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Comprehensive Approaches to Multiphase Flows in Geophysics—Application to nonisothermal, nonhomogenous, unsteady, large-scale, turbulent dusty clouds
I. Hydrodynamic and Thermodynamic RANS and LES Models

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Comprehensive Approaches to Multiphase Flows in Geophysics—Application to nonisothermal, nonhomogenous, unsteady, large-scale, turbulent dusty clouds I. Hydrodynamic and Thermodynamic RANS and LES Models

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Abstract

The objective of this manuscript is to fully derive a geophysical multiphase model able to "accommodate" different multiphase turbulence approaches; *viz*., the Reynolds Averaged Navier-Stokes (RANS), the Large Eddy Simulation (LES), or hybrid RANS-LES. This manuscript is the first part of a larger geophysical multiphase project—lead by LANL—that aims to develop comprehensive modeling tools for large-scale, atmospheric, transient-buoyancy dusty jets and plume (e.g., plinian clouds, nuclear "mushrooms," "supercell" forest fire plumes) and for boundary-dominated geophysical multiphase gravity currents (e.g., dusty surges, diluted pyroclastic flows, dusty gravity currents in street canyons). LES is a partially deterministic approach constructed on either a spatial- or a temporal-separation between the large and small scales of the flow, whereas RANS is an entirely probabilistic approach constructed on a statistical separation between an ensemble-averaged mean and higher-order statistical moments (the so-called "fluctuating parts"). Within this specific multiphase context, both turbulence approaches are built up upon the same phasic binary-valued "function of presence." This function of presence formally describes the occurrence—or not—of any phase at a given position and time and, therefore, allows to derive the same basic multiphase Navier-Stokes model for either the RANS or the LES frameworks. The only differences between these turbulence frameworks are the closures for the various "turbulence" terms involving the unknown variables from the fluctuating (RANS) or from the subgrid (LES) parts. Even though the hydrodynamic and thermodynamic models for RANS and LES have the same set of Partial Differential Equations, the physical interpretations of these PDEs cannot be the same, i.e., RANS *models* an averaged field, while LES *simulates* a filtered field. In this manuscript, we also demonstrate that this multiphase model fully fulfills the second law of thermodynamics and fulfills the necessary requirements for a well-posed initial-value problem. In the next manuscripts, we will further develop specific closures for multiphase RANS, LES, and hybrid-LES.

“*Big whorls have little whorls,*
That feed on their velocity;
And little whorls have lesser whorls,
And so on to viscosity.”

Lewis Fry Richardson (1881–1953),
Summarizing the essence of his seminal paper “The supply of energy from and to atmospheric eddies,” *Proceedings of the Royal Society*, A97, 354–373, 1920.

1. Introduction

1.1. Scope and Objectives

Large-scale, atmospheric, transient-buoyancy dusty plumes and jets, such as plinian clouds (Figure 1 and Figure 2), nuclear "mushrooms" (Figure 3, Figure 4, and Figure 5), and "supercell" forest fire plumes [Fromm and Servrankx 2003], potentially pose a major threat to human life, livestock, the environment, and aircraft safety and, therefore, may disrupt nationwide social and economical activities [Dartevelle et al., 2002]. These geophysical flows also present a great scientific and engineering interest because their dynamic has this peculiarity of being mostly (if not solely) controlled by turbulence or by the magnitude of "mixing" with the surrounding atmosphere. Hence, dusty geophysical plumes and jets present the "ideal" multiphase flows for implementing and testing new geophysical turbulence and numerical models. In addition, many of these large-scale plumes are well constrained by observations and by remote-sensing data, allowing modelers to validate their numerical results and mathematical models. Last but not least, this project can also be applied to boundary-dominated geophysical dusty gravity currents such as base surge clouds generated by nuclear blasts (Figure 5) or surge flows following, for instance, the collapse of the twin towers in New York City (Figure 6) or the collapse of volcanic jets (Figure 7) [Wohletz 1998]. For these latter flows, the boundary (e.g., ground layer and the atmospheric boundary layer) has an important effect upon the whole flow dynamic. Therefore, multiphase gravity currents turn out to be ideal flows to further test hybrid approaches (i.e., hybrid-LES) consisting of RANS at and nearby the boundary and LES further away in the boundary-free atmosphere.

1.2. Definitions

The primary goal of this manuscript is to pave the way to a better understanding of *geophysical multiphase turbulence*. By *turbulence*, we mean that the small-scale motions (generally unknown) have a significant influence upon the large-scale motions (which are the scales of interests in geophysics). By *multiphase*, we mean that the fluid system is made of different materials, each of them having their own specific and distinct behavior over all scales [Kashiwa and Vanderheyden 2000]. By *geophysical*, we mean that the flow event may last from microsecond to several hours over spatial scales from centimeters to thousands of kilometers.

1.3. Methodologies and Organization

Because geophysical multiphase turbulence is still very much in its infancy [Dartevelle 2004; Dartevelle et al., 2004], we must devise a model flexible enough to be compatible with different approaches to turbulence (e.g., LES, RANS, or hybrid methods). Indeed, different geophysical flows may require different multiphase turbulence methodologies, and/or the same geophysical flow may be explored with different multiphase turbulence models. In other words, before getting to any specific turbulence closures and models, we must set an appropriate mathematical framework able to "nest" different turbulence models. Establishing this framework is what this manuscript wants to achieve.

This manuscript is organized as follows. First (§2), we systematically review the mathematical and physical formalisms behind multiphase flow and turbulence. In particular (§2.3), we define the exact chosen methodology of this manuscript (the function of presence) for setting a multiphase system fully compatible with different approaches to turbulence; *viz*., the ensemble averaging process (RANS in §2.5) and the filtering process (LES in §2.6). The specific mass and phasic-weighted Favre decompositions are defined for both RANS and LES approaches in §2.7. With this theoretical background reviewed, we introduce a general multiphase hydrodynamic model (§3) based upon the derivations performed in Appendix 2 for the RANS approach and in Appendix 3 for the LES approach. Next, we demonstrate that this "universal" hydrodynamic model satisfies the necessary requirement for well-posed system as an initial value problem (§5) and is fully compliant with the second law of thermodynamics (§6). In §4, we define the exact relationships between the RANS and LES stress tensors in order to rationally set hybrid turbulence models based upon both the RANS (e.g., near walls) and the LES (e.g., away from walls) models.

All the symbols, constants, operator, tensors, invariants, SI units, and acronyms are thoroughly defined in Appendix 7 and Appendix 8. The averaging and filtering mathematical rules are summarized and reviewed in §2.4 and in Appendix 1. In particular, the averaging properties within RANS are reviewed in §2.5.1 and §2.5.3, while the filtering properties within LES are reviewed in §2.6.1.

The sign convention for stress is such that it follows the same convention as Fick and Fourier laws [Bird et al., 1977; Dartevelle 2004]. In other words, viscous stress is positive in the direction of decreasing velocities. Hence, compressive stress, compressive strain, and their rates are positive. Unless specified otherwise, vectors (e.g., $\mathbf{q}$, $\mathbf{y}$, $\mathbf{u}$) and tensors (e.g., $\mathbf{T}$, $\boldsymbol{\tau}$) are denoted in bold, while scalar functions (e.g., ρ, ε, T, y) are noted in normal.

Figure 1. Mt. Pinatubo volcanic plume, Philippines, June 12, 1991. Altitude: ~12 km.

Figure 2. Ascending eruption cloud from Redoubt Volcano. View is to the west from the Kenai Peninsula. Notice that the main plume is offset from the vent. Altitude: ~10 km. (Photograph by J. Warren, April 21, 1990, USGS.)

Figure 3. Baneberry Test, Operation Emery, December 1970, Nevada (failed containment underground test in a ~280-m-deep shaft). Yield: 10 kt; Altitude: ~3 km. Because the explosive device was initially underground (and supposed to be contained), the rising plume was highly enriched in dust causing local nuclide pollution.

Figure 4. George Test, Operation Greenhouse, May–June 1951, Ruby Island, Enewetak Atoll. Yield: 225 kt.

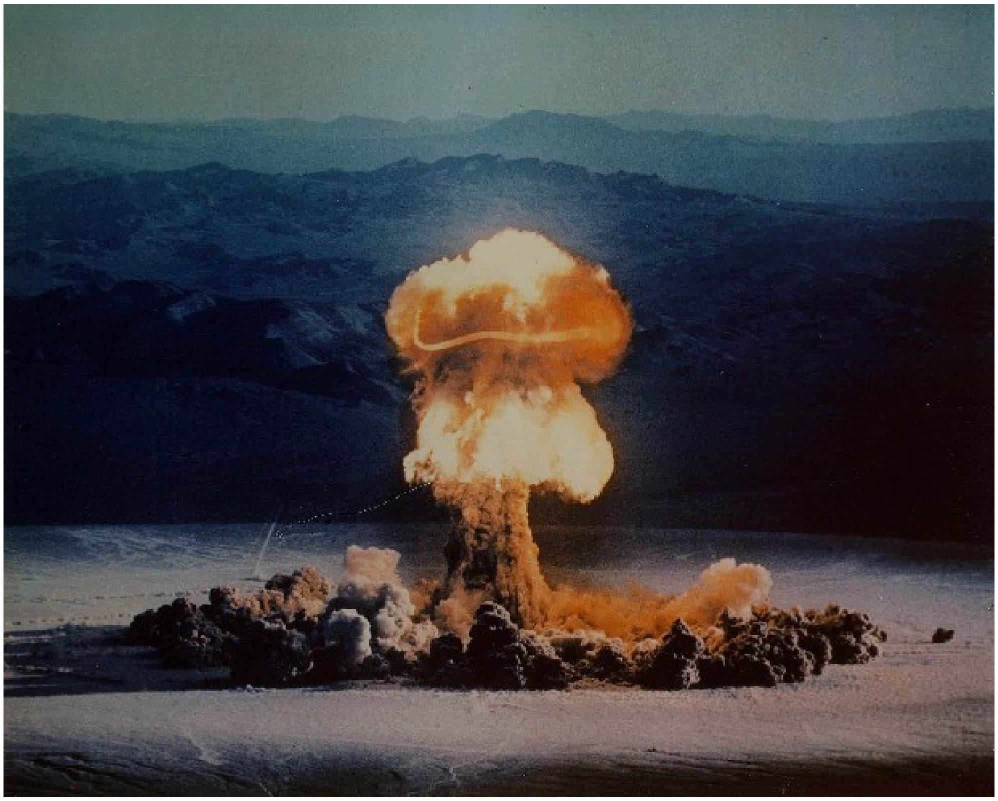

Figure 5. Grable Test, Operation Upshot-Knothole, May 1953, Nevada. Yield: 15 kt. Notice the dusty surge cloud radially spreading around the main plume.

Figure 6. Dusty gravity currents following the collapse of the Twin Towers, World Trade Center, New York City, September 11, 2001.

Figure 7. Pyroclastic flows and surges flowing the collapse of the plinian jet in Japan (exact location and time unknown).

