



# Modelling forest fires. Part I: a complete set of equations derived by extended irreversible thermodynamics

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## Abstract

In this study we derive a three-dimensional forest fire combustion model. The forest is modelled as a diphasic medium composed of a gaseous and a porous vegetal pyrolysis phase. A formal averaging method and a thermodynamic closure by use of extended irreversible thermodynamics are used to give a complete set of coupled non-linear equations for this diphasic medium. This set of equations deals with the processes of drying, the pyrolysis of the vegetal phase, and the combustion of the pyrolysis gases in this gaseous phase. A three-dimensional reaction diffusion equation for the forest fire propagation with a non-local radiation term is then derived under some simplified hypotheses. © 2002 Elsevier Science Ltd. All rights reserved.

## 1. Introduction

Every year, about 750 thousand hectares of forest are burnt in northern America versus only 40 thousand hectares of forest in Europe which is comparatively low. This destruction represents a direct cost of 2 billion dollars a year in the USA. Simulation of forest fire propagation can serve several purposes. The prevision of the fire front can help firemen in optimising the distribution of fighting means, which supposes real time simulation. Another application of simulation relates to fire prevention. Using terrain data, computer models of propagation could provide information on dangerous areas. The possibility for such models to take into account some aspects of means of fire fighting, such as chemical retardants, should be highly desirable.

However currently the fire spreading simulators are far from being scientifically satisfactory. The reason is that forest fire is a complex large scale natural phenomenon that takes into account both the chemico-physical aspect of the combustion of the forest stratum that produces heat and the local meteorological forecast.

These two aspects are coupled together because wind activates fire and fire is a heat source that induces convection above the forest. The topography of the landscape has a great importance upon forest fire prevision as well. It is worthwhile noticing that a great part of the difficulty for modelling forest fires consists in describing the physical mechanisms taking place inside the vegetal stratum.

Rothermel's model [1] gives the fire heat source and the fire straight front velocity as analytical empirical laws for a uniform forest. The computation is very fast, but the empirical laws are usually obtained from laboratory experiments, not from real fire experiments, so the transposition is sometimes difficult. Complete forest fire physical models taking better account of physical mechanisms taking place inside the vegetal stratum have been proposed by Grishin [2] and Larini et al. [3]. These models are based upon global balance laws of mass energy and momentum. They consider the forest as a porous medium, composed of a gaseous phase and a vegetal phase, i.e. the wood, the stacks, the leaves, etc., in which transfer of mass, energy and momentum takes place. With the two physical models a great effort has been exerted for modelling combustion in the vegetation. The set of equations given in Grishin's model is postulated on both basic half scale experimental data and physical balance laws governing transfer in porous media. This model is closed and is adequate for the

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| Nomenclature                  |  | Subscripts                     |  |
|-------------------------------|--|--------------------------------|--|
| <i>Macroscopic quantities</i> |  | c                              | char   |
| $d$                           | occupation density (dimensionless)   | F                              | gaseous fuel   |
| $E$                           | internal energy (J kg <sup>-1</sup> )  | f                              | fluid phase in vegetal phase   |
| $\mathbf{F}^{jk}$             | momentum transfer from phase $j$ toward phase $k$ (kg m <sup>-2</sup> s <sup>-2</sup> )      | g                              | gas in porous phase  |
| $H$                           | internal enthalpy (J kg <sup>-1</sup> )  | $i$                            | $i$ th gas species   |
| $I$                           | radiative source term (W m <sup>-4</sup> sr <sup>-1</sup> )                                  | $j, k$                         | generic subscripts for gas in porous phase   |
| $\mathbf{J}$                  | flux of mass diffusion (kg m <sup>-2</sup> s <sup>-1</sup> )                                 | l                              | liquid (water)   |
| $K^{jk}$                      | internal mass transfer from phase $j$ toward phase $k$ (kg m <sup>-3</sup> s <sup>-1</sup> ) | O                              | oxygen   |
| $L$                           | spectral intensity (W m <sup>-3</sup> sr <sup>-1</sup> )                                     | p                              | porous phase (vegetal)   |
| $P$                           | pressure (Pa)  | R                              | residues of combustion   |
| $\mathbf{Q}$                  | heat flux (W m <sup>-2</sup> )   | r                              | radiation term   |
| $Q_i$                         | puissance produced by chemical reaction number $i$ (W kg <sup>-1</sup> )                     | s                              | mesoscopic solid phase (union of wood and char components)                                   |
| $R_c$                         | chemical reaction source term (W m <sup>-3</sup> )   | T                              | tar  |
| Sa                            | saturation of solid or fluid elements (dimensionless)  | v                              | vapour   |
| $T$                           | temperature (K)  | w                              | wood   |
| $\mathbf{V}$                  | intrinsic velocity (m s <sup>-1</sup> )  | –                              | variable under the vegetation layer  |
| $W$                           | molar mass (kg kmol <sup>-1</sup> )  | <i>Mesososcopic quantities</i> |  |
| $X^{jk}$                      | puissance transfer from phase $j$ toward phase $k$ (W m <sup>-3</sup> )                      | $e$                            | internal energy (J kg <sup>-1</sup> )  |
| $Y$                           | mass fraction (dimensionless)  | $h$                            | internal enthalpy (J kg <sup>-1</sup> )  |
| <i>Greek symbols</i>          |  | $\mathbf{f}_{jk}$              | momentum transfer from phase $j$ toward phase $k$ (kg m <sup>-2</sup> s <sup>-2</sup> )      |
| $\varepsilon^p$               | porosity of the wood as a porous medium (dimensionless)                                      | $\mathbf{j}$                   | flux of mass diffusion (kg m <sup>-2</sup> s <sup>-1</sup> )                                 |
| $\kappa$                      | permeability tensor (m <sup>2</sup> )  | $k_{jk}$                       | internal mass transfer from phase $j$ toward phase $k$ (kg m <sup>-3</sup> s <sup>-1</sup> ) |
| $\rho$                        | intrinsic mass density (kg m <sup>-3</sup> )   | $\mathbf{k}$                   | permeability tensor (m <sup>2</sup> )  |
| $\mathcal{S}$                 | total stress tensor (N m <sup>-2</sup> )   | $p$                            | pressure (Pa)  |
| $\mathcal{T}$                 | viscous stress tensor (N m <sup>-2</sup> )   | $\mathbf{q}$                   | heat flux (W m <sup>-2</sup> )   |
| $\Phi$                        | porosity of the vegetal combustible phase (dimensionless)                                    | Sa                             | saturation (dimensionless)   |
| $\psi$                        | rate of mole production (kmol m <sup>-3</sup> s <sup>-1</sup> )                              | $\mathbf{v}$                   | intrinsic velocity (m s <sup>-1</sup> )  |
| $\dot{\omega}_i$              | rate of mass production of the species number $i$ (kg m <sup>-3</sup> s <sup>-1</sup> )      | $y$                            | mass fraction (dimensionless)  |
| $\Omega$                      | space region   | $\varepsilon^p$                | porosity of the wood as a porous medium (dimensionless)                                      |
| <i>Superscripts</i>           |  | $\bar{\rho}$                   | intrinsic mass density (kg m <sup>-3</sup> )   |
| –                             | variable above the vegetation layer  | $\sigma$                       | total stress tensor (N m <sup>-2</sup> )   |
| ~                             | mesoscopic quantities  | $Y_{Ff}$                       | viscous stress tensor in the gaseous phase (N m <sup>-2</sup> )                              |
| ˆ                             | vegetal combustible phase extended functions   | $\dot{\omega}_i$               | rate of mass production of the species number $i$ (kg m <sup>-3</sup> s <sup>-1</sup> )      |

prediction of general forest fire propagation. The closure is obtained by physical intuition and experimental observations. Nevertheless, it is very difficult to derive physical laws from laboratory experiments such that the similarity conditions are satisfied. On the other hand, the model of Larini et al. is derived by use of the formal averaging method and the closure is obtained after some restrictive assumptions, for example that the gaseous

heat conduction is so that negligible, and invoking some empirical laws. Moreover, the derived set of equations is not closed because coupled small scale flow resolution is still needed.

It is therefore of interest to completely derive again a closed set of equations for the combustion inside the forest, as that of Grishin, by use of a general closing tool, i.e. by the derivation of a combustion model of

forest vegetation. We adapt Marle [4] general mathematical closing method. This closed set of equations deals with gaseous heat conduction and considers the porous character of the vegetal phase, i.e. of the wood, and pyrolysis gases convection into it so that this model should better take into account the mechanisms involved at branch scale, such as drying and pyrolysis, that the model of Larini does. To our best knowledge, macroscopic equations for such a porous medium, the solid part of which is a porous medium too, are not known so that we derive such an equivalent medium for the forest combustion by a general method of scale changing. We use extended irreversible thermodynamics because of the probable large size of the averaging volume. Let us recall that thermodynamics is qualified to be “extended” if there are differential fluxes in Gibbs relation [5]. Extended thermodynamics adds relaxation coefficients in phenomenological closure relations that become differential. We would like to get such relaxation coefficients in our macroscopic equations because they are suspected to be of importance in porous medium heat and mass transfers [6].

In Section 2 we will analyse the different scales of the system and the physical mechanisms involved at these scales. This is the first essential basic stage of modelling. The mesoscopic description of the vegetation is given too. In Section 3 we will derive the equations for the vegetal combustible phase from this mesoscopic set of equations by homogenisation tool and include discussion on the closure hypotheses. In Section 4 we will give the equations for above the forest, into the ground and interface conditions between the forest and above it. Then in Section 5 we will simplify the model, and obtain a reaction diffusion equation.

## 2. Analysis of the scales and mesoscopic description

### 2.1. Geometry and scales description of the forest fire

If we consider a small intensity developed fire, the range of fire sizes is several hundred meters to several kilometres. In this scale, that we call “gigascope” scale, the vegetation appears as a thin layer and the fire front is

a one-dimensional line moving along a two-dimensional surface and the fire interacts with the topography and meteorology.

The typical size of the forest structure description is the thickness of the vegetation layer or the height of the flames. In this scale, that we call “macroscopic” scale and denote  $l_f$ , we consider three regions (Fig. 1). The region above the vegetation, denoted by  $\bar{\Omega}$  and called “ambient air”, is composed of a gaseous phase. Tall flames can develop in this region. The quantities associated with this region will be overlined. The region under the vegetation, i.e. ground, is denoted by  $\underline{\Omega}$ . The quantities associated with this region will be underlined. The vegetation layer is finally denoted by  $\Omega$ .

The forest is stratified due to the different types of vegetation at different altitudes. For the sake of simplicity we will consider a forest with only one stratum and the ground will be considered as adiabatic. Horizontal heterogeneity of vegetation repartition may appear at the macroscopic scale if the vegetation layer is composed of a “vegetal combustible phase” (bushes) and a non-combustible one with no bushes (Fig. 2, macroscopic scale). “Occupation density”  $d$  characterises this repartition at gigascope scale. It is the proportion of area occupied by the vegetation. In this scale the fire interacts with the local wind into the vegetation layer. Interface balances between the vegetation stratum and the gas above must be used.

The vegetal combustible phase (called vegetal phase in the rest of the paper) must be modelled. It is considered as a macroscopic porous medium composed of the vegetation and of a gaseous component. The typical size of its structure description is the “mesoscopic” scale, denoted by  $l_v$  (Fig. 2). This is a diphasic medium composed of a “gaseous phase” or f phase with the index f (fluid), and of the “vegetation” or p phase with the index p (porous, we will see later that the vegetation is considered as a porous medium). The geometry of the p phase in the meso- to macroscopic elementary cell plays a prominent part in the energy exchange. Let  $V_f$  and  $V_p$  be the volumes of the f phase and of the p phase and  $V = V_f + V_p$  the volume of the elementary cell. In addition to the porosity  $\Phi = V_f/V$ , the ratio  $\sigma$  of the surface to the volume of the pieces of vegetation is of great

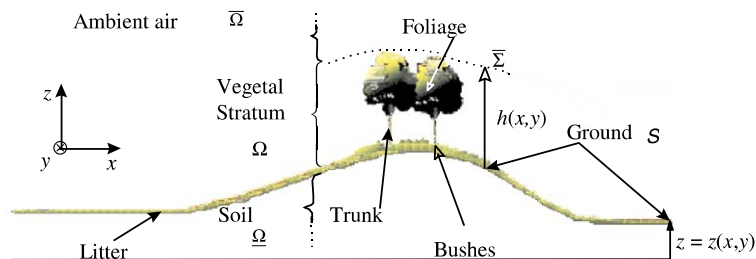


Fig. 1. Different forest regions.

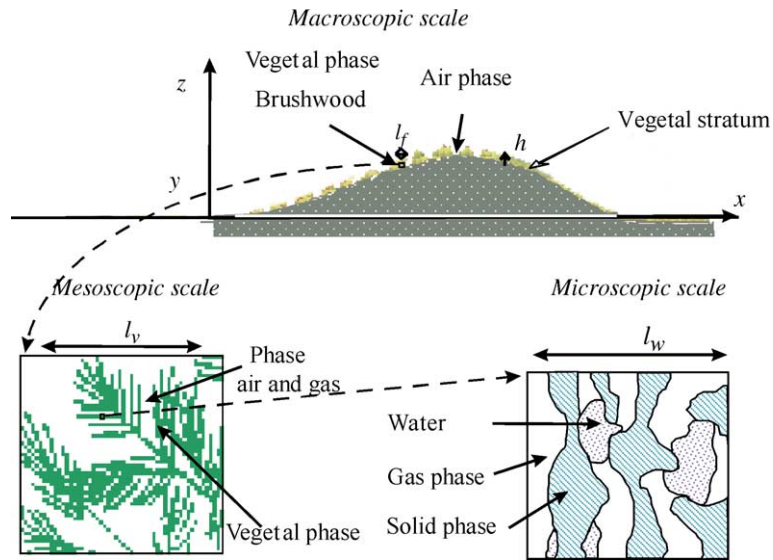


Fig. 2. Link between macroscopic, mesoscopic and microscopic scales.

importance. The greater the  $\sigma$ , the more the energy transfer that is increased between the solid and the faster the fire advances. If we compute the Reynolds number  $Re$ , with the pore size as length scale, we can estimate that  $38 < Re < 1900$ . These values are obtained for air at  $800\text{ }^\circ\text{C}$ , for a velocity of  $0.5\text{ m s}^{-1}$  and a characteristic length between  $10^{-2}$  and  $5 \times 10^{-1}\text{ m}$ . Therefore if the vegetation is very “compact” the flow, at the pore level, is not turbulent and the main reason for the oscillations of the velocity is the porous character of the forest medium.

