

Contents

Acknowledgments	iii
Main contributions	ix
Introduction	1
1 Continuous model	3
1.1 Preliminaries and notations	6
1.2 Averaging process and mathematical results	9
1.3 Basic hypotheses	10
1.4 Mass conservation	11
1.5 Momentum balance	14
1.5.1 Inertial term	16
1.5.2 Stress term	17
1.5.3 Drag force. Darcy's and Forchheimer's models	17
1.5.4 Brinkman's model	23
1.5.5 General equations for the fluid phase	24
1.5.6 Solid phase	25
1.6 Energy equation	26
1.6.1 Effective conduction tensor	31
1.6.2 Dispersion modelling	31
1.7 Conservation of the extent of conversion	34
1.8 Constitutive equations	36
1.9 Conclusion	36
2 Micro-Macro model	39
2.1 Introduction	40
2.2 Development of a micro-macro model for a porous medium	41
2.2.1 Connector model	43
2.2.2 Junction model	43
2.2.3 Network model	44
2.3 Numerical results	45

2.4	Momentum conservation	46
2.5	Perspectives	49
3	Experimental analysis	53
3.1	Conception and principles	54
3.1.1	Medium	54
3.1.2	Apparatus	55
3.2	Measurements and results	56
3.2.1	Permeability	56
3.2.2	Dispersion	59
3.3	Conclusions	63
4	Numerical tools	65
4.1	Numerical problem identification	66
4.2	Decoupled iterative strategy	67
4.3	Space and time discretization	68
4.3.1	The Finite Element Method (FEM) and related notations	69
4.3.2	Some time integration schemes	71
4.3.3	Numerical stability and coercivity	71
4.4	Stabilized methods	72
4.4.1	Stabilized method and classical tools	73
4.4.2	Bubble function strategy	74
4.4.3	Multiscale approach	77
4.5	Link between stabilized, bubble function and multiscale approaches	79
4.6	Application : the advection-diffusion operator	80
4.6.1	SUPG method	81
4.6.2	Bubble function method	83
4.6.3	Link with the multiscale approach	88
4.6.4	Conclusions	89
4.7	Bubble function-SUPG method	90
4.7.1	An original RFB approximation	90
4.7.2	Numerical results	93
4.7.3	Computational cost	94
4.7.4	3D Extension	98
4.8	Moving front issue	99
5	Flow in a thin plate, application to RTM and SRIM processes	101
5.1	Flow in a thin porous plate	101
5.1.1	Homogeneous media	102
5.1.2	Stratified media	104
5.2	Permeability and dispersion in a transversely isotropic medium	106
5.2.1	Modelling of transversely isotropic media	107

5.2.2	Mass transfer : competition between dispersion and mass transfer	110
5.3	Reactive processes	113
5.3.1	Reaction Kinetics	116
5.3.2	Viscosity	118
5.4	Remark : Thermal and material moving fronts	118
6	Cartilage behaviour modelling	121
6.1	Introduction	122
6.1.1	Cartilage histology	122
6.1.2	Observations of Maroudas and coworkers. Motivations of the model	124
6.2	Framework and hypothesis of the modelling	125
6.2.1	Definition of the phases	125
6.2.2	Modelling hypotheses	126
6.2.3	Notations for geometrical properties and concentrations	128
6.3	Balance equations	131
6.3.1	Mass balance	131
6.3.2	Momentum balance	132
6.4	Clausius-Duhem inequality and constitutive equations. Problem closure	133
6.4.1	Helmoltz free energy : chemical potential, stress and homogeneous problem closure	135
6.4.2	Transfer in intrafibrillar compartment	139
6.4.3	Fluxes and transfer in extrafibrillar compartment	140
6.4.4	Closure of the non-equilibrium problem	141
6.4.5	Possible improvements of the model	142
6.5	Solution	143
6.5.1	A reduced equation set	143
6.5.2	Solution method	145
6.5.3	FEM method	146
6.5.4	Numerical results on oedometrical test	146
6.6	Conclusions	150
	Conclusions	159
A	Viscous dissipation in a Darcy flow	161
B	Flow in a curved pipe with a low curvature in front of its diameter	163
B.1	Notations	163
B.2	Problem description, length scales and dimensionless numbers	164
B.3	Supplementary assumptions	165
B.4	Mass conservation	165
B.5	Momentum conservation	166

