

**Analytical solution for wall-bounded flow
with thermo-chemical ablation**

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Abstract

The steady, laminar two-dimensional analytical solution of a multicomponent compressible binary mixture flowing over a surface undergoing thermo-chemical ablation is presented. A special attention is given to the configuration set-up which allows to tackle the unsteady characteristic of surface recession. The idea consists in considering a channel problem in which a surface is the lieu of ablation process whereas the other one is the lieu of deposition. No specific assumption is made concerning the nature of the species involved in the problem. Within this framework, the density/velocity/concentration profiles are derived, and discussed for three particular cases.

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Analytical solutions of the compressible multicomponent Navier-Stokes equations is most of the time difficult to establish mainly because of the complex nature of the flow (due for instance to unsteady behavior, turbulence, chemical reactions or multicomponent transport properties), or because the boundary conditions of the problem can be geometrically and physically very difficult to integrate into the analytical solution. When the analytical solution is tractable, it can be used to better understand the physics and easily analyze the influence of some physical parameters onto the studied phenomena. Moreover, analytical solutions are of wide interest for experimentalists or computational fluid dynamics users to validate their experimental/numerical procedure.

For simple two-dimensional laminar flows it is sometimes possible to find the analytical solution of the system of partial differential equations that governs the physics. For instance, the well-know Poiseuille flow configuration allows to give the analytical velocity/temperature profiles under the assumption of streamwise-developed steady flow[1]. Introducing the transpiring surface effects, Koh and Hartnett[2] have shown that the analytical solution can also be recovered for flow over permeable wedges. Hamza[3] also presented the solution of channel flow with transpiring and moving walls for biomechanics-fluid interest. Concerning reacting wall effects, Rosner[4] introduced a set of solutions for surface catalyzed problems. Duan and Martín[5] also make use of an analytical solution for a diffusion-tube sidearm reactor in order to validate their numerical simulation of airflow over purely catalytic wall. To our knowledge, surface ablation has received little attention in the literature. Libby & Blake[6] developed an analytical solution for ablation but their case of study was purely diffusive : study of a carbon spherical particle interacting with a frozen flow.

The surface ablation problem can be seen as a combination between the transpiring surface and catalysis effects. Indeed, contrary to a catalytic wall, the ablative surface has an effect on the flow because the products of the heterogeneous reactions include atoms that were originally embedded in the wall lattice. As a consequence, the surface geometry is changed according to the reaction rates at the surface. This feature makes the derivation of the solution more challenging, especially when a steady state solution is sought for. As presented hereafter, the configuration set-up has to be properly thought to handle this undesirable effect.

To simply the derivation, one seeks for a solution that satisfies the following assumptions:

- two-dimensional laminar flow,
- steady state,
- channel flow developed in streamwise direction (periodic boundary conditions),
- non-reacting binary mixture,
- constant Schmidt numbers,
- pure ablation (no pyrolysis or sublimation of the wall material),
- isothermal ablated surface with finite reaction rates,
- constant pressure and temperature.

In such a configuration, a special attention must be given to the chemical scheme retained for the heterogeneous surface reactions. Indeed, if the same scheme is applied to the two surfaces, this leads to a flow that similarly behaves at the wall surfaces. This means that the two convective wall normal velocity vectors induced by surface ablation are pointing towards opposite directions. This translates into a mass increasing (or decreasing) configuration, not compatible with the steady state assumption. For this reason, one sets up a configuration in which one of the surface is the lieu of an oxidation scheme while the facing surface is the lieu of the reverse reaction. In others words, one of the surface is subjected to ablation whereas the other to deposition in such a way that the distance between the two surfaces remains constant.

The set-up retained is summarized in Fig. 1. The flow is supposed to evolved in a streamwise periodic channel between two plates separated by the distance h . The wall normal direction is referenced by the letter y whereas x is used for the streamwise direction. Making use of the assumption of steady developed non-reacting flow, one can write the multicomponent Navier-Stokes mass/species/momentum conservation equations as:

$$\frac{\partial(\rho v)}{\partial y} = 0 \quad (1)$$

$$\frac{\partial}{\partial y} (\rho (v + V_{k,y}) Y_k) = 0, \quad k \in \{1, 2\} \quad (2)$$

$$\frac{\partial(\rho uv)}{\partial y} = \frac{\partial \tau_{xy}}{\partial y} + \mathcal{S} \quad (3)$$

