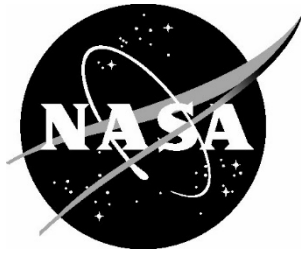


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Development of a One-Domain Volume-Averaged Navier–Stokes Solver

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Constants

k_B	Boltzmann constant	$1.38 \times 10^{-23} \text{ J/K}$
N_A	Avogadro number	$6.02 \times 10^{23} / \text{mol}$
$\mathcal{R}$	universal gas constant, $\mathcal{R} = k_B N_A$	8.31 J/(K mol)

Roman Symbols

$\mathcal{D}$	binary diffusion coefficient	m^2/s
D	multicomponent diffusion coefficient	m^2/s
d	driving force	$1/\text{m}^2$
e	energy	J/kg
E	total energy	J/kg
h	enthalpy	J/kg
$\mathcal{H}$	set of heavy species	—
$\mathcal{A}$	set of atoms	—
$\mathcal{M}$	set of molecules	—
$\mathcal{G}$	set of gas species	—
$\mathcal{S}$	set of all species	—
$\bar{\mathbf{I}}$	identity matrix	—
$\bar{\mathbf{K}}$	permeability tensor	m^2
$\bar{\mathbf{F}}$	Forchheimer tensor	m^2
$\mathbf{J}$	diffusive mass flux	$\text{kg}/(\text{m}^2 \text{ s})$
M	molecular weight	kg/mol
p	pressure	Pa
$\mathbf{q}$	convective heat flux	W/m^2
$\mathbf{q}^{\text{Diff}}$	diffusive heat flux	W/m^2
$\mathbf{q}^{\text{Cond}}$	conductive heat flux	W/m^2
T	temperature	K
$\mathbf{u}$	hydrodynamic velocity	m/s
$\mathbf{V}$	diffusion velocity	m/s
x	mole fraction	—
$\mathbf{u}_\Gamma$	surface recession velocity	m/s
B'	non-dimensional mass blowing rate	—

$\mathbf{F}^{\text{drag}}$	drag force	Pa/m
$\mathbf{F}^{\text{inv}}$	inviscid fluxes	—
$\tilde{\mathbf{F}}^{\text{inv}}$	dispersion inviscid fluxes	—
$\mathbf{F}^{\text{vis}}$	viscous fluxes	—
$\tilde{\mathbf{F}}^{\text{vis}}$	dispersion viscous fluxes	—
$\mathbf{S}$	volumetric source term	—
$\mathbf{S}^{\text{surf}}$	surface source term	—
$\mathbf{F}^{\Gamma}$	surface source term	—
$\mathbf{U}$	conservative quantities	—
m	filter function	—
E_a	Activation energy	kJ/mol
A_f	pre-exponential factor	m/s
Re	Reynolds number	
$\dot{m}$	mass flux	kg/(m ² s)
$\mathcal{S}$	surface area	1/m

Greek Symbols

μ	shear viscosity	kg/(m s)
ν	kinematic viscosity	m ² /s
λ	thermal conductivity	W/(K m)
$\bar{\tau}$	viscous stress tensor	Pa
$\dot{\omega}^{\text{chem}}$	mass production rate due to chemical reactions	kg/(m ³ s)
$\dot{\omega}^{\text{het}}$	surface source term due to heterogeneous reactions	kg/(m ² s)
ρ	mass density	kg/m ³
ψ	generic property	—
δ	Dirac delta function	—
ε	volume fraction coefficient	—
γ	phase-indicator function	—
φ	compressibility parameter	s ² /m ²

Acronyms

CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Lewy
FV	Finite Volume
GSI	Gas-Surface Interaction
NASA	National Aeronautics and Space Administration
ARC	Ames Research Center
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
MOL	Method-Of-Lines
BE	Backward-Euler
REV	Representative Elementary Volume
RVE	Representative Volume Element
AEV	Arbitrary Elementary Volume
GE	Governing equations
ATR	Ablator Thermal Response
MSL	Mars Science Laboratory
TOF	time-of-flight
ICP	Inductively coupled plasma
EOS	Equation-of-state
TT	Through-Thickness
IP	In-Plane
TPS	Thermal Protection System
PATO	Porous-material Analysis Toolbox based on OpenFOAM
PuMA	Porous Microstructure Analysis
VANS	Volume Average Navier-Stokes
TPM	Thermal Protection Materials
SEB	Surface Energy Balance
SMB	Surface Mass Balance
DSMC	Direct Simulation Monte Carlo
VKI	von Karman Institute for fluid dynamics
UIUC	University of Illinois Urbana-Champaign
PICA	Phenolic Impregnated Carbon Ablator
LES	Large eddy simulation
DNS	Direct numerical simulation
ZA	Zhukhov-Abe
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations

SIMPLEC	Semi-Implicit Method for Pressure-Linked Equations Consistent
PISO	Pressure Implicit with Splitting of Operators

Preface

The interaction between a high-enthalpy flow and a thermal protection material is inherently multiscale and multiphysics. In conventional aerothermal analyses, the external flow and material response are generally modeled using separate computational domains coupled through boundary conditions at the material surface. Although this approach has supported many practical applications, it requires assumptions about the location and behavior of the interface and may become difficult to apply when material decomposition, internal reactions, and surface recession substantially alter the porous structure.

This report presents the development of a one-domain formulation in which the free-fluid and porous-material regions are represented within a single computational domain. The formulation is based on the volume-averaged Navier–Stokes (VANS) equations, derived from the governing equations for reacting, compressible flow and condensed material. Volume averaging transfers the influence of the unresolved material microstructure to the macroscale equations through effective transport properties, interfacial source terms, and dispersion fluxes. Particular attention is given to regions in which porosity and permeability vary rapidly, including the diffuse transition between a porous material and the surrounding fluid.

The resulting equations are implemented in the Porous-material Analysis Toolbox based on OpenFOAM (PATO). The report describes the pressure–velocity coupling strategy used by the solver, examines spatial filtering techniques for deriving effective properties, and evaluates the influence of a smoothly varying interface permeability. Numerical demonstrations include canonical porous-flow configurations, a flow-tube configuration representative of FiberForm® permeability experiments, and the oxidation of a porous carbon material.

The purpose of this work is to establish a mathematical and computational foundation for a unified treatment of flow and thermal protection material response. The present formulation is intended to support the progressive inclusion of additional physical processes, including multicomponent transport, finite-rate gas–surface chemistry, pyrolysis, internal oxidation, and material recession. It also provides a framework for connecting pore-scale simulations and microstructural characterization with macroscale aerothermal-response calculations.

This report is intended for researchers and engineers working in computational fluid dynamics, porous-media transport, material response, and thermal protection system modeling. It documents both the theoretical development and the initial numerical assessment of the one-domain approach, while identifying the closure of effective and dispersion terms as an important subject for continued investigation.

Chapter 1

Statement of problem

The discovery of the unknown has always been rooted in humankind since the dawn of modern civilization, driving us toward new exploratory endeavors. In the 20th century, this curiosity was directed toward exploration beyond the confines of Earth, mainly landing on the moon, driven by the Soviet and American space programs. Currently, in addition to the return from the Moon, our aspirations go beyond the reach of Earth’s natural satellite, as they include exploring other planets and sampling cosmic bodies, such as asteroids.

The success of space exploration demands much planning and engineering design. The payload essential for exploration missions increases proportionally with their ambitious objectives; e.g., to populate Mars, it will require the transportation of equipment necessary to sustain life. Moreover, when the spacecraft returns to our planet with extreme velocities, it will endure intense conditions during reentry, causing high heat loads onto the vehicle and thus posing the highest failure risk to the mission. One way to mitigate this risk is to use an ablative **Thermal Protection System (TPS)**. Ablators are designed to degrade while protecting the spacecraft and its payload.

The **TPS** can represent up to 50% of the total spacecraft mass – e.g., the Galileo probe [Laub and Venkatapathy, 2004] – penalizing the maximum onboard payload. Therefore, the **TPS** must be sized appropriately and made of light thermal resistant materials to enable mission success. In the '90s, researchers at **National Aeronautics and Space Administration (NASA)** have developed a new class of lightweight material made of a porous carbon fiber preform impregnated in phenolic resin. This material, known as the **Phenolic Impregnated Carbon Ablator (PICA)** [Tran et al., 1997], was used effectively in missions such as Stardust (2006) [Willcockson, 1999] and Mars Science Laboratory (MSL) (2012) [Edquist et al., 2014].

Figure 1.1 illustrates an atmospheric entry, specifically, the impact of the highly energetic flow on the material. As the temperature in the material rises, the phenolic resin decomposes in a process known as pyrolysis. Pyrolysis of the phenolic produces gases that percolate through the material and react with the carbon preform, generating chemical species. The blowing of these gases into the boundary layer creates a protective film between the material and the environment as well as react with the chemical species in the boundary layer, altering the heat flux at the surface. Besides, atmospheric gases react with the carbon fibers leading to oxidation and nitridation reactions causing the ablator’s surface to recess. Finally, the weakening of the fibers near the surface leads to surface spallation, where large particles are ejected from the surface due to mechanical and thermal loads.

Considering the interactions between the aerothermal environment and the material response, the highly coupled, multi-physics problem is a key challenge in determining design margins and mission risk. The equations governing the **Thermal Protection Materials (TPM)** (the **TPM** phase) are tightly coupled to the equations governing the flow field (the environment phase) at the interface of the two domains. To date, the modeling approach decouples both phases requiring a significant number of assumptions that describe the interactions between phases, hindering the fidelity of the flow/material interface model. This procedure fails to answer questions such as “*How does the interface behave due to uneven surface recession?*” and “*What is the impact of the interface resolution on the material response?*”.

This project aims to build a detailed model from first principles that allow solving the flow and material in a unified approach by correctly deriving the governing equations suitable for both material and flow,

considering a physics-based interface representation. We will solve these equations numerically, where both phases will be considered in the same computational domain. The proposed unified approach will follow the derivation of [Whitaker \[1999\]](#) which is limited to a homogeneous medium, i.e., microstructures with slight porosity fluctuations. For our particular application, the material might suffer from abrupt porosity changes due to fibers recession and the presence of a sharp interface [[Quintard and Whitaker, 1994a](#)]. In this project, we will use and extend further the tools developed at, [NASA Ames Research Center \(ARC\)](#) more specifically [Porous-material Analysis Toolbox based on OpenFOAM \(PATO\)](#) [[Lachaud and Mansour, 2014](#)].

Chapter 2

Background and relevance to previous work

Historically, three general strategies have addressed the flow/material coupling problem. In increasing order of fidelity, we can enumerate these strategies (see fig. 2.1) in terms of numerical solvers [Schrooyen et al., 2018] as:

1. decoupled, standalone solvers for material and flow domains,
2. weak or strong coupling between standalone solvers, and
3. unified solvers.

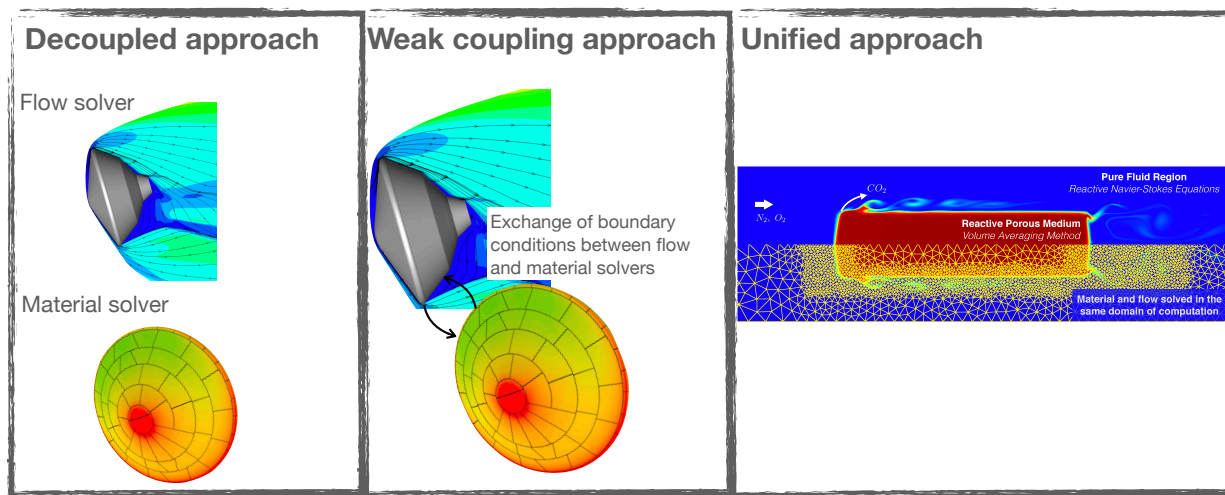


Figure 2.1: The three types of flow field and material strategies. Left and center figures courtesy of Meurisse et al. [2018], right figure courtesy of Schrooyen et al. [2016].

The first, and most popular strategy, consists of decoupling the flow field entirely from the material response and solving each domain utilizing **Computational Fluid Dynamics (CFD)** solvers for the environment and **Ablator Thermal Response (ATR)** solvers for the material, with proper boundary conditions that can represent the ablation process. This decoupling implies certain assumptions when information is needed from one domain to another. For instance, the pure flow simulation assumes that the material reaches an energetic steady-state condition and relies on an empirical relation between the material's in-depth mass production (such as the production of pyrolysis gas) and surface ablation. Moreover, this approach relies on a surface chemical equilibrium assumption which might not be reached in certain conditions. On the other hand, the

ATR solver depends on transfer coefficients to emulate the flow field properties. Among several ATR solvers, one of the most complete is PATO [Lachaud and Mansour, 2014] which includes type (3) models. It considers element [Lachaud et al., 2015, 2017] or species governing equations, pyrolysis decomposition and in-depth fiber oxidation within the material, and Darcy’s law instead of solving the complete momentum equation. This solver’s incredible flexibility and performance allowed Meurisse et al. [2018] to model a full-scale MSL heatshield, including the tiles architecture.

The second strategy consists of loosely coupling the flow, and material response [Schrooyen et al., 2018, Chen and Gökçen, 2014, Dias et al., 2020]. This strategy is a first step to reducing the number of assumptions by exchanging the information inherent to each domain through boundary conditions. Typically, this coupling strategy relies on time scale separation of both phases, i.e., the flow field adapts instantaneously to material shape change. This assumption allows us to consider that the flow field quickly reaches a steady-state; hence, its properties can be transferred to the ATR solver. The transient behavior of the ATR solver is then considered, and after a specific physical time-step, its solution (surface temperature, geometry) is transferred back to the CFD flow field solver.

The third and most complex strategy relies on generalizing the governing equations to solve the flow field and the material in a unified approach. In the works of Schrooyen et al. [2016], Weng and Martin [2017], and Duzel and Martin [2020], the interface progression between both domains naturally appears as a cause of material degradation. These authors have used heuristic models to define the porous medium’s effective properties, typically derived from ordered porous structures. Due to the strong coupling between both phases, this latter approach mitigates the modeling assumptions mentioned in the previous strategies. Moreover, this strategy makes it possible to distinguish volume and surface ablation, which is impossible with the former two methods.

2.1 Volume Average Navier-Stokes (VANS) equations

This section describes the governing equations that solve both the fluid phase and the porous medium in the same computational domain and how to estimate their closure.

Volume-averaging technique

To consider both phases in the same computational domain, one must account for the multi-scale aspects of porous media structures. Since it is not feasible with current computational resources to resolve the macro and microscale in the same domain, one must locally average the governing equations using Volume Average Navier-Stokes (VANS) equations [Whitaker, 1999]. The VANS equations determine the macroscale properties of the flow and contain effective transport properties to consider the microscale due to the porous media [Quintard and Whitaker, 1994a,b]. The VANS methodology is inspired by turbulence modeling [Pope, 2012], where filtering approaches such as Large eddy simulation (LES) [Mansour et al., 1979] can be utilized to describe the average behavior of the porous medium. Direct numerical simulation (DNS) [Moser et al., 1999] is used to simulate the porous structure and obtain closure properties to macroscale equations. The filtering procedure presumes the *decomposition of length scales*, i.e., the porous scale property is decomposed into large and small length scale quantities [Gray, 1975]. The former represents the average field over an integration volume, and the latter depicts the microscale interaction between the flow and porous structure.

The filter size is critical in the volume-averaging technique, and several definitions are given by various authors when defining the averaging volume. As shown in fig. 2.2, if the filter of radius r_0 is smaller than $r_{\min}$ then micro-heterogeneities can be observed, i.e., the averaged property will result in a noisy signal due to the interaction between the flow and a solid phase. Differently, if r_0 is more significant than $r_{\max}$, then the average quantity will be affected by the large-scale variations of the domain (macro-heterogeneities). Bachmat and Bear [1986] says that, in principle, any Arbitrary Elementary Volume (AEV) could be used to average the quantities. Still, one would get distinct averaged properties for each quantity, and they would need to be categorized by their averaging volume. Therefore, one needs to define a universal criterion such as a Representative Elementary Volume (REV) where all quantities remain constant over an averaging volume. Davit et al. [2013] mentions that the REV definition typically implies the smallest representative volume that can be evaluated, i.e., in the case of fig. 2.2 the smallest volume would be determined by $r_{\min}$. The primary concern with this description is that the averaging of each property – permeability, tortuosity, and

effective conductivity– may result in different $r_{\min}$ and REV. Davit et al. [2013] introduces the concept of Representative Volume Element (RVE) where the averaging volume is defined anywhere between $r_{\min}$ and $r_{\max}$.

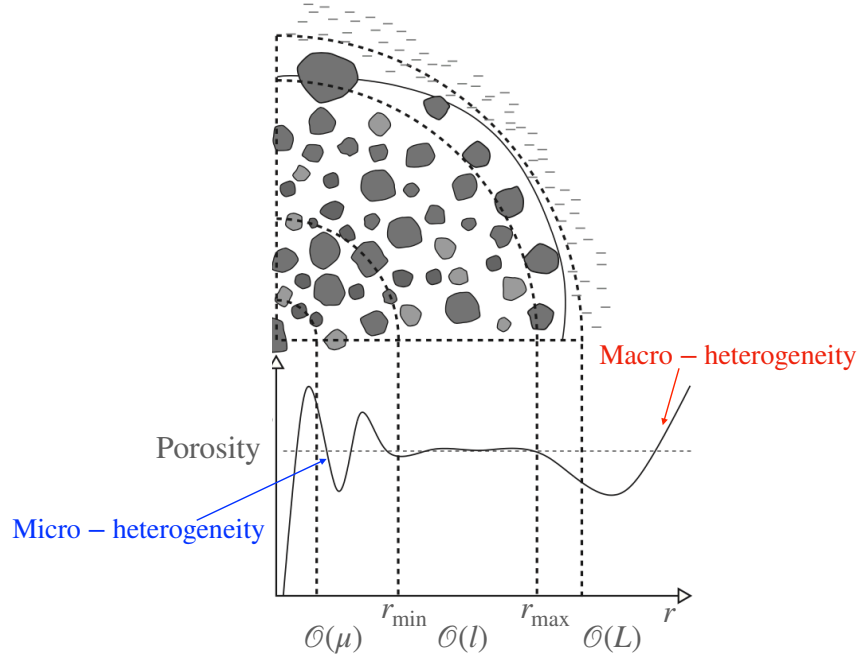


Figure 2.2: RVE illustration where $l = 2r_0$ is the filter diameter, μ and L are the microscale and macroscale characteristic lengths. Figure adapted from Davit et al. [2013].

To summarize, the volume-averaging technique results in macroscale equations that represent the average behavior of a porous domain, including the porous structure. The size of the filter is paramount for these equations to be well behaved over an RVE (or REV as commonly defined). However, these equations require closure that enables consideration of the porous structure; therefore, the microscale information is expressed in terms of effective transport properties [Davarzani et al., 2021], which can only be derived from DNS-type simulations at the porous scale.

VANS closure

The closure of effective transport properties is done at the porous scale, where several upscaling methods can be used [Quintard, 2016]. The most common methods are volume-averaging [Quintard and Whitaker, 1994c] and the formal multi-scale asymptotic analysis [Sanchez-Palencia, 1980, Keller, 1980]. The former approach is made via a spatial convolution with a smoothing function with compact support, and it is widely used due to its simplicity and flexibility. It is easily adapted to new problems. The latter is based on a perturbative decomposition of the micro-and macro-lengthscales. Although the different scales appear naturally – without the need to enforce a spatial decomposition – it requires a detailed derivation of the equations, especially for non-linear problems. Davit et al. [2013] gives an excellent review and comparison of these two methods, and in this work, we will focus on the volume-averaging technique.

It is essential to consider the filter’s kernel and size (REV) to obtain well-behaved average properties. The filter type depends on the porous structure, i.e., if the porous medium is ordered or disordered. For ordered porous medium, Quintard and Whitaker [1994a,b,d,e] observed that cellular filters (pyramid shape) are optimum, canceling the spatial higher-order terms owed to the periodicity of the structure. Moreover, this finding also leads to a filter size of the same order as the porous length scale. In the case of a disordered porous medium, a top-hat filter suffices to provide well-behaved averaged properties. Still, in this case, the size of the filter has to be much larger than the porous scale to have proper scale separations. Davit and

Quintard [2017] has carried out a thorough study on different kernels and sizes for periodic and quasi-periodic porous structures, observing a substantial impact on the averaging properties.

The effective properties can be derived over a unit cell for periodic and homogeneous porous medium. If the problem is linear, the closure properties can be derived in terms of mapping variables that are solved as a boundary-value problem in a unit REV [Whitaker, 1999, Quintard and Whitaker, 1993]. Using that methodology, Whitaker [1986, 1996] derived the permeability and Forchheimer tensor based on Darcy’s law, and Carbonell and Whitaker [1984] derived effective thermal conductivity and tortuosity coefficient for a heat and mass transfer problem. Conversely, if the porous structure is highly complex and the problem is non-linear, these properties can only be derived from porous scale simulations.

The recent evolution of computational methods and numerical tools allowed the properties’ inference based on 3D images obtained with X-ray microtomography. An example is the Porous Microstructure Analysis (PuMA) software [Ferguson et al., 2018] developed at NASA, which is extensively used to deduce effective properties from samples of relevant materials for TPS design. For instance, Semeraro et al. [2020, 2021], and Ferguson et al. [2022] inferred effective thermal conductivity and tortuosity of FiberForm[®] samples.

2.1.1 Unified treatment of the interface

It is challenging to capture the interface separating the pure fluid, and porous medium since the porosity changes significantly in a small length. From a microscale standpoint, one would define the interface of the different solid phases at the transition between the porous medium and fluid phase. From a mesoscopic perspective, this transition occurs smoothly in a certain thickness as depicted in fig. 2.3. When building a one-domain model, the main difficulty is determining the effective properties across the interface where the variation is considerable. This section summarizes the state-of-the-art interface treatment between the fluid and porous medium from a decoupled and coupled point of view.