2. The Making of a Multiphase Model

2.1. Turbulence Approaches

What would be the best turbulence model to properly capture geophysical multiphase jets, plumes, and boundary-dominated geophysical multiphase gravity currents? The answer is far from obvious because many multiphase turbulence models available in computational fluid dynamics (CFD) have not been thoroughly tested in geophysics[1]. In addition, knowing the large span of temporal and spatial scales covered by multiphase geophysical flows, we may reasonable expect that there would be no universal and unique turbulence approach. Rather, we should aim a unique mathematical model able to accommodate different approaches to turbulence.

Generally speaking, four major approaches are available to capture turbulence phenomenon:

1. The most traditional approach in multiphase-CFD is the Reynolds Averaged Navier-Stokes framework (RANS), which is an entirely statistical approach in that only a statistical mean (e.g., by ensemble-average) of a given variable is computed, while all the higher-order statistical moments are modeled. In other words, only the mean part of a quantity is "simulated," whereas the "small-scale" effects from turbulent fluctuations must be somehow modeled. Although RANS approaches have received considerable attention these past decades, these models have led to disappointing results with computer costs being higher and higher as the RANS models become more and more sophisticated [e.g., Sagaut et al., 1997; Lakehal 2002]. RANS approaches have been quite extensively developed for multiphase flows [e.g., Besnard et al., 1987, 1992; Simonin 1996; Kashiwa and Vanderheyden 2000; Peirano et al., 2001]. However, to the best of our knowledge, these multiphase models have never been applied to large-scale geophysical multiphase flows.
2. The Direct Numerical Simulations approach (DNS) is purely deterministic because it solves all spatial and temporal scales of motions from the largest to the smallest ones. The smallest scales may be related, for instance, to the Kolmogorov dissipation scales or any other dissipation scales (e.g., boundary layer) [Lesieur 1997]. DNS therefore must require extremely small time-steps and mesh size in order to fully capture the smallest dynamical scales of the flow. In other words, DNS can only be achieved with a prohibitive computational cost and, therefore, may never have been applicable (or not for long) for any geophysical flows developing upon large spatial scales and over long times.

[1] It should be noted, however, that the LES framework of single-phase turbulence is the most common way to capture turbulence effects in atmospherical sciences. It is also generally admitted in engineering literature (particularly in aeronautics) that highly unsteady and nonuniform (large-scale) turbulence is better captured by LES than RANS models.

3. LES is partially deterministic because it is constructed on a spatial or a temporal separation between the large scales and the small scales within the subgrid. Typically, large scales are strongly anisotropic and need to be directly simulated in a way similar to DNS, while small (subgrid) scales of the flow are assumed to be much more isotropic and universal so that simple scaling subgrid models can be used to model their effects. The separation between *simulated* large scales and *modeled* subgrid scales is achieved using filter functions ("kernels"). The filtered ("known") variables will be solved with the Navier-Stokes equations, and the effects from the unfiltered ("unknown") subgrid scales will be somehow modeled with supplementary source terms. At first glance, it may seem that LES should be far superior to the RANS approach because RANS models all scales, while LES only models the subgrid scales (the large scales are directly simulated). However, as we will show in this manuscript, the mathematical development of all the LES subgrid terms is far more complicated that in the RANS approach. Modeling all the LES terms is challenging[2], particularly within the multiphase framework. In addition, some further complications arise with LES methods when dealing with nonisotropic and nonhomogenous grid.
4. In many engineering applications (e.g., aeronautic, naval engineering sciences), LES usually has the favor as it better captures all the large-scale turbulent features of a given flow. However, near a boundary wall, the spatial resolution must often be increased in order to properly capture turbulent unsteadiness and instabilities near and at the wall. The spatial resolution needed at the wall must be so high in highly turbulent flows that the wall-LES model practically becomes a DNS model with prohibitive computer costs. Therefore, it may be more practical (and less computer demanding) to use a RANS model at the wall and to simulate the turbulent large-scale features with a LES approach far from the wall. These hybrid-turbulent approaches (often named "hybrid-LES") are gaining in popularity in aeronautic engineering sciences but present the challenge to properly "connect" averaged values of a given variables (from RANS) with its filtered values (from LES).

Because LES and RANS are based upon different mathematical and physical methodologies, it is necessary to systematically review these approaches first. Later, this manuscript devises a mathematical approach to derive a multiphase Navier-Stokes model compatible with both the statistical (RANS) and the filtering (LES) approaches. Specific turbulence closures will be developed in other manuscripts.

[2] It is not rare to find LES models not very well set (e.g., non-Galilean invariant) because of a poor choice of approximations [e.g., see discussion in Speziale 1985].

2.2. Multiphase Formalism

Because the system is made up of a large number of particles, it is impractical to solve the motion of each individual particle; hence, we have chosen Implicit Multi-Field formalism (IMF), which treats all phases in the system as interpenetrating continua. Each instantaneous local point variable (mass, velocity, temperature, pressure, and so forth) must be, *by some means*, "treated" to acknowledge the fact that any given arbitrary volume can be co-shared by different phases at the same time. This treatment may involve, for instance, an "averaging" or a "smoothing" process. The fact that we have averaged out or smoothed out some details is not worrisome as we are mostly concerned with the bulk flow behavior and as we rather want to know how the system works as a whole instead of knowing the exact history of a particular grain within the flow [Kashiwa and Vanderheyden 2000; Dartevelle 2003; Dartevelle 2004].

The process of deriving a *single-phase* Navier-Stokes system of equations into a *multiphase* system is far from being an obvious task, and yet it is a critical one, particularly when multiphase turbulence must be accounted for. Setting the multiphase Navier-Stokes equations alongside the appropriate turbulence closures has two basic approaches: the "*double-step*" and the "*single-step*" techniques[3]. This manuscript is only concerned with the single-step technique, which is by far the most efficient and compatible technique with the different approaches to turbulence: LES, RANS, and hybrid-LES.

1. The most common and somehow intuitive approach is the *double-step technique*. The first step involves a volume-average of all instantaneous local point variables in order to determine how much of a control volume (CV) is co-shared by all phases making up the multiphase system. This volume-average step must be achieved over a region that is large compared with the particle spacing but much smaller than the overall flow domain [Anderson and Jackson 1967]. In carefully specifying the mass, momentum, and heat transfer between phases alongside the jump conditions at their interfaces, it is easy to deduce a full set of Navier-Stokes equations for each phase. The most common volume-averaged approach for granular flows is from Anderson and Jackson [1967]. Afterwards, the second step consists of making the turbulence terms explicit within the volume-averaged equations by either averaging again (RANS framework) or filtering (LES framework). In this second step, each volume-averaged variable is decomposed into mean and fluctuating

[3] It should be noted that many modelers do not worry that much about averaging/smoothing processes and directly deduce the macroscopic equations. However, when it comes to the exact formulation of a multiphase turbulence model, many terms may be "forgotten," leading to unknown but critical assumptions regarding a given turbulence model, or even worse, leading to not very well-posed problems.

parts within the RANS framework or decomposed into filtered and subgrid parts within the LES framework. The *double-step method* is widely used within the RANS framework [e.g., Besnard et al., 1987; Besnard and Harlow 1988; Besnard et al., 1992; Cao and Ahmadi 1995; Zhang and Reese 2001; Boulet and Moisette 2002] but somewhat uncommon within LES because it becomes rather confusing to deal with both a volume-averaged and then a filtered variable. The *double-step method* is also inconvenient because the algebra during the second step is quite cumbersome.

2. The *single-step technique* relies on the phasic "function of presence" that formally describes the space occupation within any CV by a given phase [Drew 1983; Lhuillier 1996; Enwald et al., 1996; Lakehal et al., 2002]. The use of the *function of presence* saves us from the first step (i.e., the volume-averaged step) and allows us to directly derive a set of Navier-Stokes PDEs either by ensemble averaging (RANS framework) or by filtering (LES framework). This *single-step* method is clearly gaining in popularity [e.g., Simonin et al., 1995; Simonin 1996; Tran 1997; Kashiwa and VanderHeyden 2000; Milelli et al., 2001; Lakehal et al., 2002] because it offers an easier, clearer, and "handier" set of Navier-Stokes equations, which, in addition, are potentially compatible with different turbulence frameworks—RANS, LES, and hybrid-LES.

Because we aim to set a mathematical model that offers enough versatility to be compatible with different turbulence approaches, we are only concerned with the *single-step technique*, which is systematically reviewed in the next sections.

2.3. The Phasic and Interfacial Function of Presence

In a multiphase flow system, more than one phase may coexist in any CV. Therefore, let the i^{th} phase *function of presence*, $X_i(\mathbf{x},t)$, at location **x** and at time t be [Drew 1983]

$$X_i(\mathbf{x},t) = \begin{cases} 1 & \text{if location } \mathbf{x} \text{ is inside phase i at time t,} \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

Hence, in a two-phase gas-solid flow, we must have $X_g=1–X_s$. In addition to being a unique material identifier, X_i has some important properties [Drew 1983; Lhuillier 1996; Drew and Passman 1999].

a. First Property

$$\nabla X_i = -\mathbf{n}_i \delta_{Int} \tag{2}$$

where $\mathbf{n}_i$ is a unit normal vector pointing outward to the i^{th} phase at the location **x** and time t. The gradient of the phase function must be zero everywhere except exactly at the interface between phases. This gradient vector points towards the direction of maximum increase that is towards phase i itself in a direction opposite to $\mathbf{n}_i$. Obviously, at location **x** and time t in a two-phase flow, we have $\nabla X_g = -\nabla X_s$, or more generally, $\sum_{i=1}^{n} \nabla X_i = 0$. In Eq. (2), δ_{Int} is Dirac delta function at the interface location as it directly results from the step-like behavior of the interface as seen in Eq. (1). Hence, δ_{Int} acts as a function of presence of the interface itself (it is zero at any location where there is no interface).