B.6	Non-dimensionalization process	166
B.6.1	Mass conservation	167
B.6.2	Momentum conservation	168
B.7	Conclusion	169
B.7.1	Mass conservation	169
B.7.2	Momentum conservation	169
C	Detailed experimental results	171
D	Semi-positive definite character of the dispersion tensor	173
D.1	Isotropic case	173
D.2	Transversely isotropic case	174
E	Diffusion matrix detail	177
F	Values of the parameters used in order to perform numerical results	179
	Bibliography	183

List of Figures

1.1	$\mathcal{U}^1, \mathcal{U}^2, \mathcal{U}^3$, different examples of REV for a porous medium (1).	4
1.2	REV scale determination for the porosity (cf. Fig.1.1). Three main regions are distinguished. A correct REV lies in the middle zone, where the calculated porosity is quite constant when the sample volume varies (1).	5
1.3	Definition sketch for volume averaging. Difference between microscopic and macroscopic coordinates (1).	8
1.4	Meaning of the phase averaged and the intrinsic phase averaged velocities ; v_r is defined such that $v_r S_f = Q$, S_f being the surface crossed by the fluid and Q the flow rate [m^3/s]; $U_0 = SL$ is the total volume.	13
1.5	Example of a porous medium with a fluid volume fraction gradient. The hydrostatic pressure in the fluid generates a force on the internal surface which acts in the direction opposite to $\nabla \varepsilon_f = -\frac{1}{V} \int_{S_{fs}} n_{fs} dS$.	15
1.6	Relationship between molecular diffusion (see Section 1.7) and convective dispersion (2). $\mathcal{D}$ is the molecular diffusivity (equivalent to the conductivity tensor k_e) $V d$ is the Darcy velocity times the particle diameter and thus $Pe = V d / \mathcal{D}$ is a non-dimensional number, D_L is the sum of the molecular diffusivity and of the dispersion diffusivity (equivalent to $k_e + K_D$).	33
2.1	Micro-scale model for the flow in a porous medium, as consisting of a network of connectors and junctions	41
2.2	Geometry of an elementary cell as a set of connectors.	45
2.3	Comparison of the macroscopic relations between pressure gradient and seepage velocity for different values of ε .	46
2.4	Linear model. Solid force acting on the fluid at a junction.	47
2.5	Modified model. Same problem as in Fig. 2.4 . Decrease of the force acting on the fluid at the junction.	47
2.6	Same problem as in Figs. 2.4 and 2.5. Values of ε_{ij} as generated by the modified algorithm for $\alpha \in [0, \pi]$. ε_{14} is plotted with '+' symbols, ε_{42} with 'o' symbols, and ε_{43} with 'x' symbols.	50