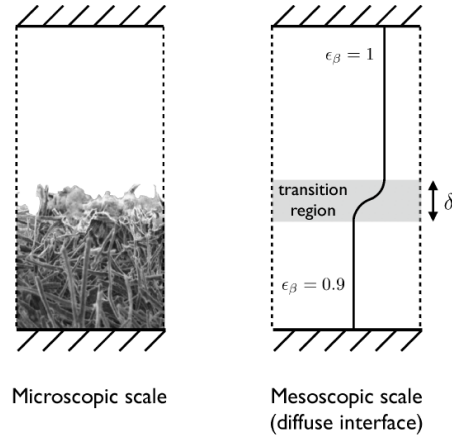
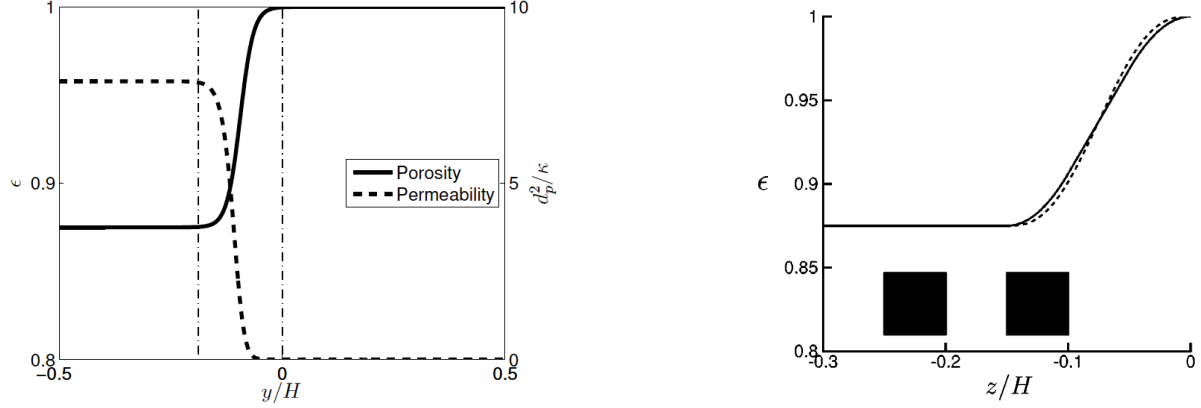


Figure 2.3: Diffuse interface illustration at a mesoscopic scale. The figure is taken from Schroyen [2016].

When defining fluid and porous medium as decoupled entities, one must regard proper boundary conditions between each phase. Betchen et al. [2006] utilized a Finite Volume (FV) method to solve the porous medium and the fluid in a conjugated manner, imposing continuity of velocity, normal and tangent stress, pressure, temperature, and heat flux as boundary conditions at the interface. Ochoa-Tapia and Whitaker [1995a,b] considered a momentum jump between both phases to deem the presence of the interface thickness. They derived the momentum jump in terms of slip coefficients to model the excess of the viscous stress in this thickness. Alazmi and Vafai [2001] have carried out a parametric study on diverse interface models regarding slip and no-slip boundary conditions under different flow conditions, both for momentum and energy. They have observed small disparities in the velocity field between the two types of boundary conditions and almost none for the temperature field.

When deeming an intrinsic coupling between each phase, one must consider the transition thickness and

the variation of effective properties at the macroscale. [Schrooyen \[2016\]](#) modeled the macroscale change of the porosity using a Heaviside step function based on a computational mesh size constraint and utilized the Carman-Kozeny model [\[Dullien, 2012\]](#) to estimate permeability (fig. 2.4a). Using filtering techniques, [Breugem \[2004\]](#) derived porosity and permeability across the interface for a ordered porous medium made of cartesian grid of cubes (fig. 2.4b) utilizing DNS-type simulations [\[Breugem et al., 2004\]](#). Using the cellular filter, they have estimated an interface thickness of three times the cube length, asserting that one can expect a much more extensive interface thickness for a disordered porous medium. Moreover, [Breugem \[2004\]](#) derived the slip coefficients based on DNS-type simulations for an ordered porous medium. Finally, [Breugem and Boersma \[2005\]](#), [Breugem et al. \[2006\]](#) have studied the interface behavior in turbulent conditions, allowing them to deduce Forchheimer terms.



(a) Porosity and permeability across the interface taken from [Schrooyen \[2016\]](#)

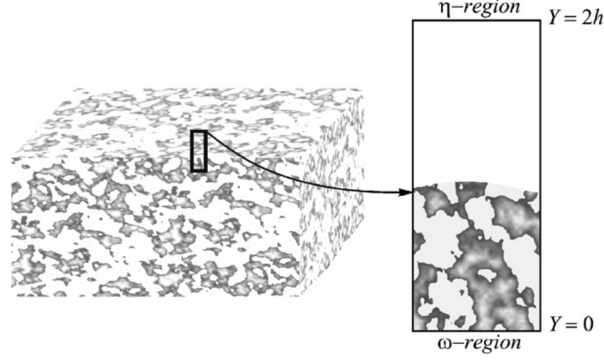
(b) Porosity across the interface for a grid of cubes. Figure taken from [Breugem and Boersma \[2005\]](#)

Figure 2.4: Porosity variation across the interface

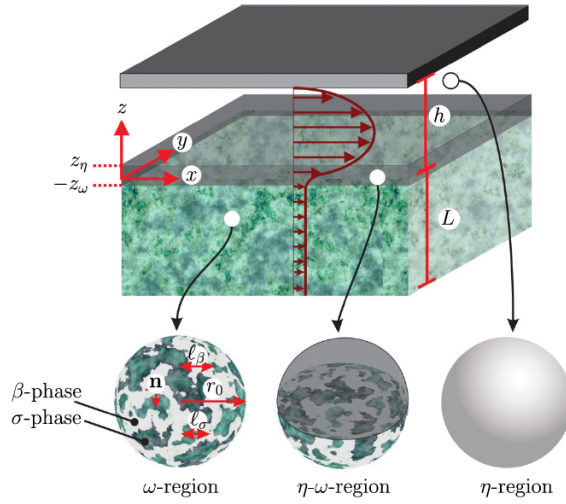
Using a one-domain approach, [Valdés-Parada et al. \[2007, 2010\]](#) derived effective diffusion coefficient including tortuosity effects. They solved the porous-scale concentration equation as a boundary-value problem in the interface region as in fig. 2.5a, obtaining the so-called mapping variables allowing them to close the macroscale equations. [Valdés-Parada et al. \[2009\]](#) derived the jump coefficients at the interface for the Beavers-Joseph problem from one-domain simulations. They deduced that these coefficients occur due to the velocity gradient from the different phases thanks to a change in porosity and permeability. [Valdés-Parada and Lasseux \[2021\]](#) derived effective permeability across the interface for a simplified microstructure considering rarefied effects in the porous medium. As depicted in fig. 2.5b, the domain was divided into three regions, a homogeneous fluid and porous medium and an interface region. By solving the porous-scale equations in the three areas, they derived a spatial distribution of the permeability. Finally, they concluded that the porous microstructure greatly affects the flow within the homogeneous porous medium and the interface region.

2.1.2 TPS modeling

We have highlighted the different modeling strategies concerning the flow and material coupling for TPS design at the beginning of chapter 2. An essential feature of this coupling is the **Gas-Surface Interaction (GSI)**, leading to the ablation phenomenon. The ablation phenomenon considers both the phenolic resin decomposition and the carbon fiber's recession in the case of **PICA**, or only the latter in the case of **FiberForm®**. Many researchers have modeled phenolic resin decomposition through a series of competitive reactions [\[Lachaud et al., 2017, Park et al., 2010\]](#). The decomposition reaction rates have been derived experimentally for different heating rates by [Bessire and Minton \[2017\]](#) and [Torres-Herrador et al. \[2019, 2020a\]](#), and calibrated through an optimization procedure by [Torres-Herrador et al. \[2020b\]](#). This section will focus on the state-of-the-art concerning TPS ablation, specifically, the modeling and experimental research on carbon fibers'



(a) One-domain approach at the interface. Figure taken from [Valdés-Parada et al. \[2007\]](#)



(b) One-domain approach for the Beavers-Joseph problem. Figure taken from [Valdés-Parada and Lasseux \[2021\]](#)

Figure 2.5: One-domain approach to derive effective properties.

oxidation.

Fiber oxidation

Since the beginning of **TPS** design and modeling, the heat of ablation model was one of the first engineering models used. It predicts the material recession rate based on the net heat flux and the material's effective heat of ablation [[Milos and Rasky, 1994](#)]. This model gives good approximations at high-heating conditions and for low thermal conductivity materials – where the steady-state is a good approximation – but it fails to provide a surface temperature estimation.

A need for more accurate predictions led to the thermochemical ablation model, often known as the *B'* model. Currently, it is one of the most general and widely applicable **TPS** ablation models primarily for the decoupled [[Meurisse et al., 2018](#), [Lachaud et al., 2017](#), [Chen and Milos, 2005](#)] and weak coupling approach [[Chen et al., 2019](#)]. This model assumes that the material and the surrounding environment are in thermochemical equilibrium [[Milos and Chen, 1997](#)] coupled with **Surface Mass Balance (SMB)** and **Surface Energy Balance (SEB)** written in terms of thin-film coefficients. Although this model does not require detailed gas-surface reactions, it often over-predicts the surface recession [[Bianchi et al., 2010, 2011](#), [Candler, 2019](#)] due to the equilibrium assumption, especially in low-pressure conditions. Another shortcoming

of this model is the low fidelity prediction of the chemical species created at the surface and blown into the flow field, impacting the surrounding environment. Moreover, these gas species, such as carbonaceous and polyaromatic hydrocarbons, have a strong radiative signature, increasing the surface radiative heat flux and altering the surface temperature [Johnston et al., 2012, Brandis and Johnston, 2014, Johnston and Brandis, 2015, Soucasse et al., 2016, Brandis et al., 2020].

For the last 30 years, GSI models have been shifting towards a finite-rate approach that can better predict the chemical species created due to ablation. An SMB is written for each chemical species and directly coupled to the flow solver as boundary conditions [MacLean et al., 2011, Bianchi et al., 2013, Turchi, 2013], requiring a closure to represent the surface ablation. The *Park model* [Park, 1993, Park et al., 2001] is one of the most used closures. This phenomenological model is based on the premise that a flux of particles (oxygen and nitrogen) impinges on the surface and reacts with a certain probability – where the probability coefficients can be derived with a experimental-numerical approach [Helber et al., 2015a] – causing oxidation and nitridation of the carbonaceous surface. The phenomenological *Park model* is too simplistic in describing the surface reactions. Inspired by catalysis modeling, Zhukov and Abe [1999] derived a finite-rate model (Zhukov-Abe (ZA) model) that considers adsorption-desorption, Eley-Rideal, and Langmuir-Hinshelwood reactions. The ZA model considers active sites [Guerra, 2007] – a region on the surface where chemical reactions occur, and they can be empty or not – as pseudo-species into the gas-surface reactions. This approach allows modeling simultaneously catalysis and ablation and considers inert phases. Later, Marshall and MacLean [2011] generalized the ZA model and derived accurate oxidation rates from experimental data. Based on the ZA model, Poovathingal et al. [2017] derived oxidation rates that include surface-coverage dependence from molecular beam experiments carried out by Murray et al. [2015]. Using the Direct Simulation Monte Carlo (DSMC) method, Swaminathan-Gopalan et al. [2018], Swaminathan-Gopalan and Stephani [2019] improved the oxidation model derived by Poovathingal et al. [2017] by accurately representing the time-of-flight (TOF) and angular distributions from the molecular beam experimental data.

Oxidation experiments

Flight experiments are an expensive approach to obtaining experimental data that allows the validation of physical models and computational tools. Therefore, ground test facilities, able to reproduce the flight aerothermodynamic environment [Barbante and Chazot, 2006], are the best invaluable tool a researcher has to obtain validation data [Chazot and Panerai, 2015]. Amid the different facilities, plasma wind tunnels (arc-jet and Inductively coupled plasma (ICP) facilities) are used to reproduce the aerothermodynamic environment and the GSI phenomena. ICP facilities are known for creating a pure flow with little contamination. Among several, we can highlight the von Karman Institute for fluid dynamics (VKI) Plasmatron (currently the most powerful in the world [Bottin et al., 1999]) and the recently built University of Illinois Urbana-Champaign (UIUC) PlasmatronX. The former has been widely used to study the ablation phenomena for carbonaceous materials [Helber et al., 2014a,b, 2015b]. Arc-jet facilities allow bigger-sized models and higher heating rates, but the flow is not entirely pure due to electrode erosion. Since the beginning of space exploration, the NASA ARC arc-jet [Tran, 1994] has been one of the most extensive facilities for the heatshield design [Smith and Younker, 2005, Gokcen et al., 2010, Hiester and Clark, 1968]. Although, in principle, these facilities can reproduce the flight conditions, it is often difficult to understand their operating conditions. Moreover, considering all the coupled physical aspects inherent to hypersonic flows, it is pretty challenging to validate a specific physical model such as the carbon fibers’ oxidation. Therefore, experiments in a controlled environment are needed to study particular problems that can help to interpret the experiments in large facilities.

The experiment carried out by Murray et al. [2015] is a great example where a molecular beam of O and O₂ was directed at a heated vitreous carbon surface. The scattering and reactive products such as O, O₂, CO, and CO₂ were measured for different TOF and angular distributions. These experiments are a reference for the derivation of oxidation rates. Another example of a controlled experiment is the flow-tube experiment carried out by Panerai et al. [2014a], where a cylinder FiberForm[®] sample was inserted into a quartz main tube. The sample was subjected to a pure oxygen environment where the mass flow was carefully measured. These experiments enabled time-resolved experimental data of the fibers’ oxidation and a better insight into the competition between volume and surface ablation. Using the same experimental set-up, Panerai et al. [2016] derived FiberForm[®] permeability in an argon flow at low pressures, which allowed them to deduce

the Klinkenberg parameters.

Chapter 3

Derivation of the Volume Average Navier-Stokes (VANS) equations

3.1 Governing equations (GE) for hypersonic flows

The conservation equations for a reacting gas flow – also denoted as β phase from hereafter – yield,

$$\partial_t \begin{pmatrix} \rho_i \\ \rho \mathbf{u} \\ \rho E \end{pmatrix}^\beta + \nabla \cdot \begin{pmatrix} \rho_i \mathbf{u} \\ \rho \mathbf{u} \otimes \mathbf{u} + p \bar{\mathbf{I}} \\ \rho \mathbf{u} E + p \mathbf{u} \end{pmatrix}^\beta + \nabla \cdot \begin{pmatrix} \mathbf{J}_i \\ \bar{\boldsymbol{\tau}} \\ \bar{\boldsymbol{\tau}} \cdot \mathbf{u} + \mathbf{q} \end{pmatrix}^\beta = \begin{pmatrix} \dot{\omega}_i^{\text{chem}} \\ 0 \\ 0 \end{pmatrix}^\beta, \quad (3.1)$$

where the first, second and third equation are respectively the mass for species $i \in \mathcal{G}$, the mixture momentum and the mixture total energy. Equation (3.1) is valid both in thermal equilibrium where the energy of the internal modes is characterized with same temperature as the translational mode $T = T^R = T^V = T^E = T_e$. In this case, we say that the internal energy levels of the atoms and molecules follow a Maxwell-Boltzmann distribution at temperature T .

The total energy per unit volume is written as

$$\rho E = \rho e + \rho \frac{\mathbf{u} \cdot \mathbf{u}}{2}$$

with ρ being the mixture mass density and the total internal energy of the mixture is defined as,

$$\rho e = \sum_{i \in \mathcal{H}} \rho_i e_i(T) + \rho_e e_e^T(T),$$

where ρ_e and e_e^T are respectively the electron density and the electron internal energy. The internal energy for the heavy species $\mathcal{H}$ is defined as,

$$\begin{cases} e_i^T(T) + e_i^E(T) + e_i^F, & \forall i \in \mathcal{A}, \\ e_i^T(T) + e_i^R(T) + e_i^V(T) + e_i^E(T) + e_i^F, & \forall i \in \mathcal{M}, \end{cases} \quad (3.2)$$

where the superscripts T, V, R, and E represent the translational, vibrational, rotational, and electronic modes, $\mathcal{A}$ represents the set of atoms, and $\mathcal{M}$ is the set of molecules. The term e_i^F represents the formation energy of the species i at 298 K. The pressure is retrieved with the perfect gas law as $p = \sum_{i \in \mathcal{H}} \rho_i R_i T + \rho_e R_e T$, where R_i is the perfect gas constant of the species i .

The viscous stress tensor reads,

$$\bar{\boldsymbol{\tau}} = \mu \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} \nabla \cdot \mathbf{u} \bar{\mathbf{I}} \right]. \quad (3.3)$$

where μ is the multicomponent shear viscosity obtained through a multiscale Chapman-Enskog perturbative solution of the Boltzmann equation [Vincenti and Kruger, 1965, Ferziger and Kaper., 1972]. The heat flux yields,

$$\mathbf{q} = \sum_{j \in \mathcal{S}} \mathbf{J}_j h_j + \left(\lambda^{\text{T}_h} + \lambda^{\text{R}} + \lambda^{\text{V}} + \lambda^{\text{E}} + \lambda^{\text{T}_e} \right) \nabla T \quad (3.4)$$

where $\mathbf{J}_i = \rho_i \mathbf{V}_i$ corresponds to the diffusion flux of species i . The diffusion velocity $\mathbf{V}_i$ is obtained by solving the Stefan-Maxwell system [Magin, 2004] or by considering the multicomponent diffusion matrix D_{ij} , as shown by Giovangigli [1999],

$$\mathbf{V}_i = \sum_{j \in \mathcal{G}} D_{ij} \mathbf{d}_j, \quad \forall i \in \mathcal{G}. \quad (3.5)$$

where the driving forces, neglecting thermo- and baro-diffusion, are written as,

$$\mathbf{d}_i = \nabla x_i, \quad \forall i \in \mathcal{G}. \quad (3.6)$$

Finally, λ^{R} , λ^{V} , and λ^{E} are the rotational, vibrational, electronic and electron (translational motion) thermal conductivities, respectively. The thermal conductivity for each internal mode is given by the Eucken correction,

$$\begin{aligned} \lambda^{\text{R}} &= \sum_{j \in \mathcal{M}} \frac{\rho_j c_j^{\text{R}}}{\sum_{j \in \mathcal{H}} x_j / \mathcal{D}_{ij}}, \\ \lambda^{\text{V}} &= \sum_{j \in \mathcal{M}} \frac{\rho_j c_j^{\text{V}}}{\sum_{j \in \mathcal{H}} x_j / \mathcal{D}_{ij}}, \\ \lambda^{\text{E}} &= \sum_{j \in \mathcal{H}} \frac{\rho_j c_j^{\text{E}}}{\sum_{j \in \mathcal{H}} x_j / \mathcal{D}_{ij}}, \end{aligned}$$

where c_i^{R} , c_i^{V} and c_i^{E} are the rotational, vibrational, and electronic species specific heats per particle, respectively. Expressions for the thermal conductivity of the heavy particles λ^{T_h} and of the electron translational mode λ^{T_e} are provided by Magin [2004] and Scoggins [2017].

In multiphase flows, one must consider the governing equations for the condensed phase, i.e., the solid and liquid phase. Therefore, we write the mass, momentum and energy conservation equations for the condensed phase – denoted as σ from hereafter – such that,

$$\partial_t \begin{pmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{pmatrix}^\sigma + \nabla \cdot \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \otimes \mathbf{u} + p \bar{\mathbf{I}} \\ \rho \mathbf{u} E + p \mathbf{u} \end{pmatrix}^\sigma + \nabla \cdot \begin{pmatrix} 0 \\ \bar{\boldsymbol{\tau}} \\ \bar{\boldsymbol{\tau}} \cdot \mathbf{u} + \mathbf{q} \end{pmatrix}^\sigma = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}^\sigma, \quad (3.7)$$

in the case of a solid phase, the velocity vector $\mathbf{u}$ is zero.

Equations (3.1) and (3.7) are cast in a compact form yielding,

$$\partial_t \mathbf{U} + \nabla \cdot \mathbf{F}^{\text{inv}} + \nabla \cdot \mathbf{F}^{\text{vis}} = \mathbf{S} \quad (3.8)$$

where the vector $\mathbf{U}$ denotes the volume-specific balance quantities, $\mathbf{F}^{\text{inv}}$ are the inviscid fluxes, $\mathbf{F}^{\text{vis}}$ are the viscous fluxes and $\mathbf{S}$ the source terms.

3.2 VANS equations

In this section, we first derive the VANS operators, allowing us to average the governing equations. The VANS equations are general for any porous material made of carbon fibers subjected to ablation. Moreover, it is trivial to include additional macroscale phases such as phenolic resin and melting materials with the present formulation.

Derivation of the **VANS** operators

Let us consider a **Representative Elementary Volume (REV)** (depicted in fig. 3.1) of radius r_0 – composed by a σ - and a β -phase such that $V = V_\beta + V_\sigma$ – centered at a location $\mathbf{x}$, $\boldsymbol{\zeta}$ it is the local coordinate and

$$\mathbf{r} = \mathbf{x} + \boldsymbol{\zeta}.$$

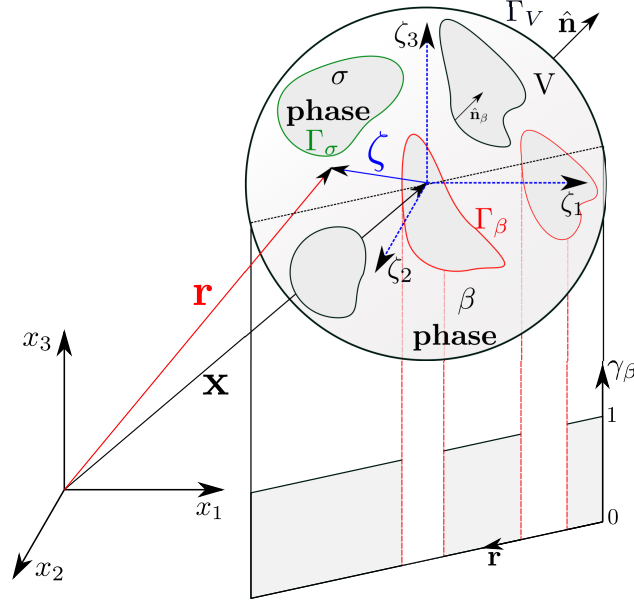


Figure 3.1: Local volume V contains β , and σ phases, and the phase-indicator function γ of the β phase.