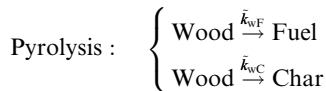
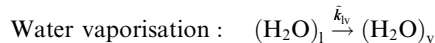
At the lowest level, that is in the microscopic scale, denoted by  $l_w$ , the p phase is a multiphasic medium itself. It is composed of three phases: the solid phase, the liquid phase, and a gaseous phase. The main physical effects involved at this scale are pyrolysis and drying. Di Blasi [7] has already given a mesoscopic model of such a vegetation medium so that we will use it and we will disregard the microscopic description in the following.

At virgin state, the solid component of the vegetation is made essentially of hemicellulose, cellulose, and lignin, the liquid component is water and the gaseous component is air. For the sake of simplicity we define the lumped “wood” species as: hemicellulose, cellulose, and lignin. Under heating, the vegetation dries firstly, and then the wood pyrolysis starts. This decomposition of wood modelling, i.e. pyrolysis modelling, was made tractable by defining the following mesoscopic lumped species [7]: “char”, “flammable gases”, and “tar”. Char is a carbon rich non-volatile pyrolysis residues, flammable gases are low molecular weight products that are gas phase species at room temperature, and tar is a high molecular weight product that is a vapour at pyrolysis

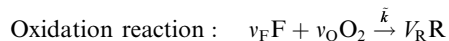
temperature but condenses near room temperature. They are secondary reactions which describe the tar decomposition into flammable gases and char. Thus the components of the vegetation or porous phase are:

1. the solids: wood indexed by w, char indexed by c;
2. the gases: air,  $(\text{H}_2\text{O})_v$ , flammable gases F or fuel, indexed by Fp and vp, respectively;
3. the liquid: water  $(\text{H}_2\text{O})_l$  indexed by lp.

For the sake of simplicity we neglect secondary reactions involving tar. Moreover, we assume that oxygen does not oxidise the wood inside the p phase (branches of vegetation). The chemical reactions which take place in the mesoscopic scale for the p phase are:



The components of the gaseous phase, or f phase, are (5 species numbered from 1 to 5): oxygen  $\text{O}_2$ , indexed by O, nitrogen  $\text{N}_2$  indexed by N; steam  $(\text{H}_2\text{O})_v$  indexed by vf (vapour in the fluid), flammable gases, i.e. fuel F indexed by Ff (fuel in the fluid) and combustion residue R indexed by Rf (residue in the fluid). There is no tar in the gaseous phase in our study because we have neglected its production in the vegetation. In the gaseous phase f oxidation of the flammable gases take place:



Let  $V_{w_p}$ ,  $V_{c_p}$ ,  $V_{g_p}$  and  $V_{f_p}$  be the volumes occupied, respectively, by the wood, the char, the gas and the

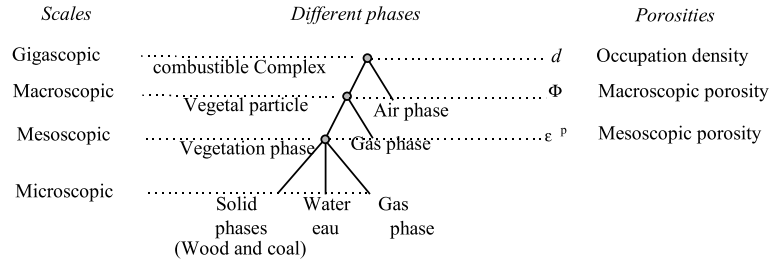


Fig. 3. Different scales and the associated phases and porosities.

liquid phases of the p phase. Then  $V_{sp} = V_{wp} + V_{cp}$ ,  $V_p = V_{gp} + V_{lp}$ , and  $V_p = V_{sp} + V_{fp}$  are the volumes occupied, respectively, by the solid, the fluid and the total part of the p phase. The porosity  $\epsilon^p$  of the p phase is defined by  $\epsilon^p = V_{fp}/V_p$ . The saturations of solid components of the p phase are  $Sa_{wp} = V_{wp}/V_{sp}$  for the wood and  $Sa_{cp} = V_{cp}/V_{sp}$  for the char component. Likewise the saturations of the fluid component are  $Sa_{gp} = V_{gp}/V_{fp}$  for the gas and  $Sa_{lp} = V_{lp}/V_{fp}$  for the liquid components.

The different scales, the different phases, the different porosities and their relationship are summarised in Fig. 3.

2.2. Mesoscopic system of equations for the different phases of the vegetation stratum

The mesoscopic set of equations for the f phase and the p phase will be described now. The mesoscopic jump conditions between these two phases will be given too. This set of equations is needed for the homogenisation of Section 3.

2.2.1. Inside the gaseous phase or f phase

Equations are the equations for the mixing of perfect gases, which are [8]:

- the balance of mass for species number  $i$

$$\frac{\partial}{\partial t} (\tilde{\rho}_f y_{if}) + \nabla \cdot (\tilde{\rho}_f y_{if} \mathbf{v}_f + \mathbf{j}_{if}) = \dot{\omega}_{if} \quad (1)$$

with  $\sum_i y_{if} = 1$ , and  $\sum_i \mathbf{j}_{if} = 0$ ,  $i = O_2, N_2, (H_2O)_v$ , fuel F and residue R,

- the balance of momentum

$$\frac{\partial}{\partial t} (\tilde{\rho}_f \mathbf{v}_f) + \nabla \cdot (\tilde{\rho}_f \mathbf{v}_f \otimes \mathbf{v}_f - \tau_f) = \tilde{\rho}_f \mathbf{g} - \nabla p_f, \quad (2)$$

- the balance of energy

$$\frac{\partial}{\partial t} \left( \tilde{\rho}_f \left( e_f + \frac{1}{2} \mathbf{v}_f^2 \right) \right) + \nabla \cdot \left( \tilde{\rho}_f \left( e_f + \frac{1}{2} \mathbf{v}_f^2 \right) \mathbf{v}_f + \mathbf{q}_f - \sigma_f \cdot \mathbf{v}_f \right) = \tilde{\rho}_f \mathbf{g} \cdot \mathbf{v}_f, \quad (3)$$

where  $\mathbf{g}$  is the gravity vector and the usual thermodynamic state equations.

2.2.2. Inside the vegetation or p phase

Di Blasi [7] has given a model of such a porous medium that we are going to use, taking into account diffusive transport of fluid species, water vaporisation and gravity. We use intrinsic density description. For example wood density  $\tilde{\rho}_{wp}$  is defined by  $\tilde{\rho}_{wp} = M_{wp}/V_{wp}$ , where  $M_{wp}$  is the mass of wood species inside the volume  $V_{wp}$ .

For the solid phase, the balances of mass for the wood and the char are

$$\frac{\partial}{\partial t} \left( (1 - \epsilon^p) Sa_{wp} \tilde{\rho}_{wp} \right) = -k_{wpFgp} - k_{wpcp} \quad (4)$$

and

$$\frac{\partial}{\partial t} \left( (1 - \epsilon^p) Sa_{cp} \tilde{\rho}_{cp} \right) = -k_{cpwp} \quad (5)$$

with  $Sa_{wp} + Sa_{cp} = 1$ . The  $k_{ij}$  are the internal mass transfers from species  $i$  to species  $j$  and  $k_{ij} = -k_{ji}$ . The union of these two solid phases will be indexed by  $s$  in the following.

For the gaseous constituents the balances of mass of the flammable gases and the water vapour are

$$\frac{\partial}{\partial t} \left( \epsilon^p Sa_{gp} \tilde{\rho}_{gp} y_{Fgp} \right) + \nabla \cdot \left( \epsilon^p Sa_{gp} \tilde{\rho}_{gp} y_{Fgp} \mathbf{v}_{gp} + \mathbf{j}_{Fgp} \right) = -k_{Fgpwp} \quad (6)$$

and

$$\frac{\partial}{\partial t} \left( \epsilon^p Sa_{gp} \tilde{\rho}_{gp} y_{vgp} \right) + \nabla \cdot \left( \epsilon^p Sa_{gp} \tilde{\rho}_{gp} y_{vgp} \mathbf{v}_{gp} + \mathbf{j}_{vgp} \right) = -k_{vgp1p} \quad (7)$$

with  $y_{Fgp} + y_{vgp} = 1$  and  $\mathbf{j}_{Fgp} + \mathbf{j}_{vgp} = 0$ , and the balance of mass of the liquid constituent is

$$\frac{\partial}{\partial t} \left( \epsilon^p Sa_{lp} \tilde{\rho}_{lp} y_{lp} \right) + \nabla \cdot \left( \epsilon^p Sa_{lp} \tilde{\rho}_{lp} y_{lp} \mathbf{v}_{lp} \right) = -k_{lpvgp} \quad (8)$$

with  $Sa_{gp} + Sa_{lp} = 1$ .

The p phase is a porous medium of small porosity  $\epsilon^p$ , so that there is no, strictly speaking, equation for the balance of momentum, in the gaseous and liquid constituents. Velocities are ruled by the Darcy law that we

write here in a balance form which is more adequate for the average procedure than the classical Darcy law form

$$\begin{aligned}\nabla\left(\varepsilon^p\text{Sa}_{g_p}p_{g_p}\right) &= \varepsilon^p\text{Sa}_{g_p}\tilde{\rho}_{g_p}\mathbf{g} - \mathbf{f}_{g_p s_p} - \mathbf{f}_{g_p l_p}, \\ \nabla\left(\varepsilon^p\text{Sa}_{l_p}p_{l_p}\right) &= \varepsilon^p\text{Sa}_{l_p}\tilde{\rho}_{l_p}\mathbf{g} - \mathbf{f}_{l_p s_p} - \mathbf{f}_{l_p g_p}\end{aligned}\quad (9)$$

with the momentum transfers  $\mathbf{f}_{g_p s_p}$  and  $\mathbf{f}_{g_p l_p}$ , respectively, from gas phases toward solid (wood and char) and liquid phases, and  $\mathbf{f}_{l_p s_p}$  and  $\mathbf{f}_{l_p g_p}$ , respectively, from liquid phases toward solid and gas phases, giving by the constitutive relations

$$\begin{aligned}\mathbf{v}_{g_p} &= -\frac{\mathbf{k}_{g_p}}{\left(\varepsilon^p\text{Sa}_{g_p}\right)^2\mu_{g_p}}\left(\mathbf{f}_{g_p s_p} + \mathbf{f}_{g_p l_p} + p_{g_p}\nabla\left(\varepsilon^p\text{Sa}_{g_p}\right)\right), \\ \mathbf{v}_{l_p} &= -\frac{\mathbf{k}_{l_p}}{\left(\varepsilon^p\text{Sa}_{l_p}\right)^2\mu_{l_p}}\left(\mathbf{f}_{l_p s_p} + \mathbf{f}_{l_p g_p} + p_{l_p}\nabla\left(\varepsilon^p\text{Sa}_{l_p}\right)\right)\end{aligned}$$

and the action reaction relation  $\mathbf{f}_{g_p l_p} + \mathbf{f}_{l_p g_p} + k_{l_p v_{g_p}}\mathbf{v}_{g_p} + k_{v_{g_p l_p}}\mathbf{v}_{l_p} = 0$ . The two tensors  $\mathbf{k}_{g_p}$  and  $\mathbf{k}_{l_p}$  are permeability tensors and  $\mathbf{v}_{g_p}$  and  $\mathbf{v}_{l_p}$  are the intrinsic mesoscopic velocities. Seepage velocities are  $\varepsilon^p\text{Sa}_{g_p}\mathbf{v}_{g_p}$  and  $\varepsilon^p\text{Sa}_{l_p}\mathbf{v}_{l_p}$ .

One can define the mass densities  $\tilde{\rho}_{s_p}$ ,  $\tilde{\rho}_{f_p}$  and  $\tilde{\rho}_p$  of the solid and fluid components and of the p phase by

$$\begin{aligned}\tilde{\rho}_{s_p} &= s_{w_p}\tilde{\rho}_{w_p} + s_{c_p}\tilde{\rho}_{c_p}, \\ \tilde{\rho}_{f_p} &= s_{g_p}\tilde{\rho}_{g_p} + s_{l_p}\tilde{\rho}_{l_p},\end{aligned}$$

and

$$\tilde{\rho}_p = \varepsilon^p\tilde{\rho}_{f_p} + (1 - \varepsilon^p)\tilde{\rho}_{s_p}.$$

The barycentric velocity  $\mathbf{v}_{f_p}$  of the p phase fluid component and the pressure  $p_{f_p}$  are defined by

$$\tilde{\rho}_{f_p}\mathbf{v}_{f_p} = s_{g_p}\tilde{\rho}_{g_p}\mathbf{v}_{g_p} + s_{l_p}\tilde{\rho}_{l_p}\mathbf{v}_{l_p}$$

and

$$p_{f_p} = s_{g_p}p_{g_p} + s_{l_p}p_{l_p}.$$

We have assumed in the preceding relations that the solid constituent is at rest. We can define the dissipating force  $\mathbf{f}_{f_p s_p}$  by  $\mathbf{f}_{f_p s_p} = \mathbf{f}_{g_p s_p} + \mathbf{f}_{l_p s_p}$  so that Eq. (9) leads to

$$\nabla\left(\varepsilon^p p_{f_p}\right) = \varepsilon^p\tilde{\rho}_{f_p}\mathbf{g} - \mathbf{f}_{f_p s_p}. \quad (10)$$

We can now write the following energy balance relation:

$$\begin{aligned}\frac{\partial}{\partial t}\left(\tilde{\rho}_p e_p\right) + \nabla\cdot\left(\varepsilon^p\tilde{\rho}_{f_p}e_{f_p}\mathbf{v}_{f_p} + \mathbf{q}_p + \varepsilon^p p_{f_p}\mathbf{v}_{f_p}\right) \\ - \varepsilon^p\tilde{\rho}_{f_p}\mathbf{v}_{f_p}\cdot\mathbf{g} = 0\end{aligned}\quad (11)$$

with mesoscopic p phase internal energy  $e_p$  defined by  $\tilde{\rho}_p e_p = \varepsilon^p\tilde{\rho}_{f_p}e_{f_p} + (1 - \varepsilon^p)\tilde{\rho}_{s_p}e_{s_p}$ .