2.7	Same problem as in Figs. 2.4 and 2.5. Objective function $\mathcal{F}$ for $\alpha \in [0, \pi]$. The continuous curve represents the objective reached by means of the modified algorithm, while symbols '+' refer to the case $\varepsilon_{14} = 1$; $\varepsilon_{42} = 0$; $\varepsilon_{43} = 0$, and symbols 'x' to the case $\varepsilon_{14} = 1$; $\varepsilon_{42} = 0$; $\varepsilon_{43} = 1$.	51
2.8	Same problem as in Figs. 2.4 and 2.5. Flow rates obtained with the modified algorithm for $\alpha \in [0, \pi]$. Q_{14} is plotted with '+' symbols, Q_{42} with 'o' symbols, and Q_{43} with 'x' symbols.	52
2.9	Same problem as in Figs. 2.4 and 2.5. Head generated at junction 4 by the modified algorithm for $\alpha \in [0, \pi]$. The '+' symbols represent the head generated by the linear model.	52
3.1	Experimental scheme - Flow rate resulting from an imposed pressure difference.	56
3.2	(a) Siphon system in order to avoid void formation and to maintain a constant exit pressure. (b) Separated zones at the entry and the exit of the porous medium.	57
3.3	Experiment scheme and boundary conditions for the determination of dispersion. (a) Flow perpendicular to the needle direction ; (b) Flow aligned with the needle direction.	60
3.4	Concentration distribution at the exit of the porous block in twelve separated zones (3). The flow is perpendicular to the medium symmetry axis (Fig. 3.3 (a)). The experiments were performed with the first and with the second block (left and right figures).	61
3.5	Flow perpendicular to the medium symmetry axis (Fig. 3.3 (a)). Similar results are obtained for the concentration distribution in both media (3).	62
3.6	Concentration distribution at the exit of the porous block in twelve separated zones (3). The flow is parallel to the medium symmetry axis (Fig. 3.3 (b)). The experiments were performed with the first and with the second block (left and right figures).	63
4.1	Global iterative algorithm. The entries follow the arrows. The superscripts refer to the time step while the subscripts refer to the iteration of the global scheme. The field variables with only a superscript represent the converged solution at the time associated with the superscript. Tol_* indicate the error tolerances relative to the searched fields.	67
4.2	Approximation of the domain Ω by Ω_h and example of discretization in elements e_k . Here $\bar{p}_i$ are the nodes belonging to the boundary Γ_h , (with i in $\bar{P}$), while p_i are the nodes belonging to the domain interior with in this case $i \in P^\circ$.	70
4.3	Different relative orientations of the elements with respect to the velocity field (cases (a) and (b)). Determination of the largest segment parallel to the velocity and entirely contained in the element.	87

4.4	Example of piecewise linear bubble function, third generation. The bubble function vanishes on the element boundary	91
4.5	Different generations of bubble functions	92
4.6	Initial cone, calculation domain and mesh, together with initial position and height of the cone top.	93
4.7	Rotating cone test for $Pe_h = 1.56$ on a 33×33 node mesh. Comparison between the results obtained by means of Galerkin, SUPG and first generation of bubble function (Gen1) methods, without or with SUPG effect inside the subelements. Position and height of the cone top after one rotation.	95
4.8	Rotating cone test for $Pe_h = 156$ on a 33×33 node mesh. Comparison between the results obtained by means of Galerkin, SUPG and first generation of bubble function (Gen1) methods, without or with SUPG effect inside the subelements. Position and height of the cone top after one rotation.	96
4.9	Rotating cone test for $Pe_h = 156$ on a 33×33 node mesh. Comparison between results obtained by means of second, third and fourth generation of bubble function (Gen2, Gen3, Gen4) methods, without or with SUPG effect inside the subelements. Decreasing of the oscillations near the cone basis when choosing a higher generations. Position and height of the cone top after one rotation.	97
5.1	Scheme and dimensions of the thin porous plate. Sketch of the problem	102
5.2	Scheme of a thin stratified porous plate with two layers. Sketch of the problem	105
5.3	Path-lines of two selected material points through a 2-layered porous medium.	106
5.4	Sketch of the problem and cross-sections of the mesh for $x = 0.5\text{m}$ and $y = 0.1\text{m}$	111
5.5	Cross-section of the velocity field for $x = 0.5\text{m}$	112
5.6	Cross-sections of the velocity field for $z = 2.5\text{mm}$ and $z = 7.5\text{mm}$. . .	112
5.7	Cross-sections of the relative conversion degree for $y = 0.1\text{m}$ and $x = 0.5\text{m}$ at different times from 0 to 20s (from 0.25 : dark gray, to 0.75 : light gray). All L_{ijkl} coefficients are 0 except $L_{\perp\parallel} = 0.17\text{mm}$	114
5.8	Same as Fig.5.7 with $L_{\perp\parallel} = 0.017\text{mm}$	115
5.9	Typical evolution of the degree of conversion under isothermal operating conditions for an unsaturated polyester (4).	116
5.10	Evolution of the temperature field when a cold polyurethane resin fills an initially hot medium (5).	117
5.11	Difference between material and thermal fronts. After 1 second, the material front has already reached the cavity extremity, while the thermal front has almost reached the middle of the cavity.	119