We define a generic quantity ψ^α in the α -phase [Gray and Lee, 1977] as

$$\psi_\alpha(\mathbf{r}, t) = \psi^\alpha(\mathbf{r}, t) \gamma_\alpha(\mathbf{r}, t), \quad \text{where } \alpha = \{\beta, \sigma\}, \quad (3.9)$$

and γ_α is the phase indicator, i.e.,

$$\gamma_\alpha(\mathbf{r}, t) = \begin{cases} 1, & \mathbf{r} \text{ in } \alpha\text{-phase} \\ 0, & \text{Otherwise,} \end{cases} \quad (3.10)$$

and the phase average is the convolution product of the filter weighting function m and the quantity ψ in the α -phase yielding,

$$\langle \psi_\alpha \rangle|_{\mathbf{x}}^{\mathbf{V}} \equiv m * \psi_\alpha|_{\mathbf{x}} = \frac{1}{V} \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \psi^\alpha(\mathbf{r}, t) \gamma_\alpha(\mathbf{r}, t) d^3\mathbf{r}, \quad (3.11)$$

where the filter weighting function for disordered porous media is [Quintard and Whitaker, 1994a,c],

$$m(\mathbf{x} - \mathbf{r}) = \begin{cases} 1, & |\mathbf{x} - \mathbf{r}| < r_0 \\ 0, & |\mathbf{x} - \mathbf{r}| \geq r_0. \end{cases} \quad (3.12)$$

The **REV** volume fraction of the α -phase (or porosity for the gas phase) is defined as,

$$\varepsilon_\alpha \equiv m * \gamma_\alpha|_{\mathbf{x}} = \frac{1}{V} \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \gamma_\alpha(\mathbf{r}, t) d^3\mathbf{r} = \frac{V_\alpha}{V} \quad (3.13)$$

Finally, the intrinsic average is

$$\langle \psi_\alpha \rangle|_{\mathbf{x}} \equiv \frac{m * \psi_\alpha|_{\mathbf{x}}}{m * \gamma_\alpha|_{\mathbf{x}}} = \frac{1}{V_\alpha} \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \psi^\alpha(\mathbf{r}, t) \gamma_\alpha(\mathbf{r}, t) d^3\mathbf{r}, \quad (3.14)$$

leading to the relation between the phase and intrinsic average,

$$\langle \psi_\alpha \rangle^{\mathbf{V}} = \varepsilon_\alpha \langle \psi_\alpha \rangle. \quad (3.15)$$

An essential ingredient of the VANS equations is the average of the differential operators (spatial and temporal) that appear in the governing equations. We first determine the average gradient of a quantity ψ^α as,

$$\langle \nabla \psi_\alpha \rangle_{\mathbf{x}}^{\mathbf{V}} \equiv m * \nabla \psi_\alpha|_{\mathbf{x}} = \frac{1}{V} \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \nabla_{\mathbf{r}} \psi^\alpha(\mathbf{r}, t) \gamma_\alpha(\mathbf{r}, t) d^3 \mathbf{r}$$

and from eq. (3.9), we write the equation above as,

$$\langle \nabla \psi_\alpha \rangle_{\mathbf{x}}^{\mathbf{V}} = \frac{1}{V} \int_{\mathbb{R}^3} m(-\zeta) \nabla_{\zeta} \psi^\alpha(\mathbf{x} + \zeta, t) \gamma_\alpha(\mathbf{x} + \zeta, t) d^3 \zeta$$

and since m is an even function,

$$\begin{aligned} \langle \nabla \psi_\alpha \rangle_{\mathbf{x}}^{\mathbf{V}} &= \frac{1}{V} \int_{\mathbb{R}^3} m(\zeta) \nabla_{\zeta} \psi^\alpha(\mathbf{x} + \zeta, t) \gamma_\alpha(\mathbf{x} + \zeta, t) d^3 \zeta \\ &= \frac{1}{V} \int_{\mathbb{R}^3} \nabla_{\zeta} [m(\zeta) \psi^\alpha(\mathbf{x} + \zeta, t) \gamma_\alpha(\mathbf{x} + \zeta, t)] d^3 \zeta \\ &\quad - \frac{1}{V} \int_{\mathbb{R}^3} m(\zeta) \psi^\alpha(\mathbf{x} + \zeta, t) \nabla_{\zeta} \gamma_\alpha(\mathbf{x} + \zeta, t) d^3 \zeta \\ &\quad - \frac{1}{V} \int_{\mathbb{R}^3} \nabla_{\zeta} m(\zeta) \psi^\alpha(\mathbf{x} + \zeta, t) \gamma_\alpha(\mathbf{x} + \zeta, t) d^3 \zeta. \end{aligned} \quad (3.16)$$

If we make another change of variables and consider the chain rule such that,

$$\partial_x(\bullet) = -\partial_{\zeta}(\bullet) \quad \text{and} \quad \partial_r(\bullet) = \partial_{\zeta}(\bullet) \quad (3.17)$$

eq. (3.16) can be written as,

$$\begin{aligned} \langle \nabla \psi_\alpha \rangle_{\mathbf{x}}^{\mathbf{V}} &= \frac{1}{V} \int_{\Gamma_{\mathbf{V}}} m(\zeta) \psi^\alpha(\mathbf{x} + \zeta, t) \gamma_\alpha(\mathbf{x} + \zeta, t) \hat{\mathbf{n}} d\Gamma_{\mathbf{V}} \\ &\quad - \frac{1}{V} \int_{\mathbb{R}^3} m(\mathbf{r} - \mathbf{x}) \psi^\alpha(\mathbf{r}, t) \nabla_{\mathbf{r}} \gamma_\alpha(\mathbf{r}, t) d^3 \mathbf{r} \\ &\quad + \frac{1}{V} \int_{\mathbb{R}^3} \nabla_{\mathbf{x}} m(\mathbf{r} - \mathbf{x}) \psi^\alpha(\mathbf{r}, t) \gamma_\alpha(\mathbf{r}, t) d^3 \mathbf{r} \end{aligned} \quad (3.18)$$

where the first term on the right-hand side cancels due to the compact support definition given by eq. (3.12).

The gradient of a step function, such as the γ_α , yields,

$$\nabla \gamma_\alpha(\mathbf{r}) = -\hat{\mathbf{n}}_\alpha \delta_\alpha(\mathbf{r} - \mathbf{r}_{\Gamma_\alpha})$$

where δ is the Dirac delta function and substituting the relation above into eq. (3.18) yields,

$$\begin{aligned} \langle \nabla \psi_\alpha \rangle_{\mathbf{x}}^{\mathbf{V}} &= \nabla_x \left[\frac{1}{V} \int_{\mathbb{R}^3} m \psi^\alpha \gamma_\alpha d^3 \mathbf{r} \right] + \frac{1}{V} \int_{\mathbb{R}^3} m \psi^\alpha \hat{\mathbf{n}}_\alpha \delta_\alpha d^3 \mathbf{r} \\ &= \nabla_x \left[\frac{1}{V} \int_{\mathbb{R}^3} m \psi^\alpha \gamma_\alpha d^3 \mathbf{r} \right] - \frac{1}{V} \oint_{\Gamma_\alpha} m(\mathbf{r}_{\Gamma_\alpha}) \psi_\alpha(\mathbf{r}_{\Gamma_\alpha}) d\Gamma_{\varphi \setminus \alpha} \\ &= \nabla_x \left[\frac{1}{V} \int_{\mathbb{R}^3} m \psi^\alpha \gamma_\alpha d^3 \mathbf{r} \right] - \frac{1}{V} \oint_{\Gamma_\varphi} m \psi_\alpha \hat{\mathbf{n}}_\varphi d\Gamma_\varphi \\ &= \nabla_x \left[\frac{1}{V} \int_{\mathbb{R}^3} m \psi^\alpha \gamma_\alpha d^3 \mathbf{r} \right] + \frac{1}{V} \oint_{\Gamma_\alpha} m \psi_\alpha \hat{\mathbf{n}}_\alpha d\Gamma_\alpha \\ &= \nabla \langle \psi_\alpha \rangle^{\mathbf{V}} + \frac{1}{V} \oint_{\Gamma_\alpha} m \psi_\alpha \hat{\mathbf{n}}_\alpha d\Gamma_\alpha. \end{aligned} \quad (3.19)$$

The same averaging theorem can be applied to the divergence operator leading to,

$$\langle \nabla \cdot \psi_\alpha \rangle_{\mathbf{x}}^{\mathbf{V}} = \nabla \cdot \langle \psi_\alpha \rangle^{\mathbf{V}} + \frac{1}{V} \oint_{\Gamma_\alpha} m \psi_\alpha \cdot \hat{\mathbf{n}}_\alpha d\Gamma_\alpha. \quad (3.20)$$

The last step consists in deriving the time derivative operator, and as in the previous examples, we start by defining,

$$\begin{aligned} \langle \partial_t \psi_\alpha \rangle_{\mathbf{x}}^{\mathbf{V}} &\equiv m * \partial_t \psi_\alpha|_{\mathbf{x}} = \frac{1}{V} \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \partial_t \psi^\alpha(\mathbf{r}, t) \gamma_\alpha(\mathbf{r}, t) d^3\mathbf{r} \\ &= \frac{1}{V} \int_{\mathbb{R}^3} m \partial_t(\psi^\alpha \gamma_\alpha) d^3\mathbf{r} - \frac{1}{V} \int_{\mathbb{R}^3} m \psi^\alpha \partial_t \gamma_\alpha d^3\mathbf{r}. \end{aligned} \quad (3.21)$$

In a reference frame attached to the surface where the observer sees no change, the material derivative yields,

$$\begin{aligned} \frac{d\gamma_\alpha}{dt} &= 0 = \frac{\partial \gamma_\alpha}{\partial t} + \mathbf{u}_\Gamma \cdot \nabla \gamma_\alpha \Rightarrow \\ \frac{\partial \gamma_\alpha}{\partial t} &= -\mathbf{u}_\Gamma \cdot \nabla \gamma_\alpha \\ &= \mathbf{u}_\Gamma \cdot \hat{\mathbf{n}}_\alpha \delta_\alpha. \end{aligned} \quad (3.22)$$

Considering the equation above and the fact that the volume V is time-independent eq. (3.21) can be written as,

$$\begin{aligned} \langle \partial_t \psi_\alpha \rangle_{\mathbf{x}}^{\mathbf{V}} &= \partial_t \langle \psi_\alpha \rangle^{\mathbf{V}} + \frac{1}{V} \int_{\mathbb{R}^3} m \psi^\alpha \mathbf{u}_\Gamma \cdot \nabla \gamma_\alpha d^3\mathbf{r} \\ &= \partial_t \langle \psi_\alpha \rangle^{\mathbf{V}} - \frac{1}{V} \int_{\mathbb{R}^3} m \psi^\alpha \mathbf{u}_\Gamma \cdot \hat{\mathbf{n}}_\alpha \delta_\alpha d^3\mathbf{r} \\ &= \partial_t \langle \psi_\alpha \rangle^{\mathbf{V}} + \frac{1}{V} \oint_{\Gamma_\alpha} m \psi_\alpha \mathbf{u}_\Gamma \cdot d\Gamma_{\varphi \setminus \alpha} \\ &= \partial_t \langle \psi_\alpha \rangle^{\mathbf{V}} - \frac{1}{V} \oint_{\Gamma_\alpha} m \psi_\alpha \mathbf{u}_\Gamma \cdot \hat{\mathbf{n}}_\alpha d\Gamma_\alpha. \end{aligned} \quad (3.23)$$

The porous-scale quantity is decomposed into an average and a dispersion term [Quintard and Whitaker, 1994a, Gray, 1975], yielding,

$$\psi_\alpha(\mathbf{r}, t) = \gamma_\alpha(\mathbf{r}, t) \langle \psi_\alpha \rangle(\mathbf{r}, t) + \tilde{\psi}_\alpha(\mathbf{r}, t), \quad (3.24)$$

also known as *decomposition of length scales*, where the average and the dispersion represent the quantity variation at the large and small length scales [Whitaker, 1999], respectively.

It is important to remark on two aspects:

- since ψ_α is a discontinuous quantity, due to the presence of condensed phases, it is essential to include the phase indicator γ in eq. (3.24), as pointed out by Mansour et al. [2022],
- it is paramount to consider the intrinsic average in eq. (3.24); otherwise, the dispersion term is non-zero even if the porous scale quantity is uniform [Gray, 1975].

Since the terms evaluated at $\mathbf{r}$ are not constant within the volume, one has to expand the terms on the right-hand side of eq. (3.24) using a Taylor series such that any property ψ is written as,

$$\langle \psi_\alpha \rangle_{\mathbf{r}} = \langle \psi_\alpha \rangle_{\mathbf{x}} + (\mathbf{r} - \mathbf{x}) \cdot \nabla \langle \psi_\alpha \rangle_{\mathbf{x}} + \frac{1}{2} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) : \nabla \nabla \langle \psi_\alpha \rangle_{\mathbf{x}}. \quad (3.25)$$

By intrinsically averaging eq. (3.24),

$$\langle \psi_\alpha \rangle_{\mathbf{x}} = \langle \gamma_\alpha \langle \psi_\alpha \rangle_{\mathbf{r}} \rangle + \left\langle \tilde{\psi}_\alpha \right\rangle_{\mathbf{r}} \quad (3.26)$$

and inserting eq. (3.25) in the above, one gets the intrinsic average of the dispersion terms,

$$\begin{aligned} \overline{\langle \psi_\alpha \rangle_{\mathbf{r}}} &= \overline{\langle \psi_\alpha \rangle_{\mathbf{x}}} + \langle (\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \psi_\alpha \rangle_{\mathbf{x}} + \frac{1}{2} \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle : \nabla \nabla \langle \psi_\alpha \rangle_{\mathbf{x}} + \left\langle \tilde{\psi}_\alpha \right\rangle_{\mathbf{r}} \Rightarrow \\ \left\langle \tilde{\psi}_\alpha \right\rangle_{\mathbf{r}} &= -\langle (\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \psi_\alpha \rangle_{\mathbf{x}} - \frac{1}{2} \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle : \nabla \nabla \langle \psi_\alpha \rangle_{\mathbf{x}}. \end{aligned} \quad (3.27)$$

where the average of the dispersion is commonly referred to as the residual.

Note

Using the intrinsic average definition given by eq. (3.14), the average of the average in eq. (3.24) yields,

$$\langle \gamma_\alpha \langle \psi_\alpha \rangle \rangle|_{\mathbf{x}} = \frac{1}{V_\alpha} \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \langle \psi_\alpha \rangle(\mathbf{r}, t) \gamma_\alpha^2(\mathbf{r}, t) d^3\mathbf{r},$$

and by definition [Mansour et al., 2022],

$$\gamma_\alpha^n = \gamma_\alpha.$$

The phase indicator function γ will be omitted from the average integral to ease the notation.

Applying the convolution from eq. (3.11) to the governing equation in eq. (3.8) one obtains,

$$\begin{aligned} m*[\partial_t \mathbf{U}_\beta + \nabla \cdot \mathbf{F}_\beta^{\text{inv}} + \nabla \cdot \mathbf{F}_\beta^{\text{vis}} = \mathbf{S}_\beta] &\Rightarrow \\ \langle \partial_t \mathbf{U}_\beta \rangle^{\mathbf{V}} + \langle \nabla \cdot \mathbf{F}_\beta^{\text{inv}} \rangle^{\mathbf{V}} + \langle \nabla \cdot \mathbf{F}_\beta^{\text{vis}} \rangle^{\mathbf{V}} &= \langle \mathbf{S}_\beta \rangle^{\mathbf{V}}. \end{aligned} \quad (3.28)$$

and utilizing the averaging properties describe above,

$$\begin{aligned} \partial_t \langle \mathbf{U}_\beta \rangle^{\mathbf{V}} - \frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{F}_\beta^\Gamma \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta + \nabla \cdot \langle \mathbf{F}_\beta^{\text{inv}} \rangle^{\mathbf{V}} + \frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{F}_\beta^{\text{inv}} \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta \\ + \nabla \cdot \langle \mathbf{F}_\beta^{\text{vis}} \rangle^{\mathbf{V}} + \frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{F}_\beta^{\text{vis}} \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \langle \mathbf{S}_\beta \rangle^{\mathbf{V}}. \end{aligned} \quad (3.29)$$

where,

$$\mathbf{F}^\Gamma = [\rho \mathbf{u}_\Gamma, \rho \mathbf{u} \otimes \mathbf{u}_\Gamma, \rho E \mathbf{u}_\Gamma]^T$$

Finally, utilizing the definition in eq. (3.15), eq. (3.29) becomes,

$$\begin{aligned} \partial_t \varepsilon_\beta \langle \mathbf{U}_\beta \rangle - \frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{F}_\beta^\Gamma \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta + \nabla \cdot \varepsilon_\beta \langle \mathbf{F}_\beta^{\text{inv}} \rangle + \frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{F}_\beta^{\text{inv}} \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta \\ + \nabla \cdot \varepsilon_\beta \langle \mathbf{F}_\beta^{\text{vis}} \rangle + \frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{F}_\beta^{\text{vis}} \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \varepsilon_\beta \langle \mathbf{S}_\beta \rangle. \end{aligned} \quad (3.30)$$

The equation above can be further simplified to account for surface balances such that,

$$\begin{aligned} \partial_t \varepsilon_\beta \langle \mathbf{U}_\beta \rangle + \nabla \cdot \varepsilon_\beta \langle \mathbf{F}_\beta^{\text{inv}} \rangle \\ + \nabla \cdot \varepsilon_\beta \langle \mathbf{F}_\beta^{\text{vis}} \rangle + \frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{S}_\beta^{\text{surf}} \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \varepsilon_\beta \langle \mathbf{S}_\beta \rangle. \end{aligned} \quad (3.31)$$

where the vector $\mathbf{S}^{\text{surf}}$ is the surface mass, momentum, and energy balance,

$$\frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{S}_\beta^{\text{surf}} \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \frac{1}{V} \oint_{\Gamma_\beta} m [\mathbf{F}_\beta^{\text{inv}} - \mathbf{F}^\Gamma + \mathbf{F}_\beta^{\text{vis}}]_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta, \quad (3.32)$$

as shown by Delhaye [1974], Ishii and Hibiki [2011], Whitaker [1992], and $[\]_\beta$ corresponds to the surface properties from the β -phase.

We apply the same methodology to the condensed phase σ , yielding,

$$\begin{aligned} \partial_t \varepsilon_\sigma \langle \mathbf{U}_\sigma \rangle + \nabla \cdot \varepsilon_\sigma \langle \mathbf{F}_\sigma^{\text{inv}} \rangle \\ + \nabla \cdot \varepsilon_\sigma \langle \mathbf{F}_\sigma^{\text{vis}} \rangle + \frac{1}{V} \oint_{\Gamma_\sigma} m \mathbf{S}_\sigma^{\text{surf}} \cdot \hat{\mathbf{n}}_\sigma d\Gamma_\sigma = 0. \end{aligned} \quad (3.33)$$

It is essential to separate the different equations since various up-scaling terms appear from this point on.

Species continuity equation

We now use the general **VANS** equation shown in eq. (3.31) to write the species continuity equation,

$$\begin{aligned} \partial_t \varepsilon_\beta \langle \rho_{i\beta} \rangle + \nabla \cdot \varepsilon_\beta \langle \rho_{i\beta} \mathbf{u}_\beta \rangle + \nabla \cdot \varepsilon_\beta \langle \mathbf{J}_{i\beta} \rangle + \\ \frac{1}{V} \oint_{\Gamma_\beta} m [\rho_i(\mathbf{u} - \mathbf{u}_\Gamma) + \mathbf{J}_i]_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \varepsilon_\beta \langle \dot{\omega}_{i,\beta}^{\text{chem}} \rangle, \quad \forall i \in \mathcal{G} \end{aligned} \quad (3.34)$$

we can decompose the second term on the left-hand side of eq. (3.34) by applying the spatial decomposition given by eq. (3.24), such that,

$$\begin{aligned} \langle \rho_{i\beta} \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \left\langle \left(\langle \rho_{i\beta} \rangle|_{\mathbf{r}} + \tilde{\rho}_{i\beta}|_{\mathbf{r}} \right) \left(\langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} + \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \right) \right\rangle \\ &= \left\langle \langle \rho_{i\beta} \rangle|_{\mathbf{r}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} + \langle \rho_{i\beta} \rangle|_{\mathbf{r}} \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} + \tilde{\rho}_{i\beta}|_{\mathbf{r}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} + \tilde{\rho}_{i\beta}|_{\mathbf{r}} \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \right\rangle, \quad \forall i \in \mathcal{G} \end{aligned} \quad (3.35)$$

leading to,

$$\begin{aligned} \langle \rho_{i\beta} \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \underbrace{\left\langle \langle \rho_{i\beta} \rangle|_{\mathbf{r}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} \right\rangle}_{\text{1st term}} + \underbrace{\left\langle \langle \rho_{i\beta} \rangle|_{\mathbf{r}} \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \right\rangle}_{\text{2nd term}} \\ &\quad + \underbrace{\left\langle \tilde{\rho}_{i\beta}|_{\mathbf{r}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} \right\rangle}_{\text{3rd term}} + \underbrace{\left\langle \tilde{\rho}_{i\beta}|_{\mathbf{r}} \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \right\rangle}_{\text{4th term}}, \quad \forall i \in \mathcal{G} \end{aligned} \quad (3.36)$$

where all terms are expanded such that,

1st term

$$\begin{aligned} \left\langle \langle \rho_{i\beta} \rangle|_{\mathbf{r}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} \right\rangle &= \left\langle \left[\langle \rho_{i\beta} \rangle|_{\mathbf{x}} + (\mathbf{r} - \mathbf{x}) \cdot \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} + \frac{1}{2}(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) : \nabla \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \right] \right. \\ &\quad \left. \left[\langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + (\mathbf{r} - \mathbf{x}) \cdot \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \frac{1}{2}(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) : \nabla \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \right] \right\rangle^\beta \end{aligned}$$

2nd term

$$\begin{aligned} \left\langle \langle \rho_{i\beta} \rangle|_{\mathbf{r}} \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \right\rangle &= \left\langle \left[\langle \rho_{i\beta} \rangle|_{\mathbf{x}} + (\mathbf{r} - \mathbf{x}) \cdot \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} + \frac{1}{2}(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) : \nabla \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \right] \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \right\rangle^\beta \\ &= \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \langle \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \rangle + \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \cdot \langle (\mathbf{r} - \mathbf{x}) \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \rangle + \\ &\quad \frac{1}{2} \nabla \nabla \left(\langle \rho_{i\beta} \rangle|_{\mathbf{x}} \right)^\text{T} : \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \rangle \end{aligned}$$

3rd term

$$\begin{aligned} \left\langle \tilde{\rho}_{i\beta}|_{\mathbf{r}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} \right\rangle &= \left\langle \tilde{\rho}_{i\beta}|_{\mathbf{r}} \right\rangle \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \left\langle \tilde{\rho}_{i\beta}|_{\mathbf{r}} (\mathbf{r} - \mathbf{x}) \right\rangle \cdot \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \\ &\quad \frac{1}{2} \left\langle \tilde{\rho}_{i\beta}|_{\mathbf{r}} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \right\rangle : \nabla \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \end{aligned}$$

Putting all terms together and regarding eq. (3.27), the final expression of eq. (3.35) is written as,

$$\begin{aligned} \langle \rho_{i\beta} \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \langle \tilde{\rho}_{i\beta}|_{\mathbf{r}} \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \rangle + (\nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} + \\ &\quad \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \cdot \langle (\mathbf{r} - \mathbf{x}) \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \rangle + \frac{1}{2} \left(\nabla \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \right)^T : \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \tilde{\mathbf{u}}_\beta|_{\mathbf{r}} \rangle + \\ &\quad \langle \tilde{\rho}_{i\beta}|_{\mathbf{r}}(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \frac{1}{2} \langle \tilde{\rho}_{i\beta}|_{\mathbf{r}}(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle : \nabla \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}}, \quad \forall i \in \mathcal{G}. \end{aligned} \quad (3.37)$$

$$\begin{aligned} \langle \mathbf{J}_{i\beta} \rangle|_{\mathbf{x}} &= \langle \rho_{i\beta} \mathbf{V}_{i\beta} \rangle|_{\mathbf{x}} = \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \langle \mathbf{V}_{i\beta} \rangle|_{\mathbf{x}} + \langle \tilde{\rho}_{i\beta}|_{\mathbf{r}} \tilde{\mathbf{V}}_{i\beta}|_{\mathbf{r}} \rangle + (\nabla \langle \mathbf{V}_{i\beta} \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} + \\ &\quad \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \cdot \langle (\mathbf{r} - \mathbf{x}) \tilde{\mathbf{V}}_{i\beta}|_{\mathbf{r}} \rangle + \frac{1}{2} \left(\nabla \nabla \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \right)^T : \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \tilde{\mathbf{V}}_{i\beta}|_{\mathbf{r}} \rangle + \\ &\quad \langle \tilde{\rho}_{i\beta}|_{\mathbf{r}}(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \mathbf{V}_{i\beta} \rangle|_{\mathbf{x}} + \frac{1}{2} \langle \tilde{\rho}_{i\beta}|_{\mathbf{r}}(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle : \nabla \nabla \langle \mathbf{V}_{i\beta} \rangle|_{\mathbf{x}}, \quad \forall i \in \mathcal{G}. \end{aligned} \quad (3.38)$$

$$\begin{aligned} \langle \mathbf{V}_{i\beta} \rangle|_{\mathbf{x}} &= \sum_{j \in \mathcal{G}} \langle D_{ij\beta} \nabla x_{j\beta} \rangle|_{\mathbf{x}} = \sum_{j \in \mathcal{G}} \left[\langle D_{ij\beta} \rangle|_{\mathbf{x}} \langle \nabla x_{j\beta} \rangle|_{\mathbf{x}} + \langle \widetilde{D}_{ij\beta}|_{\mathbf{r}} \nabla \tilde{x}_{j\beta}|_{\mathbf{r}} \rangle + \right. \\ &\quad \left. (\nabla \langle \nabla x_{j\beta} \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle D_{ij\beta} \rangle|_{\mathbf{x}} + \right. \\ &\quad \left. \nabla \langle D_{ij\beta} \rangle|_{\mathbf{x}} \cdot \langle (\mathbf{r} - \mathbf{x}) \nabla \tilde{x}_{j\beta}|_{\mathbf{r}} \rangle + \right. \\ &\quad \left. \frac{1}{2} \left(\nabla \nabla \langle D_{ij\beta} \rangle|_{\mathbf{x}} \right)^T : \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \nabla \tilde{x}_{j\beta}|_{\mathbf{r}} \rangle + \right. \\ &\quad \left. \langle \widetilde{D}_{ij\beta}|_{\mathbf{r}}(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \nabla x_{j\beta} \rangle|_{\mathbf{x}} + \right. \\ &\quad \left. \frac{1}{2} \langle \widetilde{D}_{ij\beta}|_{\mathbf{r}}(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle : \nabla \nabla \langle \nabla x_{j\beta} \rangle|_{\mathbf{x}} \right], \quad \forall i \in \mathcal{G}. \end{aligned} \quad (3.39)$$