The gradient in Eq. (2) can be used to sort out mass, molecular, and heat fluxes (and their directions) at the interface between gas and solid phases. Indeed, let us use an "angular operator," $\langle\rangle$, which will be thoroughly defined in the next sections (within RANS, it will be an ensemble averaged operator; within LES, it will be a filter operator). Ensemble-averaging or filtering Eq. (2), we have

$$\begin{aligned} \langle \nabla X_i \rangle &= \langle -\mathbf{n}_i \delta_{Int} \rangle \\ &= \nabla \langle X_i \rangle = \nabla \varepsilon_i \end{aligned} , \tag{3}$$

where ε_i is a "bulk" volumetric concentration of phase i (which will be thoroughly defined hereafter—see RANS §2.5.2 and LES §2.6.4). Clearly, the product of any property ϕ with the gradient of the phase function, e.g., $\left\langle \phi_i \nabla X_i \right\rangle$, must give a bulk contributory effect of fluxes of ϕ of phase i at its "bulk" interface over the whole domain of integration. By definition, in a two-phase system at location **x** and time t, we must have $\nabla \varepsilon_g = -\nabla \varepsilon_s$, or more generally, $\sum_{i=1}^{n} \nabla \varepsilon_i = 0$.

b. Second Property

The volumetric concentration of the interfacial area, A_i, can be defined as the "angular operator" upon the scalar product of $\mathbf{n}_i$ and ∇X_i:

$$A_i = \left\langle -\mathbf{n}_i \cdot \nabla X_i \right\rangle \quad . \tag{4}$$

Again, the angular operator may be either an ensemble-averaged operator (RANS) or a filter operator (LES). Clearly, in a system made of two phases (gas and solid) at location **x** and time t, we have $A_s = A_g$.

c. Third Property

$$\begin{aligned} &\frac{\partial X_i}{\partial t} + \mathbf{u}_{Int} \cdot \nabla X_i = 0 \\ \Leftrightarrow &\frac{\partial X_i}{\partial t} = \mathbf{u}_{Int} \cdot \mathbf{n}_i \delta_{Int} \end{aligned} \quad , \tag{5}$$

where $\mathbf{u}_{Int}$ is the velocity of the interface between phases. Eq. (5) indicates that the material (Lagrangian) derivative of X_i is always nil ($\frac{dX_i}{dt} = 0$) no matter where it occurs. Indeed, being exactly at the interface and moving with its local velocity ($\mathbf{u}_{Int}$), X_i represents a *constant* jump, and Eq. (5) must equal zero [Lhuillier 1996]. Being at any a location other than the interface, then either X_i=1 (inside the material) or X_i=0 (outside the material), and therefore all the partial derivatives (time and space) must vanish [Drew and Passman 1999]. This result, of course, justifies the second line of Eq. (5) because the transient term of X_i ($\frac{\partial X_i}{\partial t}$) must vanish at any location except when an interface crosses that specific location.

d. Fourth Property

In a multiphase flow made of two and only two phases, the interface is straightforward to define (e.g., between the solid particles and the gas phase). In a mixture made of n phases (n>2), one must distinguish n-1 interfaces separating each phase from each other. Let us write the function of presence of interfaces in Eq. (2) between phase i and j as $\delta_{Int,i,j}$ where $i \neq j$; then the function of presence of *all interfaces between all phases* in the system is

$$\delta_{Int} = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \delta_{Int,i,j} \quad . \tag{6}$$

And the function of presence of the interface between *phase i only and all the other phases* in the system is

$$\delta_{Int,i} = \sum_{\substack{j=1 \\ j \neq i}}^{n} \delta_{Int,i,j} \quad . \tag{7}$$

Hence each phase's interface can be easily tracked without any confusion between different interfaces of different phases. With these new definitions, $\mathbf{u}_{Int}$ in Eq. (5) would represent a "bulk mean" interfacial velocity of *all interfaces between all phases* making up the multiphase system.

2.4. Core Properties of the Angular Operator $\langle\rangle$

In order to properly manipulate the multiphase Navier-Stokes equations within different turbulence frameworks (RANS and LES), we must define a mathematical operator that must own *at least* the three following properties. The exact mathematical nature of $\langle\rangle$ will be analyzed in the RANS (§2.5) and in the LES sections (§2.6).

a. First Property: conservation of constant

Let c be a constant, then

$$\left\langle c \right\rangle = c \quad . \tag{8}$$

b. ***Second Property:*** linearity

Let α and β be scalars, vectors, or tensors, then

$$\left\langle \alpha + \beta \right\rangle = \left\langle \alpha \right\rangle + \left\langle \beta \right\rangle \quad . \tag{9}$$

c. Third Property: commutativity with respect to derivations

Let 'ι' be either a space (x) or time (t) variable. Let α be a scalar, vector, or tensor, then

$$\left\langle \frac{\partial \alpha}{\partial \iota} \right\rangle = \frac{\partial \left\langle \alpha \right\rangle}{\partial \iota} \quad . \tag{10}$$

As we will see hereafter, the commutativity property is guaranteed within the RANS framework but required some discussions and further work within LES.

Generally speaking and unlike the RANS angular operator, a LES angular operator is not a Reynolds operator. This is an important difference between LES and RANS, leading to a different Navier-Stokes set of equations. Appendix 1 develops and demonstrates additional properties that will be extensively used throughout this manuscript.

2.5. Averaging Process – RANS Framework

2.5.1. Definition of the RANS operator ⟨⟩

Let $\phi(\mathbf{x},t)$ be an instantaneous local (microscopic) fluid property at some specific punctual position $\mathbf{x}$ in space and at time t (ϕ can be a scalar, vector, or tensor). Let us achieve N identical experiments (replicas) with the same initial and boundary conditions. For each replica, we systematically measure at the same location $\mathbf{x}$ and time t the property $\phi(\mathbf{x},t)$. Of course, we may expect to measure slightly different values of $\phi(\mathbf{x},t)$ in each of these experiments. However, our prime interest is to capture a *bulk* property of the system or an *averaged* value of $\phi(\mathbf{x},t)$, which would be a "macroscopic" characteristic value for the whole ensemble of experiments. This ensemble average over the N replicas is

$$\left\langle \phi(\mathbf{x},t) \right\rangle = \begin{cases} \lim\limits_{N\to\infty} \sum\limits_{n=1}^{N} \phi_n(\mathbf{x},t)\, P_n \\ \int\limits_{-\infty}^{\infty} \phi(\mathbf{x},t)\, dF(\phi) \end{cases} , \tag{11}$$

where $\phi_n(\mathbf{x},t)$ is the n^{th} realization of $\phi(\mathbf{x},t)$ with an observed probability P_n (if each realization of ϕ is equiprobable[4], then $P_n = 1/N$); $dF(\phi)$ is the element of probability of observing a given specific realization of ϕ (F is the cumulative distribution function of ϕ); and the integration takes over the whole set of possible values of ϕ. Both definitions (sum vs. integral) are strictly identical depending on whether $\phi(\mathbf{x},t)$ is seen as a continuous or discrete random function[5].

Other averaging methods are possible, such as volume-averaged, which is performed *around* a fixed point $\mathbf{x}$ at time t, or the time-averaged, which is performed at the location $\mathbf{x}$ in a *time interval* around t. However, in many instances, time and volume average may be seen as a special case of the ensemble average. For instance, if the flow is homogenous (on the average, the flow is uniform in all directions) and stationary (on the average, the flow does not vary with time), time, volume, and ensemble are just identical averages (this is the ergodicity hypothesis).

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[4] Which is very likely the case because N tends to infinity.

[5] Ensemble average is a molecular dynamic concept, whereas, in classical statistics, Eq. (11) is named the *expectation* of a random variable or random function.

2.5.2. The RANS operator $\langle\rangle$ upon the function of presence and density

The ensemble average of the function of presence of a given phase, X_i, must give the probability of presence of the ith phase at **x** and t as it represents the averaged occurrence of phase i:

$$\varepsilon_i = \left\langle X_i(\mathbf{x},t)\right\rangle = \int_{-\infty}^{+\infty} X_i(\mathbf{x},t)\,dF(X_i) \quad , \tag{12}$$

where ε_i is the volumetric concentration of the ith phase[6]. We may now define the phasic bulk density as

$$\hat{\rho}_i = \varepsilon_i \overline{\rho}_i = \left\langle X_i(\mathbf{x},t)\ \rho_i(\mathbf{x},t)\right\rangle \quad , \tag{13}$$

where the ensemble-averaged density of the ith phase is weighted by the ensemble-averaged phasic function of presence, i.e.,

$$\overline{\rho}_i = \frac{\left\langle X_i(\mathbf{x},t)\ \rho_i(\mathbf{x},t)\right\rangle}{\left\langle X_i(\mathbf{x},t)\right\rangle} = \frac{\left\langle X_i(\mathbf{x},t)\ \rho_i(\mathbf{x},t)\right\rangle}{\varepsilon_i} = \frac{1}{\varepsilon_i}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} X_i(\mathbf{x},t)\ \rho_i(\mathbf{x},t)\,dF(X_i,\rho_i), \tag{14}$$

where ρ_i is the microscopic density of the ith phase (for the solid phase, it will be assumed to be constant). Averaging processes have very important properties that are entirely demonstrated in Appendix 1. These properties will be extensively used to set up the multiphase Navier-Stokes equation system.

2.5.3. The RANS operator $\langle\rangle$ as a Reynolds operator

Let $\alpha(\mathbf{x},t)$ and $\beta(\mathbf{x},t)$ be two random variables, c a constant, and $\langle\rangle$ defined by Eq. (11). The angular-operator acts as a Reynolds operator within the RANS framework if and only if all the properties seen in §2.4 hold and if, in addition, we have

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[6] Eq. (12) is not exactly the volume average or the volumetric concentration of the ith phase. The only correct interpretation of Eq. (12) is that it represents the "expected value" of the ratio of the volume occupied by phase i to the total control volume, if the limit of the total volume approaches zero. If the spatial distribution of phase i is homogenous, then Eq. (12) represents exactly a volume-averaged concentration [Drew and Passman 1999].

$$\left\langle c\ \alpha\left(\mathbf{x},t\right)\right\rangle = c\ \left\langle \alpha\left(\mathbf{x},t\right)\right\rangle \tag{15}$$

$$\left\langle \left\langle \alpha\right\rangle\ \beta\right\rangle = \left\langle \alpha\right\rangle \left\langle \beta\right\rangle . \tag{16}$$

Consequently, we also find

$$\begin{aligned} &\left\langle \left\langle \alpha\left(\mathbf{x},t\right)\right\rangle\right\rangle = \left\langle \alpha\left(\mathbf{x},t\right)\right\rangle \\ &\left\langle \alpha'\right\rangle = \left\langle \alpha - \left\langle \alpha\right\rangle\right\rangle = 0 \end{aligned} , \tag{17}$$

where α' is the turbulent fluctuation or the deviation from the expectation of $\alpha(\mathbf{x},t)$ (i.e., $\left\langle \alpha \right\rangle$). For more details on these properties, see Appendix 1.

2.6. Filtering Process — LES framework

2.6.1. Definition of the LES operator ⟨⟩

A key idea of LES is the separation of the simulated large-scale properties of the flow from the modeled (subgrid, SG) small-scale properties. The limit[7] between large scales and subgrid scales is "supposed" to take place in the inertial subrange. This decomposition is obtained using a spatial filter with a characteristic width, ξ, equal to (or of the order of) the computational mesh-size[8] or using a temporal filter with a characteristic time, τ, equal to (or of the order of) the time interval.

As in §2.3, let $\phi(\mathbf{x},t)$ be an instantaneous local (microscopic) fluid property at some specific punctual position $\mathbf{x}$ in space and at time t. The LES space- and time-filtering process of ϕ is formally defined as [Sagaut 1998]

$$\left\langle \phi(\mathbf{x},t) \right\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} G(\xi,\tau)\,\phi(\mathbf{x}',t')\,dt'd\mathbf{x}' \quad , \tag{18}$$

where the spatial integration is produced over the entire flow domain, Ω (or any of its subdomains of constant grid-size), at any time. Eq. (18) filters $\phi(\mathbf{x},t)$ at a point $\mathbf{x}=\mathbf{x}'$ (spatial filtering) and at a time t=t' (time filtering) and weighted $\phi(\mathbf{x},t)$ by $G(\xi,\tau)$. In mathematics, this process is called the "mollification" of $\phi(\mathbf{x},t)$. Eq. (18) defines a "regulariser" or "mollifier" [Galdi 1994]. The filter kernel, $G(\xi,\tau)$, is defined by its spatial width ξ, $\xi=\mathbf{x}-\mathbf{x}'$, over which the smoothing process take place, and by its time interval τ, $\tau=t-t'$ during which the filtering process occurs. It can be seen that for the most commonly used spatial filters (e.g., box, Gaussian, or spectral filters), G is centered in ξ, symmetric around ξ, and keeping the same shape in space as $\mathbf{x}'$ varies[9].

