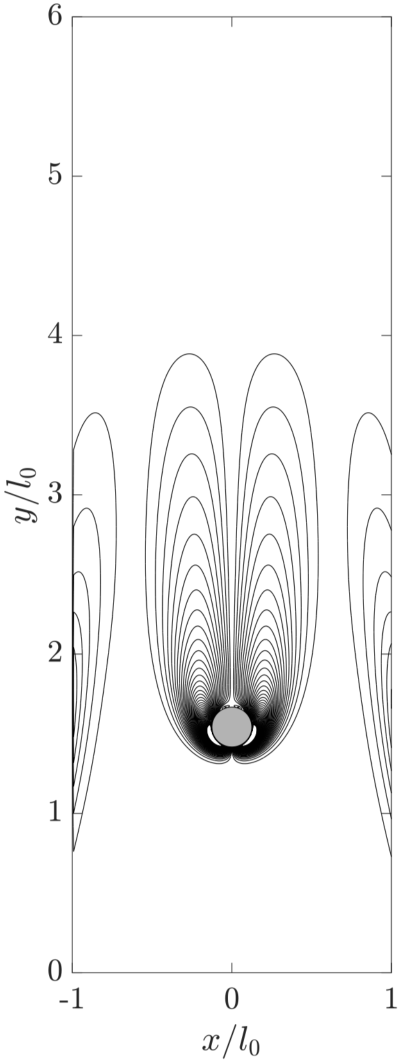
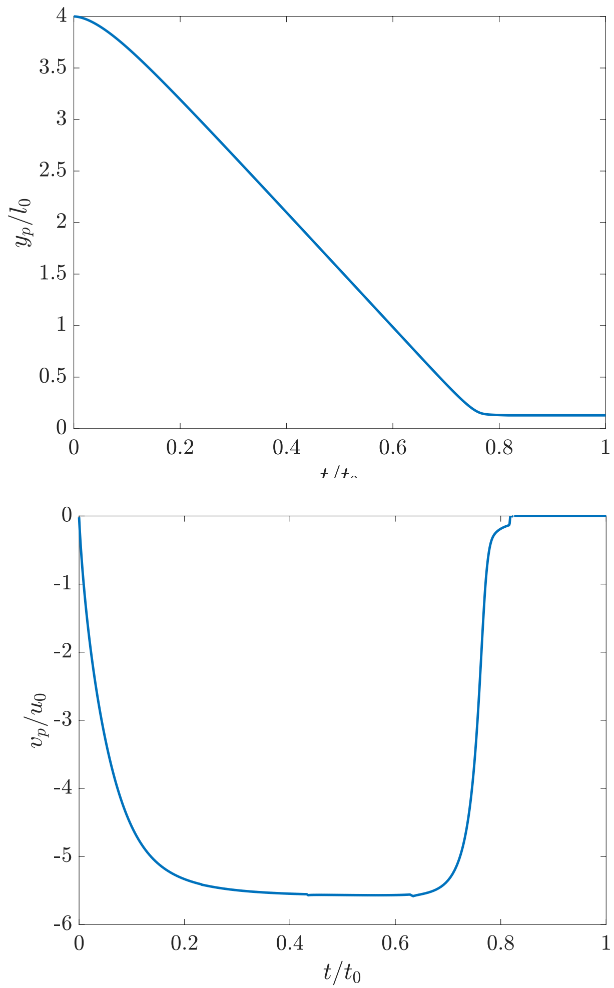
Computational resources were provided by the Consortium des Équipements de Calcul Intensif – CÉCI

Back-up slides

Validation of the solid-fluid coupling : sedimentation problem





Measure terminal particle Reynolds number :