Using eq. (3.15), we write the intrinsic average of the driving forces as,

$$\langle \nabla x_{i\beta} \rangle^{\mathbf{V}} = \varepsilon_\beta \langle \nabla x_{i\beta} \rangle, \quad \forall i \in \mathcal{G}, \quad (3.40)$$

and utilizing eq. (3.19),

$$\langle \nabla x_{i\beta} \rangle^{\mathbf{V}} = \nabla \langle x_{i\beta} \rangle^{\mathbf{V}} + \frac{1}{V} \oint_{\Gamma_\beta} m x_{i\beta} \hat{\mathbf{n}}_\beta d\Gamma_\beta, \quad \forall i \in \mathcal{G}$$

and considering the spatial decomposition in eq. (3.24) the equation above is written as,

$$\langle \nabla x_{i\beta} \rangle^{\mathbf{V}} = \nabla(\varepsilon_\beta \langle x_{i\beta} \rangle) + \frac{1}{V} \oint_{\Gamma_\beta} m \langle x_{i\beta} \rangle|_{\mathbf{r}} \hat{\mathbf{n}}_\beta d\Gamma_\beta + \frac{1}{V} \oint_{\Gamma_\beta} m \tilde{x}_{i\beta}|_{\mathbf{r}} \hat{\mathbf{n}}_\beta d\Gamma_\beta \quad (3.41)$$

and using the Taylor series for the second term on the right-hand side of the previous equation,

$$\begin{aligned} \langle \nabla x_{i\beta} \rangle^{\mathbf{V}} &= \varepsilon_\beta \nabla \langle x_{i\beta} \rangle + \cancel{\langle x_{i\beta} \rangle \nabla \varepsilon_\beta} \\ &\quad + \frac{1}{V} \oint_{\Gamma_\beta} m \hat{\mathbf{n}}_\beta d\Gamma_\beta \langle x_{i\beta} \rangle|_{\mathbf{x}} + \frac{1}{V} \oint_{\Gamma_\beta} m(\mathbf{r} - \mathbf{x}) \hat{\mathbf{n}}_\beta d\Gamma_\beta \cdot \nabla \langle x_{i\beta} \rangle|_{\mathbf{x}} \\ &\quad + \frac{1}{2} \frac{1}{V} \oint_{\Gamma_\beta} m(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \hat{\mathbf{n}}_\beta d\Gamma_\beta : \nabla \nabla \langle x_{i\beta} \rangle|_{\mathbf{x}} \\ &\quad + \frac{1}{V} \oint_{\Gamma_\beta} m \tilde{x}_{i\beta}|_{\mathbf{r}} \hat{\mathbf{n}}_\beta d\Gamma_\beta \end{aligned} \quad (3.42)$$

since from eq. (3.19) it follows,

$$\nabla \varepsilon_\beta = -\frac{1}{V} \oint_{\Gamma_\beta} m \hat{\mathbf{n}}_\beta d\Gamma_\beta$$

assuming constant porosity within the volume of integration, and finally,

$$\begin{aligned} \langle \nabla x_{i\beta} \rangle &= \nabla \langle x_{i\beta} \rangle + \frac{1}{V_\beta} \oint_{\Gamma_\beta} m (\mathbf{r} - \mathbf{x}) \hat{\mathbf{n}}_\beta d\Gamma_\beta \cdot \nabla \langle x_{i\beta} \rangle|_{\mathbf{x}} \\ &+ \frac{1}{2} \frac{1}{V_\beta} \oint_{\Gamma_\beta} m (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \hat{\mathbf{n}}_\beta d\Gamma_\beta : \nabla \nabla \langle x_{i\beta} \rangle|_{\mathbf{x}} \\ &+ \frac{1}{V_\beta} \oint_{\Gamma_\beta} m \tilde{x}_{i\beta}|_{\mathbf{r}} \hat{\mathbf{n}}_\beta d\Gamma_\beta \end{aligned} \quad (3.43)$$

Assuming the surface between the σ and β reaches a steady state, the mass balance is equal to the surface heterogeneous reactions [Schrooyen, 2016, Ishii and Hibiki, 2011, Whitaker, 1992] such that,

$$\begin{aligned} \sum_{i \in \mathcal{G}} \frac{1}{V} \oint_{\Gamma_\beta} m [\rho_i (\mathbf{u} - \mathbf{u}_\Gamma) + J_i]_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta &= \frac{1}{V} \oint_{\Gamma_\sigma} m [\rho (\mathbf{u} - \mathbf{u}_\Gamma)]_\sigma \cdot \hat{\mathbf{n}}_\sigma d\Gamma_\sigma = \\ &= \sum_{i \in \mathcal{G}} \frac{1}{V} \oint_{\Gamma_\beta} m \dot{\omega}_i^{\text{het}} d\Gamma_\beta = \langle \dot{\omega}^{\text{het}} \rangle^{\mathbf{V}}, \end{aligned} \quad (3.44)$$

Solid-phase mass equation

We must consider a governing equation for the solid phase σ due to the decomposition of the fibers. The sum of the gas and solid volume fractions yields,

$$\varepsilon_\beta + \varepsilon_\sigma = 1,$$

thus, the governing equation describing the fiber decomposition can be written as,

$$\partial_t \varepsilon_\sigma \rho_\sigma = \langle \dot{\omega}^{\text{het}} \rangle^{\mathbf{V}}.$$

Since the density of the fibers ρ_σ is constant, the equation above yields,

$$\partial_t \varepsilon_\sigma = \frac{\langle \dot{\omega}^{\text{het}} \rangle^{\mathbf{V}}}{\rho_\sigma}, \quad (3.45)$$

which depicts the decomposition rate of the solid volume fraction ε_σ .

Note

In the case of carbon/phenolic materials σ -region can represent both the fibers f-region and the phenolic resin p-region such that,

$$\varepsilon_\sigma = \varepsilon_f + \varepsilon_p,$$

and,

$$\varepsilon_\sigma \rho_\sigma = \varepsilon_f \rho_f + \varepsilon_p \rho_p.$$

Therefore, the surface source term $\dot{\omega}^{\text{het}}$ corresponds to the sum of fibers ablation and the phenolic resin decomposition contributions.

Mixture momentum equation

We now use the general VANS equation shown in eq. (3.31) to write the mixture momentum equation,

$$\begin{aligned} \partial_t \varepsilon_\beta \langle \rho_\beta \mathbf{u}_\beta \rangle + \nabla \cdot \varepsilon_\beta \langle \rho_\beta \mathbf{u}_\beta \otimes \mathbf{u}_\beta \rangle + \nabla \varepsilon_\beta \langle p_\beta \rangle \bar{\mathbf{I}} + \nabla \cdot \varepsilon_\beta \langle \bar{\boldsymbol{\tau}}_\beta \rangle + \\ \frac{1}{V} \oint_{\Gamma_\beta} m [\rho \mathbf{u} \otimes (\mathbf{u} - \mathbf{u}_\Gamma) + p \bar{\mathbf{I}} + \bar{\boldsymbol{\tau}}]_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = 0. \end{aligned} \quad (3.46)$$

The following step consists in analyzing each average term; thus, we first decompose the inviscid flux similarly to the species continuity equation,

$$\begin{aligned}\langle \rho_\beta \mathbf{u}_\beta \otimes \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \left\langle \left(\langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{r}} + \widetilde{\rho_\beta \mathbf{u}_\beta}|_{\mathbf{r}} \right) \otimes \left(\langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} + \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} \right) \right\rangle \\ &= \left\langle \langle \rho_\beta \otimes \mathbf{u}_\beta \rangle|_{\mathbf{r}} \otimes \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} + \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{r}} \otimes \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} + \widetilde{\rho_\beta \mathbf{u}_\beta}|_{\mathbf{r}} \otimes \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}} + \widetilde{\rho_\beta \mathbf{u}_\beta}|_{\mathbf{r}} \otimes \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} \right\rangle,\end{aligned}\quad (3.47)$$

leading to

$$\begin{aligned}\langle \rho_\beta \mathbf{u}_\beta \otimes \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \underbrace{\langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{r}} \otimes \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}}}_{\text{1st term}} + \underbrace{\langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{r}} \otimes \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}}}_{\text{2nd term}} \\ &\quad + \underbrace{\langle \widetilde{\rho_\beta \mathbf{u}_\beta}|_{\mathbf{r}} \otimes \langle \mathbf{u}_\beta \rangle|_{\mathbf{r}}}_{\text{3rd term}} + \underbrace{\langle \widetilde{\rho_\beta \mathbf{u}_\beta}|_{\mathbf{r}} \otimes \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}}}_{\text{4th term}},\end{aligned}\quad (3.48)$$

and finally,

$$\begin{aligned}\langle \rho_\beta \mathbf{u}_\beta \otimes \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} \otimes \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta}|_{\mathbf{r}} \otimes \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} \right\rangle + \\ &\quad (\nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \\ &\quad \nabla \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} \cdot \langle (\mathbf{r} - \mathbf{x}) \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} \rangle + \\ &\quad \frac{1}{2} (\nabla \nabla \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}})^T : \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} \rangle + \\ &\quad \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta}|_{\mathbf{r}} (\mathbf{r} - \mathbf{x}) \right\rangle \cdot \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \\ &\quad \frac{1}{2} \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta}|_{\mathbf{r}} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \right\rangle : \nabla \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}}\end{aligned}\quad (3.49)$$

where $\langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}}$ is obtained through eq. (3.37).

The average of the viscous stress tensor yields,

$$\langle \bar{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}} = \langle \boldsymbol{\mu} \nabla \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \langle \boldsymbol{\mu} (\nabla \mathbf{u}_\beta)^T \rangle|_{\mathbf{x}} - \frac{2}{3} \langle \boldsymbol{\mu} \nabla \cdot \mathbf{u}_\beta \rangle|_{\mathbf{x}} \bar{\mathbf{I}}. \quad (3.50)$$

where the viscous term can be decomposed as,

$$\begin{aligned}\langle \boldsymbol{\mu} \nabla \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \langle \boldsymbol{\mu}_\beta \rangle|_{\mathbf{x}} \langle \nabla \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \left\langle \widetilde{\boldsymbol{\mu}_\beta}|_{\mathbf{r}} \nabla \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} \right\rangle + \\ &\quad (\nabla \langle \nabla \mathbf{u}_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \boldsymbol{\mu}_\beta \rangle|_{\mathbf{x}} + \\ &\quad \nabla \langle \boldsymbol{\mu}_\beta \rangle|_{\mathbf{x}} \cdot \langle (\mathbf{r} - \mathbf{x}) \nabla \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} \rangle + \\ &\quad \frac{1}{2} (\nabla \nabla \langle \boldsymbol{\mu}_\beta \rangle|_{\mathbf{x}})^T : \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \nabla \widetilde{\mathbf{u}_\beta}|_{\mathbf{r}} \rangle + \\ &\quad \left\langle \widetilde{\boldsymbol{\mu}_\beta}|_{\mathbf{r}} (\mathbf{r} - \mathbf{x}) \right\rangle \cdot \nabla \langle \nabla \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \\ &\quad \frac{1}{2} \left\langle \widetilde{\boldsymbol{\mu}_\beta}|_{\mathbf{r}} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \right\rangle : \nabla \nabla \langle \nabla \mathbf{u}_\beta \rangle|_{\mathbf{x}}\end{aligned}\quad (3.51)$$

and the average of the velocity gradient together with a no-slip boundary condition can be written as,

$$\begin{aligned}\langle \nabla \mathbf{u}_\beta \rangle^{\mathbf{V}} &= \nabla \langle \mathbf{u}_\beta \rangle^{\mathbf{V}} + \frac{1}{V} \oint_{\Gamma_\beta} \cancel{m \mathbf{u}_\beta \hat{\mathbf{n}}_\beta} d\Gamma_\beta, \\ &= \nabla (\varepsilon_\beta \langle \mathbf{u}_\beta \rangle) \\ &= \varepsilon_\beta \nabla \langle \mathbf{u}_\beta \rangle + \langle \mathbf{u}_\beta \rangle \nabla \varepsilon_\beta\end{aligned}\quad (3.52)$$

and using the definition in eq. (3.15) leads to the following intrinsic average,

$$\langle \nabla \mathbf{u}_\beta \rangle = \nabla \langle \mathbf{u}_\beta \rangle + \frac{1}{\varepsilon_\beta} \langle \mathbf{u}_\beta \rangle \nabla \varepsilon_\beta$$

Without loss of generality, the aforementioned equations can be extended to the divergence operator in eq. (3.69).

Mixture energy equation

We now use the general VANS equation shown in eq. (3.31) to write the mixture energy equation in the gas phase,

$$\begin{aligned} \partial_t \varepsilon_\beta \langle \rho_\beta E_\beta \rangle + \nabla \cdot \varepsilon_\beta \langle \rho_\beta \mathbf{u}_\beta H_\beta \rangle + \nabla \cdot \varepsilon_\beta \langle \bar{\boldsymbol{\tau}}_\beta \cdot \mathbf{u}_\beta \rangle + \nabla \cdot \varepsilon_\beta \langle \mathbf{q}_\beta \rangle + \\ \frac{1}{V} \oint_{\Gamma_\beta} m \llbracket \rho E(\mathbf{u} - \mathbf{u}_\Gamma) + p\mathbf{u} + \bar{\boldsymbol{\tau}} \cdot \mathbf{u} + \mathbf{q} \rrbracket_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = 0. \end{aligned} \quad (3.53)$$

And applying the same average decomposition as above, we define the convective energy average as,

$$\begin{aligned} \langle \rho_\beta \mathbf{u}_\beta E_\beta \rangle|_{\mathbf{x}} = \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} \langle E_\beta \rangle|_{\mathbf{x}} + \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta} \Big|_{\mathbf{r}} \widetilde{E_\beta} \Big|_{\mathbf{r}} \right\rangle + (\nabla \langle E_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \\ \nabla \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} \cdot \left\langle (\mathbf{r} - \mathbf{x}) \widetilde{E_\beta} \Big|_{\mathbf{r}} \right\rangle + \frac{1}{2} (\nabla \nabla \langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}})^T : \left\langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \widetilde{E_\beta} \Big|_{\mathbf{r}} \right\rangle + \\ \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta} \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x}) \right\rangle \cdot \nabla \langle E_\beta \rangle|_{\mathbf{x}} + \frac{1}{2} \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta} \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \right\rangle : \nabla \nabla \langle E_\beta \rangle|_{\mathbf{x}}. \end{aligned} \quad (3.54)$$

From eq. (3.4), the average heat flux is defined by two contributions such that,

$$\langle \mathbf{q}_\beta \rangle|_{\mathbf{x}} = \langle \mathbf{q}_\beta^{\text{Diff}} \rangle|_{\mathbf{x}} + \langle \mathbf{q}_\beta^{\text{Cond}} \rangle|_{\mathbf{x}}, \quad (3.55)$$

where the first term on the right-hand side is the average diffusive heat flux and the second corresponds to the average conductive heat flux.

The average diffusive heat flux is written as,

$$\begin{aligned} \langle \mathbf{q}_\beta^{\text{Diff}} \rangle|_{\mathbf{x}} = \sum_{i \in \mathcal{G}} \left[\langle \mathbf{J}_{i\beta} h_{i\beta} \rangle|_{\mathbf{x}} \right] = \sum_{i \in \mathcal{G}} \left[\langle \mathbf{J}_{i\beta} \rangle|_{\mathbf{x}} \langle h_{i\beta} \rangle|_{\mathbf{x}} + \left\langle \tilde{\mathbf{J}}_{i\beta} \Big|_{\mathbf{r}} \tilde{h}_{i\beta} \Big|_{\mathbf{r}} \right\rangle \right. \\ + (\nabla \langle h_{i\beta} \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \mathbf{J}_{i\beta} \rangle|_{\mathbf{x}} \\ + \nabla \langle \mathbf{J}_{i\beta} \rangle|_{\mathbf{x}} \cdot \left\langle (\mathbf{r} - \mathbf{x}) \tilde{h}_{i\beta} \Big|_{\mathbf{r}} \right\rangle \\ + \frac{1}{2} (\nabla \nabla \langle \mathbf{J}_{i\beta} \rangle|_{\mathbf{x}})^T : \left\langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \tilde{h}_{i\beta} \Big|_{\mathbf{r}} \right\rangle + \\ \left\langle \tilde{\mathbf{J}}_{i\beta} \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x}) \right\rangle \cdot \nabla \langle h_{i\beta} \rangle|_{\mathbf{x}} \\ \left. + \frac{1}{2} \left\langle \tilde{\mathbf{J}}_{i\beta} \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \right\rangle : \nabla \nabla \langle h_{i\beta} \rangle|_{\mathbf{x}} \right], \end{aligned} \quad (3.56)$$

where $\langle \mathbf{J}_{i\beta} \rangle|_{\mathbf{x}}$ is defined by eq. (3.38).

The average conductive heat flux,

$$\begin{aligned}
\langle \mathbf{q}_\beta^{\text{Cond}} \rangle|_{\mathbf{x}} &= \langle \lambda_\beta \nabla T_\beta \rangle|_{\mathbf{x}} = \langle \lambda_\beta \rangle|_{\mathbf{x}} \langle \nabla T_\beta \rangle|_{\mathbf{x}} + \left\langle \tilde{\lambda}_\beta \Big|_{\mathbf{r}} \nabla \tilde{T}_\beta \Big|_{\mathbf{r}} \right\rangle + \\
&\quad (\nabla \langle \nabla T_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \lambda_\beta \rangle|_{\mathbf{x}} + \\
&\quad \nabla \langle \lambda_\beta \rangle|_{\mathbf{x}} \cdot \left\langle (\mathbf{r} - \mathbf{x}) \nabla \tilde{T}_\beta \Big|_{\mathbf{r}} \right\rangle + \\
&\quad \frac{1}{2} (\nabla \nabla \langle \lambda_\beta \rangle|_{\mathbf{x}})^T : \left\langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \nabla \tilde{T}_\beta \Big|_{\mathbf{r}} \right\rangle + \\
&\quad \left\langle \tilde{\lambda}_\beta \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x}) \right\rangle \cdot \nabla \langle \nabla T_\beta \rangle|_{\mathbf{x}} + \\
&\quad \frac{1}{2} \left\langle \tilde{\lambda}_\beta \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \right\rangle : \nabla \nabla \langle \nabla T_\beta \rangle|_{\mathbf{x}},
\end{aligned} \tag{3.57}$$

and, similarly to eq. (3.43), the average temperature gradient writes,

$$\begin{aligned}
\langle \nabla T_\beta \rangle &= \nabla \langle T_\beta \rangle + \frac{1}{V_\beta} \oint_{\Gamma_\beta} m(\mathbf{r} - \mathbf{x}) \hat{\mathbf{n}}_\beta d\Gamma_\beta \cdot \nabla \langle T_\beta \rangle|_{\mathbf{x}} \\
&\quad + \frac{1}{2} \frac{1}{V_\beta} \oint_{\Gamma_\beta} m(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \hat{\mathbf{n}}_\beta d\Gamma_\beta : \nabla \nabla \langle T_\beta \rangle|_{\mathbf{x}} \\
&\quad + \frac{1}{V_\beta} \oint_{\Gamma_\beta} m \tilde{T}_\beta \Big|_{\mathbf{r}} \hat{\mathbf{n}}_\beta d\Gamma_\beta.
\end{aligned} \tag{3.58}$$

Finally, the average of the work done on the fluid due to viscous force yields,

$$\begin{aligned}
\langle \bar{\boldsymbol{\tau}}_\beta \cdot \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \langle \bar{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}} \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \left\langle \tilde{\boldsymbol{\tau}}_\beta \Big|_{\mathbf{r}} \cdot \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \right\rangle + \\
&\quad (\nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \bar{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}} + \\
&\quad (\nabla \langle \bar{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x}) \cdot \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \rangle + \\
&\quad \frac{1}{2} (\nabla \nabla \langle \bar{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}})^T : \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \cdot \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \rangle + \\
&\quad \left\langle \tilde{\boldsymbol{\tau}}_\beta \Big|_{\mathbf{r}} \cdot (\mathbf{r} - \mathbf{x}) \right\rangle \cdot \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \\
&\quad \frac{1}{2} \left\langle \tilde{\boldsymbol{\tau}}_\beta \Big|_{\mathbf{r}} \cdot (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \right\rangle : \nabla \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}}.
\end{aligned} \tag{3.59}$$

and the pressure work can be written as,

$$\begin{aligned}
\langle p_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} &= \langle p_\beta \rangle|_{\mathbf{x}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \langle \tilde{p}_\beta \Big|_{\mathbf{r}} \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \rangle + \\
&\quad (\nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle p_\beta \rangle|_{\mathbf{x}} + \\
&\quad (\nabla \langle p_\beta \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x}) \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \rangle + \\
&\quad \frac{1}{2} (\nabla \nabla \langle p_\beta \rangle|_{\mathbf{x}})^T : \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \rangle + \\
&\quad \langle \tilde{p}_\beta \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \\
&\quad \frac{1}{2} \langle \tilde{p}_\beta \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle : \nabla \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}}.
\end{aligned} \tag{3.60}$$

The energy conservation for the solid phase read as,

$$\partial_t \varepsilon_\sigma \langle \rho_\sigma E_\sigma \rangle + \nabla \cdot \varepsilon_\sigma \langle \mathbf{q}_\sigma \rangle - \frac{1}{V} \oint_{\Gamma_\beta} m \llbracket \rho E(-\mathbf{u}_\Gamma) + \mathbf{q} \rrbracket_\sigma \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = 0. \tag{3.61}$$

where the average conductive heat flux is defined as,

$$\begin{aligned}
\langle \mathbf{q}_\sigma \rangle|_{\mathbf{x}} &= \langle \lambda_\sigma \nabla T_\sigma \rangle|_{\mathbf{x}} = \langle \lambda_\sigma \rangle|_{\mathbf{x}} \langle \nabla T_\sigma \rangle|_{\mathbf{x}} + \left\langle \tilde{\lambda}_\sigma \Big|_{\mathbf{r}} \nabla \tilde{T}_\sigma \Big|_{\mathbf{r}} \right\rangle + \\
&\quad (\nabla \langle \nabla T_\sigma \rangle|_{\mathbf{x}})^T \cdot \langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \rangle \cdot \nabla \langle \lambda_\sigma \rangle|_{\mathbf{x}} + \\
&\quad \nabla \langle \lambda_\sigma \rangle|_{\mathbf{x}} \cdot \left\langle (\mathbf{r} - \mathbf{x}) \nabla \tilde{T}_\sigma \Big|_{\mathbf{r}} \right\rangle + \\
&\quad \frac{1}{2} (\nabla \nabla \langle \lambda_\sigma \rangle|_{\mathbf{x}})^T : \left\langle (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \nabla \tilde{T}_\sigma \Big|_{\mathbf{r}} \right\rangle + \\
&\quad \left\langle \tilde{\lambda}_\sigma \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x}) \right\rangle \cdot \nabla \langle \nabla T_\sigma \rangle|_{\mathbf{x}} + \\
&\quad \frac{1}{2} \left\langle \tilde{\lambda}_\sigma \Big|_{\mathbf{r}} (\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \right\rangle : \nabla \nabla \langle \nabla T_\sigma \rangle|_{\mathbf{x}},
\end{aligned} \tag{3.62}$$

and the average temperature gradient,

$$\begin{aligned}
\langle \nabla T_\sigma \rangle &= \nabla \langle T_\sigma \rangle + \frac{1}{V_\sigma} \oint_{\Gamma_\sigma} m(\mathbf{r} - \mathbf{x}) \hat{\mathbf{n}}_\sigma d\Gamma_\sigma \cdot \nabla \langle T_\sigma \rangle|_{\mathbf{x}} \\
&\quad + \frac{1}{2} \frac{1}{V_\sigma} \oint_{\Gamma_\sigma} m(\mathbf{r} - \mathbf{x})(\mathbf{r} - \mathbf{x}) \hat{\mathbf{n}}_\sigma d\Gamma_\sigma : \nabla \nabla \langle T_\sigma \rangle|_{\mathbf{x}} \\
&\quad + \frac{1}{V_\sigma} \oint_{\Gamma_\sigma} m \tilde{T}_\sigma \Big|_{\mathbf{r}} \hat{\mathbf{n}}_\sigma d\Gamma_\sigma.
\end{aligned} \tag{3.63}$$

3.2.1 Simplification of the VANS equations

Here, we regard the length scale analysis done by [Quintard and Whitaker, 1994a, Whitaker, 1996, Carbonell and Whitaker, 1984] resulting in $\mu_\beta \ll r_0 \ll L$, where μ_β is the porous length, r_0 is the radius of the filtering volume, and L is the macro-scale length of interest. Considering this separation of scales, the higher-order terms derived from the Taylor series expansion are null, and the average dispersion (residual) equals zero. Therefore, the size of the filter is essential, so the average of the porous scale quantities becomes well behaved.

