Study of the boundary layer for a solid particle combustion : a Robin boundary condition application

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General context

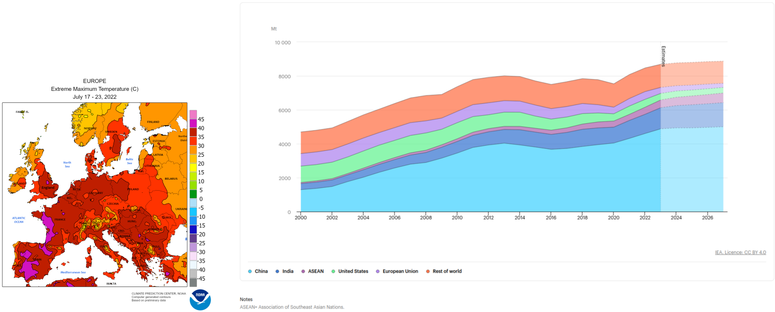


Figure 1: (Left) Heat wave 2022 in Europe, (Right) Global coal consumption, 2000-2026 (*International Energy Agency, 2025*)

Physical problem

We want to simulate the combustion of a solid particle of Char. The following equations are the one solve by (*Hassan et al, 2021*)

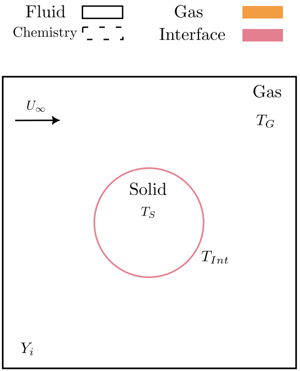


Figure 2: U_∞ velocity far from the sphere. T_S, T_G, T_{int} are respectively the temperature of the Solid, the Gas and the Interface. Y_i denote all the species in the gas.

Physical problem

For this study we simplify the problem by only solving at the interface and in the gas.

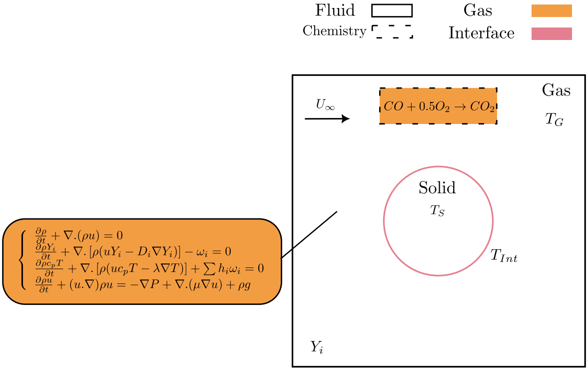


Figure 3: D_i is the diffusivity coefficient of the species i. ω_i are the product of the combustion, h_i, λ, the transfer and thermal coefficients. ρ, μ, are the density and the viscosity in the gas.

Physical problem

We have to consider the reaction at the interface, this is expressed by a robin boundary condition.

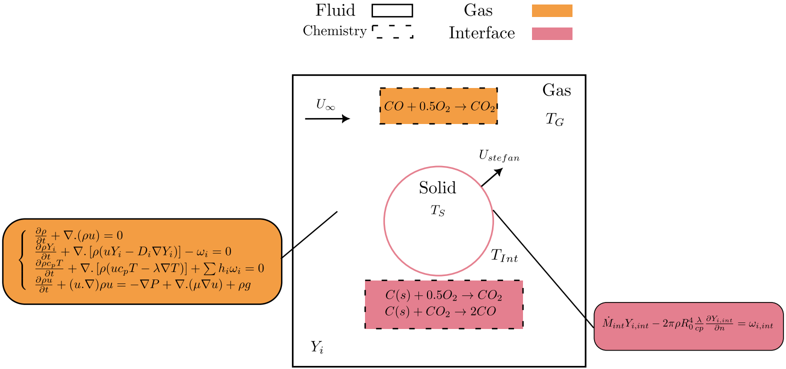


Figure 4: The subscript (s) qualify the solid. At the interface two reaction occurs resulting in the production of CO_2. $\dot{M}_{int}$ is the particle burning rate, R_0 the radius of the particle.

Definition

Let w a scalar field define on a domain Ω of surface Γ. We impose on the boundary surface Γ a robin boundary condition define as follow :

$$\alpha w + \beta \nabla w \cdot \mathbf{n}_\Gamma = \gamma \tag{1}$$

with α, β and γ three parameters.

State of the art in Basilisk

Work has been done by A.Van Hooft, T.Fullana, Yong Hui (among others). The definition is based on the ghost cells.