$e_{f_p}$  and  $e_{s_p}$  are the internal energies of the p phase fluid and solid phases and  $\mathbf{q}_p$  is the p phase heat flux. The usual thermodynamic state equations are assumed to be valid. In particular,  $\tilde{\rho}_{w_p}$ ,  $\tilde{\rho}_{c_p}$ , and  $\tilde{\rho}_{l_p}$  are assumed to

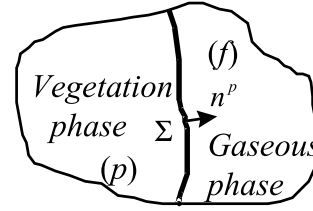


Fig. 4. The direction for the jump across the interface.

be constants and  $\tilde{\rho}_{g_p}$  is given by perfect gas state equation.

### 2.2.3. Jump conditions between the p phase and the gaseous phase

All the mesoscopic quantities can be considered as continuous, each one in its own phase, but there are jump conditions across the interface between the p phase and the gaseous phase. For a detailed derivation of such conditions, see [9,10]. Let us denote  $\mathbf{n}_p$ , the normal to  $\Sigma$  in the direction from p to f (Fig. 4), and  $\mathbf{w}_\Sigma$ , the velocity of the interface.

Of course  $\mathbf{n}_p = -\mathbf{n}_f$ , and the jump conditions can be written:

for the mass balance of the gaseous species number  $i$  ( $i = \text{F}, v, \text{O}_2, \text{N}_2$  and  $\text{R}$ ):

$$\begin{aligned}\left[\varepsilon^p\text{Sa}_{g_p}\tilde{\rho}_{g_p}y_{i g_p}\left(\mathbf{v}_{g_p} - \mathbf{w}_\Sigma\right) + \mathbf{j}_{i g_p}\right]\cdot\mathbf{n}_p \\ + \left[\tilde{\rho}_f y_{i f}\left(\mathbf{v}_f - \mathbf{w}_\Sigma\right) + \mathbf{j}_{i f}\right]\cdot\mathbf{n}_f = 0,\end{aligned}\quad (12)$$

We suppose here that no fluid water is flowing from the p phase.

for the balance of momentum:

$$-\varepsilon^p p_{f_p}\cdot\mathbf{n}_p + \left[\tilde{\rho}_f\left(\mathbf{v}_f - \mathbf{w}_\Sigma\right) \otimes \mathbf{v} + \sigma_f\right]\cdot\mathbf{n}_f = 0, \quad (13)$$

for the balance of energy, with the appropriate notations for the indices:

$$\begin{aligned}\left[\varepsilon^p\tilde{\rho}_{f_p}e_{f_p}\mathbf{v}_{f_p} + \mathbf{q}_p + \varepsilon^p p_{f_p}\mathbf{v}_{f_p} - \tilde{\rho}_p e_p \mathbf{w}_\Sigma\right]\cdot\mathbf{n}_p \\ + \left[\tilde{\rho}_f\left(e_f + \frac{1}{2}\mathbf{v}_f^2\right)\left(\mathbf{v}_f - \mathbf{w}_\Sigma\right) - \left(\mathbf{q}_f - \sigma_f\cdot\mathbf{v}_f\right)\right]\cdot\mathbf{n}_f \\ = 0.\end{aligned}\quad (14)$$

## 3. Averaging procedure and macroscopic vegetal phase equations

### 3.1. Average procedure choice

There are several methods for deriving the equations of an equivalent medium. One which is typically used in porous medium theory is the method of volume averaging [11,12]. We use here the one developed by Marle

[4] because it is the more simple general method that leads to a closed set of equations. The method can be summarised as follows:

1. Describe the mesoscopic system of balance equations for the bulk phases and the interface jump conditions between these phases.
2. Use distribution theory for writing the equations, so that interface jump conditions and bulk phase equations are not separated.
3. Take the average by convolution of the equations with a kernel with compact support and choose macroscopic quantity definitions. At this step, we get more macroscopic quantities than macroscopic balance equations.
4. Close the system of equations using a thermodynamic second principle.

The main difference between this study and Marle's one is the use of extended irreversible thermodynamics in place of irreversible thermodynamics.

### 3.2. Averaging procedure and definition of the macroscopic quantities

The quantities involved in the preceding equations are defined only on subdomains of the vegetal phase. Before averaging them, let us extend these functions to all spaces of the vegetal phase, setting their values equal to 0 outside their definition domain. These new extended functions are denoted by superscript  $\hat{\cdot}$ . For example, the mass density  $\hat{\rho}_{ep}$  of gas in the p phase is extended to  $\hat{\rho}_{ep} = \tilde{\rho}_{ep}$  inside the p phase and to  $\hat{\rho}_{ep} = 0$  outside. These new functions have derivatives which are no longer functions but are distributions. We consider the following equations relating the different derivatives:

$$\nabla \hat{f} = \nabla \tilde{f} + \tilde{f} \mathbf{n}_a \delta_{\Sigma_a},$$

$$\nabla \cdot \hat{\mathbf{f}} = \nabla \cdot \tilde{\mathbf{f}} + \tilde{\mathbf{f}} \cdot \mathbf{n}_a \delta_{\Sigma_a},$$

$$\frac{\partial}{\partial t} \hat{f} = \frac{\partial}{\partial t} \tilde{f} - \tilde{f} \mathbf{w}_{\Sigma_a} \cdot \mathbf{n}_a \delta_{\Sigma_a},$$

where  $\Sigma_a$  is the boundary of the definition domain of  $\tilde{f}$  or  $\tilde{\mathbf{f}}$ ,  $\mathbf{w}_{\Sigma_a}$  is the velocity of the interface, and  $\delta_{\Sigma_a}$  is the Dirac measure on  $\Sigma_a$ . We can write the system of Eqs. (1)–(11) with the extended quantities, so that Eq. (1), for example, becomes

$$\begin{aligned} \frac{\partial}{\partial t} (\hat{\rho}_f \hat{y}_{if}) + \nabla \cdot (\hat{\rho}_f \hat{y}_{if} \hat{\mathbf{v}}_f + \hat{\mathbf{j}}_{if}) \\ = \hat{\omega}_{if} + [\hat{\rho}_f \hat{y}_{if} (\hat{\mathbf{v}}_f - \mathbf{w}_{\Sigma_p}) + \hat{\mathbf{j}}_{if}] \cdot \mathbf{n}_f \delta_{\Sigma_p}. \end{aligned} \quad (15)$$

Therefore the new system of equations incorporates the boundary conditions. To proceed to the averaging of equations we must consider a function  $m(\mathbf{x})$ , positive with a compact support, indefinitely derivable and such that

$$\int m(\mathbf{x}) d\mathbf{x} = 1.$$

The function

$$m(\mathbf{x}) = \begin{cases} C \exp -(1 - (|\mathbf{x}|/r)^2)^{-1} & \text{if } |\mathbf{x}|/r < 1, \\ 0 & \text{if } |\mathbf{x}|/r \geq 1 \end{cases}$$

is a good candidate. The radius  $r$  must be of the size of the elementary representative volume, and represents the size of the macroscopic particle. The average value  $G(\mathbf{x}, t)$  of a quantity  $g$  is then obtained by taking the convolution product of  $g$  and  $m$ :

$$G(\mathbf{x}, t) = (g * m)(\mathbf{x}, t) = \int g(\mathbf{y}, t) m(\mathbf{x} - \mathbf{y}) d\mathbf{y}.$$

Whatever the smoothness of  $g$  the average value  $G$  is as smooth as the kernel  $m$ .

Let us consider  $\chi_p(\mathbf{x}, t)$  and  $\chi_f(\mathbf{x}, t)$  as the characteristic functions for each phase. The porosity  $\Phi$  can be written as

$$\Phi = \chi_f * m. \quad (16)$$

Now all Eqs. (1)–(11) are written as Eq. (15) and we take the convolution product with the kernel  $m$ , Eq. (1) gives, for example,

$$\frac{\partial}{\partial t} (\Phi \rho_f Y_{if}) + \nabla \cdot (\Phi \rho_f Y_{if} \mathbf{V}_f + \mathbf{J}_{if}) = \Phi \dot{\omega}_{if} - K_i^{fp} \quad (17)$$

and the following macroscopic quantities (between brackets) are defined:

$$\Phi[\rho_f] = \hat{\rho}_f * m,$$

$$\Phi \rho_f[\mathbf{V}_f] = \hat{\rho}_f \hat{\mathbf{v}}_f * m,$$

$$\Phi \rho_f[Y_{if}] = \hat{\rho}_f \hat{y}_{if} * m,$$

$$\Phi \rho_f Y_{if} \mathbf{V}_f + [\mathbf{J}_{if}] = (\hat{\rho}_f \hat{y}_{if} \hat{\mathbf{v}}_f + \hat{\mathbf{j}}_{if}) * m,$$

$$\Phi[\dot{\omega}_{if}] = \hat{\omega}_{if} * m,$$

$$[K_i^{fp}] = (\hat{\rho}_f \hat{y}_{if} (\hat{\mathbf{v}}_f - \mathbf{w}_{\Sigma_f}) \cdot \mathbf{n}_{\Sigma_f} \delta_{\Sigma_f}) * m.$$

The term  $K_i^{fp}$  represents the rate of mass transfer of the species number  $i$  from phase f to phase p. The total mass transfer is  $K^{fp} = \sum_i K_i^{fp}$ . Note that the macroscopic diffusion  $\mathbf{J}_{if}$  is by no means the average of the mesoscopic diffusion  $\hat{\mathbf{j}}_{if}$ .

From the balance of momentum equation (2), we obtain

$$\begin{aligned} \frac{\partial}{\partial t} (\Phi \rho_f \mathbf{V}_f) + \nabla \cdot (\Phi \rho_f \mathbf{V}_f \otimes \mathbf{V}_f - \mathcal{S}_f) \\ = \Phi \rho_f \mathbf{g} - K^{fp} \mathbf{V}_f - \mathbf{F}^{fp}. \end{aligned} \quad (18)$$

with the following definitions for macroscopic quantities:

$$\Phi \rho_f \mathbf{V}_f \otimes \mathbf{V}_f - [\mathcal{S}_f] = \left( \widehat{\rho}_f \widehat{\mathbf{v}}_f \otimes \widehat{\mathbf{v}}_f - \widehat{\sigma}_f \right) * m,$$

$$K^{\text{fp}} \mathbf{V}_f + [\mathbf{F}^{\text{fp}}] = \left( \widehat{\rho}_f \widehat{\mathbf{v}}_f (\widehat{\mathbf{v}}_f - \mathbf{w}_{\Sigma_f}) - \widehat{\sigma}_f \right) \cdot \mathbf{n}_{\Sigma_f} \delta_{\Sigma_f} * m.$$

For the balance of energy equation (3), we get

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \Phi \rho_f \left( E_f + \frac{1}{2} \mathbf{V}_f^2 \right) \right) \\ & + \nabla \cdot \left( \Phi \rho_f \left( E_f + \frac{1}{2} \mathbf{V}_f^2 \right) \mathbf{V}_f + \mathbf{Q}_f - \mathcal{S}_f \cdot \mathbf{V}_f \right) \\ & = \Phi \rho_f \mathbf{g} \cdot \mathbf{V}_f - P_f \frac{\partial \Phi}{\partial t} - \left( E_f + \frac{1}{2} \mathbf{V}_f^2 + \frac{P_f}{\rho_f} \right) K^{\text{fp}} - X^{\text{fp}} \end{aligned} \quad (19)$$

with

$$\begin{aligned} \Phi \rho_f \left( [E_f] + \frac{1}{2} \mathbf{V}_f^2 \right) &= \widehat{\rho}_f \left( \widehat{e}_f + \frac{1}{2} \widehat{\mathbf{v}}_f^2 \right) * m, \\ \Phi \rho_f \left( E_f + \frac{1}{2} \mathbf{V}_f^2 \right) \mathbf{V}_f + [\mathbf{Q}_f] - \mathcal{S}_f \cdot \mathbf{V}_f &= \left( \widehat{\rho}_f \left( \widehat{e}_f + \frac{1}{2} \widehat{\mathbf{v}}_f^2 \right) \widehat{\mathbf{v}}_f + \widehat{\mathbf{q}}_f - \widehat{\sigma}_f \cdot \widehat{\mathbf{v}}_f \right) * m, \\ \left( E_f + \frac{1}{2} \mathbf{V}_f^2 + \frac{P_f}{\rho_f} \right) K^{\text{fp}} + P_f \frac{\partial \Phi}{\partial t} + [X^{\text{fp}}] &= \left( \left[ \widehat{\rho}_f \left( \widehat{e}_f + \frac{P_f}{\rho_f} + \frac{1}{2} \widehat{\mathbf{v}}_f^2 \right) (\widehat{\mathbf{v}}_f - \mathbf{w}_{\Sigma_f}) + \widehat{\mathbf{q}}_f - \widehat{\sigma}_f \cdot \widehat{\mathbf{v}}_f \right. \right. \\ & \left. \left. + \widehat{p}_f \mathbf{w}_{\Sigma_f} \right] \cdot \mathbf{n}_{\Sigma_f} \delta_{\Sigma_f} \right) * m. \end{aligned}$$