Species continuity equation

Under the constraints mentioned above, and assuming that the dispersion multicomponent diffusion matrix is negligible eq. (3.34) yields,

$$\begin{aligned}
\partial_t \varepsilon_\beta \langle \rho_{i\beta} \rangle &+ \nabla \cdot \varepsilon_\beta \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \nabla \cdot \varepsilon_\beta \left\langle \tilde{\rho}_{i\beta} \Big|_{\mathbf{r}} \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \right\rangle \\
&+ \nabla \cdot \varepsilon_\beta \langle \rho_{i\beta} \rangle|_{\mathbf{x}} \sum_{j \in \mathcal{G}} \left[\left\langle D_{ij\beta} \right\rangle|_{\mathbf{x}} \left(\nabla \langle x_{i\beta} \rangle + \frac{1}{V_\beta} \oint_{\Gamma_\beta} m \tilde{x}_{i\beta} \hat{\mathbf{n}}_\beta d\Gamma_\beta \right) \right] \\
&+ \nabla \cdot \varepsilon_\beta \left\langle \tilde{\rho}_{i\beta} \Big|_{\mathbf{r}} \tilde{\mathbf{V}}_{i\beta} \Big|_{\mathbf{r}} \right\rangle \\
&= \varepsilon_\beta \langle \dot{\omega}_{i,\beta}^{\text{chem}} \rangle - \langle \dot{\omega}_i^{\text{het}} \rangle^{\mathbf{V}}, \quad \forall i \in \mathcal{G}.
\end{aligned} \tag{3.64}$$

The diffusive flux on the fourth term of the left-hand side look is approximated as,

$$\begin{aligned}
\varepsilon_\beta \langle \mathbf{J}_{i\beta} \rangle &= \varepsilon_\beta \langle \rho_{i\beta} \rangle \sum_{j \in \mathcal{G}} \left[\left\langle D_{ij\beta} \right\rangle \left(\nabla \langle x_{i\beta} \rangle + \frac{1}{V_\beta} \oint_{\Gamma_\beta} m \tilde{x}_{i\beta} \hat{\mathbf{n}}_\beta d\Gamma_\beta \right) \right] \\
&= \varepsilon_\beta \langle \rho_{i\beta} \rangle \sum_{j \in \mathcal{G}} D_{ij\beta}^{\text{effect}} \nabla \langle x_{i\beta} \rangle
\end{aligned} \tag{3.65}$$

where $\bar{\mathbf{D}}^{\text{effect}}$ is the effective multicomponent diffusion matrix.

Solid-phase mass equation

The final expression of the σ -phase mass equation yields,

$$\partial_t \varepsilon_\sigma = \frac{\langle \dot{\omega}^{\text{het}} \rangle^{\mathbf{V}}}{\rho_\sigma}. \quad (3.66)$$

Mixture momentum equation

Using the same constraints as above and considering that the dispersion of the transport coefficients is approximately equal to zero, eq. (3.46) yields,

$$\begin{aligned} \partial_t \varepsilon_\beta \langle \rho_\beta \mathbf{u}_\beta \rangle + \nabla \cdot \varepsilon_\beta \left[\langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} \otimes \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta} \Big|_{\mathbf{r}} \otimes \widetilde{\mathbf{u}_\beta} \Big|_{\mathbf{r}} \right\rangle \right] + \varepsilon_\beta \nabla \langle p_\beta \rangle \bar{\mathbf{I}} + \nabla \cdot \langle \bar{\boldsymbol{\tau}}_\beta \rangle \\ + \frac{1}{V} \oint_{\Gamma_\beta} m \llbracket \rho \mathbf{u} \otimes (\mathbf{u} - \mathbf{u}_\Gamma) \rrbracket_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \mathbf{F}^{\text{drag}} \end{aligned} \quad (3.67)$$

where the drag force is defined as [Whitaker, 1996, Breugem et al., 2006, Ganesan and Poirier, 1990],

$$\mathbf{F}^{\text{drag}} = \frac{1}{V} \oint_{\Gamma_\beta} m [p\bar{\mathbf{I}} + \bar{\boldsymbol{\tau}}] \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta - \langle p_\beta \rangle \nabla \varepsilon_\beta = -\mu^{\text{effect}} \bar{\mathbf{K}}^{-1} (\bar{\mathbf{I}} + \bar{\mathbf{F}}) \varepsilon_\beta^2 \langle \mathbf{u}_\beta \rangle. \quad (3.68)$$

where $\bar{\mathbf{K}}$ and $\bar{\mathbf{F}}$ are the permeability and the Forchheimer tensor, respectively. Additionally, the permeability tensor $\bar{\mathbf{K}}$ must be corrected in the high Knudsen number regime to account for the Klinkenberg effects [Borner et al., 2017].

The average viscous stress tensor yields,

$$\begin{aligned} \langle \bar{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}} = \langle \mu_\beta \rangle|_{\mathbf{x}} \nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \frac{\langle \mu_\beta \rangle|_{\mathbf{x}}}{\varepsilon_\beta} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \nabla \varepsilon_\beta + \left\langle \tilde{\mu}_\beta \Big|_{\mathbf{r}} \nabla \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \right\rangle \\ + \langle \mu_\beta \rangle|_{\mathbf{x}} (\nabla \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}})^T + \frac{\langle \mu_\beta \rangle|_{\mathbf{x}}}{\varepsilon_\beta} (\langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \nabla \varepsilon_\beta)^T + \left\langle \tilde{\mu}_\beta \Big|_{\mathbf{r}} (\nabla \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}})^T \right\rangle \\ - \frac{2}{3} \left[\langle \mu_\beta \rangle|_{\mathbf{x}} \nabla \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \frac{\langle \mu_\beta \rangle|_{\mathbf{x}}}{\varepsilon_\beta} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \cdot \nabla \varepsilon_\beta + \left\langle \tilde{\mu}_\beta \Big|_{\mathbf{r}} \nabla \cdot \tilde{\mathbf{u}}_\beta \Big|_{\mathbf{r}} \right\rangle \right] \bar{\mathbf{I}}. \end{aligned} \quad (3.69)$$

The viscous stress tensor above can be decomposed in three contributions,

$$\langle \bar{\boldsymbol{\tau}}_\beta \rangle = \varepsilon_\beta \langle \bar{\boldsymbol{\tau}}_\beta^{\text{A}} \rangle + \varepsilon_\beta \langle \bar{\boldsymbol{\tau}}_\beta^{\text{I}} \rangle + \varepsilon_\beta \langle \bar{\boldsymbol{\tau}}_\beta^{\text{D}} \rangle$$

where the first term on the right-hand side represents the average viscous stress tensor,

$$\langle \bar{\boldsymbol{\tau}}_\beta^{\text{A}} \rangle = \langle \mu_\beta \rangle \nabla \langle \mathbf{u}_\beta \rangle + \langle \mu_\beta \rangle (\nabla \langle \mathbf{u}_\beta \rangle)^T - \frac{2}{3} \langle \mu_\beta \rangle \nabla \cdot \langle \mathbf{u}_\beta \rangle \bar{\mathbf{I}} \quad (3.70)$$

the second the represents the interface viscous stress tensor contribution,

$$\langle \bar{\boldsymbol{\tau}}_\beta^{\text{I}} \rangle = \frac{\langle \mu_\beta \rangle}{\varepsilon_\beta} \langle \mathbf{u}_\beta \rangle \nabla \varepsilon_\beta + \frac{\langle \mu_\beta \rangle}{\varepsilon_\beta} (\langle \mathbf{u}_\beta \rangle \nabla \varepsilon_\beta)^T - \frac{2}{3} \frac{\langle \mu_\beta \rangle}{\varepsilon_\beta} \langle \mathbf{u}_\beta \rangle \cdot \nabla \varepsilon_\beta \bar{\mathbf{I}}, \quad (3.71)$$

and the two expressions above can be further simplified such that,

$$\varepsilon_\beta \langle \bar{\boldsymbol{\tau}}_\beta^{\text{A}} \rangle + \varepsilon_\beta \langle \bar{\boldsymbol{\tau}}_\beta^{\text{I}} \rangle = \langle \mu_\beta \rangle \nabla \varepsilon_\beta \langle \mathbf{u}_\beta \rangle + \langle \mu_\beta \rangle (\nabla \varepsilon_\beta \langle \mathbf{u}_\beta \rangle)^T - \frac{2}{3} \langle \mu_\beta \rangle \nabla \cdot \varepsilon_\beta \langle \mathbf{u}_\beta \rangle \bar{\mathbf{I}} \quad (3.72)$$

The final term represents the dispersion viscous stress tensor contribution,

$$\langle \bar{\boldsymbol{\tau}}_\beta^{\text{D}} \rangle = \langle \tilde{\mu}_\beta \nabla \tilde{\mathbf{u}}_\beta \rangle + \left\langle \tilde{\mu}_\beta (\nabla \tilde{\mathbf{u}}_\beta)^T \right\rangle - \frac{2}{3} \langle \tilde{\mu}_\beta \nabla \cdot \tilde{\mathbf{u}}_\beta \rangle \bar{\mathbf{I}}. \quad (3.73)$$

Ultimately, we seek an approximate solution of the average viscous stress tensor such that,

$$\langle \bar{\boldsymbol{\tau}}_\beta \rangle = \mu^{\text{effect}} \nabla \varepsilon_\beta \langle \mathbf{u}_\beta \rangle + \mu^{\text{effect}} (\nabla \varepsilon_\beta \langle \mathbf{u}_\beta \rangle)^T - \frac{2}{3} \mu^{\text{effect}} \nabla \cdot \varepsilon_\beta \langle \mathbf{u}_\beta \rangle \bar{\mathbf{I}}. \quad (3.74)$$

where μ^{effect} is an effective viscosity containing the information at the macro and microscale.

Energy equation

Using the same constraints as above and considering that the dispersion of the transport coefficients is approximately equal to zero, eq. (3.53) yields,

$$\begin{aligned}
& \partial_t \varepsilon_\beta \langle \rho_\beta E_\beta \rangle + \nabla \cdot \varepsilon_\beta \left[\langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} \langle E_\beta \rangle|_{\mathbf{x}} + \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta} \Big|_{\mathbf{r}} \widetilde{E_\beta} \Big|_{\mathbf{r}} \right\rangle \right] \\
& + \nabla \cdot \varepsilon_\beta \left[\langle p_\beta \rangle|_{\mathbf{x}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \langle \widetilde{p_\beta} \Big|_{\mathbf{r}} \widetilde{\mathbf{u}_\beta} \Big|_{\mathbf{r}} \rangle \right] \\
& + \nabla \cdot \varepsilon_\beta \left[\langle \tilde{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}} \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \langle \tilde{\boldsymbol{\tau}}_\beta \Big|_{\mathbf{r}} \cdot \tilde{\mathbf{u}_\beta} \Big|_{\mathbf{r}} \rangle \right] \\
& + \nabla \cdot \varepsilon_\beta \sum_{i \in \mathcal{G}} \left[\langle \mathbf{J}_{i\beta} \rangle|_{\mathbf{x}} \langle h_{i\beta} \rangle|_{\mathbf{x}} + \left\langle \tilde{\mathbf{J}}_{i\beta} \Big|_{\mathbf{r}} \tilde{h}_{i\beta} \Big|_{\mathbf{r}} \right\rangle \right] \\
& + \nabla \cdot \varepsilon_\beta \langle \lambda_\beta \rangle|_{\mathbf{x}} \left[\nabla \langle T_\beta \rangle + \frac{1}{V_\beta} \oint_{\Gamma_\beta} m \tilde{T}_\beta \Big|_{\mathbf{r}} \hat{\mathbf{n}}_\beta d\Gamma_\beta \right] \\
& + \frac{1}{V} \oint_{\Gamma_\beta} m [\rho E(\mathbf{u} - \mathbf{u}_\Gamma) + p\mathbf{u} + \tilde{\boldsymbol{\tau}} \cdot \mathbf{u} + \mathbf{q}]_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = 0.
\end{aligned} \tag{3.75}$$

and the energy equation for the solid phase writes as,

$$\begin{aligned}
& \partial_t \varepsilon_\sigma \langle \rho_\sigma E_\sigma \rangle + \nabla \cdot \varepsilon_\sigma \langle \lambda_\sigma \rangle|_{\mathbf{x}} \left[\nabla \langle T_\sigma \rangle + \frac{1}{V_\sigma} \oint_{\Gamma_\sigma} m \tilde{T}_\sigma \Big|_{\mathbf{r}} \hat{\mathbf{n}}_\sigma d\Gamma_\sigma \right] \\
& - \frac{1}{V} \oint_{\Gamma_\beta} m [\rho E(-\mathbf{u}_\Gamma) + \mathbf{q}]_\sigma \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = 0.
\end{aligned} \tag{3.76}$$

If we assume local thermal equilibrium, i.e., an equal temperature within both phases, we can sum eqs. (3.75) and (3.76), yielding the total average energy of the porous medium as,

$$\begin{aligned}
& \partial_t (\varepsilon_\beta \langle \rho_\beta E_\beta \rangle + \varepsilon_\sigma \langle \rho_\sigma E_\sigma \rangle) + \nabla \cdot \varepsilon_\beta \left[\langle \rho_\beta \mathbf{u}_\beta \rangle|_{\mathbf{x}} \langle E_\beta \rangle|_{\mathbf{x}} + \left\langle \widetilde{\rho_\beta \mathbf{u}_\beta} \Big|_{\mathbf{r}} \widetilde{E_\beta} \Big|_{\mathbf{r}} \right\rangle \right] \\
& + \langle p_\beta \rangle|_{\mathbf{x}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \cdot \nabla \varepsilon_\beta + \varepsilon_\beta \nabla \cdot \langle p_\beta \rangle|_{\mathbf{x}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \nabla \cdot \varepsilon_\beta \langle \widetilde{p_\beta} \Big|_{\mathbf{r}} \widetilde{\mathbf{u}_\beta} \Big|_{\mathbf{r}} \rangle \\
& + \langle \tilde{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}} \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \cdot \nabla \varepsilon_\beta + \varepsilon_\beta \nabla \cdot \langle \tilde{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}} \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} + \nabla \cdot \varepsilon_\beta \langle \tilde{\boldsymbol{\tau}}_\beta \Big|_{\mathbf{r}} \cdot \tilde{\mathbf{u}_\beta} \Big|_{\mathbf{r}} \rangle \\
& + \nabla \cdot \varepsilon_\beta \sum_{i \in \mathcal{G}} \left[\langle \mathbf{J}_{i\beta} \rangle|_{\mathbf{x}} \langle h_{i\beta} \rangle|_{\mathbf{x}} + \left\langle \tilde{\mathbf{J}}_{i\beta} \Big|_{\mathbf{r}} \tilde{h}_{i\beta} \Big|_{\mathbf{r}} \right\rangle \right] \\
& + \nabla \cdot \langle \mathbf{q}^{\text{Cond}} \rangle + \mathcal{E} = 0.
\end{aligned} \tag{3.77}$$

The last term on the left-hand side in eq. (3.77) corresponds to an energy balance between both phases and the average conductive heat flux can be written as,

$$\begin{aligned}
\langle \mathbf{q}^{\text{Cond}} \rangle &= (\varepsilon_\beta \langle \lambda_\beta \rangle \nabla \langle T_\beta \rangle + \varepsilon_\sigma \langle \lambda_\sigma \rangle \nabla \langle T_\sigma \rangle) \\
&+ \left(\varepsilon_\beta \langle \lambda_\beta \rangle \frac{1}{V_\beta} \oint_{\Gamma_\beta} m \tilde{T}_\beta \hat{\mathbf{n}}_\beta d\Gamma_\beta + \varepsilon_\sigma \langle \lambda_\sigma \rangle \frac{1}{V_\sigma} \oint_{\Gamma_\sigma} m \tilde{T}_\sigma \hat{\mathbf{n}}_\sigma d\Gamma_\sigma \right) \\
&= (\varepsilon_\beta \langle \lambda_\beta \rangle \nabla \langle T_\beta \rangle + \varepsilon_\sigma \langle \lambda_\sigma \rangle \nabla \langle T_\sigma \rangle) \\
&+ \left(\langle \lambda_\beta \rangle \frac{1}{V} \oint_{\Gamma_\beta} m \tilde{T}_\beta \hat{\mathbf{n}}_\beta d\Gamma_\beta - \langle \lambda_\sigma \rangle \frac{1}{V} \oint_{\Gamma_\beta} m \tilde{T}_\sigma \hat{\mathbf{n}}_\beta d\Gamma_\beta \right)
\end{aligned} \tag{3.78}$$

Finally, we look for an approximate solution of the average conductive heat flux such that,

$$\langle \mathbf{q}^{\text{Cond}} \rangle = \lambda^{\text{effect}} \nabla \langle T \rangle \tag{3.79}$$

where λ^{effect} is an effective thermal conductivity containing the information at the macro and microscale.

The energy balance writes as follows,

$$\mathcal{E} = \frac{1}{V} \oint_{\Gamma_\beta} m [\rho E(\mathbf{u} - \mathbf{u}_\Gamma) + p\mathbf{u} + \bar{\boldsymbol{\tau}} \cdot \mathbf{u} + \mathbf{q}]_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta - \frac{1}{V} \oint_{\Gamma_\beta} m [\rho E(-\mathbf{u}_\Gamma) + \mathbf{q}]_\sigma \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta$$

considering that,

$$E_\beta = e_\beta + \frac{\mathbf{u}_\beta \cdot \mathbf{u}_\beta}{2}, \quad \text{and} \quad e_\beta \gg \frac{\mathbf{u}_\beta \cdot \mathbf{u}_\beta}{2}, \quad \text{and} \quad e_\sigma = E_\sigma, \quad (3.80)$$

and with eq. (4.20), the energy balance above can be written as,

$$\begin{aligned} \mathcal{E} = & \frac{1}{V} \oint_{\Gamma_\beta} m \dot{\omega}^{\text{het}} \Delta e \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta \\ & + \frac{1}{V} \oint_{\Gamma_\beta} m [(p\bar{\mathbf{I}} + \bar{\boldsymbol{\tau}}) \cdot \mathbf{u}]_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta \\ & + \frac{1}{V} \oint_{\Gamma_\beta} m ([\mathbf{q}^{\text{Diff}} + \mathbf{q}^{\text{Cond}}]_\beta - [\mathbf{q}^{\text{Cond}}]_\sigma) \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta, \end{aligned} \quad (3.81)$$

where Δe is the energy difference between both phases. The first and last terms cancel each other due to heat flux continuity at the surface between both phases. The second term on the right-hand side can be approximated as,

$$\begin{aligned} \frac{1}{V} \oint_{\Gamma_\beta} m [p_\beta \bar{\mathbf{I}} + \bar{\boldsymbol{\tau}}_\beta] \cdot \mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = & -\langle p_\beta \rangle|_{\mathbf{x}} \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \cdot \nabla \varepsilon_\beta - \langle \bar{\boldsymbol{\tau}}_\beta \rangle|_{\mathbf{x}} \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \nabla \varepsilon_\beta \\ & + \frac{1}{V} \oint_{\Gamma_\beta} m [\tilde{p}_\beta \bar{\mathbf{I}} + \tilde{\boldsymbol{\tau}}_\beta] \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} \\ & + \frac{1}{V} \oint_{\Gamma_\beta} m [p_\beta \bar{\mathbf{I}} + \bar{\boldsymbol{\tau}}_\beta] \cdot \tilde{\mathbf{u}}_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta \end{aligned} \quad (3.82)$$

where the first term on the right-hand side cancels with the third term in eq. (3.75).

Neglecting the last term of the equation above, the work due to the drag force can be written as,

$$\mathbf{F}^{\text{drag}} \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}} = \frac{1}{V} \oint_{\Gamma_\beta} m [\tilde{p}_\beta \bar{\mathbf{I}} + \tilde{\boldsymbol{\tau}}_\beta] \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta \cdot \langle \mathbf{u}_\beta \rangle|_{\mathbf{x}}. \quad (3.83)$$

Note

As mentioned before, the energy equation derived above assumes thermal equilibrium. To consider thermal non-equilibrium, one should follow the work of Duval et al. [2004] and solve an average energy equation of each phase with proper boundary conditions.

No-slip boundary condition assumption

We now go back to eq. (3.52), to evaluate the no-slip boundary condition assumption, more precisely,

$$\frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = 0.$$

The velocity at the surface can be decomposed into two components, a normal and a tangential, such that,

$$\mathbf{u}_\beta = (\mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta) \hat{\mathbf{n}}_\beta + (\mathbf{u}_\beta - (\mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta) \hat{\mathbf{n}}_\beta),$$

where the last term cancels due to the no-slip condition, the first term is different from zero due to ablation.

Therefore, the velocity at the surface can be written as,

$$\frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \frac{1}{V} \oint_{\Gamma_\beta} m (\mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta) \hat{\mathbf{n}}_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta,$$

and from eq. (4.20),

$$\mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta \approx \frac{\dot{\omega}^{\text{het}}}{\rho_\beta}$$

and using the spatial decomposition, we can write the velocity at the surface as,

$$\frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \left\langle \frac{\dot{\omega}^{\text{het}}}{\rho_\beta} \right\rangle_{\mathbf{x}} \frac{1}{V} \oint_{\Gamma_\beta} m \varepsilon_\beta \hat{\mathbf{n}}_\beta d\Gamma_\beta,$$

which, according to [Carbonell and Whitaker, 1984], can be simplified as,

$$\frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \varepsilon_\beta \left\langle \frac{\dot{\omega}^{\text{het}}}{\rho_\beta} \right\rangle_{\mathbf{x}} \frac{4}{3} \pi \vartheta_0^2 \bar{\mathbf{I}},$$

where ϑ_0 is the fiber radius.