[7] This limit is often named "cutoff."
[8] Although it does not have to be, the width may even be totally independent of the grid size. However, for finite volume codes, the most natural way is to relate ξ with the grid size.
[9] There are other filters that do not have these properties.

2.6.2. Properties of the LES operator ⟨⟩

1. The filter kernel is normalized to preserve the constants (First Property in §2.4); hence, over the whole domain, Ω (or any of its subdomains), during the whole time under consideration, we must have $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} G(\xi,\tau)\; dt'd\mathbf{x}' = 1$.

2. The space and time filter kernel, G(ξ,τ) in $\Re^4$, is initially obtained by tensorizing two kernels in space, $G_x(\xi)$ in $\Re^3$, and in time, $G_t(\tau)$ in ℜ [Sagaut 1998]

$$G(\xi,\tau) = G_x(\xi)\, G_t(\tau) \tag{19}$$

3. At the limit of ξ and τ going to zero, Eq. (18) becomes a Dirac delta sequence function [Weber and Arfken 2004]

$$\begin{array}{ccc} \lim\limits_{\substack{\xi\to 0\\ \tau\to 0}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} G_x(\xi)\, G_t(\tau)\, \phi(\mathbf{x}',t')\; dt'd\mathbf{x}' & = & \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} \delta(\xi)\,\delta(\tau)\,\phi(\mathbf{x}',t')\; dt'd\mathbf{x}' \\ \left\langle \phi(\mathbf{x},t) \right\rangle & = & \phi(\mathbf{x},t) \end{array} , \tag{20}$$

so that, when the grid size and/or the time step becomes smaller and smaller, near **x=x′** and t=t', we must have $\left\langle \phi(\mathbf{x},t) \right\rangle \approx \phi(\mathbf{x},t)$ as expected, wanted, and shown by Eq. (20).

2.6.3. Explicit spatial filters

In LES engineering and single-flow atmospherical literatures, it is by far more common to use a spatial filter rather than a time filter[10] because the time filter separates spatial scales (large vs. subgrid) with an obvious ease. This is formally expressed as

$$\lim_{\tau\to 0} G_x(\xi)\, G_t(\tau) = G_x(\xi)\,\delta(\tau) \quad . \tag{21}$$

[10] We should, however, mention that time filtering has numerous advantages, particularly filtering within a nonuniform grid domain and when applied to hybrid LES-RANS turbulence approaches.

It should be kept in mind that whenever a spatial filtering is achieved, an implicit (and often "forgotten") time filtering is also achieved as well [Sagaut 1998], which imposes supplementary conditions over the time step of any LES simulations.

Let us define a cutoff length, $\overleftrightarrow{\Delta}_k$, in the x_k^{th} direction (k=1, 2, 3 or x_k=X, Y, Z),

$$\overleftrightarrow{\Delta}_k = n \; \Delta x_k \quad , \tag{22}$$

where Δx_k is the mesh size in the X-, Y-, and Z-directions and 'n' is an integer usually taken between 1 and 3 (i.e., the filter length is two to three times coarser than the grid size in any given direction).

One of the most commonly used filters in space is the Gaussian spatial filter, e.g., in the x_k^{th} direction [Ferziger 1976; Piomelli et al., 1991],

$$G_x\,(\xi_k) = \frac{1}{\overleftrightarrow{\Delta}_k} \sqrt{\frac{\gamma}{\pi}} \; e^{-\frac{\gamma\,\xi_k^2}{\overleftrightarrow{\Delta}_k^2}} \quad , \tag{23}$$

where γ is a constant usually taken to be equal to 6 [Sagaut 1998; Pope 2000] and the filter width in the x_k^{th} direction is $\xi_k = x_k - x'$.

Another filter often used in finite-volume methods is the box spatial filter, e.g., in the x_k^{th} direction [Deardorff 1970; Piomelli et al., 1991],

$$G_x\,(\xi_k) = \begin{cases} \dfrac{1}{\overleftrightarrow{\Delta}_k} & \text{if } \left\|\xi_k\right\| < \dfrac{\overleftrightarrow{\Delta}_k}{2} \\ 0 & \text{otherwise} \end{cases} \quad . \tag{24}$$

With the box filter, $\left\langle \phi(\mathbf{x}, t) \right\rangle$ is the weighted-average of $\phi(\mathbf{x},t)$ over an interval ξ smaller than half of ΔX, ΔY, or ΔZ (Figure 8A).

Both filters are shown in Figure 8[11].

[11] There are many other filters [see Pope 2000]. We will review them in the next manuscript on multiphase LES approaches (under preparation).

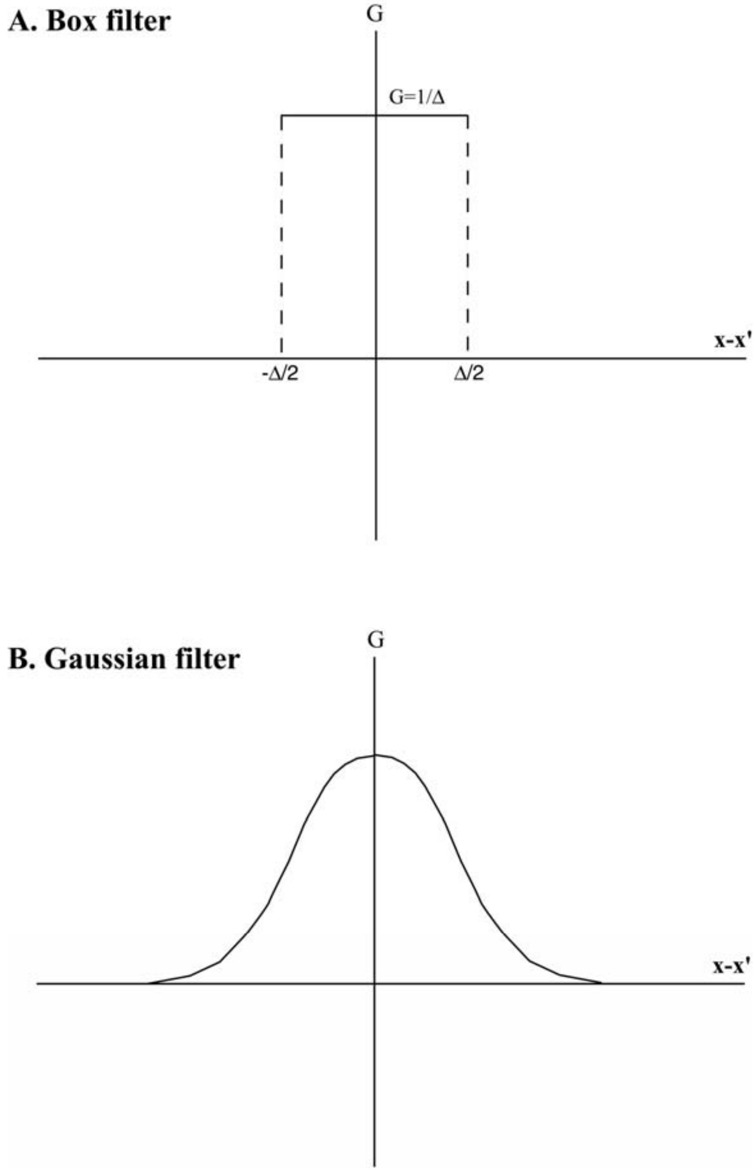

Figure 8

Two possible and common spatial filters: **A**. the box filter and **B**. the Gaussian filter.

2.6.4. *The LES operator $\langle\,\rangle$ upon the function of presence and density*

Let us use the i$^{\text{th}}$ phase function of presence, $X_i(\mathbf{x},t)$, as defined in Eq. (1) of §2.3. Then the spatial-filtering of X_i must give the filtered occurrence of phase i at the $\vec{\boldsymbol{\Delta}}$-scale over the whole domain Ω,

$$\varepsilon_i = \left\langle X_i\,(\mathbf{x},t)\right\rangle = \iiint_{\Omega} G_x\,(\xi)\,X_i\,(\mathbf{x}',t)\;d\mathbf{x}' \quad , \tag{25}$$

where ε_i is the volumetric concentration of the i$^{\text{th}}$ phase [compare with Eq. (12)]. Hereafter in this manuscript, we will not make any symbolic difference between the volumetric concentrations obtained by an ensemble averaging (RANS) or by a filtering (LES) process. The filtered phasic bulk density is

$$\underset{\smile}{\hat{\rho}_i} = \varepsilon_i\,\underset{\smile}{\overline{\rho}_i} = \left\langle X_i\,(\mathbf{x},t)\;\rho_i\,(\mathbf{x},t)\right\rangle \quad , \tag{26}$$

where the "bottom upside-down hat" is used to emphasize that the variable has been filtered (instead of being averaged as in RANS). The filtered density of the i$^{\text{th}}$ phase is weighted by the filtered phasic function of presence,

$$\underset{\smile}{\overline{\rho}_i} = \frac{\left\langle X_i\,(\mathbf{x},t)\;\rho_i\,(\mathbf{x},t)\right\rangle}{\left\langle X_i\,(\mathbf{x},t)\right\rangle} = \frac{\left\langle X_i\,(\mathbf{x},t)\;\rho_i\,(\mathbf{x},t)\right\rangle}{\varepsilon_i} = \frac{1}{\varepsilon_i}\iiint_{\Omega} G_x\,(\xi)\Big(X_i\,(\mathbf{x}',t)\,\rho_i\,(\mathbf{x}',t)\Big)\,d\mathbf{x}' \;, \tag{27}$$

where ρ_i is the microscopic density of the i$^{\text{th}}$ phase.

2.6.5. *Anisotropic and nonhomogenous explicit spatial filters*

In many engineering and geophysical applications, the grid size, $\Delta\mathbf{x}$, (hence the spatial-filter width, ξ) may not be homogenous over the whole computational domain (i.e., $\Delta\mathbf{x}$ varies in some directions) and/or may not be isotropic (i.e., $\Delta x_1 \neq \Delta x_2 \neq \Delta x_3$). The latter is not a problem, but the former is quite a matter of concern as it does pose a problem for the commutativity property with respect to space derivation [Third Property of §2.4, Eq. (10)].

The most common and classical way to deal with anisotropic filter width is the Deardorff [1970] method, which takes the geometric mean of the grid length between the 3 directions of space (Δ) to evaluate a "geometric-averaged" filter cutoff length,

$$\overleftrightarrow{\Delta} = n\ \Delta = n\ \sqrt[3]{\prod_{k=1}^{3} \Delta x_k} \quad , \tag{28}$$

where 'n' is a constant (usually between 1 and 3) and Δx_k is the grid width in the x_k^{th} direction of space. Many modifications of Deardroff's original model [see Sagaut 1998] and other models have also been proposed [e.g., Scotti et al., 1993, 1997]. Those will be reviewed in a future manuscript on multiphase LES.