We solve 1 dimension Poisson equation : $\frac{\partial^2 w}{\partial x^2} = 1 - 2x^2$ with

$$\alpha_l w + \beta_l \frac{\partial w}{\partial x} = \gamma_l, \qquad \alpha_r w + \beta_r \frac{\partial w}{\partial x} = \gamma_r \tag{2}$$

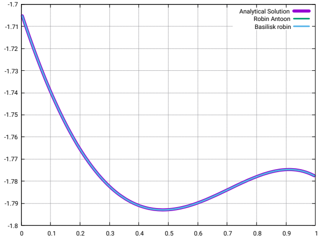


Figure 5: Solution of 1D Poisson equation with $\alpha_l = 2$, $\beta_l = -1$, $\gamma_l = -3$ and $\alpha_r = 1$, $\beta_r = 3$, $\gamma_l = -2$

Robin boundary on the computation domain : Analytical problem 1/2

We solve a Poisson equation on a squared box $\Omega = \{0 \leq x \leq a\} \times \{0 \leq y \leq b\}$

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = \Phi\left(x, y\right) \tag{3}$$

with the following boundaries :

$$\frac{\partial w}{\partial x} - \alpha_1 w = f_1\left(y\right) \quad \text{left } x = 0; \qquad \frac{\partial w}{\partial x} + \alpha_2 w = f_2\left(y\right) \quad \text{right } x = a$$

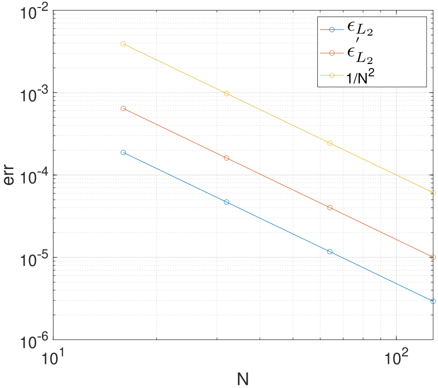
$$\frac{\partial w}{\partial y} - \alpha_3 w = f_3\left(x\right) \quad \text{bottom } \; y = 0; \qquad \frac{\partial w}{\partial y} + \alpha_4 w = f_4\left(x\right) \quad \text{top } y = b$$

This is the problem 7.2.2-14. from *Polyanin Handbook of Linear Partial Differential Equations for Engineers and Scientists*.

Robin boundary on the computation domain : Analytical problem 2/2

We define $\epsilon_{L_2} = \sqrt{\frac{\int_\Omega |\epsilon|^2 d\Omega}{\Omega}}, \quad \epsilon'_{L_2} = \sqrt{\frac{\int_\Omega |\epsilon|^2 d\Omega}{\int_\Omega |w_{analytique}|^2 d\Omega}}$ with

$$\epsilon = w_{analytique} - w_{basilisk}$$



How to compute a robin boundary condition ?

We are following the path taken by M.Tavares, T.Fullana and J-M.Lopez, they are using the *Johansen and Colella, 1998* method to recover the gradient and impose the correct value on the solid boundary condition.

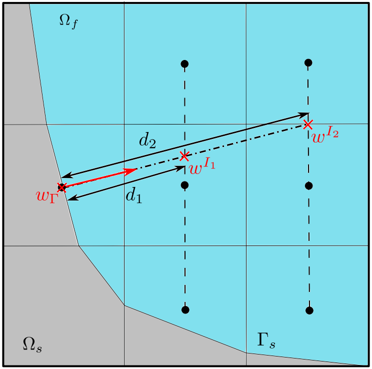


Figure 6: Gradient calculation in the embedded boundary method depending on the normal orientation n. (copy of fig from *Tavares et al, 2024*).

Johansen and Colella equation 1/2

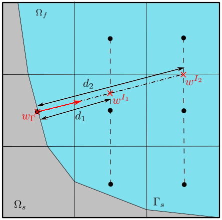
$$\nabla w|_\Gamma = \frac{1}{d_2 - d_1}\left[\frac{d_2}{d_1}(w_\Gamma - w^{I_1}) - \frac{d_1}{d_2}(w_\Gamma - w^{I_2})\right]. \tag{4}$$

The previous equation can be rewritten as :

$$\nabla w|_\Gamma = a_0 w_\Gamma + a_1 w^{I_1} + a_2 w^{I_2}, \tag{5}$$

where the constants a_0, a_1, a_2 are given by

$$a_0 = \frac{1}{(d_2 - d_1)}\left(\frac{d_2}{d_1} - \frac{d_1}{d_2}\right); \quad a_1 = -\frac{d_2}{(d_2 - d_1)\, d_1}; \quad a_2 = \frac{d_1}{(d_2 - d_1)\, d_2}. \tag{6}$$



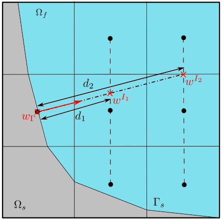
Johansen and Colella equation 1/2

Reminder : Robin boundary condition :

$$\alpha w_\Gamma + \beta \frac{\partial w}{\partial n}\bigg|_\Gamma = \gamma, \quad \nabla w|_\Gamma = a_0 w_\Gamma + a_1 w^{I_1} + a_2 w^{I_2}, \tag{7}$$

Combining the previous equation leads to :

$$w_\Gamma = \frac{-\beta(a_1 w^{I_1} + a_2 w^{I_2}) + \gamma}{\alpha + \beta a_0}. \tag{8}$$