A similar term appearing in the average viscous stress tensor in eq. (3.69) can be written as,

$$\frac{1}{V} \oint_{\Gamma_\beta} m \mathbf{u}_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta = \frac{1}{V} \oint_{\Gamma_\beta} m \frac{\dot{\omega}^{\text{het}}}{\rho_\beta} d\Gamma_\beta = \left\langle \frac{\dot{\omega}^{\text{het}}}{\rho_\beta} \right\rangle_{\mathbf{x}}.$$

3.2.2 Final form of the VANS equations

Gathering all the terms previously derived, the final form of the VANS equations are cast in the differential form as,

$$\partial_t \mathbf{U} + \nabla \cdot \mathbf{F}^{\text{inv}} + \nabla \cdot \tilde{\mathbf{F}}^{\text{inv}} + \nabla \cdot \mathbf{F}^{\text{vis}} + \nabla \cdot \tilde{\mathbf{F}}^{\text{vis}} = \mathbf{S} + \mathbf{S}^{\text{surf}} \quad (3.84)$$

where each vector is defined as,

$$\begin{aligned} \mathbf{U} &= [\varepsilon_\beta \langle \rho_{i\beta} \rangle, \varepsilon_\beta \langle \rho_\beta \mathbf{u}_\beta \rangle, \varepsilon_\beta \langle \rho_\beta E_\beta \rangle + \varepsilon_\sigma \langle \rho_\sigma E_\sigma \rangle, \varepsilon_\sigma]^T, \\ \mathbf{F}^{\text{inv}} &= [\varepsilon_\beta \langle \rho_{i\beta} \rangle \langle \mathbf{u}_\beta \rangle, \varepsilon_\beta \langle \rho_\beta \mathbf{u}_\beta \rangle \otimes \langle \mathbf{u}_\beta \rangle, \varepsilon_\beta \langle \rho_\beta \mathbf{u}_\beta \rangle \langle E_\beta \rangle, 0]^T, \\ \tilde{\mathbf{F}}^{\text{inv}} &= [\varepsilon_\beta \langle \tilde{\rho}_{i\beta} \tilde{\mathbf{u}}_\beta \rangle, \varepsilon_\beta \langle \tilde{\rho}_\beta \tilde{\mathbf{u}}_\beta \otimes \tilde{\mathbf{u}}_\beta \rangle, \varepsilon_\beta \langle \tilde{\rho}_\beta \tilde{\mathbf{u}}_\beta \tilde{E}_\beta \rangle + \varepsilon_\beta \langle \tilde{p}_\beta \tilde{\mathbf{u}}_\beta \rangle, 0]^T, \\ \mathbf{F}^{\text{vis}} &= \left[\varepsilon_\beta \langle \mathbf{J}_{i\beta} \rangle, 0, \langle \mathbf{q}^{\text{Cond}} \rangle + \varepsilon_\beta \sum_{i \in \mathcal{G}} \langle \mathbf{J}_{i\beta} \rangle \langle h_{i\beta} \rangle, 0 \right]^T, \\ \tilde{\mathbf{F}}^{\text{vis}} &= [\varepsilon_\beta \langle \tilde{\rho}_{i\beta} \tilde{\mathbf{V}}_{i\beta} \rangle, 0, \varepsilon_\beta \langle \tilde{\tau}_\beta \cdot \tilde{\mathbf{u}}_\beta \rangle + \varepsilon_\beta \langle \tilde{\mathbf{J}}_{i\beta} \tilde{h}_{i\beta} \rangle, 0]^T, \\ \mathbf{S} &= [\varepsilon_\beta \langle \dot{\omega}_{i,\beta}^{\text{chem}} \rangle, \varepsilon_\beta (\nabla \langle p_\beta \rangle \bar{\mathbf{I}} + \nabla \cdot \langle \bar{\tau}_\beta \rangle), \varepsilon_\beta (\nabla \cdot \langle p_\beta \rangle \langle \mathbf{u}_\beta \rangle + \nabla \cdot \langle \bar{\tau}_\beta \rangle \cdot \langle \mathbf{u}_\beta \rangle), 0]^T, \\ \mathbf{S}^{\text{surf}} &= \left[\varepsilon_\beta \langle \dot{\omega}_i^{\text{het}} \rangle, \mathbf{F}^{\text{drag}}, \mathbf{F}^{\text{drag}} \cdot \langle \mathbf{u}_\beta \rangle, \frac{\langle \dot{\omega}^{\text{het}} \rangle}{\rho_\sigma} \right]^T, \end{aligned}$$

and the average viscous flux yield,

$$\begin{aligned} \langle \mathbf{J}_{i\beta} \rangle &= \langle \rho_{i\beta} \rangle \sum_{j \in \mathcal{G}} D_{ij\beta}^{\text{effect}} \nabla \langle x_{i\beta} \rangle, \\ \varepsilon_\beta \langle \bar{\tau}_\beta \rangle &= \mu^{\text{effect}} \nabla \varepsilon_\beta \langle \mathbf{u}_\beta \rangle + \mu^{\text{effect}} (\nabla \varepsilon_\beta \langle \mathbf{u}_\beta \rangle)^T - \frac{2}{3} \mu^{\text{effect}} \nabla \cdot \varepsilon_\beta \langle \mathbf{u}_\beta \rangle \bar{\mathbf{I}}, \\ \langle \mathbf{q}^{\text{Cond}} \rangle^{\mathbf{V}} &= \lambda^{\text{effect}} \nabla \langle T \rangle, \end{aligned}$$

and the drag force is written as,

$$\mathbf{F}^{\text{drag}} = -\mu^{\text{effect}} \bar{\mathbf{K}}^{-1} \cdot (\bar{\mathbf{I}} + \bar{\mathbf{F}}) \cdot \varepsilon_\beta^2 \langle \mathbf{u}_\beta \rangle.$$

The primary challenge in solving the equations above consists in finding a proper closure for the effective properties and, finding closure for the dispersion fluxes. On the former, the closure has to be found via

DNS-type simulations capable of solving the flow quantities at the porous scale. The difficulty of this task increases with the complexity of the porous structure. It is almost impossible to determine a closure for the dispersion terms, although [Whitaker \[1999\]](#), [Breugem et al. \[2006\]](#) have shown that some are negligible and can be disregarded.

Chapter 4

The Unified Solver in the Porous-material Analysis Toolbox based on OpenFOAM (PATO)

4.1 Discretization of the GE

As the Mach number approaches zero, compressible flow solvers encounter efficiency and accuracy challenges. Two fundamental approaches address low Mach number flows. The first involves adapting compressible solvers (density-based) to handle low Mach numbers, while the second entails extending incompressible solvers (pressure-based) to cover this regime.

Regarding density-based solvers, the time integration eq. (3.1) is a *Herculean task* due to the severe time-step constraints. For stability reasons, explicit schemes are constrained to lower Courant-Friedrichs-Lewy (CFL) number than one, leading to a time-step of the order of infinitesimal volume to the square. On the other hand, implicit methods suffer from stiffness due to a high condition number of the linear system caused by a significant disparity in the eigenvalues as the Mach number approaches the incompressible limit Liou and Edwards [1999]. A popular remedy to this problem is to precondition the linear system such that the magnitude of the eigenvalues is of the same order. Effectively, this approach alters the time integration of the GE, leading to time-inaccurate results. In such situations, one can use a dual-time stepping scheme Jameson [2015] to reduce these errors.

In contrast, based on projection methods, pressure-based solvers are characterized by an instantaneous propagation of the acoustic wave, alleviating the time-step constraints. Fractional-step methods have been developed initially for time-accurate incompressible flow Kim and Moin [1985], Perot [1993] while segregated iterative methods such as Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) Patankar and Spalding [1972] and Semi-Implicit Method for Pressure-Linked Equations Consistent (SIMPLEC) Van Doormaal and Raithby [1984] have been developed for steady-state flows.

Pressure Implicit with Splitting of Operators (PISO) Issa [1986], Issa et al. [1986, 1991] is a non-iterative method segregated method developed for time-accurate flows with small time-step. In this method, the non-linear terms are less relevant than temporal terms, eliminating the need for sub-iterations Perot et al. [2020]. Fractional-step and PISO Tuković et al. [2018] are constrained to small time-step integration, while SIMPLE and SIMPLEC allow for more significant time steps. PIMPLE is a combination between PISO and SIMPLE (or SIMPLEC), allowing for a larger time-step while keeping an accurate transient pressure-velocity coupling. Moreover, the original PISO is first-order accurate in time because it uses the mass flow from the previous time step. When PISO is merged with the SIMPLE method, the mass flow is estimated in an iterative procedure, allowing an overall second-order converge Tuković et al. [2018]. In this work, we adapted the original PIMPLE method developed in OpenFOAM based on our system of equations in eq. (3.1). PIMPLE is a combination between PISO Issa [1986], Issa et al. [1986, 1991] and SIMPLE Patankar and Spalding [1972] (or SIMPLEC Van Doormaal and Raithby [1984]), allowing for a larger time-step while keeping an accurate transient pressure-velocity coupling.

The discretized momentum equation using a second-order backward differentiation yields,

$$\frac{3\varepsilon_\beta(\rho\mathbf{u})^{n+1} - 4\varepsilon_\beta(\rho\mathbf{u})^n + \varepsilon_\beta(\rho\mathbf{u})^{n-1}}{2\Delta t} = \mathcal{C}(\mathbf{u}^{n+1}) + \mathcal{D}(\mathbf{u}^{n+1}) + \varepsilon_\beta\mathcal{G}(p^{n+1}) + \mathcal{S}(\mathbf{u}^{n+1}, \mathbf{u}^n) \quad (4.1)$$

where $\mathcal{C}$, $\mathcal{D}$, and $\mathcal{G}$ are the inviscid, viscous and gradient operators, and $\mathcal{S}$ is an implicit/explicit source term. For consistency, we follow the same notation as Ferziger et al. [2020] where m is the iteration counter leading to $n + 1$ when the iterative procedure converges. The non-linear terms are linearized using the Picard-iteration scheme, where the volumetric momentum and momentum flux yield,

$$(\rho\mathbf{u})^{n+1} \approx \rho^{m-1}\mathbf{u}^m, \quad (4.2)$$

$$(\rho\mathbf{u} \otimes \mathbf{u})^{n+1} \approx (\rho\mathbf{u})^{m-1} \otimes \mathbf{u}^m. \quad (4.3)$$

The linearized momentum equation for the velocity component j is written as a linear system – using a pressure estimate from the previous iteration or time step – such that,

$$\mathbf{M}u_j^m = \mathbf{RHS}^{m-1} - \varepsilon_\beta\mathcal{G}_j(p^{m-1}), \quad (4.4)$$

where the right-hand side $\mathbf{RHS}$ represent the explicit terms, and the matrix $\mathbf{M}$ can be decomposed into,

$$\mathbf{M}u_j^m = \mathbf{A}u_j^m + \mathbf{A}_{\text{OD}}u_j^m, \quad (4.5)$$

where $\mathbf{A}$ is a diagonal matrix, and $\mathbf{A}_{\text{OD}}$ is a matrix containing all off-diagonal terms – i.e., the information of the neighboring cells – and eq. (4.4) with eq. (4.5) leads to,

$$u_j^m = \mathbf{A}^{-1}\mathbf{H}(u_j^m) - \mathbf{A}^{-1}\varepsilon_\beta\mathcal{G}_j(p^{m-1}), \quad (4.6)$$

where

$$\mathbf{H}(u_j^m) = -\mathbf{A}_{\text{OD}}u_j^m + \mathbf{RHS}^{m-1}. \quad (4.7)$$

The motivation behind the pressure-based solver is to predict a flow variable ψ^* (prediction-step) and to correct it ψ' (correction-step) in an iterative procedure such that

$$\begin{aligned} u_j^m &= u_j^* + u_j' \\ p^m &= p^* + p' \\ \rho^m &= \rho^* + \rho' \end{aligned} \quad (4.8)$$

and the mass flux reads,

$$\begin{aligned} \dot{m}_j^m &= \varepsilon_\beta \rho^m u_j^m \\ &= \varepsilon_\beta (\rho^* + \rho') (u_j^* + u_j') \\ &= \underbrace{\varepsilon_\beta \rho^* u_j^*}_{\dot{m}_j^*} + \underbrace{\varepsilon_\beta (\rho' u_j^* + \rho^* u_j' + \rho' u_j')}_{\dot{m}_j'} \end{aligned} \quad (4.9)$$

where the last term on the right-hand side is often neglected due to its small magnitude.

The momentum predictor of eq. (4.6) yields,

$$u_j^* = \mathbf{A}^{-1}\mathbf{H}(u_j^*) - \mathbf{A}^{-1}\varepsilon_\beta\mathcal{G}_j(p^*), \quad (4.10)$$

and subtracting to eq. (4.6) leads to the correction equation,

$$u_j' = \mathbf{A}^{-1}\mathbf{H}(u_j') - \mathbf{A}^{-1}\varepsilon_\beta\mathcal{G}_j(p'), \quad (4.11)$$

In the case of SIMPLE method, the first term on the right-hand side is neglected, requiring under-relaxation of the linear system, leading to a slower convergence and requiring more interactions Ferziger et al. [2020], Moukalled et al. [2016]. The SIMPLEC algorithm is a modified version of the SIMPLE algorithm that

approximates the velocity correction at cell-center as a weighted average of the velocity correction of the neighboring cells [Moukalled et al. \[2016\]](#), leading to faster convergence of the linear system,

$$u'_j = (1 - \mathbf{H}_c)^{-1} \mathbf{A}^{-1} \varepsilon_\beta \mathcal{G}_j(p'). \quad (4.12)$$

The discretized mass equation using a second-order backward differentiation yields,

$$\frac{3\varepsilon_\beta \rho^m - 4\varepsilon_\beta \rho^n + \varepsilon_\beta \rho^{n-1}}{2\Delta t} = \nabla \cdot (\dot{\mathbf{m}}^m), \quad (4.13)$$

and utilizing eqs. (4.8) and (4.9) and the Equation-of-state (EOS) [Ferziger et al. \[2020\]](#),

$$\rho' = \varphi p',$$

where φ is a compressibility factor, the pressure correction equation yields,

$$\begin{aligned} \frac{3\varepsilon_\beta \varphi p' + 3\varepsilon_\beta \rho^* - 4\varepsilon_\beta \rho^n + \varepsilon_\beta \rho^{n-1}}{2\Delta t} &= \nabla \cdot (\dot{\mathbf{m}}_j^*) + \nabla \cdot (\dot{\mathbf{m}}_j') \\ &= \nabla \cdot [\varepsilon_\beta \rho^* (\mathbf{A}^{-1} \mathbf{H}(u_j^*) - \mathbf{A}^{-1} \varepsilon_\beta \mathcal{G}_j(p^*))] + \nabla \cdot (\varepsilon_\beta \varphi p' u_j^*) + \nabla \cdot (\varepsilon_\beta \rho^* (1 - \mathbf{H}_c)^{-1} \mathbf{A}^{-1} \varepsilon_\beta \mathcal{G}_j(p')), \end{aligned} \quad (4.14)$$

the second term on the right-hand side transforms the pressure-correction equation from an elliptic into a hyperbolic equation when the compressibility effects are considerable. For low Mach number, the third term dominates, turning the pressure-correction into an elliptic equation as the **SIMPLE** version for incompressible flows.

Algorithm 1 shows the pressure-velocity coupling procedure for each time step. The procedure consists of two main loops: an outer correction loop, which corresponds to the **SIMPLEC** or **SIMPLE** methods, and an inner loop corresponding to the **PISO** algorithm. The inner loop focuses on the pressure-velocity coupling without updating the non-linear coefficients in eq. (4.5). Typically, five iterations are sufficient to converge it [Ferziger et al. \[2020\]](#). The outer loop allows updating the non-linear terms, such as transport and thermodynamic properties, in the **GE**. This requires more iterations based on the non-linearity of the system. Fifty iterations are enough for a highly non-linear problem.

Algorithm 1 Pressure-velocity coupling for each time-step

```

while Outer corrections (SIMPLEC) do
  assemble and solve momentum predictor eq. (4.4) for a prediction state *
  solve species equation in eq. (3.1)
  solve energy equation in eq. (3.1)
  update compressibility factor  $\varphi$ 
  while Inner corrections (PISO) do
    solve pressure correction eq. (4.14)
    correct the momentum by estimating a new velocity prediction state  $\mathbf{u}^{\text{new} *}$   $\leftarrow$  eq. (4.10) + eq. (4.11)
    update  $\mathbf{H}(u_j^*)$ 
  end while
   $p^m \leftarrow p^* + p'$ 
   $\rho^m \leftarrow \rho^* + \rho'$ 
   $\mathbf{u}^m \leftarrow \mathbf{u}^* + \mathbf{u}'$ 
end while

```

4.2 Property filtering and **VANS** closure

Apart from the size, it is also essential to consider the filter's kernel to obtain well-behaved average properties and cancel the residual derived in eq. (3.27). The filter type depends on the porous structure, i.e., if the porous medium is ordered, disordered, periodic, quasi-periodic [Davit and Quintard \[2017\]](#) and :

- it acts as a low pass filter,

- it doesn't change the **GE** conservative properties since $\frac{1}{V} \int_{\mathbb{R}^3} m \, d^3\mathbf{r} = 1$,
- it has a compact support,
- it is symmetric.

In the case of a disordered porous medium, a top-hat filter [Quintard and Whitaker, 1994a,c],

$$m_{\square}(\mathbf{x} - \mathbf{r}) = \begin{cases} \frac{1}{V}, & |\mathbf{x} - \mathbf{r}| < r_i \\ 0, & |\mathbf{x} - \mathbf{r}| \geq r_i. \end{cases} \quad (4.15)$$

suffices to provide well-behaved averaged properties. Still, Whitaker [1999], Carbonell and Whitaker [1984] have carried out a scaling analysis of the residual terms in eq. (3.27) showing the size of the filter has to be much larger than the porous scale to have proper scale separations, i.e.,

$$\mu \ll l \ll L, \quad (4.16)$$

where μ and L are the microscale and macroscale characteristic lengths.

For ordered porous medium, Quintard and Whitaker [1994a,b,d,e] observed that cellular filters (pyramid shape)

$$m_{\wedge}(\mathbf{x} - \mathbf{r}) = \begin{cases} \prod_{i=1}^3 (r_i - |\mathbf{x} - \mathbf{r}|) / r_i^2, & |\mathbf{x} - \mathbf{r}| < r_i \\ 0, & |\mathbf{x} - \mathbf{r}| \geq r_i, \end{cases} \quad (4.17)$$

are optimum, canceling the spatial higher-order terms owed to the periodicity of the structure. Moreover, this finding also leads to a filter size of the same order as the porous length scale, i.e.,

$$l \sim \mathcal{O}(\mu). \quad (4.18)$$

Figure 4.1 shows the normalized kernel of the filters mentioned above.

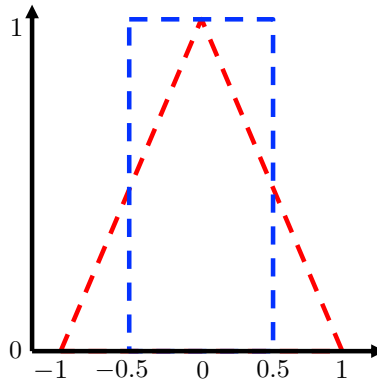


Figure 4.1: Illustration of the normalized kernels: cellular filter $m_{\wedge}$ (---) and top-hat filter $m_{\square}$ (---).

Davit and Quintard [2017] have conducted a thorough study on different kernels and sizes for periodic and quasi-periodic porous structures, observing a substantial impact on the averaging properties. They have concluded that the top-hat and cellular filters are equivalent regarding a unitary **REV** due to the normalization condition. Still, when used as a spatial convolution, the former shows significant fluctuations errors (eq. (3.27)) due to the flow/microstructure interaction.

To summarize, the volume-averaging technique results in macroscale equations that represent the average behavior of a porous domain, including the porous structure. The size and kernel of the filter are paramount for these equations to be well behaved over an **Representative Volume Element (RVE)** (or **REV** as commonly defined), especially in regions with considerable porosity variation, such as the interface between pure fluid and porous medium. However, these equations require closure that enables consideration of the porous structure; therefore, the microscale information is expressed as effective transport properties [Davarzani et al., 2021] – such as the permeability tensor derived in eq. (3.68). These effective properties can only be derived from porous scale simulations for complex microstructures and heterogeneous porous media.

4.2.1 Results

In this section, we infer the interface permeability for an isotropic microstructure using the filtering techniques mentioned above. Afterward, we include the permeability into the macroscopic equations derived in section 3.2.1 and analyze its effects compared to a sharp variation of the permeability at the interface.

Permeability derivation through porous scale numerical simulations

As mentioned before, one objective of this work is to study the impact of a variable permeability that can be derived from a microstructure using filtering techniques. For that purpose, we deem the geometry proposed by Breugem et al. [2004], i.e., a 3D Cartesian grid of cubes porous structure inserted into a viscous channel as depicted in fig. 4.2 – known in the literature as the Beavers & Joseph problem. The size of the cube d_s and the void between them is $5.00\text{ }\mu\text{m}$, leading to a porosity of 0.875. The ratio between the cube size and the height d_s/H is 0.0625. Moreover, in the current study, we neglect any turbulence effect and consider a flow Reynolds number equal to one. Since this porous structure is isotropic and periodic, we can reduce our computational domain to the pink region¹ depicted in fig. 4.2.

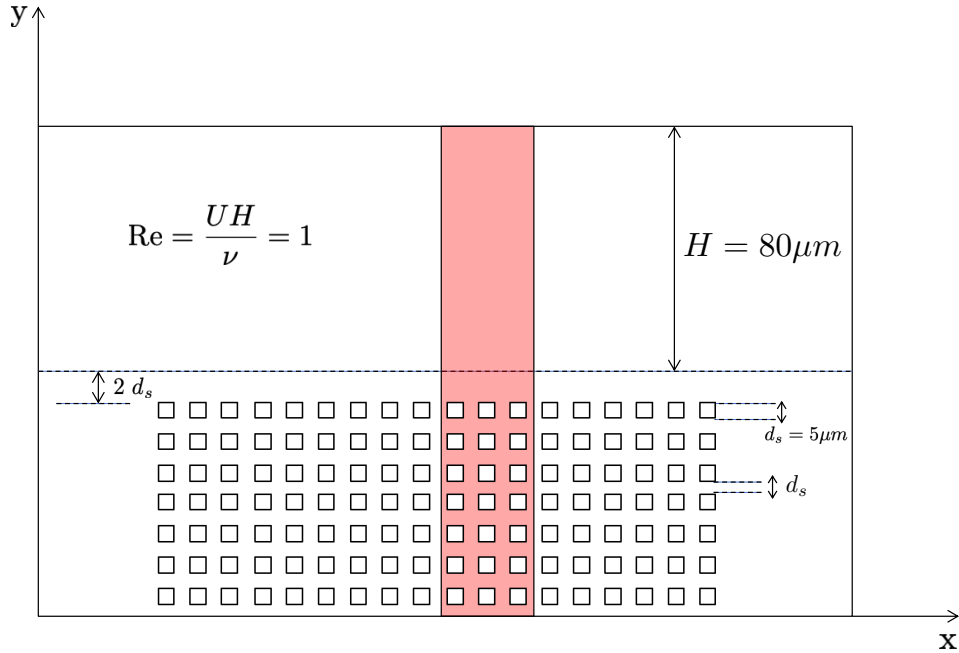


Figure 4.2: Beavers & Joseph problem over a 3D cartesian grid of cubes. The simulation domain is reduced to the pink area because this porous structure is isotropic and periodic.

We utilize the steady-state incompressible flow solver *simpleFoam* from PATO to solve the flow field of the domain depicted in fig. 4.2. This solver uses the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm Patankar and Spalding [1972]. Since our environment is periodic in the x-direction, we impose a mass flux corresponding to the unity Reynolds number. The solver computes the equivalent pressure gradient in the same direction, which ensures that mass is conserved. We enforce the no-slip boundary condition for the channel's top and bottom walls and at the surfaces of the cubes². Figure 4.3 shows the non-dimensional velocity field in the periodic computational domain. The velocity is nearly zero in the porous region and has a parabolic shape in the free-fluid part, identical to the Poiseuille Flow.

The average quantity is obtained from the convolution of the porous scale flow field with a filter function m . Figure 4.4 illustrates the convolution, or moving average, where the gray square box corresponds to the filter, also shown in fig. 4.5. Using the convolution definition from eqs. (3.11), (3.13) and (3.15), we derive

¹Note that to derive the permeability, the flow on top of the porous medium must be fully developed.