To deal with nonhomogenous filter characteristic length, i.e., $\overleftrightarrow{\mathbf{\Delta}}$ is nonconstant within the computational domain, Ω, let Ω_i and Ω_j be two subdomains of Ω ($\forall\ i, j \in \mathbb{N}_0\ \cap\ i \neq j$), each characterized by constant grid sizes (Δx_k) in any direction (hence constant filter cutoff lengths, i.e., $\overleftrightarrow{\mathbf{\Delta}}_i$ and $\overleftrightarrow{\mathbf{\Delta}}_j$); let $\partial\Omega_{i,j}$ be the boundary between these subdomains; and let G_i and G_j be the spatial-filter kernels associated with Ω_i and Ω_j.

Let us examine first what happens to the filtering process with these nonhomogenous filters. Because $\overleftrightarrow{\mathbf{\Delta}}$ is nonconstant, the space-filter kernel becomes a function of $\overleftrightarrow{\mathbf{\Delta}}$ itself, i.e., $G_x(\xi, \overleftrightarrow{\mathbf{\Delta}})$ over Ω. We note that differentiating $\phi(\mathbf{x},t)$ with respect to space becomes

$$\begin{aligned} \nabla \left\langle \phi(\mathbf{x}, t) \right\rangle &= \nabla \left[\iiint_{\Omega} G_x(\xi, \overleftrightarrow{\mathbf{\Delta}})\, \phi(\mathbf{x}', t)\ d\mathbf{x}' \right] \\ &= \iiint_{\Omega} G_x(\xi, \overleftrightarrow{\mathbf{\Delta}})\, \nabla \left[\phi(\mathbf{x}', t) \right] d\mathbf{x}' + \iiint_{\Omega} \nabla \left[G_x(\xi, \overleftrightarrow{\mathbf{\Delta}}) \right] \phi(\mathbf{x}', t)\ d\mathbf{x}' \quad . \\ &= \left\langle \nabla \phi(\mathbf{x}, t) \right\rangle + \iiint_{\Omega} \nabla \left[G_x(\xi, \overleftrightarrow{\mathbf{\Delta}}) \right] \phi(\mathbf{x}', t)\ d\mathbf{x}' \end{aligned} \tag{29}$$

The second term of Eq. (29) would have been zero over a strictly homogenous domain; therefore, it represents a source of errors if not properly accounted for. This term can be further expanded into

$$\iiint_{\Omega} \frac{\partial}{\partial \mathbf{x}} \Big[G_x(\xi, \vec{\boldsymbol{\Delta}}) \Big] \phi(\mathbf{x}', t)\ d\mathbf{x}' = \frac{\partial G_x(\xi, \vec{\boldsymbol{\Delta}})}{\partial \vec{\boldsymbol{\Delta}}} \frac{\partial \vec{\boldsymbol{\Delta}}}{\partial \mathbf{x}} + \iint_{\partial\Omega} \Big[G_x(\xi, \vec{\boldsymbol{\Delta}})\, \phi(\mathbf{x}', t) \Big] \mathbf{n}(\mathbf{x}')\ d\mathbf{s} \quad , \tag{30}$$

where the first term on the RHS represents the error that is due to the spatial variation of the filter length and the second term represents the error from the flux of $\left\langle \phi(\mathbf{x}, t) \right\rangle$ through the surface of the boundary $\partial\Omega_{i,j}$ between the subdomain Ω_i and Ω_j. In Eq. (30), **n** represents an unit vector normal to $\partial\Omega_{i,j}$ pointing in the positive direction of the flux of $\left\langle \phi(\mathbf{x}, t) \right\rangle$.

As thoroughly seen in the next paragraph (§2.7), any instantaneous local fluid property at some specific punctual position **x** and at time t, $\phi(\mathbf{x},t)$, can be decomposed into a filtered (simulated and known) part (e.g., $\tilde{\phi} = \left\langle \phi \right\rangle$) and a subgrid (unfiltered and unknown) part (e.g., ϕ'') and this in each subdomain i and j of Ω (i.e., Ω_i and Ω_j) as follows:

$$\begin{array}{lccccc} & \text{within } \Omega_i & . & \text{within } \Omega_j & \\ \phi = & \tilde{\phi}_i + \phi_i'' & = & \tilde{\phi}_j + \phi_j'' & . \end{array} \tag{31}$$

Because each domain has different spatial resolution (hence different filter characteristics and filter length) but the same kernel function, we may define

$$\begin{aligned} \tilde{\phi}_{i,j} &= \tilde{\phi}_i - \tilde{\phi}_j \\ &= \iiint_{\Omega_i} G_i(\xi_i)\, \phi(\mathbf{x}', t)\ d\mathbf{x}' - \iiint_{\Omega_j} G_j(\xi_j)\, \phi(\mathbf{x}', t)\ d\mathbf{x}' \quad , \\ &= \iiint_{\Omega_{i,j}} \Big(G_i(\xi_i) - G_j(\xi_j) \Big) \phi(\mathbf{x}', t)\ d\mathbf{x}' \end{aligned} \tag{32}$$

where $\tilde{\phi}_{i,j}$ becomes a new complementary field allowing the transfer of information between Ω_i and Ω_j at $\partial\Omega_{i,j}$. The key information points that must now be tracked at all times are (1) the flux directions of $\phi(\mathbf{x},t)$ between the subdomains (if $\Omega_i \to \Omega_j$, then $\tilde{\phi}_j = \tilde{\phi}_i - \tilde{\phi}_{i,j}$ at $\partial\Omega_{i,j}$ or if $\Omega_j \to \Omega_i$, then $\tilde{\phi}_i = \tilde{\phi}_j + \tilde{\phi}_{i,j}$ at $\partial\Omega_{i,j}$) and (2) the exact location of the boundaries between subdomains, $\partial\Omega_{i,j}$.

The method to achieve LES simulation with multiresolution subdomains will mostly depend on the exact geometry configuration: either the finer grid subdomain is surrounded by a coarser subdomain [Kravchenko et al., 1996; Sullivan et al., 1996; Boersma et al., 1997], or, in the more general case, there is no specific geometric configuration between fine resolution and coarse resolution subdomains [Sagaut 1998; Quemere et al., 2001]. In the former case, the solution is solved either first in each Ω_i independently from the other subdomains (a separate time step for each Ω_i) and, afterwards, all solutions are coupled between all subdomains at their respective boundaries [Sullivan et al., 1996; Boersma et al., 1997], or the solution is solved within a unique time step over the whole Ω and all its subdomains with appropriate subdomain coupling [Kravchenko et al., 1996]. In the latter and more general case, the time integration must be achieved within a unique time step over the whole Ω. We should also mention the application of LES approaches to adaptative grids by Cook [2001] and Mitran [2001]. All these methods will not be reviewed herewith—our main point was simply to show that anisotropic, multigrid domains and adaptative grids can be dealt within the LES framework, even though it raises the level of complexity in code development.

It can be seen that with a box-filter [Eq. (24)] the problem is rather simple as it reduces itself to a simple factor multiplication of the variables at the boundary subdomain (rescaling ϕ through $\partial\Omega_{i,j}$)[12].

Therefore, we assume hereafter that the 3rd Property of §2.4 [Eq.(10)] is fully valid within the LES framework.

---

[12] For instance, let Ω_1 be the fine grid subdomain and Ω_2 the coarse grid domain, so that $\Delta_1 = \frac{\Delta_2}{\sqrt[3]{6}}$ (each mesh length is two times coarser in Ω_2 than in Ω_1). Hence, we have

from Ω_1 (fine) to Ω_2 (coarse) flux at $\partial\Omega_{1,2}$: $\tilde{\phi}_2 = \frac{\tilde{\phi}_1}{\sqrt[3]{6}}$ and

from Ω_2 (coarse) to Ω_1 (fine) flux at $\partial\Omega_{1,2}$: $\tilde{\phi}_1 = \sqrt[3]{6}\ \tilde{\phi}_2$.

2.7. RANS and LES Favre Decompositions

Within the RANS framework (§2.5), each time an idealized experiment is achieved, we may measure deviations (fluctuations) between the calculated ensemble average over all the experiments and the instantaneous local variable measured at position **x** and t. As we are mostly interested in the bulk flow, the approach of taking the ensemble average of each variable in the system is fully justified. However, the ensemble-averaged value of a given variable and its factual instantaneous local value may greatly differ. Hence, it becomes critical to "properly" recover the lost information during the averaging process that will be supplied by a RANS model. Each instantaneous local variable, $\phi(\mathbf{x},t)$, is broken into an ensemble-averaged part ($\overline{\phi}$ or $\tilde{\phi}$) and a fluctuating part (ϕ' or ϕ'') using two Favre decompositions (density-weighted and volumetric concentration-weighted) [Favre 1965].

Within the LES framework (§2.6), a formal scale separation by means of filter functions is achieved between the anisotropic large scales and the more isotropic small scales. The filtering process between scales can be achieved either in space (spatial filter, the most common approach) or in time (temporal filter). Each instantaneous local variable, $\phi(\mathbf{x},t)$, is broken into a filtered (or resolved, simulated) part ($\underset{\smile}{\overline{\phi}}$ or $\underset{\smile}{\tilde{\phi}}$) and an unresolved (or unfiltered within the subgrid) part ($\underset{\smile}{\phi}'$ or $\underset{\smile}{\phi}''$) that needs to be modeled. The same two Favre decompositions used in RANS—mass-weighted and phasic-weighted [Favre 1965]—complete this decomposition. The unresolved part can be seen as all the fluctuations caused by, for instance, turbulence within the subgrid. However, it should be kept in mind that the unresolved part exists only because of the finite cutoff scale, $\vec{\boldsymbol{\Delta}}$, of the filter[13].

In this manuscript, and within the LES framework only, all Favre decompositions are noted by a "bottom upside-down hat" under the variable (e.g., $\underset{\smile}{\overline{\phi}}, \underset{\smile}{\tilde{\mathbf{u}}}, \underset{\smile}{\overline{\rho}}, \underset{\smile}{\overline{\mathbf{T}}}, \ \ldots$).