6.1	Cartilage composition scheme (6)	123
6.2	Characteristic dimensions of collagen fibers in side view (left) and cross-section (right). Only small molecules, like water and Na^+ , can enter the space between the collagen fibrils (6).	123
6.3	Cartilage species partition and exchange schemes (6)	126
6.4	Definition of ε_I . Definition and meaning of p^{eff} as function of the salinity.	137
6.5	Oedometrical test with variation of the bath salinity.	147
6.6	Experimental measurements at equilibrium from oedometrical tests (7).	148
6.7	Numerical results from oedometrical tests. Normal stress versus longitudinal deformation in the 4-step cycle.	149
6.8	Numerical results from oedometrical tests. Evolution in time and space of the extrafibrillar water mass content during the 4 steps of the cycle with $\tau_{Na} = 15.5 \cdot 10^4$ s, $\tau_w = 7.4$ s.	151
6.9	Numerical results from oedometrical tests. Evolution in time and space of the intrafibrillar water mass content during the 4 steps of the cycle with $\tau_{Na} = 15.5 \cdot 10^4$ s, $\tau_w = 7.4$ s.	152
6.10	Numerical results from oedometrical tests. Evolution in time and space of the extrafibrillar sodium mass content during the 4 steps of the cycle with $\tau_{Na} = 15.5 \cdot 10^4$ s, $\tau_w = 7.4$ s.	153
6.11	Numerical results from oedometrical tests. Evolution in time and space of the intrafibrillar sodium mass content during the 4 steps of the cycle with $\tau_{Na} = 15.5 \cdot 10^4$ s, $\tau_w = 7.4$ s.	154
6.12	Numerical results from oedometrical tests. Evolution in time and space of the pressure p_I during the 4 steps of the cycle with $\tau_{Na} = 15.5 \cdot 10^4$ s, $\tau_w = 7.4$ s.	155
6.13	Numerical results from oedometrical tests. Evolution in time and space of the electrical potential field during the 4 steps of the cycle with $\tau_{Na} = 15.5 \cdot 10^4$ s, $\tau_w = 7.4$ s.	156
6.14	Numerical results from oedometrical tests. Comparison of the evolution in space and time of the water and EFC sodium mass contents during the first step of the cycle with different characteristic time scales : (a) $\tau_{Na} = 15.5 \cdot 10^4$ s, $\tau_w = 7.4$ s and (b) $\tau_{Na} = 15.5 \cdot 10^6$ s, $\tau_w = 7.4$ s.	157
6.15	Numerical results from oedometrical tests. Comparison of the evolution in space and time of the IFC sodium mass content, of the pressure p_I and of the electrical potential during the first step of the cycle with different characteristic time scales : (a) $\tau_{Na} = 15.5 \cdot 10^4$ s, $\tau_w = 7.4$ s and (b) $\tau_{Na} = 15.5 \cdot 10^6$ s, $\tau_w = 7.4$ s.	158
B.1	Length scales of the problem	164
D.1	Vectorial decomposition of l	175

List of Tables

1.1	Momentum equation summary for the fluid phase	28
1.2	Substitution of variables in the energy equation to establish the species conservation equation for the conversion extent.	34
3.1	Mean time [s] taken by one water liter to flow across the porous medium 58	
3.2	Permeability components from the measurements	59
4.1	Parameters of the numerical solution	98
4.2	Computational cost of different refinement strategies for 2D problems.	98
6.1	Total problem unknowns for two salts and in 3D.	141
6.2	Total problem equations for two salts and in 3D	142
C.1	Time [s] required in order to let one water liter flow through a porous medium for different relative orientations of the medium with respect to the averaged velocity (Fig. 3.1) (3)	172