The pressure and the temperature have yet not been defined. We define these quantities in such a way that the macroscopic thermodynamic relations have the usual expressions, i.e.:

for the energy:

$$E_f = \sum_i H_{if} Y_{if} - \frac{P_f}{\rho_f}, \quad (20)$$

for the enthalpies:

$$H_{if} = H_{if}^0 + \int_{T_0}^{T_f} C_{p,if} dT, \quad (21)$$

for the pressure:

$$P_f = \rho_f R T_f \sum_i Y_{if} / W_i. \quad (22)$$

In the same way, we define the macroscopic quantities of the p phase. The macroscopic porosity  $\mathcal{E}^p$  is defined by

$$(1 - \Phi) [\mathcal{E}^p] = \widehat{\varepsilon}^p * m.$$

By the procedure of averaging and convolution, Eq. (4) gives

$$\begin{aligned} & \frac{\partial}{\partial t} \left( (1 - \Phi) (1 - \mathcal{E}^p) \text{Sa}_{w_p} \rho_{w_p} \right) \\ & = -(1 - \Phi) \left( K_{w_p, F_{gp}} + K_{w_p, c_p} \right) \end{aligned} \quad (23)$$

with the following definitions:

macroscopic saturation of the wood

$$(1 - \Phi) (1 - \mathcal{E}^p) [\text{Sa}_{w_p}] = (1 - \widehat{\varepsilon}^p) \widehat{\text{Sa}}_{w_p} * m,$$

macroscopic wood mass density

$$(1 - \Phi) (1 - \mathcal{E}^p) \text{Sa}_{w_p} [\rho_{w_p}] = (1 - \widehat{\varepsilon}^p) \widehat{\text{Sa}}_{w_p} \widehat{\rho}_{w_p} * m,$$

macroscopic mass transfers

$$\begin{aligned} (1 - \Phi) K_{w_p, F_{gp}} &= \left( k_{w_p, F_{gp}} - (1 - \widehat{\varepsilon}^p) \widehat{\text{Sa}}_{w_p} \widehat{\rho}_{w_p} \mathbf{w}_{\Sigma_w} \cdot \mathbf{n}_{\Sigma_w} \delta_{\Sigma_w} \right) * m, \\ (1 - \Phi) K_{w_p, c_p} &= \widehat{k}_{w_p, c_p} * m. \end{aligned}$$

Whilst the mesoscopic mass transfer follows an Arrhenius law such that  $k_{w_p, F_{gp}} = A(\theta_p) e^{-E_w/R\theta_p}$ , where  $\theta_p$  is the mesoscopic temperature, the macroscopic temperature is not the average of the mesoscopic temperature and therefore the macroscopic mass transfer does not follow, a priori, such a law. As for the phase f, the macroscopic temperature is not yet defined. Eq. (5) gives

$$\frac{\partial}{\partial t} \left( (1 - \Phi) (1 - \mathcal{E}^p) \text{Sa}_{c_p} \rho_{c_p} \right) = -(1 - \Phi) K_{c_p, w_p}, \quad (24)$$

the macroscopic saturation of the char is defined by

$$(1 - \Phi) (1 - \mathcal{E}^p) [\text{Sa}_{c_p}] = (1 - \widehat{\varepsilon}^p) \widehat{\text{Sa}}_{c_p} * m,$$

the macroscopic density

$$(1 - \Phi) (1 - \mathcal{E}^p) \text{Sa}_{c_p} [\rho_{c_p}] = (1 - \widehat{\varepsilon}^p) \widehat{\text{Sa}}_{c_p} \widehat{\rho}_{c_p} * m,$$

and the mass transfers

$$(1 - \Phi) K_{c_p, w_p} = \left( k_{c_p, w_p} - (1 - \widehat{\varepsilon}^p) \widehat{\text{Sa}}_{c_p} \widehat{\rho}_{c_p} \mathbf{w}_{\Sigma_c} \cdot \mathbf{n}_{\Sigma_c} \delta_{\Sigma_c} \right) * m.$$

In the liquid constituent, we obtain

$$\begin{aligned} & \frac{\partial}{\partial t} \left( (1 - \Phi) \mathcal{E}^p \text{Sa}_{l_p} \rho_{l_p} \right) + \nabla \cdot \left( (1 - \Phi) \mathcal{E}^p \text{Sa}_{l_p} \rho_{l_p} \mathbf{V}_{l_p} \right) \\ & = -(1 - \Phi) K_{l_p, v_{gp}}, \end{aligned} \quad (25)$$

with the saturation defined by

$$(1 - \Phi) \mathcal{E}^p [\text{Sa}_{l_p}] = \widehat{\varepsilon}^p \widehat{\text{Sa}}_{l_p} * m,$$

the mass density

$$(1 - \Phi) \mathcal{E}^p \text{Sa}_{l_p} [\rho_{l_p}] = \widehat{\varepsilon}^p \widehat{\text{Sa}}_{l_p} \widehat{\rho}_{l_p} * m,$$



the velocity

$$(1 - \Phi)\mathcal{E}^p \text{Sa}_{l_p} \rho_{l_p} [\mathbf{V}_{l_p}] = \widehat{\varepsilon}^p \widehat{\text{Sa}}_{l_p} \widehat{\rho}_{l_p} \widehat{\mathbf{v}}_{l_p} * m,$$

the mass transfer

$$(1 - \Phi)K_{l_p v_{g_p}} \\ = \left( \widehat{k}_{l_p v_{g_p}} - \widehat{\varepsilon}^p \widehat{\text{Sa}}_{l_p} \widehat{\rho}_{l_p} \left( \widehat{\mathbf{v}}_{l_p} - \mathbf{w}_{\Sigma_l} \right) \cdot \mathbf{n}_{\Sigma_l} \delta_{\Sigma_l} \right) * m.$$

We now consider the gaseous constituent, the saturation is defined by

$$(1 - \Phi)\mathcal{E}^p [\text{Sa}_{g_p}] = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{g_p} \right) * m$$

its mass density  $\rho_{g_p}$  is defined by

$$(1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} [\rho_{g_p}] = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{g_p} \widehat{\rho}_{g_p} \right) * m,$$

its velocity by

$$(1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} \rho_{g_p} [\mathbf{V}_{g_p}] = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{g_p} \widehat{\rho}_{g_p} \widehat{\mathbf{v}}_{g_p} \right) * m,$$

the mass fractions  $Y_{i_{g_p}}$  by

$$(1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} \rho_{g_p} [Y_{i_{g_p}}] = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{g_p} \widehat{\rho}_{g_p} \widehat{y}_{i_{g_p}} \right) * m,$$

and the macroscopic mass diffusion by

$$(1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} \rho_{g_p} Y_{i_{g_p}} \mathbf{V}_{g_p} + [\mathbf{J}_{i_{g_p}}] \\ = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{g_p} \widehat{\rho}_{g_p} \widehat{y}_{i_{g_p}} \widehat{\mathbf{v}}_{g_p} + \widehat{\mathbf{j}}_{i_{g_p}} \right) * m,$$

so that Eqs. (6) and (7) become

$$\frac{\partial}{\partial t} \left( (1 - \Phi)\mathcal{E}^p S_{g_p} \rho_{g_p} Y_{F_{g_p}} \right) \\ + \nabla \cdot \left( (1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} \rho_{g_p} Y_{F_{g_p}} \mathbf{V}_{g_p} + \mathbf{J}_{F_{g_p}} \right) \\ = -(1 - \Phi)K_{F_{g_p} w_p} - K_{F_{g_p}}^{pf}, \quad (26a)$$

$$\frac{\partial}{\partial t} \left( (1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} \rho_{g_p} Y_{v_{g_p}} \right) \\ + \nabla \cdot \left( (1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} \rho_{g_p} Y_{v_{g_p}} \mathbf{V}_{g_p} + \mathbf{J}_{v_{g_p}} \right) \\ = -(1 - \Phi)K_{v_{g_p} l_p} - K_{v_{g_p}}^{pf}. \quad (26b)$$

The mass transfers are defined by

$$(1 - \Phi)K_{F_{g_p} w_p} = \widehat{k}_{F_{g_p} w_p} * m,$$

$$(1 - \Phi)K_{v_{g_p} l_p} = \widehat{k}_{v_{g_p} l_p} * m,$$

$$K_i^{pf} = \left( \left[ \widehat{\varepsilon}^p \widehat{\text{Sa}}_{g_p} \widehat{\rho}_{g_p} \widehat{y}_{i_{g_p}} \left( \widehat{\mathbf{v}}_{g_p} - \mathbf{w}_{\Sigma_{g_p}} \right) \right. \right. \\ \left. \left. + \widehat{\mathbf{j}}_{i_{g_p}} \right] \cdot \mathbf{n}_{\Sigma_{g_p}} \delta_{\Sigma_{g_p}} \right) * m.$$

The total transfer of gas from phase p to phase f is  $K_g^{pf} = K_{F_{g_p}}^{pf} + K_{v_{g_p}}^{pf}$ . The total mass density of phase p and the barycentric velocity are defined by

$$\rho_p = \mathcal{E}^p \rho_{f_p} + (1 - \mathcal{E}^p) \rho_{s_p}, \quad (27) \\ \rho_{f_p} \mathbf{V}_{f_p} = \text{Sa}_{g_p} \rho_{g_p} \mathbf{V}_{g_p} + \text{Sa}_{l_p} \rho_{l_p} \mathbf{V}_{l_p}$$

with  $\rho_{f_p} = \text{Sa}_{g_p} \rho_{g_p} + \text{Sa}_{l_p} \rho_{l_p}$  and  $\rho_{s_p} = \text{Sa}_{w_p} \rho_{w_p} + \text{Sa}_{c_p} \rho_{c_p}$ . Darcy laws in Eq. (9) become

$$\nabla \cdot \left( (1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} P_{g_p} \right) - (1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} \rho_{g_p} \mathbf{g} \\ + \mathbf{F}_{g_p l_p} + \mathbf{F}_{g_p s_p} + \mathbf{F}_{g_p}^{pf} = 0, \quad (28) \\ \nabla \cdot \left( (1 - \Phi)\mathcal{E}^p \text{Sa}_{l_p} P_{l_p} \right) - (1 - \Phi)\mathcal{E}^p \text{Sa}_{l_p} \rho_{l_p} \mathbf{g} \\ + \mathbf{F}_{l_p g_p} + \mathbf{F}_{l_p s_p} + \mathbf{F}_{l_p}^{pf} = 0$$

with the following definitions:

$$(1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p} P_{g_p} = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{g_p} \widehat{p}_{g_p} \right) * m,$$

$$\mathbf{F}_{g_p s_p} = \widehat{\mathbf{f}}_{g_p s_p} * m,$$

$$(1 - \Phi)\mathcal{E}^p \text{Sa}_{l_p} P_{l_p} = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{l_p} \widehat{p}_{l_p} \right) * m,$$

$$\mathbf{F}_{l_p s_p} = \widehat{\mathbf{f}}_{l_p s_p} * m,$$

$$K_{v_{g_p} l_p} \mathbf{V}_{g_p} + \mathbf{F}_{g_p l_p} = \left( \widehat{k}_{v_{g_p} l_p} \widehat{\mathbf{v}}_{g_p} + \widehat{\mathbf{f}}_{g_p l_p} \right) * m,$$

$$\mathbf{F}_{g_p}^{pf} = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{g_p} \widehat{\rho}_{g_p} \mathbf{n}_{\Sigma_{g_p}} \delta_{\Sigma_{g_p}} \right) * m,$$

$$K_{l_p v_{g_p}} \mathbf{V}_{l_p} + \mathbf{F}_{l_p g_p} = \left( \widehat{k}_{l_p v_{g_p}} \widehat{\mathbf{v}}_{l_p} + \widehat{\mathbf{f}}_{l_p g_p} \right) * m,$$

$$\mathbf{F}_{l_p}^{pf} = \left( \widehat{\varepsilon}^p \widehat{\text{Sa}}_{l_p} \widehat{p}_{l_p} \mathbf{n}_{\Sigma_{l_p}} \delta_{\Sigma_{l_p}} \right) * m.$$

We have  $\mathbf{F}_{l_p g_p} + \mathbf{F}_{g_p l_p} + K_{v_{g_p} l_p} \mathbf{V}_{g_p} + K_{l_p v_{g_p}} \mathbf{V}_{l_p} = 0$ .