Favre *phasic*-weighted decompositions are shown below:

RANS framework	LES framework
$\phi_i = \overline{\phi}_i + \phi_i'$ (33)	$\phi_i = \underset{\smile}{\overline{\phi}_i} + \underset{\smile}{\phi_i}'$ (34)

Within the RANS framework, the prime stands for the fluctuating part and the horizontal bar stands for the mean part obtained from the Favre *phasic*-weighted ensemble averaging. Within the LES framework, the horizontal bar stands for the resolved (the filtered field that is simulated), while the

[13] In other words, it is not mathematically correct to compare the fluctuating part obtained from RANS and the subgrid part obtained from LES, even though both may be somehow connected to the small-scale (turbulent) flow fluctuations.

prime stands for the unresolved subgrid (residual) field (that needs to be modeled). The phasic-weighted ensemble-averaged and filtered decompositions are given by the following:

RANS framework:	$\overline{\phi}_i = \dfrac{\langle X_i(\mathbf{x},t)\,\phi_i(\mathbf{x},t)\rangle}{\langle X_i(\mathbf{x},t)\rangle} = \dfrac{\langle X_i(\mathbf{x},t)\,\phi_i(\mathbf{x},t)\rangle}{\varepsilon_i}$	(35)
LES framework:	$\underset{\smile}{\overline{\phi}}_i = \dfrac{\langle X_i(\mathbf{x},t)\,\phi_i(\mathbf{x},t)\rangle}{\langle X_i(\mathbf{x},t)\rangle} = \dfrac{\langle X_i(\mathbf{x},t)\,\phi_i(\mathbf{x},t)\rangle}{\varepsilon_i}$	(36)

The Favre *mass*-weighted decompositions are shown below

RANS framework		**LES framework**	
$\phi_i = \tilde{\phi}_i + \phi_i''$	(37)	$\phi_i = \underset{\smile}{\tilde{\phi}}_i + \underset{\smile}{\phi}_i''$	(38)

where the double prime stands for the fluctuating (or unresolved residual) part and the tilde stands for the mean (or resolved) part. The Favre *mass*-weighted ensemble-averaged and filtered decompositions are given by the following:

RANS framework:	$\tilde{\phi}_i = \dfrac{\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\,\phi_i(\mathbf{x},t)\rangle}{\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\rangle} = \dfrac{\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\,\phi_i(\mathbf{x},t)\rangle}{\hat{\rho}_i}$	(39)
LES framework:	$\underset{\smile}{\tilde{\phi}}_i = \dfrac{\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\,\phi_i(\mathbf{x},t)\rangle}{\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\rangle} = \dfrac{\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\,\phi_i(\mathbf{x},t)\rangle}{\underset{\smile}{\hat{\rho}}_i}$	(40)

Unless it can be shown that the microscopic density of a given phase is strictly constant (which is the case if the dispersed phase is made of solid grains), the *mass*-weighted values ($\tilde{\phi}_i$ or $\underset{\smile}{\tilde{\phi}}_i$) are not equal to the *phasic*-weighted values ($\overline{\phi}_i$ or $\underset{\smile}{\overline{\phi}}_i$). Last but not least, it is worth mentioning that filtering and averaging have two very distinct properties (see also Appendix 1):

RANS framework (Averaging)	**LES framework** (Filtering)
$\overline{\overline{\phi_i}} = \overline{\phi_i}$ $\tilde{\tilde{\phi_i}} = \tilde{\phi_i}$	$\underset{\smile}{\overline{\overline{\phi_i}}} \neq \underset{\smile}{\overline{\phi_i}}$ $\underset{\smile}{\tilde{\tilde{\phi_i}}} \neq \underset{\smile}{\tilde{\phi_i}}$
$\overline{\phi_i'} = \widetilde{\phi_i''} = 0$	$\overline{\phi_i'} \neq \widetilde{\phi_i''} \neq 0$

In other words, within the LES framework, filtering a variable twice does not give the same results as the initial filtered variable, and filtering the unresolved subgrid (residual) field of the variable will not necessarily give a nil result[14]. The consequence is that modeling subgrid fields (stress, heat flux, and so forth) will be more complicated than for the RANS approach [Ferziger 1997].

With all this in mind, it is now possible to derive in a "*one-step ensemble-averaging process*" (RANS) or in a "*one-step filtering process*" (LES) a full set of Navier-Stokes equations for all the phases in the system as demonstrated in Appendix 2, Appendix 3, and detailed in the next section (§3).

[14] It would be possible to define a filter G_x so that filtering the unresolved subgrid field leads to zero, but this is not that case with a Gaussian and the box filters.

3. RANS and LES Hydrodynamic and Thermodynamic Model

From the demonstrations in Appendix 2 (RANS) and Appendix 3 (LES), one can see that it is possible to derive hydrodynamic and thermodynamic models that would be able to accommodate both the Large-Eddy Simulation and Reynolds-Favre ensemble-averaged Navier-Stokes frameworks of turbulence. Of course, the constitutive equations for turbulent or subgrid phenomena (stress, dissipation, heat conduction, and so forth) and possibly the interfacial terms may differ.

In the following, we will not make any distinction between the LES and RANS symbols; however, we will retain the symbols for phasic-weighted decomposition ($\overline{\phi}$), mass-weighted decomposition ($\tilde{\phi}$) variables, and their subsequent fluctuating or unfiltered parts, i.e., ϕ' or ϕ'', respectively.

The equations are written in terms of the ensemble-averaged or filtered variable for each phase, where $\hat{\rho}$, $\tilde{\mathbf{u}}$, and $\tilde{y}$ pertain to averaged or filtered macroscopic density, velocity vector, and mass fraction. The indices ‘s’ and ‘g’ are for the solid and gas phase. Because each phase is modeled as a continuum, they can be present at the same time in the same control volume, CV [Harlow and Amsden 1975]. Hence, we must distinguish the microscopic density of a particular material, ρ, from the macroscopic bulk density, $\hat{\rho}_i = \varepsilon_i \overline{\rho}_i$, where ε is the volumetric fraction of the phase under consideration and $\overline{\rho}_i$ is the phasic-averaged (§2.5.2) or filtered (§2.6.4) density. Within any CV, we must have $\sum_{i=1}^{n} \varepsilon_i = 1$ for all n phases, and for all m species of a given phase, $\sum_{j=1}^{m} y_j = 1$. The gas phase needs an equation of state, which has be specified in a specific context[15], e.g.,

$$\tilde{\rho}_g = \widetilde{fct}\left(P_g, \ddot{R}, T_g, \ldots\right) \quad , \tag{41}$$

where $\ddot{R}$ is the ratio of the universal gas constant (R) and the molar mass of a gas mixture of m species,

$$\ddot{R} = R\sum_{j=1}^{m} \frac{y_j}{M_j} \quad , \tag{42}$$

where M_j is the molar mass of the j^{th} gas species.

[15] The EOS issue is thoroughly discussed in the Method of Characteristics (MOC) section (see §5).

3.1. Phasic and Species Continuity

From Appendix 2 and Appendix 3, we may write the phasic continuity equation valid within both RANS and LES frameworks as

$$\frac{\partial \hat{\rho}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i = R_i \quad , \tag{43}$$

where, for instance, i=1 for the gas phase and i≥2 for the dispersed phases and R_i is the mass exchange flux between phases at their interfaces, with $\sum_{i=1}^{n} R_i = 0$.

In the case where one of the phases would be made up of different species (e.g., for the gas phase, dry air and water vapor), the species continuity for both RANS and LES framework (see Appendix 2 and Appendix 3) is

$$\frac{\partial \hat{\rho}_i \tilde{y}_j}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{y}_j \tilde{\mathbf{u}}_i = -\nabla \cdot \hat{\rho}_i \left(\mathbf{y}_j + {}^{tur/SG}\mathbf{y}_j \right) + \varepsilon_i \overline{\Gamma}_j + C_{i,j} \quad , \tag{44}$$

where $\tilde{y}_j$ is the averaged or filtered mass fraction of the j^{th} species; $\overline{\Gamma}_j$ is the averaged/filtered mass source or sink rate because of chemical or physical processes between species; and $C_{i,j}$ is the interfacial species mass transfer rate and has two contributions—one from the mass transfer between phases and one from the diffusion of the interface belonging to species j of the i^{th} phase. The latter contribution is very often disregarded [Syamlal et al., 1993; Veynante and Poinsot 1997]; hence, in most circumstances, $C_{i,j}$ can be written as a simple function of mass transfer between phases:

$$C_{i,j} \approx \tilde{y}_j R_i \quad , \tag{45}$$

with the mean jump condition between the m species of phase i and all other phases as $\sum_{i=1}^{n} \sum_{j=1}^{m} C_{i,j} = 0$.

In Eq. (44), the species mass fraction flux has two contributions: one from the averaged or filtered flux (i.e., $\mathbf{y}_j$) and one from turbulence (RANS, ${}^{tur}\mathbf{y}_j$, 00Appendix 2: Favre-Averaged Navier-Stokes Equations) or from the subgrid (LES, ${}^{SG}\mathbf{y}_j$):

$$
\begin{aligned}
&\mathbf{y}_j = \varpi \nabla \tilde{y}_j \\
&{}^{tur}\mathbf{y}_j = \widetilde{y_j'' \mathbf{u}_i''} && \text{RANS framework} \\
&{}^{SG}\mathbf{y}_j = \left(\widetilde{\breve{\tilde{y}}_j \breve{\tilde{\mathbf{u}}}_i} - \breve{\tilde{y}}_j \breve{\tilde{\mathbf{u}}}_i \right) + \left(\widetilde{\breve{\tilde{y}}_j \breve{\mathbf{u}}_i''} + \widetilde{\breve{y}_j'' \breve{\tilde{\mathbf{u}}}_i} \right) + \left(\widetilde{\breve{y}_j'' \breve{\mathbf{u}}_i''} \right) && \text{LES framework}
\end{aligned}
\tag{46}
$$

where ϖ is the molecular diffusion coefficient of species j in the mixture. It can be recognized in ${}^{SG}\mathbf{y}_j$, from left to right between parenthesis, the LES Leonard-, Cross-, and Reynolds-terms.

Clearly, the turbulent contribution must be modeled within a specific context of turbulence (either RANS or LES).

3.2. Momentum

From Appendix 2 and Appendix 3, we may write the phasic momentum equation within both RANS and LES frameworks as

$$
\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i = -\nabla \cdot \varepsilon_i \left(\overline{\mathbf{T}}_i + {}^{tur/SG}\mathbf{T}_i \right) + \hat{\rho}_i \tilde{\mathbf{G}}_i + \mathbf{M}_i \quad , \tag{47}
$$

where $\mathbf{M}_i$ is the interfacial momentum transfer rate between phases; $\tilde{\mathbf{G}}_i$ represents a body force (e.g., gravity); and $\overline{\mathbf{T}}_i$ and ${}^{tur/SG}\mathbf{T}_i$ are respectively the phasic mean/averaged stress and the Reynolds (RANS) or the subgrid (LES) stress tensors. As seen in Appendix 4, $\mathbf{M}_i$ may be decomposed into a contribution from mass transfer between phases and a contribution from the interfacial forces at the interfaces (e.g., drag force, added mass forces, interfacial shear stress, and pressure),

$$
\mathbf{M}_i = \overline{\mathbf{u}}_{Int} R_i + \overline{P}_{Int,i} \nabla \varepsilon_i + \overline{\boldsymbol{\tau}}_{Int,i} \cdot \nabla \varepsilon_i + \mathbf{M}_i^{drag} \quad , \tag{48}
$$

where $\mathbf{M}_i^{drag}$ represents the contribution of drag forces between phase; $\overline{\mathbf{u}}_{Int}$ is the averaged/filtered bulk velocity of all interfaces (Appendix 4 discusses a few possibilities to model and simplify $\overline{\mathbf{u}}_{Int}$);

and $P_{Int,i}$ and $\tau_{Int,i}$ are the interfacial pressure and stress between phase i and all the other phases (see Appendix 4). Eq. (48) can be simplified knowing that $\left\langle \boldsymbol{\tau}_{Int,i} \cdot \nabla X_i \right\rangle$, which represents the interfacial shear stress, is expected to be important only in separated phase flows; hence, for most geophysical-atmospherical applications where all phases are well mixed, it can be safely neglected. So, Eq. (48) into Eq. (47) yields the following:

$$\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i = -\nabla \cdot \varepsilon_i \left(\overline{\mathbf{T}}_i + {}^{tur/SG}\mathbf{T}_i \right) + \hat{\rho}_i \tilde{\mathbf{G}}_i + \overline{\mathbf{u}}_{Int} R_i + \overline{P}_{Int,i} \nabla \varepsilon_i + \mathbf{M}_i^{drag}$$

$$\Leftrightarrow$$

$$\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i = -\nabla \varepsilon_i \overline{P}_i - \nabla \cdot \varepsilon_i \overline{\boldsymbol{\tau}}_i - \nabla \cdot \varepsilon_i \, {}^{tur/SG}\mathbf{T}_i + \hat{\rho}_i \tilde{\mathbf{G}}_i + \overline{\mathbf{u}}_{Int} R_i + \overline{P}_{Int,i} \nabla \varepsilon_i + \mathbf{M}_i^{drag} \quad . \tag{49}$$

$$\Leftrightarrow$$

$$\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i = \left(\overline{P}_{Int,i} \nabla \varepsilon_i - \nabla \varepsilon_i \overline{P}_i \right) - \nabla \cdot \varepsilon_i \left(\overline{\boldsymbol{\tau}}_i + {}^{tur/SG}\mathbf{T}_i \right) + \overline{\mathbf{u}}_{Int} R_i + \mathbf{M}_i^{drag} + \hat{\rho}_i \tilde{\mathbf{G}}_i$$