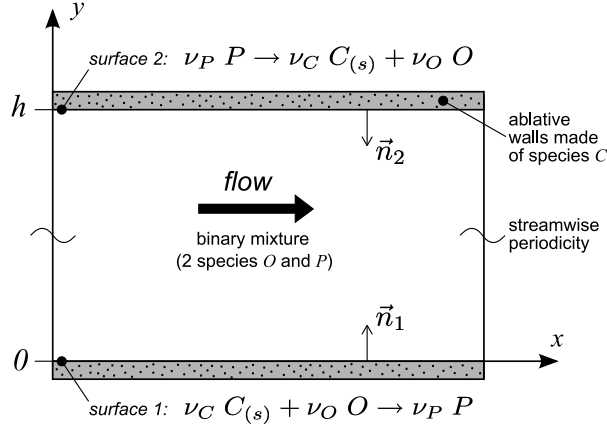


FIG. 1: Sketch of the configuration.

where ρ denotes the density, u the streamwise velocity component, v the wall normal velocity component, Y_k the mass fraction of species k , $V_{k,y}$ the wall normal diffusion velocity of species k , $\tau_{xy} = \mu du/dy$ the shear stress, and \mathcal{S} is the source term driving the flow. Note that this term must be added because the periodicity condition along x imposes $\partial p/\partial x = 0$. Note that the wall normal momentum conservation is not presented here because it does not give useful information to determine the solution. Also, the energy conservation equation does not appear since the temperature is supposed constant. Finally, the perfect gas equation of state is used to close the problem, which supposes that no real gas effects are considered:

$$\frac{p}{\rho} = \frac{R}{W}T \quad (4)$$

where R stands for the perfect gas constant and W the mean molecular weight of the mixture. The relation between W and Y_k is so that $1/W = \sum_k Y_k/W_k$, with W_k the atomic weight of species k . Equivalently, W can be expressed as a function of the molar fractions X_k , $W = \sum X_k W_k$. Under the conditions described in Fig. 1, one seeks for an analytical solution for the independent variables $\rho(y)$, $u(y)$, $v(y)$, $Y_k(y)$ (or equivalently $X_k(y)$) via the relation $X_k = Y_k W/W_k$.

In the following, the letter C , O and P denote the solid wall species (which could be for instance solid carbon), the gaseous oxidizing species and the gaseous species produced by ablation, respectively. The associated stoichiometric coefficients are noted ν_C , ν_O and ν_P . According to these notations, the following chemical schemes are applied to the surface 1 (lieu of ablation):



and to the surface 2 (lieu of deposition):



In what follows, variables subscripted by letters C , O and P refer to the associated species and subscript numbers 1 and 2 refer to space location, $y = 0$ and $y = h$, respectively. The molar progress rate of reaction 1, \mathcal{Q}_1 , can then be modeled as follows:

$$\mathcal{Q}_1 = \left(\frac{Y_{O,1}}{W_O} \rho_1 \right)^{\nu_O} K_1 = \left(X_{O,1} \frac{p}{RT} \right)^{\nu_O} K_1 \quad (7)$$

where K_1 represents the rate of reaction 1 which can be modeled by an Arrhenius law for instance. However, in the present framework it is not necessary to go deeper in the modeling of this coefficient because one assumes a constant temperature implying that K_1 can be merely seen as a parameter of the problem. Similarly, one can write the molar progress rate of reaction 2 as:

$$\mathcal{Q}_2 = \left(\frac{Y_{P,2}}{W_P} \rho_2 \right)^{\nu_P} K_2 = \left(X_{P,2} \frac{p}{RT} \right)^{\nu_P} K_2 \quad (8)$$

Moreover, the general formulation of species conservation balance at the reacting surfaces reads:

$$\left(\rho_j \vec{u}_j Y_{k,j} + \rho_j \vec{V}_{k,j} Y_{k,j} \right) \cdot \vec{n}_j = \dot{s}_{k,j} \quad (9)$$

where \vec{u}_j and $\vec{V}_{k,j}$ represent the convection and diffusion velocity vectors of species k estimated at surface j , \vec{n}_j is the unitary wall normal vector at surface j directed towards the gaseous domain (see Fig. 1), and $\dot{s}_{k,j}$ is the mass production rate of species k defined as $\dot{s}_{k,j} = \overline{\nu_{k,j}} W_k \mathcal{Q}_j$ with $\overline{\nu_{k,j}}$ the algebraic stoichiometric coefficient of species k at surface j (positive for produced species, negative for consumed species). Finally, the species conservation balance at surface 1 reads:

$$\rho_1 v_1 Y_{k,1} + \rho_1 V_{k,1} Y_{k,1} = \dot{s}_{k,1} \quad (10)$$

and at surface 2:

$$\rho_2 v_2 Y_{k,2} + \rho_2 V_{k,2} Y_{k,2} = -\dot{s}_{k,2} \quad (11)$$

Summing over all the species and making use of the mass conservation constraints $\sum_k Y_k = 1$ and $\sum_k Y_k V_k = 0$, one obtains the two relations $\rho_1 v_1 = \sum_k \dot{s}_{k,1}$ and $\rho_2 v_2 = -\sum_k \dot{s}_{k,2}$. Furthermore, the continuity equation (1) imposes that $\rho(y)v(y)$ is constant (in the forthcoming the notation $\dot{m} = \rho(y)v(y)$ will be used). As a consequence, one finds that