Equations set (28) will provide the following equation:

$$\nabla \cdot \left( (1 - \Phi)\mathcal{E}^p P_{f_p} \right) - (1 - \Phi)\mathcal{E}^p \rho_{f_p} \mathbf{g} + \mathbf{F}_{g_p s_p} \\ + \mathbf{F}_{l_p s_p} + \mathbf{F}_{g_p}^{pf} + \mathbf{F}_{l_p}^{pf} = 0 \quad (29)$$

with

$$P_{f_p} = \text{Sa}_{g_p} P_{g_p} + \text{Sa}_{l_p} P_{l_p}. \quad (30)$$

The energy balance Eq. (11) can be written as

$$\frac{\partial}{\partial t} \left( (1 - \Phi)\rho_p E_p \right) + \nabla \cdot \left( (1 - \Phi)\rho_{f_p} E_{f_p} \mathbf{V}_{f_p} + \mathbf{Q}_p \right) \\ + \nabla \cdot \left( (1 - \Phi)\mathcal{E}^p \left( \text{Sa}_{g_p} P_{g_p} \mathbf{V}_{g_p} + \text{Sa}_{l_p} P_{l_p} \mathbf{V}_{l_p} \right) \right) \\ = -P_{g_p} \frac{\partial (1 - \Phi)\mathcal{E}^p \text{Sa}_{g_p}}{\partial t} - P_{l_p} \frac{\partial (1 - \Phi)\mathcal{E}^p \text{Sa}_{l_p}}{\partial t} \\ - \frac{P_{g_p}}{\rho_{g_p}} K_{g_p l_p} - \frac{P_{l_p}}{\rho_{l_p}} K_{l_p v_{g_p}} - E_p K^{pf} \\ - (1 - \Phi)\rho_{f_p} \mathbf{V}_{f_p} \cdot \mathbf{g} - X^{pf} \quad (31)$$

with the following definitions:

$$\begin{aligned} \mathcal{E}^p \rho_{f_p} [E_{f_p}] &= \left( \widehat{\varepsilon}^p \widehat{\rho}_{f_p} \widehat{e}_{f_p} \right) * m, \\ (1 - \mathcal{E}^p) \rho_{s_p} [E_{s_p}] &= \left( (1 - \widehat{\varepsilon}^p) \widehat{\rho}_{s_p} \widehat{e}_{s_p} \right) * m, \\ \rho_p E_p &= \mathcal{E}^p \rho_{f_p} E_{f_p} + (1 - \mathcal{E}^p) \rho_{s_p} E_{s_p} \end{aligned}$$

and

$$\begin{aligned} (1 - \Phi) \rho_{f_p} E_{f_p} + (1 - \Phi) \mathcal{E}^p \text{Sa}_{g_p} P_{g_p} \cdot \mathbf{V}_{g_p} \\ + (1 - \Phi) \mathcal{E}^p \text{Sa}_{l_p} P_{l_p} \cdot \mathbf{V}_{l_p} + [\mathbf{Q}_p] \\ = \left( \widehat{\varepsilon}^p \widehat{\rho}_{f_p} \widehat{e}_{f_p} \widehat{\mathbf{v}}_{f_p} + \widehat{\mathbf{q}}_p + \widehat{\varepsilon}^p \left( \widehat{\text{Sa}}_{g_p} \widehat{\rho}_{g_p} \widehat{\mathbf{v}}_{g_p} + \widehat{\text{Sa}}_{l_p} \widehat{\rho}_{l_p} \widehat{\mathbf{v}}_{l_p} \right) \right) \\ * m, \\ P_{g_p} \frac{\partial(1 - \Phi) \mathcal{E}^p \text{Sa}_{g_p}}{\partial t} + P_{l_p} \frac{\partial(1 - \Phi) \mathcal{E}^p \text{Sa}_{l_p}}{\partial t} + \frac{P_{g_p}}{\rho_{g_p}} K_{g_p l_p} \\ + \frac{P_{l_p}}{\rho_{l_p}} K_{l_p v_{g_p}} E_p K^{pf} + [X^{pf}] \\ = \left( \left[ \widehat{\rho}_{f_p} \widehat{e}_{f_p} \widehat{\mathbf{v}}_{f_p} + \widehat{\varepsilon}^p \left( \widehat{\text{Sa}}_{g_p} \widehat{\rho}_{g_p} \widehat{\mathbf{v}}_{g_p} + \widehat{\text{Sa}}_{l_p} \widehat{\rho}_{l_p} \widehat{\mathbf{v}}_{l_p} \right) \right. \right. \\ \left. \left. - \widehat{\rho}_p \widehat{e}_p \widehat{\mathbf{w}}_{\Sigma_p} + \widehat{\mathbf{q}}_p \right] \cdot \mathbf{n}_{\Sigma_p} \delta \Sigma_p \right) * m. \end{aligned}$$

As for phase f, the temperature is not yet defined. The thermodynamical equations take the usual form:

for the internal energy:

$$\begin{aligned} \rho_p E_p = \left[ (1 - \mathcal{E}^p) \left( \text{Sa}_{w_p} \rho_{w_p} H_{w_p} + \text{Sa}_{c_p} \rho_{c_p} H_{c_p} \right) \right. \\ \left. + \mathcal{E}^p \left( \text{Sa}_{g_p} \rho_{g_p} \sum_i H_{i_{g_p}} Y_{i_{g_p}} + \text{Sa}_{l_p} \rho_{l_p} H_{l_p} - P_{f_p} \right) \right], \end{aligned} \tag{32}$$

for the enthalpies:

$$H_{i_{g_p}} = H_{i_{g_p}}^0 + \int_{T_0}^{T_p} C_{p,i_{g_p}} dT, \tag{33}$$

for the pressure:

$$P_{g_p} = \rho_{g_p} R T_p \sum_i Y_{i_{g_p}} / W_{i_{g_p}}, \tag{34}$$

$$\rho_{w_p}, \rho_{c_p} \text{ and } \rho_{l_p} = \text{constant}. \tag{35}$$

Because of compatibility and jump conditions the following relations hold:

$$\begin{aligned} \text{Sa}_{w_p} + \text{Sa}_{c_p} = 1, \quad \text{Sa}_{g_p} + \text{Sa}_{l_p} = 1, \\ \sum_i Y_{if} = 1, \quad \sum_i \mathbf{J}_{if} = 0, \quad Y_{F_{g_p}} + Y_{v_{g_p}} = 1, \\ \mathbf{J}_{F_{g_p}} + \mathbf{J}_{v_{g_p}} = 0, \end{aligned} \tag{36}$$

$$K_i^{pf} + K_i^{fp} = 0, \tag{37}$$

$$\mathbf{F}_{g_p}^{pf} + \mathbf{F}_{l_p}^{pf} + \mathbf{F}^{fp} + K^{fp} \mathbf{V}_f = 0, \tag{38}$$

$$\begin{aligned} \left( E_f + \frac{P_f}{\rho_f} + \frac{1}{2} |\mathbf{V}_f|^2 \right) K^{fp} + P_f \frac{\partial \Phi}{\partial t} + X^{fp} + E_p K^{pf} \\ + P_{g_p} \frac{\partial \Phi \mathcal{E}^p \text{Sa}_{g_p}}{\partial t} + P_{l_p} \frac{\partial \Phi \mathcal{E}^p \text{Sa}_{l_p}}{\partial t} + \frac{P_{g_p}}{\rho_{g_p}} K_{g_p}^{pf} \\ + \frac{P_{l_p}}{\rho_{l_p}} K_{l_p}^{pf} + X^{pf} = 0. \end{aligned} \tag{39}$$

### 3.3. Entropy balance

The averaging method introduces new quantities, essentially

Fluxes:  $\mathbf{J}_{if}$ ,  $\mathbf{J}_{i_{g_p}}$ ,  $\mathcal{S}_f$ ,  $\mathbf{Q}_f$  and  $\mathbf{Q}_p$ .

Sources:  $\dot{\omega}_{if}$ ,  $K_{w_p F_{g_p}}$ ,  $K_{w_p c_p}$ ,  $K_{l_p v_{g_p}}$ ,  $\mathbf{F}_{g_p l_p}$ ,  $\mathbf{F}_{g_p s_p}$ ,  $\mathbf{F}_{l_p s_p}$ ,  $K_i^{fp}$ ,  $\mathbf{F}^{fp}$ ,  $\mathbf{F}_{g_p}^{pf}$ ,  $\mathbf{F}_{l_p}^{pf}$  and  $X^{fp}$ .

For closing the system of equations, we must relate these quantities to usual mean mechanical variables. Let us write the variation of the generalised entropy  $S$  in the form

$$\rho_{ve} \frac{dS}{dt} = -\nabla \cdot \mathbf{J}_S + \sigma_S, \tag{40}$$

where  $\mathbf{J}_S$  is the entropy flux,  $\sigma_S$  is the entropy production and  $\rho_{ve} = \Phi \rho_f + (1 - \Phi) \rho_p$ . This entropy production must be positive and can be written as

$$\sigma_S = \sum_a J_a X_a, \tag{41}$$

where  $J_a$  are the fluxes and  $X_a$  are the forces.

In extended irreversible thermodynamics the generalised entropy  $S$  of the macroscopic medium may depend upon the whole set of variables. The fluxes are a function of some of the variables defining the system and of the forces  $J_a = J_a(X_1, X_2, \dots, T_p, T_f, \dots, Y_{if}, \dots)$ . As at equilibrium  $\mathbf{J}_a^{eq} = 0$ , up to first order one can write:

$$J_a = \sum_b \left( \frac{\partial J_a}{\partial X_b} \right)_{eq} X_b + O(X_b X_c). \tag{42}$$

Taking into account relation (42), the production of entropy is positive if there is a positive matrix  $\mathbf{M} = (M_{ab})$  such that  $J_a = \sum_b M_{ab} X_b$ . The coefficients  $M_{ab}$  are phenomenological coefficients. To obtain the total entropy balance we write

$$\begin{aligned} \rho_{ve} \frac{dS}{dt} = \Phi \rho_f \frac{d^f S_f}{dt} + (1 - \Phi) \rho_p \frac{d^{lp} S_{lp}}{dt} + (1 - \Phi) \rho_{gp} \\ \times \frac{d^{gp} S_{gp}}{dt}. \end{aligned}$$

The derivative are along the motion of each phase. These motions can indeed be considered as independent. Moreover we suppose that the entropies depend upon the following variables:

$$S_f = S_f(E_f, 1/\rho_f, Y_{if}, \mathbf{Q}_f)$$

and

$$S_p = S_p(E_p, 1/\rho_{gp}, 1/\rho_{lp}, Y_{igp}, \rho_{wp} \mathbf{S}a_{wp}, \rho_{cp} \mathbf{S}a_{cp}, \rho_{lp} \mathbf{S}a_{lp}, \mathbf{Q}_p, K_i^{pf}).$$

So that the differential variation of entropy are

$$d^f S = \frac{\partial S}{\partial E_f} d^f E_f - \frac{\partial S}{\partial(1/\rho_f)} \frac{d^f \rho_f}{\rho_f^2} + \sum_j \frac{\partial S}{\partial Y_{jf}} d^f Y_{jf} + \frac{\partial S}{\partial \mathbf{Q}_f} d^f \mathbf{Q}_f, \tag{43}$$

$$d^p S = \frac{\partial S}{\partial E_p} d^p E_p - \frac{\partial S}{\partial(1/\rho_{gp})} \frac{d^p \rho_{gp}}{\rho_{gp}^2} - \frac{\partial S}{\partial(1/\rho_{lp})} \frac{d^p \rho_{lp}}{\rho_{lp}^2} + \sum_a \frac{\partial S}{\partial(S_a \rho_a)} d^p(S_a \rho_a) + \sum_i \frac{\partial S}{\partial Y_{igp}} d^p Y_{igp} + \sum_i \frac{\partial S}{\partial K_i^{pf}} d^p K_i^{pf} + \frac{\partial S}{\partial \mathbf{Q}_p} d^p \mathbf{Q}_p. \tag{44}$$

We can define non-equilibrium temperature and pressure by

$$\frac{\partial S}{\partial E_f} = \frac{1}{\Theta_f}$$

and absolute non-equilibrium pressure by

$$\frac{\partial S}{\partial(1/\rho_f)} = \frac{P_f}{\Theta_f}.$$

In fact if the system is not far from equilibrium the thermodynamics temperature and pressure can be equal to the equilibrium temperature and pressure  $T_f$  and  $P_f$  [5]. We can use the same argument for the temperature and pressure of the phase p and define:

$$\frac{\partial S}{\partial E_f} = \frac{1}{T_f}, \quad \frac{\partial S}{\partial(1/\rho_f)} = \frac{P_f}{T_f}, \quad \frac{\partial S}{\partial Y_{if}} = -\frac{\mu_{if}}{T_f}, \quad \frac{\partial S}{\partial \mathbf{Q}_f} = -\frac{\mathbf{a}_f}{T_f},$$

$$\frac{\partial S}{\partial E_p} = \frac{1}{T_p}, \quad \frac{\partial S}{\partial(1/\rho_{gp})} = \frac{P_{gp}}{T_p}, \quad \frac{\partial S}{\partial(1/\rho_{lp})} = \frac{P_{lp}}{T_p},$$

$$\frac{\partial S}{\partial Y_{igp}} = -\mathcal{E}^p \frac{\rho_{gp}}{\rho_p} \frac{\mu_{igp}}{T_p},$$

$$\frac{\partial S}{\partial(S_a \rho_a)} = -(1 - \mathcal{E}^p) \frac{\rho_a}{\rho_p} \frac{\mu_a}{T_p} \quad \text{for } a = w, c, l,$$

$$\frac{\partial S}{\partial K_i^{pf}} = -\frac{\beta_i^{pf}}{T_p}, \quad \frac{\partial S}{\partial \mathbf{Q}_p} = -\frac{\mathbf{a}_p}{T_p},$$

where  $\mathbf{a}_f$  and  $\mathbf{a}_p$  are two vectors which are null when  $\mathbf{Q}_f$  and  $\mathbf{Q}_p$  are null so that we can set

$$\mathbf{a}_f = a_f(T_f, \rho_f, \dots) \mathbf{Q}_f$$

and

$$\mathbf{a}_p = a_p(T_p, \rho_p, \dots) \mathbf{Q}_p,$$

where  $a_f$  and  $a_p$  are two second-order tensors; in the same way we can set

$$\frac{\partial S}{\partial K_i^{pf}} = -\frac{b_i^{pf}}{T_p} K_i^{pf}.$$

We have to replace all differentials in (43) and (44) by the appropriate expressions calculated from relations (16)–(19) and (23)–(31). For example, Eq. (19) written with the material derivative is

$$\Phi \rho_f \frac{d^f E_f}{dt} = -\nabla \cdot \mathbf{Q}_f + \mathcal{S}_f \cdot \nabla \mathbf{V}_f - P_f / K^{fp} - X^{fp} + \mathbf{F}^{fp} \cdot \mathbf{V}_f.$$