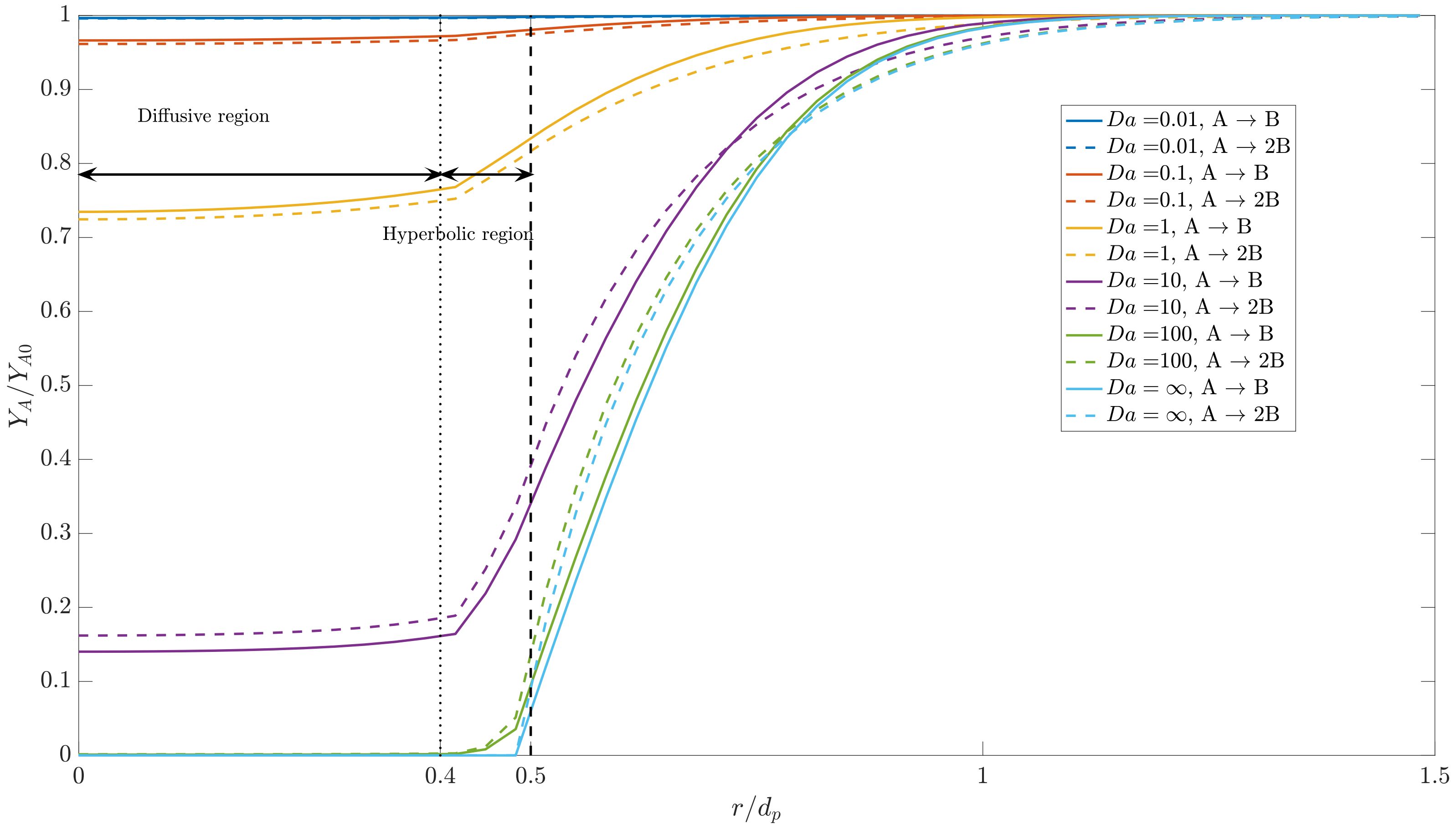
$$Re_t = 17.4$$

vs. Glowinski et al. :

$$Re_t = 17.31$$

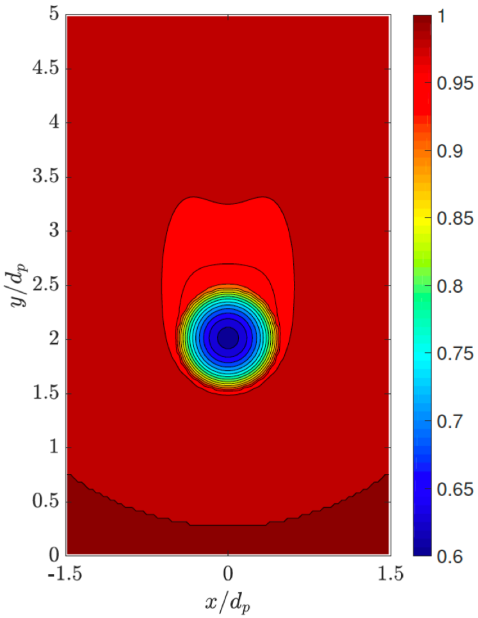
→ good agreement

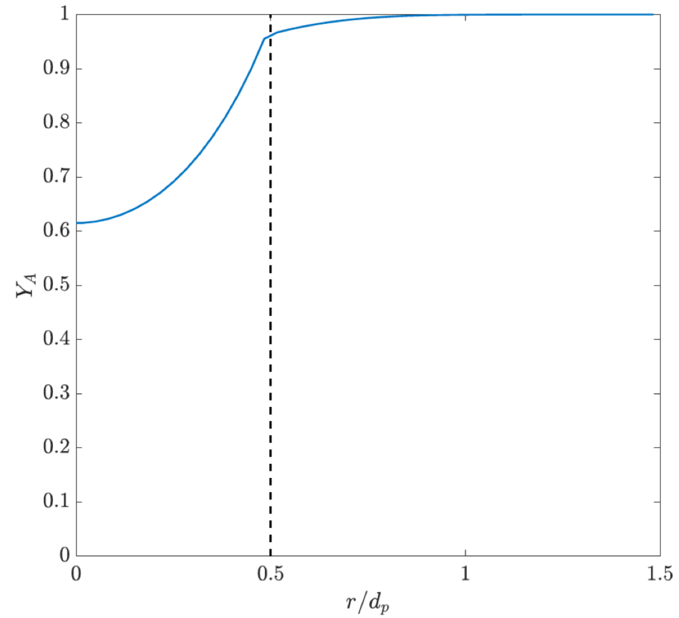
Hyperbolic and diffusive regions for characteristics propagation



Intraparticle reaction-diffusion process:

$$\frac{\partial Y_k}{\partial t} = -\mathbf{u} \cdot \nabla Y_k + \frac{1}{\rho} \nabla \cdot \left(\rho \left[(1-\chi)\mathcal{D}_f + \chi \mathcal{D}_s \right] \nabla Y_k \right) - \chi k Y_A,$$





Mass flux conservation :

$$-\rho D_S \frac{\partial Y_{A,s}}{\partial n}|_\Gamma = -\rho D_f \frac{\partial Y_{A,f}}{\partial n}|_\Gamma$$

→ The ratio between the slopes of species concentration profiles must be the inverse of the ratio between diffusivities.
For $D_S = 0.1 D_f$, we get a ratio of 9.73, i.e. a 2.3% error.