$\dot{m} = \sum_k \dot{s}_{k,1} = -\sum_k \dot{s}_{k,2}$ which leads to the relation $\mathcal{Q}_1 = \mathcal{Q}_2$ (the notation $\mathcal{Q} = \mathcal{Q}_j$ is thus retained for simplification). The two progress rates of the surface reactions are thus identical. The relation between the wall normal mass flow rate and the progress rate of reaction is thus expressed as:

$$\dot{m} = \mathcal{Q}(\nu_P W_P - \nu_O W_O) \quad (12)$$

When the species diffusion due to pressure gradients, temperature gradients (Soret effect) and volume forces are neglected, the binary diffusion between the two species O and P can be modeled by the classical relation[7] $V_k Y_k = -\mathcal{D}_{OP}^{\text{bin}} \partial Y_k / \partial y$, where $\mathcal{D}_{OP}^{\text{bin}} = \mathcal{D}_{PO}^{\text{bin}}$ is the binary diffusion coefficient. Another formulation is obtained by considering equivalent diffusion coefficients, D_k , that represents the diffusion of species k into the mixture and expressed as $D_k = (1 - Y_k) / (\sum_{l \neq k} X_l / \mathcal{D}_{kl}^{\text{bin}})$. This leads to an equivalent diffusion model which now involves the species molar fractions instead of their mass fractions, $V_k X_k = -D_k dX_k / dy$. One recalls here that when a binary mixture is considered, it is not necessary to include a correction velocity in the model to insure mass conservation[8]. This presents a strong advantage for solving the system of equations. Note also that contrary to the binary coefficient, D_k is depending on the local concentration of each species which means that $D_k = D_k(y)$. According to the previous definitions, the following relation stands for the present mixture:

$$D_O W_O = D_P W_P \quad (13)$$

Moreover, the dynamic viscosity for gases is usually assumed to be solely temperature dependent which means that in the present isothermal framework μ is a constant. Since the Schmidt numbers, $Sc_k = \mu / (\rho D_k)$, are assumed to be constant, we find that $\rho(y) D_k(y)$ is also constant. This statement allows to simplify the integration of the forthcoming partial differential equations.

In order to determine the species concentration profiles, one may concentrate on the variable X_O and to deduce the concentration of species P by the relation $X_P = 1 - X_O$. At this step, it is important to consider molar fractions instead of mass fractions because it leads to a first order partial differential equation with constant coefficients. Indeed, making use of Eq. (2), integrating once and identifying with Eq. (10), rearranging in terms of molar fractions, and making use of $\rho(y) D_O(y) = \mu / Sc_O$ yields:

$$\eta X_O - \frac{\mu}{Sc_O \dot{m}} \frac{dX_O}{dy} = \frac{\nu_O W_P}{\nu_O W_O - \nu_P W_P} \quad (14)$$

with

$$\eta = \frac{W_P (\nu_O - \nu_P)}{\nu_O W_O - \nu_P W_P} \quad (15)$$

Since $\eta = 0$ for $\nu_O = \nu_P$, the integration of this differential equation leads to two solutions depending on the values taken by ν_O and ν_P :

$$\begin{cases} X_O(y) = \left(X_{O,1} - \frac{\nu_O}{\nu_O - \nu_P} \right) \exp \left[\eta \frac{Sc_O \dot{m}}{\mu} y \right] + \frac{\nu_O}{\nu_O - \nu_P}, & \text{for } \nu_O \neq \nu_P \\ X_O(y) = - \frac{Sc_O \dot{m}}{\mu} \frac{W_P}{W_O - W_P} y + X_{O,1}, & \text{for } \nu_O = \nu_P \end{cases} \quad (16)$$

where $X_{O,1}$ is the molar fraction of species O at surface 1. The value of this constant is determined thanks to the relation between $X_{O,1}$ and $X_{O,2}$ that comes from the identity $\mathcal{Q}_1 = \mathcal{Q}_2$ which according to equations (7) and (8) gives:

$$X_{O,1}^{\nu_O} \left(\frac{p}{RT} \right)^{\nu_O - \nu_P} \frac{K_1}{K_2} = (1 - X_{O,2})^{\nu_P} \quad (17)$$