After a somewhat lengthy calculation one obtains

$$\mathbf{J}_s = \mathbf{J}_{sf} + \mathbf{J}_{sp} \tag{45}$$

with

$$\mathbf{J}_{sf} = \frac{\mathbf{Q}_f}{T_f} - \sum_i \frac{\mu_{if}}{T_f} \mathbf{J}_{if}, \tag{46}$$

$$\mathbf{J}_{sp} = \frac{\mathbf{Q}_p}{T_p} - \sum_j \frac{\mu_{jgp}}{T_p} \mathbf{J}_{jgp}.$$

The entropy production, which is a large expression, can be split into several terms:

$$\begin{aligned} \sigma_{s1} &= \nabla \mathbf{V}_f \\ &: \frac{\mathcal{S}_f}{T_f} - \sum_i \mathbf{J}_{if} \cdot \nabla \left( \frac{\mu_{if}}{T_f} \right) - \sum_i \mathbf{J}_{igp} \cdot \nabla \left( \frac{\mu_{igp}}{T_p} \right) \\ &+ \frac{\mathbf{V}_f}{T_f} \cdot (\mathbf{F}^{fp} + P_f \nabla \Phi) + \frac{\mathbf{V}_{gp}}{T_p} \cdot (\mathbf{F}_{gp,lp} + \mathbf{F}_{gp,sp} + \mathbf{F}_{gp}^{pf}) \\ &+ P_{gp} \nabla \cdot ((1 - \Phi) \mathcal{E}^p \mathbf{S}a_{gp}) + \frac{\mathbf{V}_{lp}}{T_p} \cdot (\mathbf{F}_{lp,sp} + \mathbf{F}_{lp,sp} + \mathbf{F}_{lp}^{pf} \\ &+ P_{lp} \nabla \cdot ((1 - \Phi) \mathcal{E}^p \mathbf{S}a_{lp})), \end{aligned} \tag{47}$$

$$\begin{aligned} \sigma_{s2} &= \mathbf{Q}_f \cdot \left( \nabla \frac{1}{T_f} - \frac{a_f}{T_f} \frac{d^f \mathbf{Q}_f}{dt} \right) + \mathbf{Q}_p \cdot \left( \nabla \frac{1}{T_p} - \frac{a_p}{T_p} \frac{d^p \mathbf{Q}_p}{dt} \right) \\ &- \frac{X^{fp}}{T_f} - \frac{X^{pf}}{T_p}, \end{aligned} \tag{48}$$

$$\begin{aligned} \sigma_{s3} &= -\sum_j \frac{\mu_{jf}}{T_f} \dot{\omega}_{jf} - \frac{(1 - \Phi)}{T_p} K_{w_p F_{gp}} [(Y_{F_{gp}} - 1) \mu_{F_{gp}} \\ &- \mu_{w_p} + Y_{gp} \mu_{v_{gp}}] - \frac{(1 - \Phi)}{T_p} K_{l_p v_{gp}} [(Y_{v_{gp}} - 1) \mu_{v_{gp}} \\ &- \mu_{l_p} + Y_{F_{gp}} \mu_{F_{gp}}] + \frac{(1 - \Phi)}{T_p} K_{w_p c_p} [\mu_{w_p} - \mu_{c_p}], \end{aligned} \tag{49}$$

$$\begin{aligned} \sigma_{s4} = & K_{v_{gp}}^{pf} \left[ -\frac{b_{v_{gp}}^{pf}}{T_p} \frac{d^p K_{v_{gp}}^{pf}}{dt} + \frac{\mu_{vf}}{T_f} (Y_{vf} - 1) \right. \\ & \left. - \frac{\mu_{v_{gp}}}{T_p} (Y_{v_{gp}} - 1) + \frac{\mu_{Ff}}{T_f} Y_{Ff} - \frac{\mu_{F_{gp}}}{T_p} Y_{F_{gp}} \right] \\ & + K_{F_{gp}}^{pf} \left[ -\frac{b_{F_{gp}}^{pf}}{T_p} \frac{d^p K_{F_{gp}}^{pf}}{dt} + \frac{\mu_{Ff}}{T_f} (Y_{Ff} - 1) \right. \\ & \left. - \frac{\mu_{F_{gp}}}{T_p} (Y_{F_{gp}} - 1) + \frac{\mu_{vf}}{T_f} Y_{vf} - \frac{\mu_{v_{gp}}}{T_p} Y_{v_{gp}} \right]. \end{aligned} \quad (50)$$

### 3.4. Closure relations

We must now write the phenomenological relations between macroscopic fluxes and the macroscopic quantities gradients. The determination in entropy production of what a flux is and what is its associated force is indeed a matter of choice, but the products involved in the production of entropy must be made up of independent variables. In fact, as expressed by Eq. (42) the fluxes should depend upon all the forces, provided that the force associated with a flux must be a tensor of the same rank. For example, in order that the term  $\mathbf{V}_f/T_f \cdot (\mathbf{F}^{fp} + P_f \nabla \Phi)$  is positive, we can suppose then that there is a positive second-order tensor  $\kappa_f$  such that

$$\mathbf{V}_f = \frac{\kappa_f}{\mu_f \Phi^2} (\mathbf{F}^{fp} + P_f \nabla \Phi), \quad (51)$$

where  $\mu_f$  is the macroscopic viscosity and  $\kappa_f$  is the permeability tensor.

The stress tensor has the usual form

$$\mathcal{S}_f = -[\Phi P_f + \frac{2}{3} \eta_{fb} \nabla \cdot \mathbf{V}_f] \mathbf{Id} + 2\eta_{fv} \mathbf{D}_f, \quad (52)$$

$\mathbf{D}_f = \frac{1}{2} (\nabla \mathbf{V}_f + {}^t \nabla \mathbf{V}_f)$  being the rate of strain tensor. So that the balance of momentum for the f phase is

$$\begin{aligned} \frac{\partial}{\partial t} (\Phi \rho_f \mathbf{V}_f) + \nabla \cdot (\Phi \rho_f \mathbf{V}_f \otimes \mathbf{V}_f - \sigma_f) \\ = \Phi \rho_f \mathbf{g} - K^{fp} \mathbf{V}_f + \mu_f \Phi^2 \kappa_f^{-1} \mathbf{V}_f + P_f \nabla \Phi. \end{aligned} \quad (53)$$

For analogous reasons we can consider the generalised Fourier's law:

$$\begin{aligned} \tau_p \frac{d^p \mathbf{Q}_p}{dt} + \mathbf{Q}_p = -\lambda_p \nabla T_p + \sum_i H_{i_{gp}} \mathbf{J}_{i_{gp}} + \mathbf{Q}_{pr}, \\ \tau_f \frac{d^f \mathbf{Q}_f}{dt} + \mathbf{Q}_f = -\lambda_f \nabla T_f + \sum_j H_{jf} \mathbf{J}_{jf} + \mathbf{Q}_{fr}, \end{aligned} \quad (54)$$

where  $H_{i_{gp}}(T_p)$  and  $H_{jf}(T_f)$  are the enthalpies of species number  $i$ . We have separated the radiant heat fluxes  $\mathbf{Q}_{pr}$  and  $\mathbf{Q}_{fr}$ .  $\tau_p$  and  $\tau_f$  are the relaxation coefficients and  $\lambda_p$  and  $\lambda_f$  are the conductivity coefficients. As the model contains two temperatures, there is a heat flux inside the particles given by

$$X^{pf} = \chi(T_f - T_p), \quad (55)$$

where  $\chi$  is a phenomenological coefficient.

The balance of the different chemical species during the chemical reactions gives the following relations:

$$-\dot{\omega}_{O_2f}/\nu_O W_{O_2} = -\dot{\omega}_{Ff}/\nu_F W_F = \dot{\omega}_{Rf}/\nu_R W_R = \psi, \quad (56)$$

$\psi$  is the rate of mole production. As the reactions are of total order  $\nu_F + \nu_O$ :

$$\psi = k(T_f) (\rho_f Y_F)^{\nu_F} (\rho_f Y_{O_2})^{\nu_O}. \quad (57)$$

From  $\sigma_{s4}$  Eq. (50) we can propose the following relations:

$$\begin{aligned} A_{11} \frac{b_{v_{gp}}}{T_p} \frac{d^p K_{v_{gp}}^{pf}}{dt} + K_{v_{gp}}^{pf} \\ = A_{11} \left[ \frac{\mu_{vf}}{T_f} (Y_{vf} - 1) - \frac{\mu_{v_{gp}}}{T_p} (Y_{v_{gp}} - 1) \right] \\ + A_{12} \left[ \frac{\mu_{Ff}}{T_f} Y_{Ff} - \frac{\mu_{F_{gp}}}{T_p} Y_{F_{gp}} \right], \\ A_{21} \frac{b_{F_{gp}}}{T_p} \frac{d^p K_{F_{gp}}^{pf}}{dt} + K_{F_{gp}}^{pf} \\ = A_{21} \left[ \frac{\mu_{Ff}}{T_f} (Y_{Ff} - 1) - \frac{\mu_{F_{gp}}}{T_p} (Y_{F_{gp}} - 1) \right] \\ + A_{22} \left[ \frac{\mu_{vf}}{T_f} Y_{vf} - \frac{\mu_{v_{gp}}}{T_p} Y_{v_{gp}} \right]. \end{aligned} \quad (58a)$$

where the  $A_{ij}$  are phenomenological coefficients. The right-hand side of equation set (58a) is linear in the  $Y_{ip}$  and  $Y_{if}$ , so that it can be generalised to

$$\tau_i \frac{d^p K_i^{pf}}{dt} + K_i^{pf} = f_i(T_p, T_f, Y_{Fp}, Y_{vp}, Y_{of}, \dots, Y_{pr}).$$

The  $f_i(T_p, T_f, Y_{Fp}, Y_{vp}, Y_{of}, \dots, Y_{pr})$  is a phenomenological function derived from experiments. We assume the following non-linear chemical kinetics:

$$\begin{aligned} \tau_v \frac{d^p K_{v_{gp}}^{pf}}{dt} + K_{v_{gp}}^{pf} = k_v^{pf}(T_f, T_p) l_v(Y_{v_{gp}}, Y_{vf}), \\ \tau_F \frac{d^p K_{F_{gp}}^{pf}}{dt} + K_{F_{gp}}^{pf} = k_F^{pf}(T_f, T_p) l_F(Y_{F_{gp}}, Y_{Ff}) \end{aligned} \quad (58b)$$

and  $K_{O_2}^{pf} = K_N^{pf} = K_R^{pf} = 0$ ; we can assume relations such as

$$\begin{aligned} k_i^{pf}(T_p, T_f) = A_i \exp \left( -\frac{E_i}{2R} \left( \frac{1}{T_p} + \frac{1}{T_f} \right) \right), \\ i = v_{gp}, F_{gp}. \end{aligned} \quad (59)$$

The function  $l(Y_i, Y_j)$  must be determined experimentally but we can choose  $l(Y_{v_{gp}}, Y_{vf}) = (Y_{v_{gp}} - Y_{vf})^+$  or  $l(Y_{v_{gp}}, Y_{vf}) = Y_{v_{gp}}$ ,  $f^+$  is the function equal to  $f$  if  $f$  is positive, and to 0 if  $f$  is negative, and analogously  $l(Y_{F_{gp}}, Y_{Ff}) = (Y_{F_{gp}} - Y_{Ff})^+$  or  $l(Y_{F_{gp}}, Y_{Ff}) = Y_{F_{gp}}$ .

The non-linear chemical kinetics can be interpreted as new macroscopic reactions that we call volatilising reactions:

$$\text{Volatilisation : } \begin{cases} \text{Fuel}_p \xrightarrow{k_p^{\text{pf}}} \text{Fuel}_f \\ (\text{H}_2\text{O})_{\text{vp}} \xrightarrow{k_p^{\text{vf}}} (\text{H}_2\text{O})_{\text{vf}} \end{cases}$$

We have defined the mass rate transfer from wood to fuel (for example) by  $K_{\text{wp,Fgp}} = \bar{k}_{\text{wp,Fgp}} * m$ , where  $\bar{k}_{\text{wp,Fgp}}$  defined by an Arrhenius law, is a function of the mesoscopic temperature. One expects that  $K_{\text{wp,Fgp}}$  should be expressed in the same way, but as a function of the macroscopic temperature, so that we can define

$$K_{\text{wp,Fgp}} = k_{\text{wp,Fgp}}(T_p)(1 - \mathcal{E}^p)\text{Sa}_{\text{wp}}\rho_{\text{wp}}. \quad (60)$$

By an identical reasoning we can deduce that:

$$K_{\text{wp,cp}} = k_{\text{wp,cp}}(T_p)(1 - \mathcal{E}^p)\text{Sa}_{\text{wp}}\rho_{\text{wp}}, \quad (61)$$

$$K_{\text{lp,vgp}} = k_{\text{lp,vgp}}(T_p)\mathcal{E}^p\text{Sa}_{\text{lp}}\rho_{\text{lp}} \quad (62)$$

with  $k_{ij} = A_{ij} \exp(-E_{ij}/RT_p)$ .