²Breugem et al. [2004] utilized an Immersed boundary method to simulate the boundaries of the cubes

the superficial and intrinsic velocity and the porosity. Together with the volume average Stokes equation Breugem [2004], Quintard and Whitaker [1994a], Whitaker [1986], Valdés-Parada et al. [2013], which writes as,

$$0 = \underbrace{-\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x} - \nu \frac{\langle u_x \rangle}{K}}_{\text{Darcy's terms}} + \underbrace{\frac{\nu}{\varepsilon_\beta} \frac{\partial \varepsilon_\beta}{\partial y} \frac{\partial \langle u_x \rangle}{\partial y} + \nu \frac{\partial^2 \langle u_x \rangle}{\partial y^2}}_{\text{Brinkman's correction}} \quad (4.19)$$

we derive the permeability coefficient K , where ν is the kinematic viscosity. Since this porous structure is isotropic the permeability tensor is,

$$\bar{\mathbf{K}} = K \bar{\mathbf{I}}.$$

Equation (4.19) is also known as the Darcy-Brinkman equation, where the first and second terms on the right-hand side are Darcy terms while two last are Brinkman's, usually neglected in homogeneous porous medium.

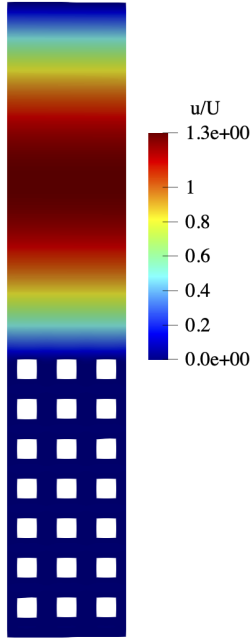


Figure 4.3: The velocity field on the periodic domain is nearly zero in the porous region and reaches a maximum at the center of the free-fluid region.

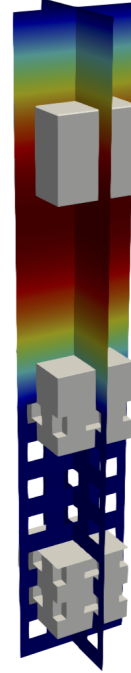


Figure 4.4: Illustration of the velocity filtering where the gray box represents the filter size.

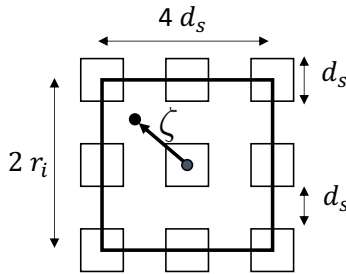
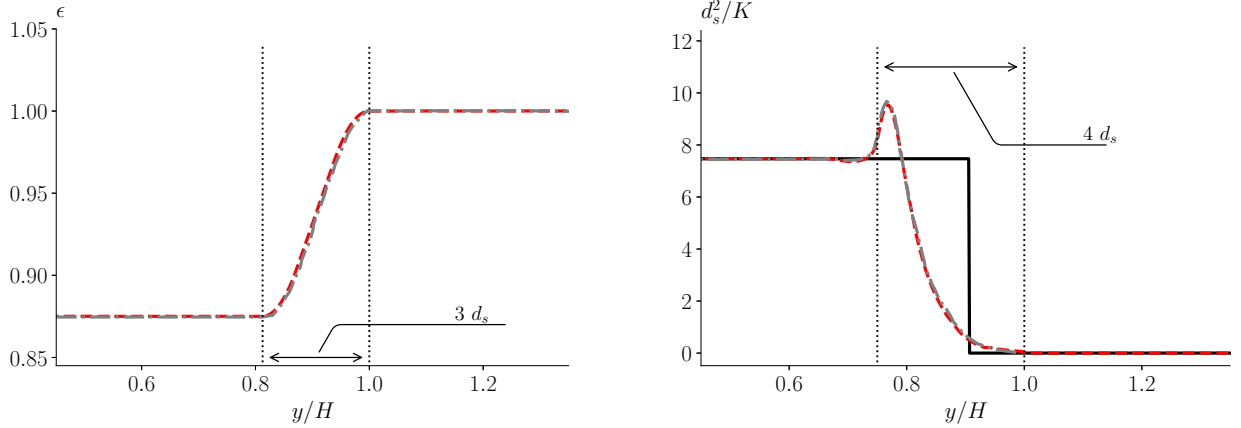


Figure 4.5: The volume of filter is $(4d_s)^3$, as the used by Breugem [2004].

Figures 4.6 and 4.7 show the porosity and permeability derived from the cellular and top-hat kernels (fig. 4.1). Figure 4.6a shows the porosity derived through the cellular filter, equal to one in the free-fluid region, 0.875 in the porous region, as predicted by Breugem [2004]. The porosity varies smoothly across the interface which has a thickness of $3d_s$. The interface thickness appears naturally from the filtering approach. Figure 4.6b shows that the non-dimensional permeability, derived with the cellular filter, varies over a length of $4d_s$ at the interface. Moreover, we observe an overshoot caused by the Brinkman terms in eq. (4.19), owing to the large velocity gradient and shear stress balance at the interface.

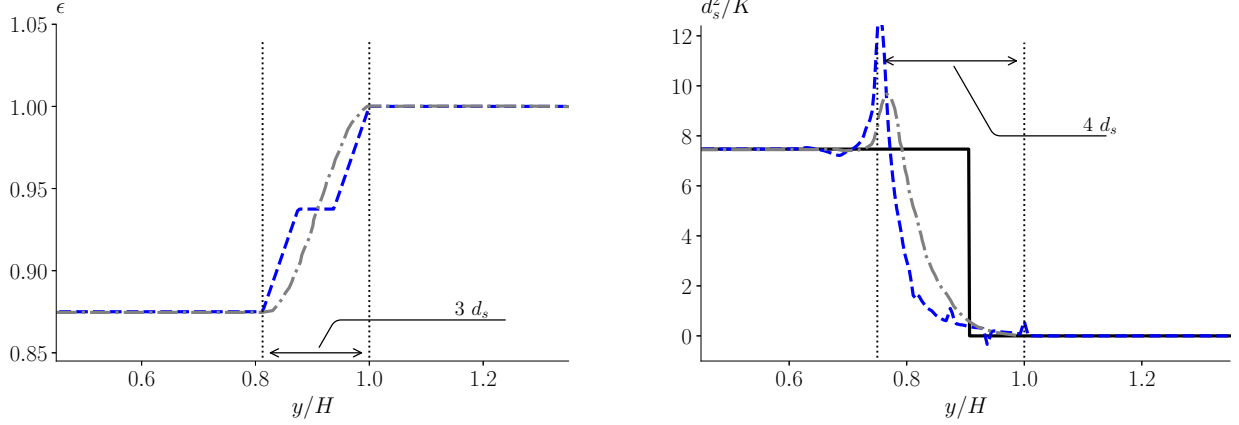
Contrarily to the cellular filter, the interface porosity derived from the top-hat filter is not smooth and shows a non-physical plateau in the middle of it. Moreover, the permeability in fig. 4.7b presents a more significant overshoot, and some fluctuations are observed due to the porosity gradient. These fluctuations are also related to the filtering errors from eq. (3.27), addressed by Davit and Quintard [2017]. Intuitively, one would predict that the permeability plateau and the overshoots can be reduced by increasing the filter size such that the *decomposition of the length scales* in eq. (4.16) is respected.



(a) The porosity has a smooth variation across the interface. The interface thickness, $3d_s$, is a result of the phase-indicator filtering.

(b) The permeability varies over $4d_s$ across the interface. Moreover, the Brinkman terms cause an overshoot of the permeability. The black line (—) corresponds to a sharp permeability variation at the interface.

Figure 4.6: Porosity and permeability derived from the cellular filter: comparison between this work (---) and Breugem [2004] (---).



(a) The porosity has a non-smooth variation across the interface with a small plateau in the middle.

(b) The permeability overshoot is more significant than the one computed with the cellular filter. Moreover, some fluctuations are observed due to the filtering error. The black line (—) corresponds to a sharp permeability variation at the interface.

Figure 4.7: Porosity and permeability derived from the top-hat filter: comparison between this work (---) and Breugem [2004] (....).

Macroscopic results

We have implemented a new module in **PATO**, which solves the **VANS** equation written in eq. (3.1) with the aforementioned permeability closure. The numerical discretization of the **GE** is based on the **Method-Of-Lines (MOL)** Hirsch [2007]. This method separates the spatial and the temporal dependence of the **Partial Differential Equation (PDE)** leading to an **Ordinary Differential Equation (ODE)**. The spatial integration of the **ODE** is performed with a cell-centered **Finite Volume (FV)** method, whereas the temporal part is integrated with the **Backward-Euler (BE)** method. All the physico-chemical properties necessary to close the **GE** are given by **Mutation⁺⁺** Scoggins et al. [2020].

This section shows the effect of considering a variable permeability at the interface through two test cases, a viscous plug and the Beavers & Joseph problem. These cases have been taken from Betchen et al. [2006], and used for verification purposes by Schrooyen [2016], Weng and Martin [2017], and Duzel and Martin [2020]. The main difference between this and previous works is that we include the permeability closure derived from the cellular filter in section 4.2.1 into the macroscale equations in section 3.2.1. All the characteristic dimensions are the same as in section 4.2.1, i.e., non-dimensional interface thickness $3d_s/H = 0.1875$.

Viscous plug

This test case simulates a porous plug inside a closed channel (fig. 4.8), with the objective of quantifying the flow deceleration and pressure drop due to the presence of a porous material and the viscous boundaries. Therefore, we consider a no-slip momentum boundary condition at the top and bottom of the channel, and a unitary Reynolds number yielding,

$$\text{Re} = \frac{\rho U H}{\mu} = 1,$$

where U is the average inlet velocity. Similarly to Betchen et al. [2006], we impose a velocity profile at the inlet to ensure a fully developed flow inside the channel.

Figure 4.9 shows the non-dimensional intrinsic velocity contour along the channel, where flow decelerates in the porous medium, accelerating again further downstream. This feature is better observed in figs. 4.10a and 4.10b, corresponding to the intrinsic and superficial velocities. In the former figure, the velocity increases in the middle of the channel due to the porosity change at the interface and material. We observe an impact of the velocity field when including the variable permeability against the sharp variation (black line in fig. 4.6b)

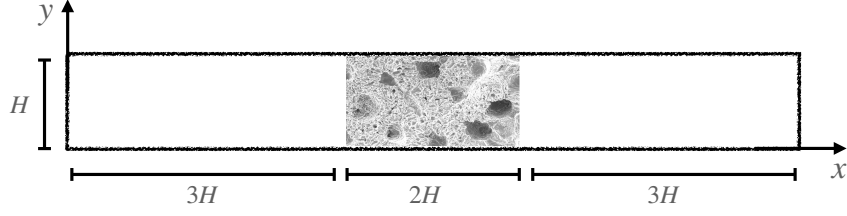


Figure 4.8: Porous plug geometry.

model at the interface. The variable permeability model predicts a more pronounced velocity overshoot inside the material, which can be owed to the permeability overshoot observed in fig. 4.6b. Ultimately, this velocity difference affects the pressure drop along the channel (fig. 4.11a) and the velocity gradient (fig. 4.11b), which is related to the shear forces. Due to its smooth variation across the interface, the variable permeability model predicts a lower pressure drop along the channel and a lower velocity gradient at the interface.

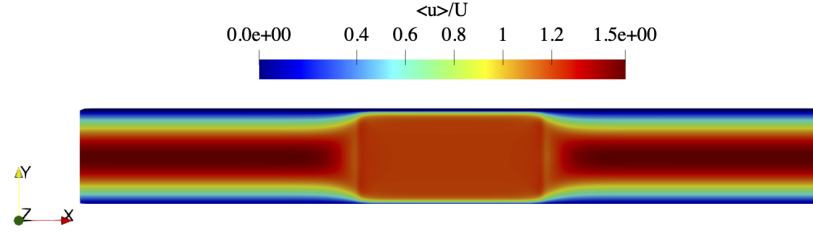
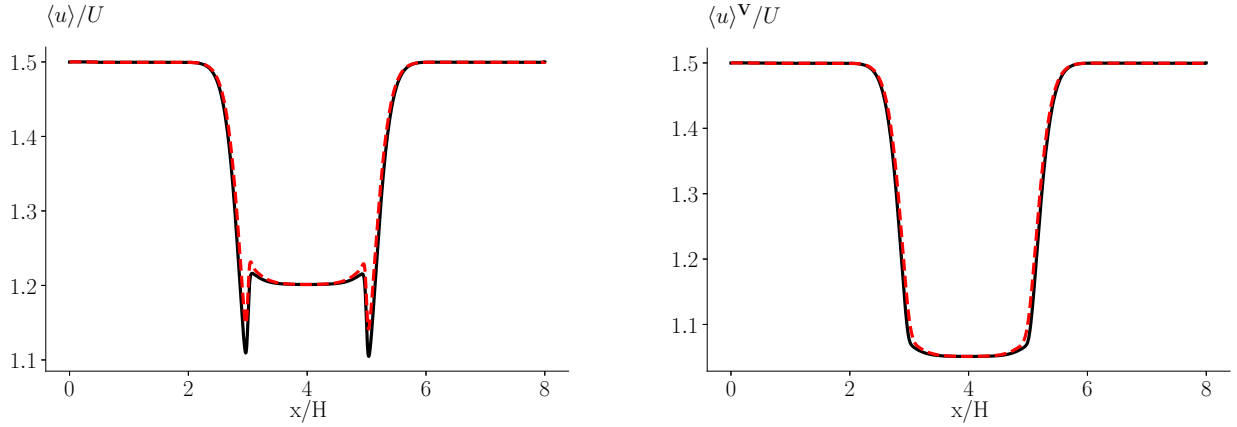


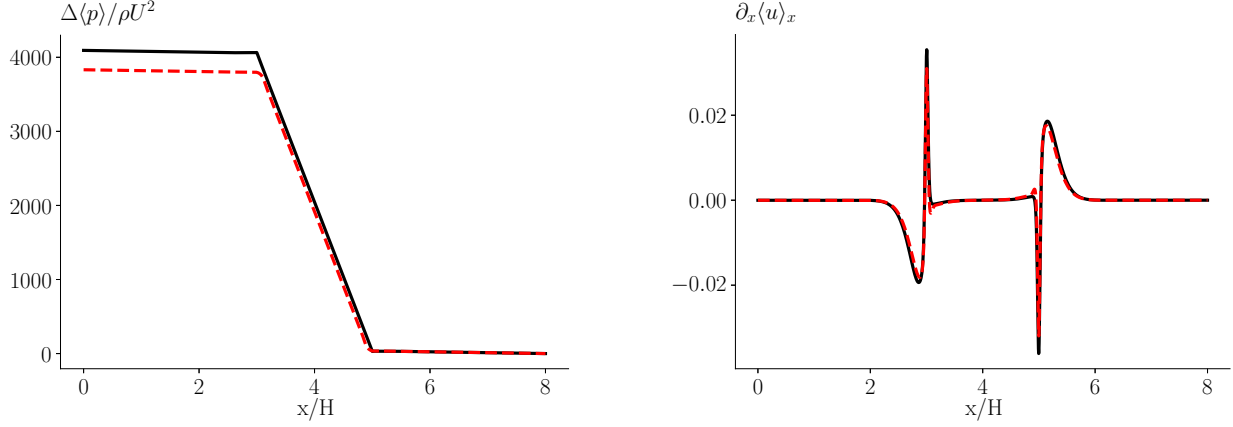
Figure 4.9: Non-dimensional intrinsic velocity ($\langle \mathbf{u} \rangle / U$) contour along the channel.



(a) Intrinsic velocity at the centerline along the channel. The increase of velocity inside the porous material is due to the decrease of porosity.

(b) Superficial velocity at the centerline along the channel. The velocity varies smoother at the interface when predicted with the variable permeability model.

Figure 4.10: Intrinsic and superficial velocity along the channel: variable permeability (---) and sharp permeability (—) model.



(a) Non-dimensional pressure at the centerline along the channel. The variable permeability model predicts a lower pressure drop compared to the sharp permeability.

(b) Velocity gradient (related to the shear forces) at the centerline along the channel. The variable permeability model predicts a lower velocity gradient due to its smooth variation across the interface.

Figure 4.11: Pressure drop and velocity gradient along the channel: variable permeability (---) and sharp permeability (—) model.

Beavers & Joseph problem

The last test case is the well-known Beavers & Joseph [Beavers and Joseph \[1967\]](#) problem, which has been widely used to derive proper boundary conditions between the pure fluid phase and the porous material phase; when considering both domains as decoupled phases. As illustrated in fig. 4.12, a semi-infinite porous plug is regarded in the middle of the channel, forcing partial blockage of the pure fluid phase. Figure 4.13 shows exactly that behavior where the flow accelerates on the top of the porous plug, resembling a Poiseuille flow. Although we do not simulate the presence of the solid phase in the porous material, the flow features in fig. 4.13 are identical to one solution presented in fig. 4.3. This behavior is because the drag term in eq. (3.1) penalizes the momentum equation.

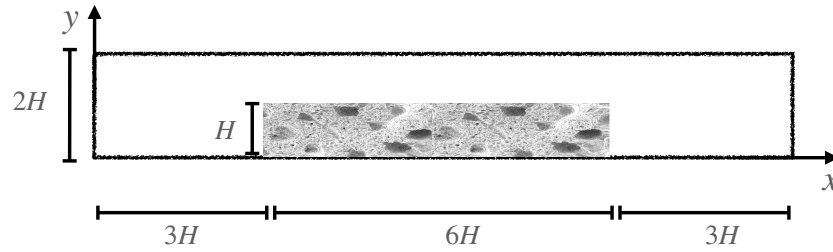


Figure 4.12: Beavers & Joseph problem geometry.

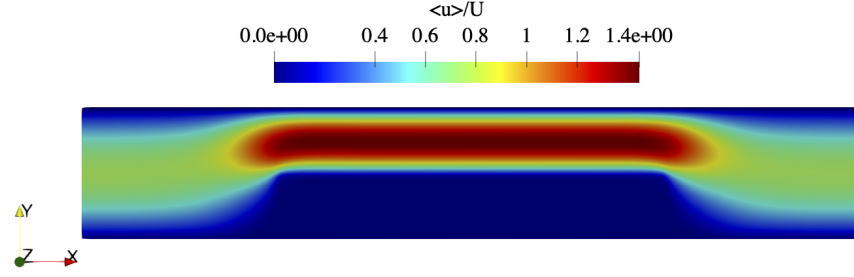
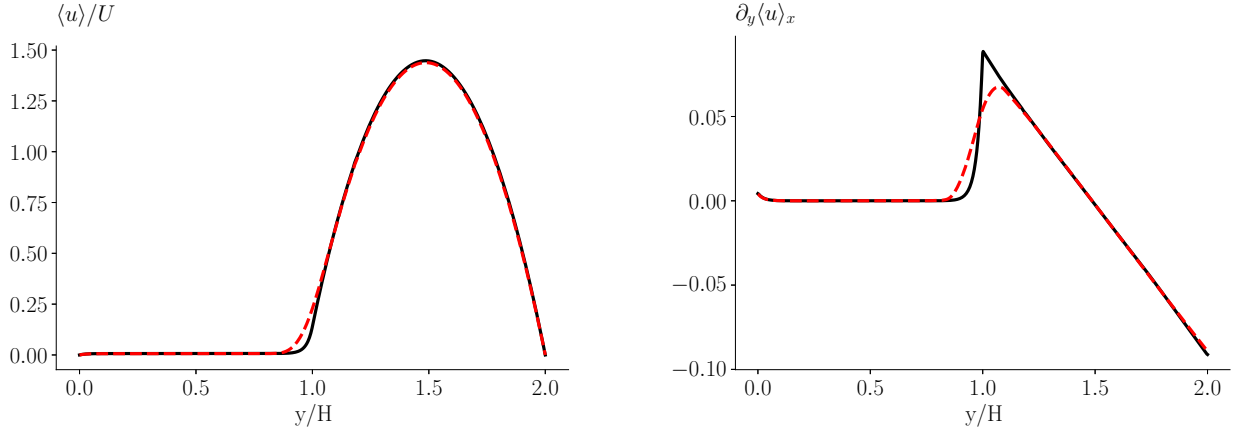


Figure 4.13: Non-dimensional intrinsic velocity ($\langle u \rangle / U$) contour along the channel. The flow deviates due to the presence of the porous material.

Figure 4.14a shows the velocity profile along the y -direction. One notes a near-zero velocity inside the porous material due to the low permeability and a parabolic profile in the plain fluid region. Moreover, the variable permeability model predicts a higher velocity inside the porous material than the sharp one. As shown in fig. 4.14b, this effect leads to a larger and smoother velocity gradient in-depth of the porous material, due to the change of porosity over a finite length and the overshoot observed previously. Ultimately, we can expect higher in-depth shear stress when considering a variable permeability across the interface.



(a) Non-dimensional intrinsic velocity profile along the y -direction. The variable permeability model predicts a smoother and higher velocity inside the material close to the interface.

(b) Velocity gradient along the y -direction. The variable permeability model predicts a smoother and non-negligible velocity gradient inside the porous material close to the interface.

Figure 4.14: Flow field properties on the transversal direction at the center of the channel $x = 6H$: variable permeability (---) and sharp permeability (—) model.

4.3 FiberForm[®] oxidation

Mass Balance: Assuming that the surface between the σ and β phases reaches a steady state, the mass balance is equal to the surface heterogeneous reactions [Schrooyen, 2016, Ishii and Hibiki, 2011, Whitaker, 1992], such that

$$\begin{aligned}
\sum_{i \in \mathcal{G}} \frac{1}{V} \oint_{\Gamma_\beta} m [\rho_i (\mathbf{u} - \mathbf{u}_\Gamma) + J_i]_\beta \cdot \hat{\mathbf{n}}_\beta d\Gamma_\beta &= \frac{1}{V} \oint_{\Gamma_\sigma} m [\rho (\mathbf{u} - \mathbf{u}_\Gamma)]_\sigma \cdot \hat{\mathbf{n}}_\sigma d\Gamma_\sigma \\
&= \sum_{i \in \mathcal{G}} \frac{1}{V} \oint_{\Gamma_\beta} m \dot{\omega}_i^{\text{het}} d\Gamma_\beta \\
&= \langle \dot{\omega}^{\text{het}} \rangle^{\mathbf{V}}.
\end{aligned} \tag{4.20}$$

For a heterogeneous carbon-oxidation reaction of the form



the heterogeneous production terms are

$$\begin{aligned}
\langle \dot{\omega}^{\text{het}}_{\text{O}_2} \rangle^{\mathbf{V}} &= \mathcal{S} \langle k_{\text{R1}}^{\text{het}} \rangle \left\langle \rho_{\text{O}_2, \beta} \right\rangle \frac{M_{\text{O}_2}}{M_{\text{O}_2}}, \\
\langle \dot{\omega}^{\text{het}}_{\text{CO}_2} \rangle^{\mathbf{V}} &= -\mathcal{S} \langle k_{\text{R1}}^{\text{het}} \rangle \left\langle \rho_{\text{O}_2, \beta} \right\rangle \frac{M_{\text{CO}_2}}{M_{\text{O}_2}}, \\
\langle \dot{\omega}^{\text{het}} \rangle^{\mathbf{V}} &= \langle \dot{\omega}^{\text{het}}_{\text{O}_2} \rangle^{\mathbf{V}} + \langle \dot{\omega}^{\text{het}}_{\text{CO}_2} \rangle^{\mathbf{V}}.
\end{aligned} \tag{4.21}$$

Here, $\langle k_{\text{R1}}^{\text{het}} \rangle$ and $\mathcal{S}$ are the reaction rate associated with Eq. (R1) and the surface area, respectively. The reaction rate follows an Arrhenius-type law:

$$\langle k_{\text{R1}}^{\text{het}} \rangle = A_f \exp \left(-\frac{E_a}{\mathcal{R}T} \right). \tag{4.22}$$

The activation energy $E_a = 42.4 \text{ kJ/mol}$ and the pre-exponential factor $A_f = 0.087 \text{ m/s}$ are taken from Panerai et al. [2014b].

We compute the surface area using the cylindrical model proposed by Lachaud et al. [2011], yielding

$$\mathcal{S} = \frac{2}{r_0} \sqrt{\varepsilon_{s,0} \varepsilon_s}, \tag{4.23}$$

where ε_s is the solid volume fraction and $r_0 = 5.5 \mu\text{m}$ is the initial fiber radius [Panerai et al., 2014b].