Furthermore, injecting Eq. (7) into the wall normal mass flow rate Eq. (12) yields the dependency relation between \dot{m} and $X_{O,1}$

$$\dot{m} = X_{O,1}^{\nu_O} \left(\frac{p}{RT} \right)^{\nu_O} K_1 (\nu_P W_P - \nu_O W_O) \quad (18)$$

Hence, Eq. (16) expressed for $y = h$ can be injected into Eq. (17), and with the use of Eq. (18) one obtains an equation in which $X_{O,1}$ is the only unknown. This manipulation allows to determine the $X_{O,1}$ constant and equations (15,16,17,18) form the analytical solution for the molar fraction of species O . The molar fraction of P is then given by the relation $X_P(y) = 1 - X_O(y)$.

Concerning the determination of the streamwise velocity profile, one introduces the newtonian fluid relation $\tau_{xy} = \mu du/dy$ into Eq. (3) which gives $\rho v du/dy - \mu d^2u/dy^2 = \mathcal{S}$. Since μ is a constant under the approximation of constant temperature, and because $\rho(y)v(y) = \dot{m}$ is a constant according to the continuity equation (1), the latter differential equation is merely of second order with constant coefficients. Its integration with the boundary conditions $u(0) = u(h) = 0$ leads to the following solution:

$$u(y) = \frac{\mathcal{S}}{\dot{m}} \left[\frac{h}{e^{\frac{\dot{m}}{\mu} h} - 1} \left(1 - e^{\frac{\dot{m}}{\mu} y} \right) + y \right] \quad (19)$$

where \dot{m} is determined with Eq. (18). It is interesting to precise that if \dot{m} tends to zero, the use of second-order Taylor series in Eq. (19) allows to demonstrate that the streamwise

velocity profile tends to the classical Poiseuille one, namely $u(y) = \mathcal{S}/(2\mu)(yh - y^2)$. Finally, the maximum streamwise velocity is expected to be observed at the wall normal distance:

$$y|_{u_{max}} = \frac{\mu}{\dot{m}} \ln \left[\frac{\mu}{h \dot{m}} \left(e^{\frac{\dot{m}}{\mu} h} - 1 \right) \right] \quad (20)$$

which differs from a classical Poiseuille profile for which the maximum velocity is observed at the channel half-height. This deviation is only due to the wall normal mass flow rate and non-sensitive to the driving pressure gradient. Note also that making use of Taylor series (for $\dot{m} \rightarrow 0$) it is easy to show that $y|_{u_{max}} \rightarrow h/2$.

The analytical solution formed by equations (4,15,16,17,18, and 19) is now discussed in a few particular cases. One investigates the three cases presented in Table I, for which $h = 10^{-3}m$, $p = 10^6 Pa$, $T = 2750K$, and $\mathcal{S} = 1000 Pa/m$. The transport coefficients are determined thanks to the EGLIB library[9]. Hence, the Schmidt numbers Sc_O and Sc_P satisfies Eq. (13), and the dynamic viscosity is set to $\mu = 8.012 \times 10^{-5} Pa \cdot s$ for cases 1 and 2, $\mu = 4.336 \times 10^{-5} Pa \cdot s$ for case 3. These three cases allow to investigate two types of oxidation schemes typically used when dealing with carbon material ablation[10]: oxidation by CO_2 species for cases 1 and 2 (corresponding to the solution $\nu_O \neq \nu_P$), and oxidation by H_2 species for case 3 (corresponding to the solution $\nu_O = \nu_P$). Cases 1 and 3 represent a solution for which the oxidation reaction is of infinite-rate type, which means that K_1 and K_2 tend to infinity. In this case the concentration of the oxidizing species is null at surface 1 and equals to unity at surface 2. On the contrary, case 2 represents a realistic case in which $K_1 = 0.5$ [MKS units] (corresponding to the order of magnitude given by the kinetics data by Chelliah *et al.*[10] for the present thermodynamic operating condition), and $K_2 = K_1/10^3$.