$E_{ij}$  is the activation energy of the reaction  $i \rightarrow j$ ,  $R$  is the ideal gas constant. Now from Eq. (47) we deduce that there are two positive tensors  $\kappa_{\text{lp}}$  and  $\kappa_{\text{gp}}$  such that

$$\mathbf{V}_{\text{lp}} = \frac{\kappa_{\text{lp}}}{\mu_{\text{lp}}((1 - \Phi)\mathcal{E}^p\text{Sa}_{\text{lp}})^2} (\mathbf{F}_{\text{lp,gp}} + \mathbf{F}_{\text{lp,sp}} + \mathbf{F}_{\text{lp}}^{\text{pf}} + P_{\text{lp}}\nabla((1 - \Phi)\mathcal{E}^p\text{Sa}_{\text{lp}})), \quad (63)$$

$$\mathbf{V}_{\text{gp}} = \frac{\kappa_{\text{gp}}}{\mu_{\text{gp}}((1 - \Phi)\mathcal{E}^p\text{Sa}_{\text{gp}})^2} (\mathbf{F}_{\text{gp,lp}} + \mathbf{F}_{\text{gp,sp}} + \mathbf{F}_{\text{gp}}^{\text{pf}} + P_{\text{gp}}\nabla((1 - \Phi)\mathcal{E}^p\text{Sa}_{\text{gp}})). \quad (64)$$

For the mass diffusion in general the law should be  $\mathbf{J}_{ia} = -L_{ia}\nabla(\mu_{ia}/T_a)$ , however usually one considers Fick's law:

$$\begin{aligned} \mathbf{J}_{if} &= -\Phi\rho_f d_{if}\nabla Y_{if}, \\ \mathbf{J}_{i\text{gp}} &= -(1 - \Phi)\mathcal{E}^p\text{Sa}_{\text{gp}}\rho_{\text{gp}} d_{i\text{gp}}\nabla Y_{i\text{gp}}. \end{aligned} \quad (65)$$

The thermodynamic state laws are given by relations (20)–(22) and (31)–(35).

### 3.5. Radiant heat fluxes

The derivation of a radiation model in a porous medium is beyond the scope of this paper (see [13] for more details on the subject), instead we consider a simplified but appropriate model. We suppose that the heat flux  $\mathbf{Q}_{\text{fr}}$  is null, because the gaseous phase is considered as a transparent medium, and the flux  $\mathbf{Q}_{\text{pr}}$  is related to the spectral intensity  $L_\lambda$  by the expression

$$\mathbf{Q}_{\text{pr}}(\mathbf{x}, t) = \int_0^\infty \int_{4\pi} L_\lambda(\mathbf{x}, \mathbf{u}, t) \mathbf{u} d\Omega d\lambda, \quad (66)$$

where  $\lambda$ , is the wavelength and  $d\Omega$  the elementary solid angle in the direction  $\mathbf{u}$ .

The spectral intensity is supposed to satisfy the equation of transfer in an absorbing and emitting medium:

$$\frac{1}{c} \frac{\partial L_\lambda}{\partial t} + \nabla \cdot \mathbf{L}_\lambda = -\mathbf{K}_\lambda \mathbf{L}_\lambda + \mathbf{I}_\lambda, \quad (67)$$

where  $c$  is the light speed. The term  $(1/c)\partial L_\lambda/\partial t$  can be neglected, because the propagation time of light is very small compared to characteristic time for transfer of mass, momentum and energy. The source term  $\mathbf{I}_\lambda(\mathbf{x}, \mathbf{u}, t)$  is given by

$$\begin{aligned} \mathbf{I}_\lambda(\mathbf{x}, \mathbf{u}, t) &= a_\lambda L_\lambda^0(T_p(\mathbf{x}, t)) + \frac{\sigma_{s\lambda}}{4\pi} \\ &\times \int_{4\pi} L_\lambda(\mathbf{x}, \mathbf{u}, t) \Phi_\lambda(\mathbf{x}, \mathbf{u}, \mathbf{u}') d\Omega'. \end{aligned} \quad (68)$$

### 3.6. Discussion

This model, although complex, is probably the simplest which takes into account the variety of scales and physical phenomena. It has several interesting features. The "vegetal particle" (corresponding to the equivalent medium) has two temperatures, so that the two phases cannot be in thermal equilibrium. As in any equivalent medium model, the size of the representative element volume, on which the average is taken, is an important parameter. This size can be important, if the forest vegetation is dispersed, so that the model should take into account the possible variation of each temperatures  $T_f$  and  $T_r$  inside the particles. Thus extended irreversible process thermodynamics has been used for the closure of the equations, to obtain generalised Fourier law allowing possible thermodynamic non-equilibrium of the particles. Moreover it is interesting to compare the model obtained by this approach to the ones obtained by other means such as homogenisation theory [14]. Homogenisation gives models with only one temperature and the thermal equation can be written as Eq. (16) in [15]

$$\begin{aligned} \langle \rho C \rangle \frac{\partial T}{\partial t} - \rho_f C_f \int_{-\infty}^t \hat{K}(t - \tau) \frac{\partial^2 T}{\partial t^2} d\tau \\ = \nabla \cdot (\lambda_{\text{eq}} \nabla T), \end{aligned} \quad (69)$$

where  $\hat{K}$  is the memory function. In many cases we can assume that there is only one temperature. If the generalised Fourier law (54) is assumed, the corresponding thermal equation will be of second order in time in our modelling. But integrating by parts in Eq. (69) will provide

$$\langle \rho C \rangle \frac{\partial T}{\partial t} - \rho_f \sum_{i>1} C_i \frac{\partial^i T}{\partial t^i} = \nabla \cdot (\lambda_{\text{eq}} \nabla T). \quad (70)$$

Indeed in the sum of Eq. (70) only a few terms should be considered. We could have considered higher-order time derivatives of heat flux for obtaining a sum as Eq. (70). Therefore the results obtained by homogenisation theory and extended irreversible thermodynamic are compatible. It can be seen from Eq. (53), that if the porosity is very small, we can neglect the right term of the balance of momentum, so that the equation for the flow reduces to Darcy's law. Therefore the flow inside the vegetation can be ruled by Darcy's law or Brinkman law depending on the size of the obstacles in the elementary cell compared to the size of the cell (see [14] for a discussion). For Brinkman's law the Navier–Stokes equation must be supplemented by a term  $\mathbf{M} \cdot \mathbf{V}$ , linear in the velocity  $\mathbf{V}$ , where the term  $m_{ij}$  of the matrix  $\mathbf{M}$  represents the components in the direction  $n^{\circ}i$  of the drag force exerted by the solid phase, when a unit pressure gradient is exerted in the direction  $n^{\circ}j$ . For both cases (Darcy's law or Brinkman's law) the matrix  $\mathbf{M}$  or the permeability tensor  $\mathbf{k}$  can be calculated or experimentally determined. A first attempt has already been made, using a fractal modelling of vegetation, to estimate these terms (see [16]).

#### 4. Macroscopic equations above the forest, into the ground and interface conditions between the forest and above it

##### 4.1. Macroscopic equations above the forest and into the ground

We consider here the equations above the vegetation and into the ground. These equations are the same at macroscopic and mesoscopic description. The gaseous phase above the vegetation or ambient air is a mixing of gases involved in combustion or the results of combustion and steam. We can consider:

1. oxygen  $O_2$ ,
2. inert gases, mainly nitrogen  $N_2$ ,
3. steam  $(H_2O)_v$ ,
4. the gaseous fuel due to pyrolysis denoted by F, and
5. the residues of combustion, denoted by R.

The mass density of the species number  $i$  will be denoted by  $\bar{\rho}_i$  and its molar mass by  $W_i$ . The total density  $\bar{\rho}$  is then defined by  $\bar{\rho} = \sum_{i=1}^5 \bar{\rho}_i$ . The mass density of  $i$ th species is  $\bar{Y}_i = \bar{\rho}_i / \bar{\rho}$ .

These species combustion kinetics are described through an overall, second-order reaction



$\dot{\omega}_i$  denotes the rate of mass production of the species number  $i$ . The balance of species gives the following relations:

$$-\dot{\omega}_{O_2} / v_O W_{O_2} = \dot{\omega}_F / v_F W_F = \dot{\omega}_R / v_R W_R = \bar{\psi}, \quad (72)$$

where  $\bar{\psi}$  is the rate of mass production in the oxidation reaction (71). This reaction is of the total order  $v_F + v_O$ , and then:  $\bar{\psi} = \bar{k}(\bar{T})(\bar{\rho} Y_F)^{v_F} (\bar{\rho} Y_{O_2})^{v_O}$

$$\bar{\psi} = \bar{k}(\bar{T})(\bar{\rho} Y_F)^{v_F} (\bar{\rho} Y_{O_2})^{v_O}, \quad (73)$$

where  $\bar{T}$  is the temperature in the ambient air. The macroscopic equations in  $\bar{\Omega}$  are the equations for the mixing of perfect gases, which are [8]:

balance of mass for the species number  $i$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_i) + \nabla \cdot (\bar{\rho} \bar{Y}_i \bar{\mathbf{V}} + \bar{\mathbf{J}}_i) = \dot{\omega}_i, \quad (74)$$

balance of momentum

$$\bar{\rho} \left( \frac{\partial \bar{\mathbf{V}}}{\partial t} + \bar{\mathbf{V}} \cdot \nabla \bar{\mathbf{V}} \right) - \nabla \cdot \bar{\mathcal{T}} = -\nabla \bar{P} + \bar{\rho} \mathbf{g}, \quad (75)$$

balance of total energy

$$\frac{\partial}{\partial t} \left[ \bar{\rho} \left( \bar{E} + \frac{1}{2} |\bar{\mathbf{V}}|^2 \right) \right] - \nabla \cdot \left[ \bar{\rho} \left( \bar{E} + \frac{1}{2} |\bar{\mathbf{V}}|^2 \right) \bar{\mathbf{V}} + \mathbf{Q} - \bar{\mathcal{T}} \cdot \bar{\mathbf{V}} \right] = \bar{\rho} \bar{\mathbf{V}} \cdot \mathbf{g} \quad (76)$$

with  $\bar{\mathbf{V}}$  the velocity of the centre of mass,  $\bar{P}$  the pressure and  $\bar{E}$  the total internal energy. Because of the definition of the mass density and the conservation of the total mass we have  $\sum_{i=1}^5 \bar{Y}_i = 1$  and  $\sum_{i=1}^5 \bar{\mathbf{J}}_i = 0$ .

The stress tensor  $\bar{\mathcal{T}} = -\bar{P} \mathbf{I} + \bar{\mathcal{T}}$  is defined by

$$\bar{\mathcal{T}} = - \left[ \bar{P} + \frac{2}{3} \bar{\mu} \nabla \cdot \bar{\mathbf{V}} \right] \mathbf{I} + 2 \bar{\mu} \bar{\mathbf{D}}, \quad (77)$$

where  $\mathbf{I}$  is the identity, and  $\bar{\mathbf{D}} = \frac{1}{2} (\nabla \bar{\mathbf{V}} + {}^t \nabla \bar{\mathbf{V}})$ . The heat flux is given by

$$\bar{\mathbf{Q}} = -\bar{\lambda} \nabla \bar{T} + \sum_{i=1}^5 \bar{H}_i \bar{\mathbf{J}}_i + \bar{\mathbf{Q}}_r. \quad (78)$$

$$\bar{H}_i(\bar{T}) = \bar{H}_i^0 + \int_{T_0}^{\bar{T}} C_{p,i} dT$$

is the enthalpy of the species  $i$  and  $\bar{\mathbf{Q}}_r$  is the radiative flux vector. The diffusive fluxes  $\bar{\mathbf{J}}_i$  are given by Fick's law

$$\bar{\mathbf{J}}_i = -\bar{\rho} \bar{d}_i \nabla \bar{Y}_i. \quad (79)$$

The state equation for the gas is that of perfect gases, that is

$$\bar{P} = R^0 \bar{T} \sum_{i=1}^5 \bar{Y}_i / \bar{W}_i. \quad (80)$$

The total mass enthalpy is  $\bar{H} = \sum_{i=1}^5 \bar{Y}_i \bar{H}_i$ , and then the total energy is

$$\bar{E} = \bar{H} - \bar{P} / \bar{\rho}. \quad (81)$$

The equations in the ground reduce to balance of energy

$$\rho \frac{\partial E}{\partial t} + \nabla \cdot \mathbf{Q} = 0 \quad (82)$$

with

$$\mathbf{Q} = -\lambda \nabla T, \quad \text{and} \quad E = C_p T + E_0. \quad (83)$$

#### 4.2. Interface conditions between the forest and above it

At the interfaces  $\bar{\Sigma}$ , there are some macroscopic interface jump conditions for the macroscopic quantities, that must be added, to relate the equations written in  $\Omega$  and  $\bar{\Omega}$  bulk phases. Let us write  $\bar{\mathbf{n}}$ , the unit normal vector to the interface  $\bar{\Sigma}$  directed from phase  $\Omega$  toward phase  $\bar{\Omega}$ , and  $[G]_{\bar{\Sigma}}^{\bar{\Sigma}} = \bar{G} - G_{\bar{\Sigma}}$  the jump of  $G$  across  $\bar{\Sigma}$ . From a rigorous point of view, these relations should be derived from mesoscopic equations in the two bulk phases  $\Omega$  and  $\bar{\Omega}$  by a thermodynamic macroscopic description of the interface  $\bar{\Sigma}$ . Volume average calculus has been done by Ochoa-Tapia and Whitaker [10,17] for the interface between a two temperature porous medium and a homogeneous fluid. Nevertheless, we assume local thermodynamic equilibrium at the interface  $\bar{\Sigma}$ . The temperature  $T_f$  is continuous across the interface, i.e.  $T_f = \bar{T}$  and the tangential component of the velocity can also be considered as continuous. Then only interfacial balances are needed. We postulate these interfacial jump conditions for our porous medium with microstructure. Let us define  $\dot{M}^f$  and  $\bar{M}_f$  by  $\dot{M}_f = \Phi \rho_f \mathbf{V}_f \cdot \bar{\mathbf{n}}$  and  $\bar{M}_f = -\bar{\rho}_f \bar{\mathbf{V}}_f \cdot \bar{\mathbf{n}}$ . Then the jump conditions are the total balance of mass

$$\bar{M}_f + \dot{M}_f = 0, \quad (84)$$

the balance of mass for the different species

$$\dot{M}_f Y_{if} + \bar{M}_f \bar{Y}_{if} + [\mathbf{J}_{if}]_{\bar{\Sigma}}^{\bar{\Sigma}} \cdot \bar{\mathbf{n}} = 0, \quad (85)$$

balance of momentum

$$\dot{M}_f [\mathbf{V}]_{\bar{\Sigma}}^{\bar{\Sigma}} - [\mathcal{S}]_{\bar{\Sigma}}^{\bar{\Sigma}} \cdot \bar{\mathbf{n}} = 0, \quad (86)$$

and balances of energy

$$\dot{M}_f \left[ E + \frac{1}{2} \mathbf{V}^2 \right]_{\bar{\Sigma}}^{\bar{\Sigma}} - [\mathbf{Q} + \mathcal{S} \cdot \mathbf{V}]_{\bar{\Sigma}}^{\bar{\Sigma}} \cdot \bar{\mathbf{n}} = \chi(T_f - T_p), \quad (87)$$

$$\mathbf{Q}_p \cdot \bar{\mathbf{n}} = \chi(T_p - T_f). \quad (88)$$

The jump conditions across the interface  $\bar{\Sigma}$  are similar to the above relations with no mass transfer and no velocity but now  $T_p = \underline{T}$ . Let us write  $\underline{\mathbf{n}}$ , the unit normal vector to the interface  $\underline{\Sigma}$  directed from phase  $\underline{\Omega}$  toward phase  $\Omega$ . Then

$$(\mathbf{Q}_f + \mathcal{S}_f \cdot \mathbf{V}_f) \cdot \underline{\mathbf{n}} = \chi(T_p - T_f), \quad (89)$$

$$(\mathbf{Q}_p - \underline{\mathbf{Q}}) \cdot \underline{\mathbf{n}} = \chi(T_f - T_p). \quad (90)$$

This achieves the derivation of the complete model.