The first two terms on the RHS need to be developed in a specific phasic context. For instance, for the gas phase, the pressure is simple to define, and it is clear that $P_i = P_g$; hence,

$$\text{Gas (carrier) phase: } \nabla \varepsilon_i \overline{P}_i \equiv \nabla \varepsilon_g \overline{P}_g = \varepsilon_g \nabla \overline{P}_g + \overline{P}_g \nabla \varepsilon_g \quad . \tag{50}$$

For the solid phase, defining the pressure is more complicated, but it is generally thought that there must be a contribution from the carrier phase and, possibly, a contribution from the dispersed phase itself. Because the concept of granular pressure in this manuscript is entirely defined from a specific turbulence context (RANS vs. LES), we formally write $\nabla \varepsilon_i \overline{P}_i$ as

$$\text{Dusty (dispersed) phase: } \nabla \varepsilon_i \overline{P}_i \cong \nabla \varepsilon_s \overline{P}_g + \nabla \varepsilon_s \overline{P}_s = \varepsilon_s \nabla \overline{P}_g + \overline{P}_g \nabla \varepsilon_s + \nabla \varepsilon_s \overline{P}_s \quad . \tag{51}$$

The first term, $\nabla \varepsilon_s \overline{P}_g$, represents three-dimensional buoyancy effects on the particle (the gas pressure gradient exerts a buoyancy force on a population of grains), and the second term, $\nabla \varepsilon_s \overline{P}_s$, represents granular pressure effects that must be defined in a specific solid-phase turbulence and/or rheological model. Within the RANS framework, either ${}^{tur}P_s$ represents the collisional part of the solid pressure (while the kinetic granular pressure would represent the true turbulent motions of the grains), or ${}^{tur}P_s$ simply represents both the kinetic and the collisional pressures[16]. A third more complete approach [e.g., Dartevelle 2004] is to consider the effects from an averaged bulk frictional plastic pressure, so that the total solid phase pressure would now read as $P_s = {}^{f}P_s + {}^{tur}P_s$, with ${}^{f}P_s$ (or $\overline{P}_s$) being a frictional pressure and ${}^{tur}P_s$ being a pressure from a turbulence model (e.g., kinetic-collisional model within RANS). Within LES, it is usually assumed that the granular subgrid pressure is negligible. In the following, we will assume that it is always possible to define a filtered or an ensemble-averaged solid-phase stress (i.e., $\overline{P}_s$ and $\overline{\boldsymbol{\tau}}_s$) from, for instance, a plastic rheology as achieved by Dartevelle [2004], but other interpretations can be given to $\overline{P}_s$ and $\overline{\boldsymbol{\tau}}_s$.

Rearranging Eq. (49) with Eq. (50) or Eq. (51) in a two-phase dusty cloud context, we systematically have a term, $\left(\overline{P}_{Int,i} - \overline{P}_g\right)\nabla\varepsilon_i$, that represents the pressure difference between the interface and the carrier phase. In a well-mixed multiphase flow system, this term is negligible [Ishii 1975]. Therefore, we finally obtain, after simplification,

$$\begin{cases} \dfrac{\partial \hat{\rho}_g \tilde{\mathbf{u}}_g}{\partial t} + \nabla\cdot\hat{\rho}_g \tilde{\mathbf{u}}_g \tilde{\mathbf{u}}_g & = -\varepsilon_g \nabla \overline{P}_g - \nabla\cdot\varepsilon_g \left(\overline{\boldsymbol{\tau}}_g + {}^{tur/SG}\mathbf{T}_g\right) + \mathbf{M}_g^{drag} + \overline{\mathbf{u}}_{Int} R_g + \hat{\rho}_g \tilde{\mathbf{G}}_g \\ \dfrac{\partial \hat{\rho}_s \tilde{\mathbf{u}}_s}{\partial t} + \nabla\cdot\hat{\rho}_s \tilde{\mathbf{u}}_s \tilde{\mathbf{u}}_s & = -\varepsilon_s \nabla \overline{P}_g - \nabla\varepsilon_s \overline{P}_s - \nabla\cdot\varepsilon_s \left(\overline{\boldsymbol{\tau}}_s + {}^{tur/SG}\mathbf{T}_s\right) + \mathbf{M}_s^{drag} + \overline{\mathbf{u}}_{Int} R_s + \hat{\rho}_s \tilde{\mathbf{G}}_s \end{cases}, \quad (52)$$

where ‘s’ represents any dispersed solid phase within the gas phase. Eq. (52) is valid for both the LES and RANS frameworks. Within a specific turbulence framework, different constitutive equations must be specified for the turbulence/subgrid stress tensor of the gas phase (${}^{tur/SG}\mathbf{T}_g$), the stress tensor of the solid phase (${}^{tur/SG}\mathbf{T}_s$), and the drag vector for all the phases ($\mathbf{M}_i^{drag}$).

Within the RANS (Appendix 2) and LES (Appendix 3) frameworks, the stress tensors from turbulence/subgrid can be defined as

[16] Defining the stress tensor of the granular (dispersed) phase, $\mathbf{T}_s$, is not difficult. Within the RANS framework, it is common to qualify the “molecular” stress tensor (i.e., not due to turbulence) as “collisional,” while the “turbulence” stress tensor would describe the kinetic behavior of the grains (possibly modified by the gas-phase turbulence). However, both granular behaviors (collisional and kinetic) are clearly due to the fluctuating and chaotic motions of the grains within the flow (whatever the reasons) [Dartevelle 2003; Dartevelle 2004; Dartevelle et al., 2004]. In this manuscript, within RANS, we will define a turbulent granular stress as being the sum of the kinetic and collisional parts, ${}^{tur}\mathbf{T}_s = {}^{k}\mathbf{T}_s + {}^{c}\mathbf{T}_s$; hence, ${}^{tur}\mathbf{T}_s$ is a full kinetic and collisional viscous stress tensor as described, for instance, in Dartevelle [2004]. Within LES, ${}^{SG}\mathbf{T}_s$ will be the sum of the Leonard-terms (strictly speaking the only true filtered part), the Cross-terms, and the Reynolds-term (strictly speaking, the “true” unresolved part from the subgrid). The nonturbulent stress ($\overline{\mathbf{T}}_s$, or $\overline{P}_s$ and $\overline{\boldsymbol{\tau}}_s$) may be, for instance, due to frictional interactions between grains, which can be described at high concentrations by a visco-plastic rheology [Dartevelle 2004].

$$ {}^{tur}\mathbf{T}_i = \bar{\rho}_i\, \widetilde{\mathbf{u}_i''\mathbf{u}_i''} \qquad \text{RANS framework} $$

$$ {}^{SG}\mathbf{T}_i = \underset{\smile}{\bar{\rho}_i}\left[\underbrace{\left(\widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i}\underset{\smile}{\tilde{\mathbf{u}}_i}} - \underset{\smile}{\tilde{\mathbf{u}}_i}\underset{\smile}{\tilde{\mathbf{u}}_i}\right)}_{\text{Leonard}} + \underbrace{\left(\widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i}\mathbf{u}_i''} + \widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i}\mathbf{u}_i''}\right)}_{\text{Cross}} + \underbrace{\left(\widetilde{\underset{\smile}{\mathbf{u}_i''}\underset{\smile}{\mathbf{u}_i''}}\right)}_{\text{Reynolds}}\right] \qquad \text{LES framework} \quad . \tag{53} $$

It should be noted that the viscous stress tensor, $\bar{\boldsymbol{\tau}}_i$, is not easy to calculate because it involves unknowns in terms of Favre phasic-weighted viscosities ($\bar{\mu}_i$ and $\overline{{}^{b}\mu_i}$) and velocities ($\bar{\mathbf{u}}_i$ instead of $\tilde{\mathbf{u}}_i$) both within the RANS and LES frameworks. As shown in Appendix 5, it is common to assume that $\bar{\boldsymbol{\tau}}_i$ may be written as

$$ \bar{\boldsymbol{\tau}}_i \approx -\mu_i\left(\nabla\tilde{\mathbf{u}}_i + \nabla\tilde{\mathbf{u}}_i^{T}\right) + \frac{2}{3}\mu_i\nabla\cdot\tilde{\mathbf{u}}_i\mathbf{I} - {}^{b}\mu_i\nabla\cdot\tilde{\mathbf{u}}_i\mathbf{I} \quad , \tag{54} $$

where the viscosities acts as a constant with respect to the LES/RANS integral operators; hence, $\bar{\mu}_i \approx \tilde{\mu}_i \approx \mu_i$ and $\overline{{}^{b}\mu_i} \approx \widetilde{{}^{b}\mu_i} \approx {}^{b}\mu_i$. Eq. (54) is, of course, a simplification that is nevertheless very common, even for compressible turbulent flows [e.g., Gatski 1997].

3.3. Energy (Enthalpy)

From Appendix 2 and Appendix 3, we may write the phasic enthalpy equation within both RANS and LES frameworks as

$$ \frac{\partial\hat{\rho}_i\tilde{h}_i}{\partial t} + \nabla\cdot\hat{\rho}_i\tilde{h}_i\tilde{\mathbf{u}}_i = \varepsilon_i W_{\boldsymbol{\tau},i} - \nabla\cdot\varepsilon_i\left(\bar{\mathbf{q}}_i + {}^{tur/SG}\mathbf{q}_i\right) + \varepsilon_i\frac{d\bar{P}_i}{dt} + \hat{\rho}_i\tilde{S}_i + {}^{h}H_i \quad , \tag{55} $$

where ${}^{h}H_i$ is the interfacial heat transfer between phases; $\tilde{S}_i$ represents any supplementary heat sources (i.e., radiation); $W_{\tau,i}$ is the viscous dissipation; $\bar{\mathbf{q}}_i$ is the intraphase heat conduction flux; and ${}^{tur/SG}\mathbf{q}_i$ is a supplementary heat flux induced by turbulence (RANS) or by the subgrid (LES). We have neglected in Eq. (55) the supplementary dissipation from turbulence (${}^{tur}W_{\tau,i}$) or from the subgrid (${}^{SG}W_{\tau,i}$), as it is universally assumed to be negligible with respect to all the other contributions in this equation.