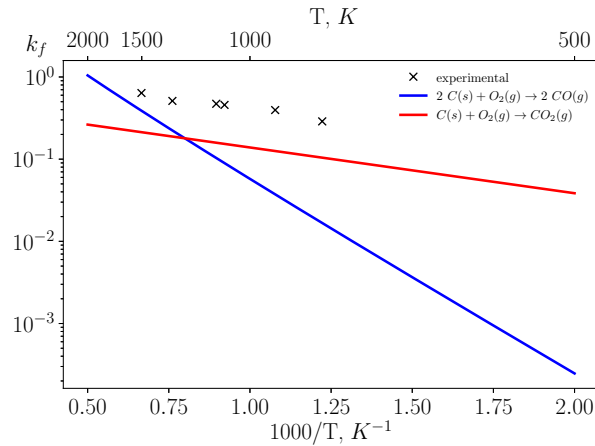


Figure 4.15: Oxidation rates.

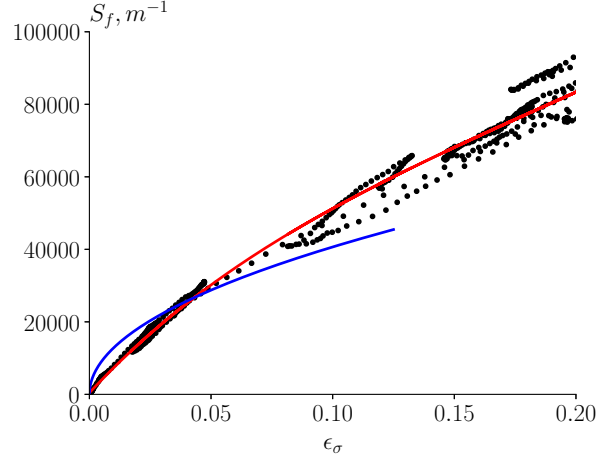


Figure 4.16: Mass-loss error.

4.3.1 Results

We have implemented a new module in **PATO**, which solves the **VANS** equation written in ?? All the physico-chemical properties necessary to close the **GE** are given by **Mutation**⁺⁺ [Scoggins et al. \[2020\]](#). This section shows two test cases where we solve the pure fluid and porous medium in the same computational domain. The first test case concerns the flow tube experiment carried out by [Panerai et al. \[2016\]](#). In the second test case, we simulate the Beavers & Joseph [Beavers and Joseph \[1967\]](#) problem for a reactive porous material made of carbon fibers.

Flow tube experiment

All the details of the flow tube experiment can be found in [Panerai et al. \[2016\]](#), but in brief, a 22 mm diameter FiberForm[®] sample was inserted in a quartz tube and pre-heated to a specific temperature. Afterward, a fixed mass flow rate of argon was injected at the inlet, and the pressure upstream and downstream of the sample was measured. From these measurements, [Panerai et al. \[2016\]](#) derived the **Through-Thickness** (TT) and **In-Plane** (IP) permeability considering Klinkenberg effects. We used the same closure properties obtained by [Panerai et al. \[2016\]](#), where the permeability tensor is written as,

$$\bar{\mathbf{K}}_{\alpha} = K_0 + (1 + b/p) \quad \text{where} \quad \alpha = \{\text{TT}, \text{IP}\}$$

where the constants b and K_0 for the **TT** and **IP**, as well as the solid density and solid thermal conductivity, are taken from [Panerai et al. \[2016\]](#) for the specific experiment.

Figure 4.17 illustrates the computational domain used to replicate the flow tube experiment. We first initialized the domain with the pressure measured on the probe downstream of the sample. We imposed the experimental temperature at the wall, and at the inlet, we imposed the mass flow rate for the specific experiment. At the outlet, we only imposed the measured downstream pressure.

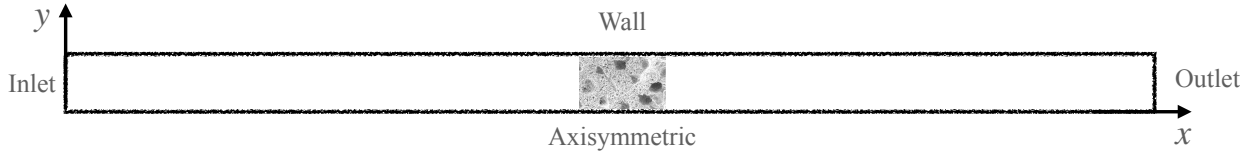


Figure 4.17: Illustration of the flow tube computational domain with a FiberForm[®] sample in the middle.

In this experiment, the sample was heated to 298 K, and the mass flow rate was equal to 1.80×10^{-5} kg/s. The solution reached a steady state after 10.0 s of the simulation. The upstream and downstream pressure were equal to 6020 Pa and 293 Pa. Figure 4.18a shows the pressure increase upstream of the sample, directly related to *Darcy's law*. The simulated pressure is 6410 Pa corresponding to a 6.00 % error. This difference can be attributed to experimental errors such as mass flow or pressure measurements from which the permeability tensor is derived.

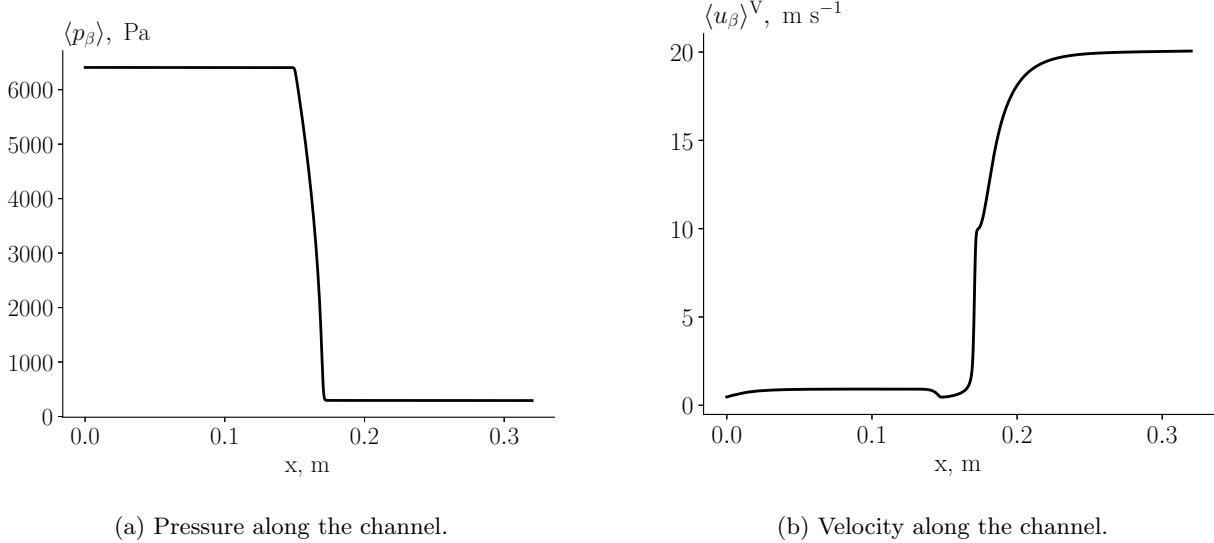


Figure 4.18: Flow field properties along the axis of the channel.

Figures 4.18b and 4.19 show the velocity along the axis of the channel where we first observe an initial increase due to the boundary layer development from the tube walls. Near the sample, the velocity first decreases due to viscous effects caused by the presence of the material (or the boundary layer effects). It then rapidly increases to almost twenty times due to the significant decrease in pressure. Figure 4.18b also shows some artifacts at the material interface caused by variation of permeability in that region. In this work, we assume a permeability variation proportional to the porosity, which is considered by using a Heaviside function. Dias et al. [2023] have shown a rigorous approach to derive the permeability at the interface using filtering techniques. In the future, this approach may be used to derive the permeability variation at the interface for FiberForm[®].

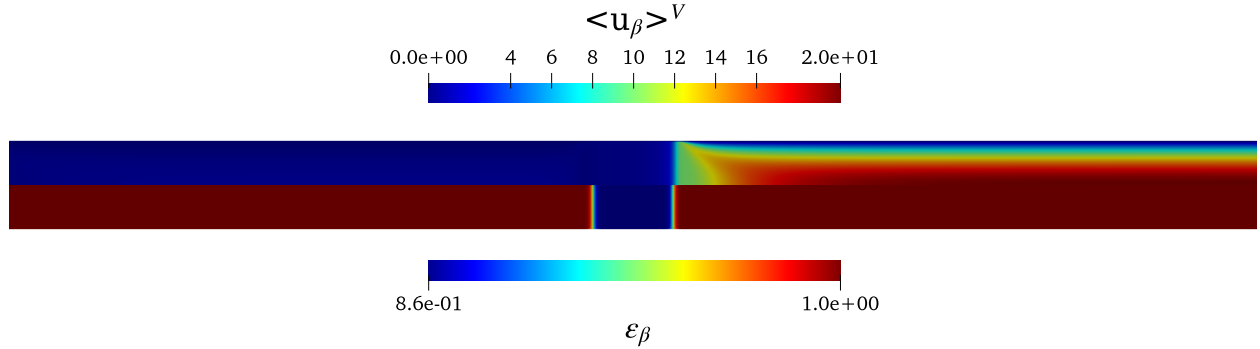


Figure 4.19: Top: Velocity contour along the channel, bottom: porosity along the channel.

Figure 4.20 shows the temperature contour along the channel where we observe a 0.200 K drop downstream of the sample due to viscous dissipation and increase of kinetic energy that can be easily related to velocity

results shown in fig. 4.19.

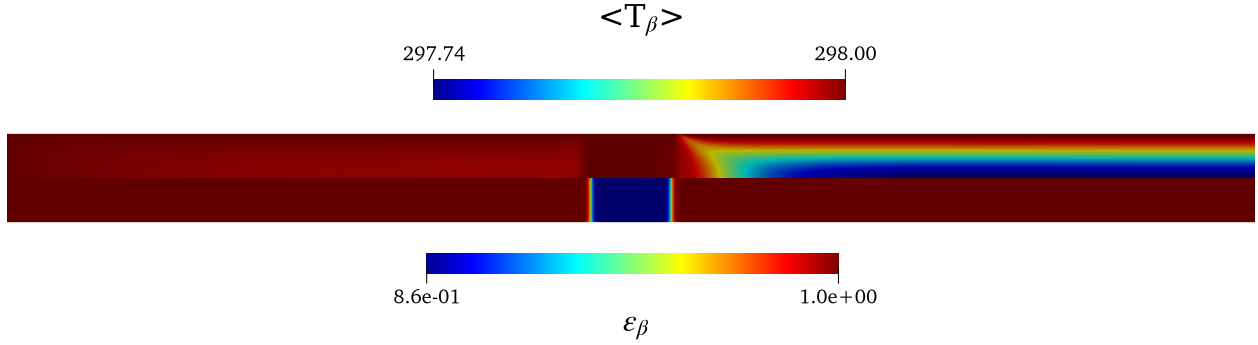


Figure 4.20: Top: Temperature contour along the channel, bottom: porosity along the channel.

TTO1 — 1500 K

In this experiment, the sample was heated to 1500 K, and the mass flow rate was equal to 1.81×10^{-5} kg/s. The solution reached a steady state after 15.0 s of the simulation. The upstream and downstream pressure were equal to 19 700 Pa and 1330 Pa and the simulated pressure is 19 600 Pa, corresponding to a 0.200 % error. Similar conclusions in terms of pressure (fig. 4.21a) fields can be drawn from the previous test case where the mass flow rate is almost the same. The major exceptions are the higher initial pressure and experimental temperature (fig. 4.22), causing a significant pressure increase upstream and a shaper velocity increase after the porous region.

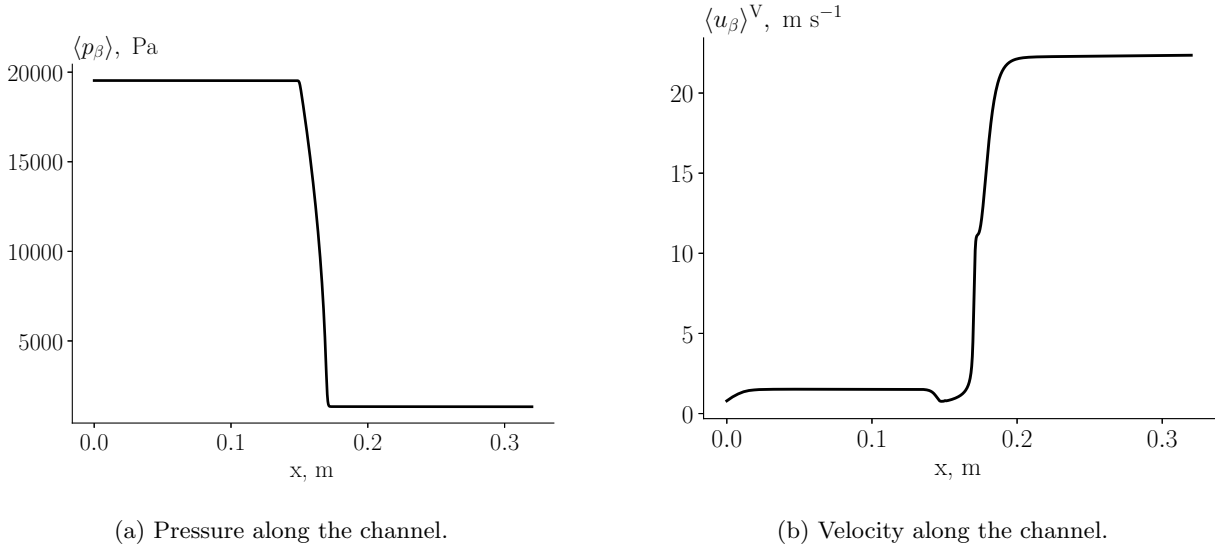


Figure 4.21: Flow field properties along the axis of the channel.

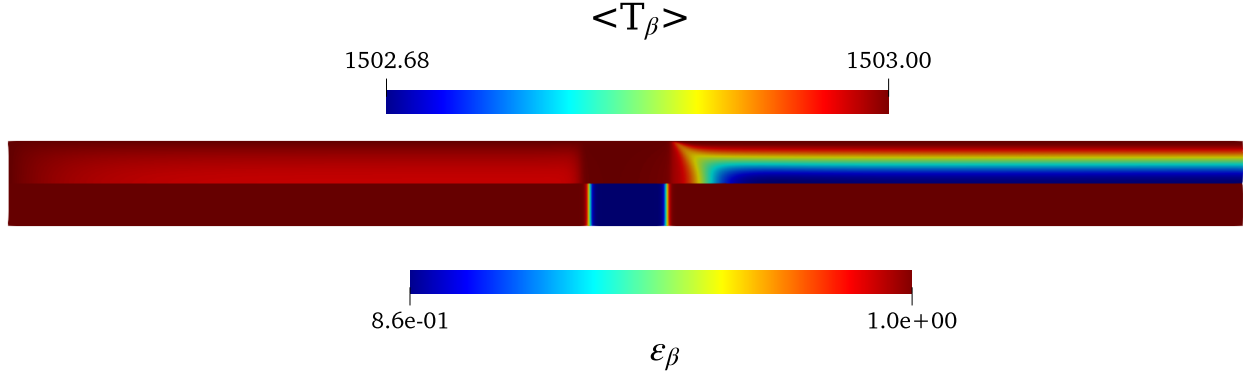


Figure 4.22: Top: Temperature contour along the channel, bottom: porosity along the channel.

Flow tube oxidation

The last test case is the well-known Beavers & Joseph [Beavers and Joseph \[1967\]](#) problem, which has been widely used to derive proper boundary conditions between the pure fluid phase and the porous material phase when considering both domains as decoupled phases. As illustrated in [fig. 4.23](#), a semi-infinite porous plug is regarded in the middle of the channel, forcing partial blockage of the pure fluid phase. Therefore, we consider a no-slip momentum boundary condition at the top and bottom of the channel and a unitary Reynolds number yielding,

$$\text{Re} = \frac{\rho U H}{\mu} = 1,$$

where U is the average inlet velocity. In this case, we consider molecular oxygen flowing along the channel at an initial temperature of 1000 K. At this temperature, the oxygen reacts with the carbon fibers in a reaction similar to [R1](#). Moreover, we include the heterogeneous production term shown in [eq. \(4.21\)](#) and used the reaction rate derived by [Panerai et al. \[2014a\]](#).

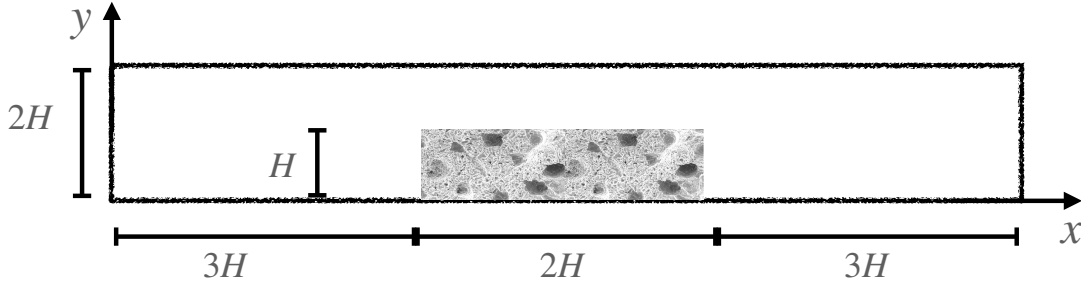


Figure 4.23: Beavers & Joseph problem geometry.

[Figures 4.24 and 4.25](#) show the CO_2 mass fraction and velocity along the channel. The former figure reveals a significant increase in CO_2 mass fraction within the porous region, leading to a subsequent decrease in the concentration of O_2 ([fig. 4.26a](#)), which then decreases the production rate, as shown in [fig. 4.26b](#). The peaks shown in [fig. 4.26b](#) indicate a higher production rate at the interface of the porous region, owing to the presence of available molecular oxygen. The velocity increases due to the channel contraction caused by the presence of the porous material, as described by [Dias et al. \[2023\]](#). Furthermore, a re-circulation bubble is observed at the back of the material.

Reaction [R1](#) is highly exothermic, meaning that it releases energy when it occurs. This release of energy increases the temperature where the production term is higher, as shown in [fig. 4.27](#). [Figure 4.27](#) shows an increase of temperature inside the material due to heat conduction caused by the increase of temperature due to reaction [R1](#). A similar behavior has been observed in the experiments of [Panerai et al. \[2014a\]](#) and also modeled by [Schrooyen et al. \[2016\]](#).

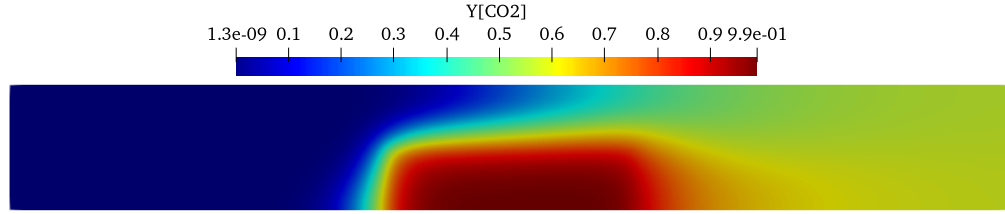


Figure 4.24: CO_2 mass fraction contour along the channel.

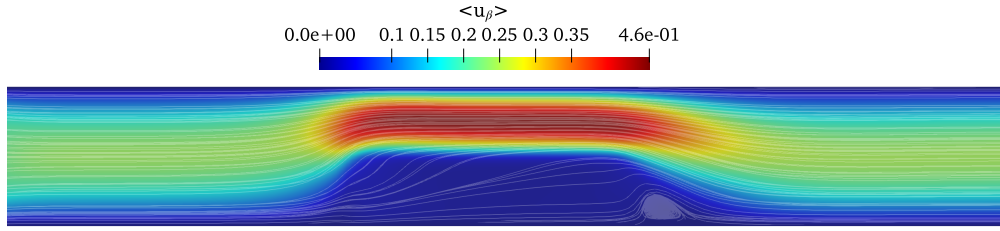
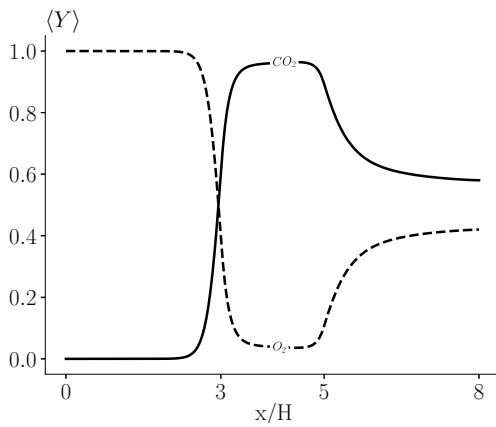
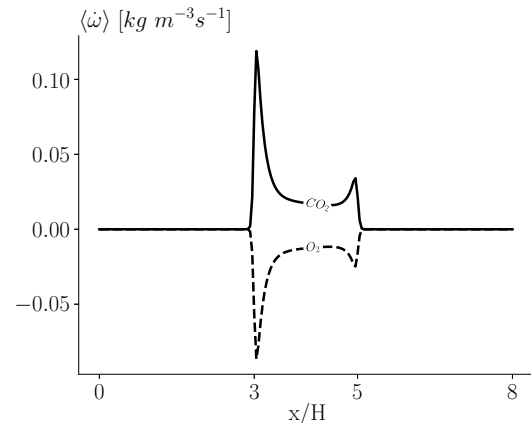


Figure 4.25: Velocity contour and streamlines along the channel.



(a) Species concentration along the x-direction.



(b) Species heterogeneous production source term along the x-direction.

Figure 4.26: Flow field properties along the channel at $y = 0.5H$

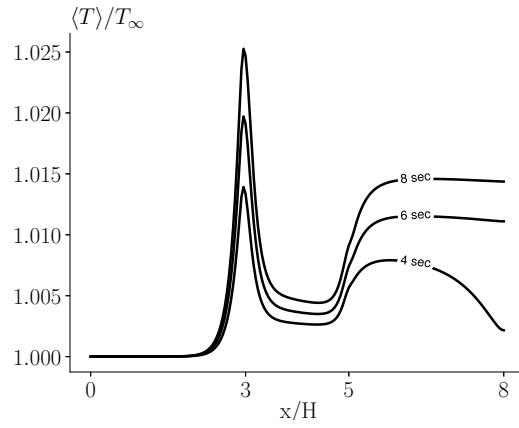


Figure 4.27: Temperature along the channel at at $y = 0.5H$ at different time.

Chapter 5

Conclusions

Using the **VANS** technique, we have derived the **GE** that enables solving a fluid and porous media in the same computational domain. With this technique, also known as filtering, the interaction between the different phases is averaged over a **REV** (or filter), allowing a single set of equations without explicitly modeling the solid phase. Instead, this averaging procedure results in effective transport properties, which map the micro-scale fluid-solid interaction onto a macro-scale effect, also perceived as upscaling. The effective properties are derived at the porous scale using DNS-type simulations, and its complexity increases with the porous structure.

The upscaling accuracy is mainly related to the averaging volume (**REV**) size, where the decomposition of length scales has to be regarded; otherwise, higher-order terms become relevant. Usually, the upscaling is done in a homogenous porous medium, i.e., the porosity is constant. In TPS modeling, that might not be the case because the phenolic resin and fibers decompose unevenly, depending on the local heat load. In this case, the filter size and kernel play an essential role in upscaling, particularly in the fluid and porous domain transition, thus requiring special attention.

For the last 40 years, most **VANS** research has focused on incompressible non-reacting problems far from aerospace applications. For those cases, a range of studies concerns the closure of the average equation and the importance of dispersion terms, which can often be neglected. In this work, we have derived the **VANS** equations from the reactive compressible Navier-Stokes equations, considering import higher-order terms that might appear at the interface. These higher-order terms are unattainable to close from a macroscale standpoint. Hence, the only possibility is to deduce the variation of effective properties at the interface using DNS-type simulations.

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