Analytical problem on embed 1/2

This is the problem 7.1.2-4. from *Polyanin Handbook of Linear Partial Differential Equations for Engineers and Scientists*.
We solve a Poisson equation on a circle of radius R in the inner domain $0 \leq r < R$

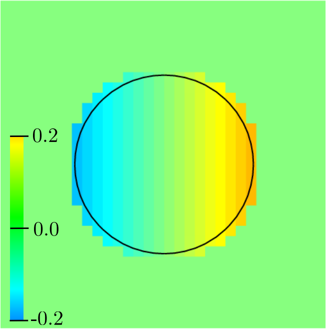
$$\alpha w + \frac{\partial w}{\partial r} = f(\theta) \tag{9}$$

The solution is given by :

$$w(r,\theta) = \frac{a_0}{2k} + \sum_{n=1}^{\infty} \frac{R}{kR+n} \left(\frac{r}{R}\right)^n \Big(a_n \cos(n\theta) + b_n \sin(n\theta)\Big), \tag{10}$$

$$\begin{aligned} a_n &= \frac{1}{\pi} \int_0^{2\pi} f(\psi) \cos(n\psi) d\psi \quad n = 0, 1, 2, \cdots \\ b_n &= \frac{1}{\pi} \int_0^{2\pi} f(\psi) \sin(n\psi) d\psi \quad n = 1, 2, 3 \cdots \end{aligned} \tag{11}$$

Analytical problem on embed 2/2



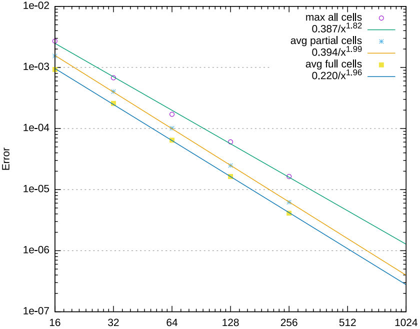


Figure 7: (Left) Analytical solution on 32x32 grid. (Right) Convergence study for norm L_∞ in green, and norm L_2 for all cells in blue and only partial in yellow.

Status of Robin BC

Done

- ✓ Works on the domain boundary
- ✓ Tested on embed in 2D
- ✓ Compatible with M.Tavares/J-M.Lopez Navier implemetation
- ✓ *robin* is exist now as a keyword in *Basilisk* like *dirichlet* or *neumann*. Let w a scalar field, the robin boundary condition is express as :

$$\alpha w + \beta \nabla w \cdot \mathbf{n} = \gamma \tag{12}$$

$$\text{The } \textit{Basilisk} \text{ syntax is : robin}(\alpha, \beta, \gamma) \tag{13}$$

To do

- ✗ Further test in 3D, parallel, and degenerate cases must be done
- ✗ A patch will be soon release

Solvers and Organisation

Outside *Basilisk*

Thermodynamic files

Transport files

KemKIN files

External programs

Canterra, FlameMaster, OpenSMOKE, etc

Kinetics files : *Basilisk* input

Solvers and Organisation

Basilisk

Low Mach approximation

Navier-Stokes solver with divergence source term

$$\nabla \cdot u = \dot{m}\frac{1}{\rho}\delta_\Gamma - \frac{1}{\rho}\frac{D\rho}{Dt}$$

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Advection-Diffusion

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \left[\rho \left(u Y_i - D_i \nabla Y_i\right)\right] = \omega_i + \omega_{i,s}$$

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Chemistry

Homogeneous

Heterogeneous

OpenSMOKE solver

Chemistry Roadmap

All credits to Edoardo Cipriano for the chemistry interface between OpenSMOKE and Basilisk.

Done

- ✓ Homogenous reaction with a diffusion problem + Robin boundary condition
- ✓ Adding the Stefan flow velocity at the interface

To do

- ✗ Coupling homogenous reactions and heterogenous one (current work)
- ✗ Solve temperature in the gas and at the interface
- ✗ Comparing with previous study (*Hassan et al, 2021*)

Conclusion

- ✓ A robin function added to Basilisk
- ✍ A better accuracy in the resolution of the boundary layer for solid particles simulation
- ✍ Toward an improvement in combustion for solid/gas interface in Basilisk
- ✍ A future generalisation of Robin/Navier in 3D, parallel, etc in the Basilisk framework.

Difficulties around the interface

Let's zoom around one interface cell and deal with the case of the temperature field:

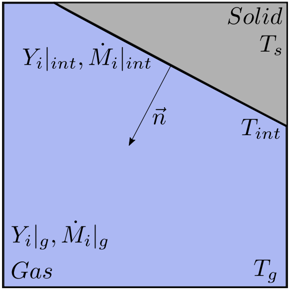

Figure 8: Zoom around the interface cell

The equation at the interface and inside the gas are coupled, to simplify we will solve the chemistry in the gas and at the interface separately. We also choose to not resolve in the solid particle.