### 5. Simplification of the previous system of equations

We describe what may be the main physical processes involved in forest fire propagation. If there is a sufficient heat source, the wood will firstly be dried. During this phase, the vaporisation of the water will use a large part of the thermal energy. Once the wood is dried the temperature will increase up to a value where pyrolysis takes place. During pyrolysis, the cellulose (and other volatile components) will decompose into flammable gases. If the outflow of flammable gases is sufficient, the gases will burn and a flame will develop above and inside the vegetal stratum. The heat released during combustion is the heat source necessary to continue the process. In the vicinity of the flames, the gases will move upward, due to the conservation of mass, and a flow of fresh air, bringing oxygen to the combustion, will occur inside and outside the vegetation. One can appreciate the importance of the permeability of the vegetal medium on the spreading of the fire.

For analysing the energy transfer in the porous phase we consider Eqs. (19) and (31) of balance of energy. At first approximation we can assume that the vegetation forming this phase is at rest, and then, that the kinetic energy is negligible. We do not consider here the possibility of oscillations for the twigs and the branches. The energy due to the mass transfer from the twigs to the fluids domain is also negligible. The ‘‘relaxation times’’ coefficients in the generalised Fourier laws Eq. (54), which are related to the memory of the media or to the lack of thermal equilibrium of the particles will also be considered as small. This hypothesis is probably very questionable because of the assumed size of particles, but the experimental determination is a very hard task. Moreover, we suppose that the Lewis number in the gas is closed to unity. We neglect advection terms, pressure and porosity variations in the porous phase. With these assumptions in mind, the energy equations (19) and (31) in each phase of the particle reduce to

$$(1 - \Phi) \rho_p C_p^p \frac{\partial T_p}{\partial t} + \nabla \cdot (-\lambda_p \nabla T_p + \mathbf{Q}_{pr}) = R_{pc} - \chi(T_f - T_p), \quad (91)$$

$$\Phi \rho_f C_p^f \left( \frac{\partial T_f}{\partial t} + \mathbf{V}_f \cdot \nabla T_f \right) + \nabla \cdot (-\lambda_f \nabla T_f + \mathbf{Q}_{fr}) = \chi(T_f - T_p) + R_{fc}. \quad (92)$$

In Eq. (92) we have neglected the dissipation  $\mathcal{T}_f : \nabla \mathbf{V}_f$  and the variation of the porosity. The coefficients  $C_p^p$  and  $C_p^f$  are the total specific heat given by

$$C_p^p = (1 - \mathcal{E}^p) \left( S_{w_p} \frac{\rho_{w_p}}{\rho_p} C_{p,w_p} + S_{c_p} \frac{\rho_{c_p}}{\rho_p} C_{p,c_p} \right) + \mathcal{E}^p \left( S_{g_p} \frac{\rho_{g_p}}{\rho_p} \sum_i Y_{i g_p} C_{p,i g_p} + S_{l_p} \frac{\rho_{l_p}}{\rho_p} C_{p,l_p} \right),$$

$$C_p^f = \sum Y_{if} C_{p,i}^f,$$

and  $R_{fc}$  and  $R_{pc}$  are the chemical energy source terms. The heat released by chemical reactions in the particle can be written:

$$R_{pc} = -(1 - \mathcal{E}^p) \left( \text{Sa}_{w_p} \rho_{w_p} Q_{w_p} + \text{Sa}_{l_p} \rho_{l_p} Q_v \right) \quad (93)$$

with

$$Q_{w_p} = k_{w_p F_{g_p}}(T_p) Q_{w_p F_{g_p}} + k_{w_p c_p}(T_p) Q_{w_p c_p},$$

$$Q_v = k_{l_p v_{g_p}}(T_p) Q_{l_p v_{g_p}},$$

where  $Q_\alpha$  are the energy produced by the reaction numbered  $\alpha$ . They are the standard heat released by the chemical  $\alpha$  reaction at temperature  $T_p$ . The only chemical reaction in the gaseous phase is the combustion of flammable gases released by pyrolysis, so that

$$R_{fc} = -k(T_f)(\rho_f Y_{Ff})^{vf} (\rho_f Y_{Of})^{vo} Q, \quad (94)$$

where  $Q$  is the energy produced by the reaction of oxidation. The mass balance relations in phase p reduce to

$$\begin{aligned} \frac{\partial}{\partial t} \left( (1 - \Phi)(1 - \mathcal{E}^p) \rho_{w_p} \text{Sa}_{w_p} \right) \\ = -(1 - \Phi)(1 - \mathcal{E}^p) \rho_{w_p} \text{Sa}_{w_p} k_{w_p}(T_p), \end{aligned} \quad (95)$$

$$\begin{aligned} \frac{\partial}{\partial t} \left( (1 - \Phi)(1 - \mathcal{E}^p) \text{Sa}_{c_p} \rho_{c_p} \right) \\ = -(1 - \mathcal{E}^p) \left( -k_l(T_p)(1 - \Phi) \text{Sa}_{w_p} \rho_{w_p} \right), \end{aligned} \quad (96)$$

$$\frac{\partial}{\partial t} \left( (1 - \Phi) \mathcal{E}^p \text{Sa}_{l_p} \right) = -k_{l_p v_{g_p}}(T_p) \mathcal{E}^p \text{Sa}_{l_p} \quad (97)$$

with  $k_{w_p}(T_p) = k_{w_p F_{g_p}}(T_p) + k_{w_p c_p}(T_p)$ .

For obtaining the quantities  $Y_{Ff}$  and  $Y_{Of}$ , let us write Eq. (17) for the fuel F and the oxygen O:

$$\begin{aligned} \frac{\partial}{\partial t} (\Phi \rho_f Y_{Ff}) + \nabla \cdot (\Phi \rho_f Y_{Ff} \mathbf{V}_f + \mathbf{J}_{Ff}) \\ = -\Phi v_F W_F \psi + K_{F_{g_p}}^{pf}, \end{aligned} \quad (98)$$

$$\frac{\partial}{\partial t} (\Phi \rho_f Y_{Of}) + \nabla \cdot (\Phi \rho_f Y_{Of} \mathbf{V}_f + \mathbf{J}_{Of}) = -\Phi v_O W_{O_2} \psi, \quad (99)$$

where the  $K_{F_{g_p}}^{pf}$  is given by Eq. (58b).

Using Eqs. (17), (51) and (52) the velocity  $\mathbf{V}_f$  satisfies the relation

$$\begin{aligned} \Phi \rho_f \left( \frac{\partial \mathbf{V}_f}{\partial t} + \mathbf{V}_f \cdot \nabla \mathbf{V}_f \right) \\ = -\Phi \nabla P_f - \nabla \cdot \left( \frac{2}{3} \eta_{fb} \nabla \cdot \mathbf{V}_f \right) - \mu_f \Phi^2 \kappa_f^{-1} \mathbf{V}_f + \Phi \rho_f \mathbf{g} \\ + K^{pf} \mathbf{V}_f + \eta_{fv} \Delta \mathbf{V}_f. \end{aligned} \quad (100)$$

Considering the thermal equations (91) and (92), the pyrolysis and vaporisation equations (95)–(97) and the balance of mass for gaseous constituent equations (98)

and (99), supplemented by the heat sources due to radiation, given by Eqs. (66)–(68), the chemical reactions (56) and (57), the thermodynamical relations (32)–(35) and the balance of momentum equation (100) we have a close model.

Vegetation can be modelled by fractals cf. [16], with a heat exchange area which can be very large. Thus the two phases of the vegetal particle should be near thermal equilibrium and  $T_p = T_f = T$  at first approximation. In this case one can consider a “one temperature model”, where there is only one balance energy equation, instead of Eqs. (91) and (92), which can be written

$$\begin{aligned} (\Phi \rho_f C_p^f + (1 - \Phi) \rho_p C_p^p) \frac{\partial T}{\partial t} + \Phi \rho_f C_p^f \mathbf{V}_f \cdot \nabla T \\ + \nabla \cdot (-\lambda_{eq} \nabla T + \mathbf{Q}_{fr} + \mathbf{Q}_{pr}) \\ = R_{fc} + R_{pc}. \end{aligned} \quad (101)$$

If we consider that the velocity of the fluid is given or imposed, we can drop the balance of momentum equation (100) and keep only equations related to conservation of mass, so that we obtain a reaction–diffusion system. This reaction–diffusion model is similar to those postulated by Weber [18] and by Albin [19].

## 6. Conclusion

The global three-dimensional model that we derived, although complex, is probably the simplest which takes into account the variety of scales and physical phenomena for the combustion of the vegetation. Defining the vegetation as a porous medium, the equations of the mean equivalent medium have been derived by the method of volume averaging. Because of the possible large size of the averaging volume the closure of equations is obtained using extended irreversible thermodynamics. This approach provides a means of estimating physical parameters such as heat conductivity or permeability, using homogenisation theory [14,20] for example, and mesoscopic values of parameters (such mesoscopic values are accessible by laboratory experiments). The permeability tensor  $\kappa_f$  in Eq. (100) is only dependent on the geometry of vegetation in the pore, does not depend on the macroscopic flow and can be calculated [16]. One feature of the model, which has not been yet exploited is the possibility for the temperature equations to be hyperbolic, which provides a finite speed for the propagation of temperature. We have seen that the equation for the balance of momentum must be supplemented by a drag term  $-K^{fp} \mathbf{V}_f - \mathbf{F}^{fp}$ , see Eq. (18), however for very compact vegetation, the flow can be ruled by Darcy’s law. Models closely related to the one presented here as the one derived by Joulin [21], for particle-laden gaseous flames, have been derived. But they do not try to include the internal structure of the



fuel, although the model presented here includes fine structure of the vegetation. The coefficients  $\tau_i$  in equation set (58b) are relaxation times involved in the migration of gases in the wood. They are related to the microstructure of the wood: if the permeability (or porosity) of the wood tends to zero,  $\tau_i$  must tend to infinity, and conversely if the permeability of the wood tends to infinity, relaxation times  $\tau_i$  must tend to zero. Note that the influence of the porosity of wood may be of some importance in the modelling of the fighting. One of the chemical additives added to the water dropped by aircrafts is a polyphosphate. Under the action of heat this product is transformed into phosphoric acid which attacks the surface of the vegetation and changes its porosity. In order to model fire fighting where retardants are used, one can consider that retardants affect the activation energy of pyrolysis reactions and combustion reactions, if the retardant action is mainly in the gaseous phase, or by decreasing the porosity of the wood, if the retardant action is mainly at interface between p phase and f phase.

However a complementary work has to be done on the modelling of radiation inside vegetation. Moreover the equations for the ambient air (above vegetation) are not completely satisfactory. They are considered as the prolongation of the equations of the fluid phase inside vegetation and then contain no consideration on a possible solid phase. Therefore if one considers that the soot is rather produced in the flame above the vegetation, its influence is not taken into account because no solid phase has been considered in Eqs. (71)–(83).

An analysis of the different scales involved in the spreading of fire has been provided in this paper, but only the microscopic to the macroscopic scales has been considered. The numerical simulation of this “complete” model is beyond the scope of this work. This calculation should include radiation heat transfer and then the system to be simulated is very complex. Such simulation would provide the position, and then the propagation, of the front flames but as the size of the fire will grow, the size of the computation domain will increase with time, rendering the computation almost impossible. Therefore it is tempting to look for simplified models tackling more specifically with the propagation. The largest scale evoked previously was the “gigascopic” scale see Fig. 2. At this scale, the fire interacts with wind and topography of the ground, the height of the vegetation may appear as a small parameter. Using some “boundary layer” hypothesis, one can derive two-dimensional models. The study of the derivation of simplified two-dimensional reaction–diffusion model, by asymptotic analysis, is the scope of part II of this paper. In fact seeing the type of the modelling of forest fire one can recognise two generic approaches of modelling (in general): a first way going from the simple to the complex where “simple” models are enlarged in order to

predict as correctly as possible the needed information. A second way going from the complex to the simple where “complete” models are reduced in order to obtain the simpler of the biggest models. One could postulate that the modelling is finished when the two approaches provide the same type of models.

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