The results are presented in figure 2 for the wall normal velocity, streamwise velocity and the mass fraction of the oxidizing species. Comparing case 1 and 2, one notably observes that the streamwise velocity profile is a bit more displaced away from the centerline in case 1. This is because the activity of the surface reactions is stronger in the latter case, which leads to a higher mass rate ($\dot{m} = 2.6 \times 10^{-2} kg \cdot m^{-2} \cdot s^{-1}$ for case 1, $\dot{m} = 6.8 \times 10^{-3} kg \cdot m^{-2} \cdot s^{-1}$ for case 2). However, these values of \dot{m} are not strong enough to modify the streamwise velocity profiles significantly. As a result, these profiles are very close to the impermeable wall solution. On the contrary, the mass flow rate is $\dot{m} = 2.8 \times 10^{-1} kg \cdot m^{-2} \cdot s^{-1}$ for case 3 and the streamwise velocity profile is clearly non symmetric. In this case, the maximum

TABLE I: Parameters of the test cases.

case	O species	P species	ν_O	ν_P	Sc_O	Sc_P	K_1	K_2
1	CO_2	CO	1	2	0.92	0.59	$\rightarrow \infty$	$\rightarrow \infty$
2	CO_2	CO	1	2	0.92	0.59	0.5 [MKS units]	$K_1/10^3$
3	H_2	C_2H_2	0.5	0.5	0.14	1.82	$\rightarrow \infty$	$\rightarrow \infty$

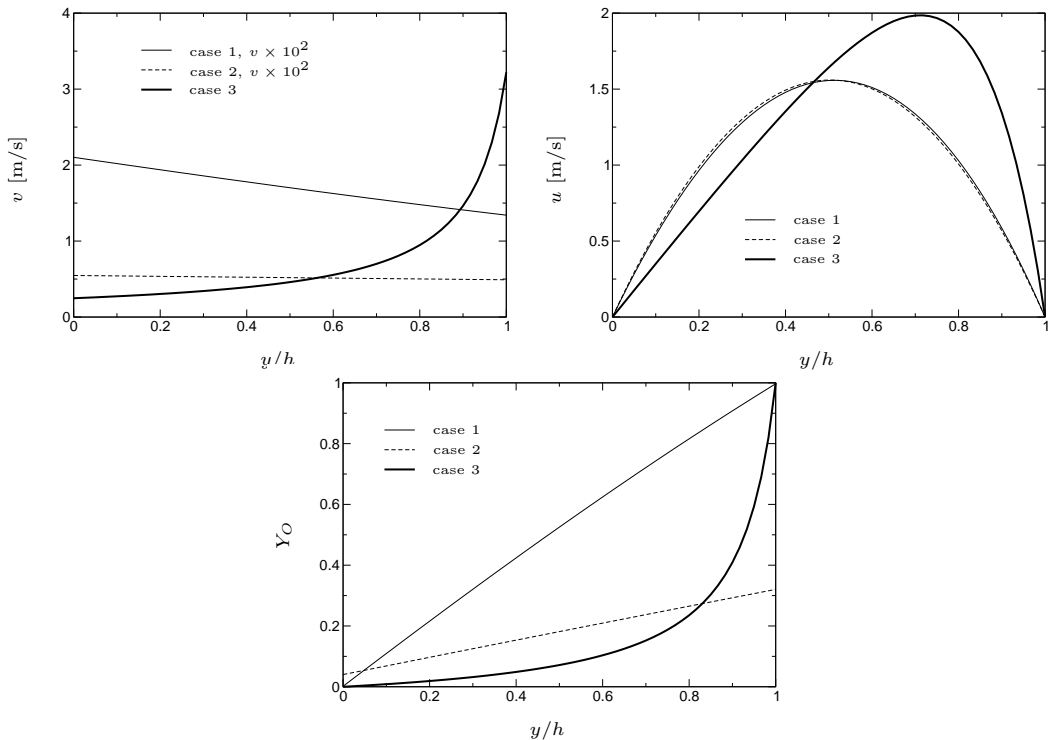


FIG. 2: Analytical solution plotted for three typical cases.

of velocity is observed at around $y/h = 0.71$ (in agreement with Eq. (20)) and the wall shear stress is strongly different at the two surfaces ($\tau_{w,2}/\tau_{w,1} = 5.2$ for case 3, against 1.1 and 1.02 for cases 1 and 2 respectively). Furthermore, the mass fraction profiles are no longer linear in case 3 because the difference between the species atomic weights is higher ($W_P/W_O = 0.63$ for cases 1 and 2, $W_P/W_O = 13$ for case 3). The diffusion process is then enhanced which leads to a different balance between convection and diffusion (see Eq. (2)). Of course, the wall normal velocity follows the same behavior since it is inversely proportional to the density variation (one recalls that the mass rate is constant) which is related to the species concentration variations.

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