${}^{h}H_i$ can be approached by (see Appendix 4)

$$ {}^{h}H_i \approx \tilde{h}_i R_i + \sum_{\substack{j=1 \\ j\neq i}}^{n} Q_j \left(T_j - T_i \right) \quad , \tag{56} $$

where Q_j represents the interfacial heat transfer coefficient, which is usually taken as a function of the Nusselt, Reynolds numbers, and phasic heat conduction coefficients, and R_i represents the total contribution of mass transfer between i and all the other phases.

The heat fluxes are

$$ \begin{aligned} &\overline{\mathbf{q}}_i && = -k_i \nabla \overline{T}_i && \\ &{}^{tur}\mathbf{q}_i && = \overline{\rho_i h_i'' \mathbf{u}_i''} = \overline{\rho}_i \widetilde{h_i'' \mathbf{u}_i''} && \text{RANS framework} \quad , \\ &{}^{SG}\mathbf{q}_i && = \left[\underset{\smile}{\overline{\rho}_i} \widetilde{\underset{\smile}{\tilde{h}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}} - \underset{\smile}{\overline{\rho}_i} \underset{\smile}{\tilde{h}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} \right] + \left[\underset{\smile}{\overline{\rho}_i} \widetilde{\underset{\smile}{\tilde{h}_i} \underset{\smile}{\mathbf{u}_i''}} + \underset{\smile}{\overline{\rho}_i} \widetilde{\underset{\smile}{h_i''} \underset{\smile}{\tilde{\mathbf{u}}_i}} \right] + \left[\underset{\smile}{\overline{\rho}_i} \widetilde{\underset{\smile}{h_i''} \underset{\smile}{\mathbf{u}_i''}} \right] && \text{LES framework} \end{aligned} \tag{57} $$

where k_i is the molecular (not affected by turbulence) thermal conductivity coefficient of phase i.

The following general definitions are used in Eq. (55) (see also Appendix 7 and Appendix 8):

$$ \begin{cases} \overline{\boldsymbol{\tau}}_i \approx 2\,\mu_i \,\widetilde{\overset{\circ}{\overline{\overline{\mathbf{D}}}}}_i - {}^{b}\mu_i \nabla\cdot\tilde{\mathbf{u}}_i \mathbf{I} = 2\,\mu_i \left[\tilde{\mathbf{D}}_i + \dfrac{1}{3}\left(\nabla\cdot\tilde{\mathbf{u}}_i \right)\mathbf{I} \right] - {}^{b}\mu_i \nabla\cdot\tilde{\mathbf{u}}_i \mathbf{I} \\ \qquad = \mu_i \left[-\left(\nabla\tilde{\mathbf{u}}_i + \nabla\tilde{\mathbf{u}}_i^{\,T} \right) + \dfrac{2}{3}\left(\nabla\cdot\tilde{\mathbf{u}}_i \right)\mathbf{I} \right] - {}^{b}\mu_i \nabla\cdot\tilde{\mathbf{u}}_i \mathbf{I} \quad , \\ W_{\boldsymbol{\tau},i} \approx -\tilde{\boldsymbol{\tau}}_i : \nabla\tilde{\mathbf{u}}_i \end{cases} \tag{58} $$

where μ and ${}^{b}\mu_i$ are the shear and bulk viscosity of phase i and $\mathbf{D}_i$ and $\overset{\circ}{\overline{\overline{\mathbf{D}}}}_i$ are the rate-of-strain tensor and its deviator.

In the two-phase dusty flow context without any phase change between the solid particles and the gas phase, Eq. (55) may be further simplified into

$$\begin{cases} \dfrac{\partial \hat{\rho}_g \tilde{h}_g}{\partial t} + \nabla \cdot \hat{\rho}_g \tilde{h}_g \tilde{\mathbf{u}}_g = \varepsilon_g W_{\boldsymbol{\tau},g} - \nabla \cdot \varepsilon_g \left(\overline{\mathbf{q}}_g + {}^{tur/SG}\mathbf{q}_g \right) + \varepsilon_g \dfrac{d\overline{P}_g}{dt} + \hat{\rho}_g \tilde{S}_g + Q\left(T_s - T_g \right) \\ \dfrac{\partial \hat{\rho}_s \tilde{h}_s}{\partial t} + \nabla \cdot \hat{\rho}_s \tilde{h}_s \tilde{\mathbf{u}}_s = \varepsilon_s W_{\boldsymbol{\tau},s} - \nabla \cdot \varepsilon_s \left(\overline{\mathbf{q}}_s + {}^{tur/SG}\mathbf{q}_s \right) + \varepsilon_s \dfrac{d\overline{P}_s}{dt} + \hat{\rho}_s \tilde{S}_s - Q\left(T_s - T_g \right) \end{cases} . (59)$$

where, in Eq. (59), for the solid phase, various interpretations can be given to $\dfrac{d\overline{P}_s}{dt}$ and are disregarded most of the time.

4. Reynolds (RANS) and Subgrid (LES) Relationships

As we have mentioned throughout this manuscript, unlike the RANS framework, the subgrid stress tensor in a multiphase system is not very well known. On the other hand, the RANS framework of turbulence is not common in geophysical-atmospherical multiphase flow applications (yet highly developed for small-scale flows as in chemical engineering). Therefore, one way or the other, it would be interesting to know the exact relationships between the Reynolds stress tensor from the RANS framework and the subgrid stress tensor from the LES framework. In addition, for the hybrid model of turbulence, knowing the exact relationship between RANS and LES variables is essential.

We know that for any instantaneous and local variable of phase i (see §2.7):

$$\mathbf{u}_i = \overset{\text{RANS}}{\tilde{\mathbf{u}}_i + \mathbf{u}_i''} \;\overset{.}{=}\; \overset{\text{LES}}{\underset{\smile}{\tilde{\mathbf{u}}}_i + \underset{\smile}{\mathbf{u}}_i''} \;. \qquad (60)$$

The stress tensor from turbulence (RANS, ${}^{tur}\mathbf{T}_i$) and from the subgrid (LES, ${}^{SG}\mathbf{T}_i$) are defined by Eq. (53). To avoid in the following any confusion between averaging and filtering operation, let us rewrite Eq. (60) as

$$\mathbf{u}_i = \overset{\text{RANS}}{\left\langle \mathbf{u}_i \right\rangle_{av} + \left.\mathbf{u}_i''\right|_{RANS}} \;\overset{.}{=}\; \overset{\text{LES}}{\tilde{\mathbf{u}}_i + \left.\mathbf{u}_i''\right|_{LES}} \;, \qquad (61)$$

where, now, in this paragraph, the tilde denotes a Favre mass-weighted <u>filtering</u> process and the angular operator with the subscript "av" indicates a Favre mass-weighted <u>ensemble-averaging</u> process. As a reminder, the double prime indicates either the fluctuating part (RANS) or the subgrid part (LES) of a variable. With this in mind, let us define the following Reynolds stress tensor, ${}^{tur}\mathbf{R}_i$, from the RANS framework and subsequently filter it with the definitions of Eq. (61)

$$\begin{aligned} {}^{tur}\mathbf{T}_i &= \left\langle \rho_i \left.\mathbf{u}_i''\right|_{RANS} \left.\mathbf{u}_i''\right|_{RANS} \right\rangle_{av} = \bar{\rho}_i \left\langle \left.\mathbf{u}_i''\right|_{RANS} \left.\mathbf{u}_i''\right|_{RANS} \right\rangle_{av} \\ \Rightarrow {}^{tur}\mathbf{R}_i &= \frac{{}^{tur}\mathbf{T}_i}{\bar{\rho}_i} \end{aligned} \;, \qquad (62)$$

and

$$
\begin{aligned}
{}^{\mathrm{tur}}\widetilde{\mathbf{R}_{\mathrm{i}}} &= \widetilde{\left\langle \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{RANS}}\, \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{RANS}} \right\rangle_{\mathrm{av}}} \\
{}^{\mathrm{tur}}\widetilde{\mathbf{R}_{\mathrm{i}}} &= \widetilde{\left\langle \left(\tilde{\mathbf{u}}_{\mathrm{i}} + \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} - \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \right)\left(\tilde{\mathbf{u}}_{\mathrm{i}} + \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} - \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \right) \right\rangle_{\mathrm{av}}} \\
{}^{\mathrm{tur}}\widetilde{\mathbf{R}_{\mathrm{i}}} &= \widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} + \widetilde{\left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} + \widetilde{\left\langle \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}}\, \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}}} \\
&\quad + 2\,\widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\, \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}}} - 2\,\widetilde{\left\langle \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} - 2\,\widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}}
\end{aligned}
\quad , \qquad (63)
$$

where we have used the fact that $\left\langle \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \right\rangle_{\mathrm{av}} = \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}$. We also know that

$$
\begin{aligned}
\widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} &= \widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} + \left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} - \left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} & .\mathrm{a} \\
2\,\widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} &= 2\,\widetilde{\left\langle \left(\mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{RANS}} + \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} - \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right) \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} & . \qquad (64) \\
&= 2\,\widetilde{\left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} - 2\,\widetilde{\left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}}} & .\mathrm{b}
\end{aligned}
$$

Eq. (64)a and Eq. (64)b into Eq. (63) yields the following:

$$
\begin{aligned}
{}^{\mathrm{tur}}\widetilde{\mathbf{R}_{\mathrm{i}}} &= \widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} + \left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} - \left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \\
&\quad + \widetilde{\left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} + \widetilde{\left\langle \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}}\, \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}}} \\
&\quad + 2\,\widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\, \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}}} \\
&\quad - 2\,\widetilde{\left\langle \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} + 2\,\widetilde{\left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}}} \\
&\quad - 2\,\widetilde{\left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}}
\end{aligned}
\quad . \qquad (65)
$$

Rearranging Eq. (65) yields the following:

$$
\begin{aligned}
\widetilde{{}^{\mathrm{tur}}\mathbf{R}_{\mathrm{i}}} \;&= \widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} - \left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} + 2\,\widetilde{\left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\ \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}}} + \widetilde{\left\langle \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}}\ \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}} \right\rangle_{\mathrm{av}}} \\
&\quad + \left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} - \widetilde{\left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}}
\end{aligned}
\quad . \tag{66}
$$

Applying the commutative property between ensemble averaging and filtering, we finally obtain

$$
\widetilde{{}^{\mathrm{tur}}\mathbf{R}_{\mathrm{i}}} = \left\langle {}^{\mathrm{SG}}\mathbf{R}_{\mathrm{i}} \right\rangle_{\mathrm{av}} + \left\langle \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} - \widetilde{\left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \mathbf{u}_{\mathrm{i}} \right\rangle_{\mathrm{av}}} \quad , \tag{67}
$$

where the LES subgrid stress tensor is as usual defined as

$$
{}^{\mathrm{SG}}\mathbf{R}_{\mathrm{i}} = \left(\widetilde{\tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}}} - \tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}} \right) + 2\,\widetilde{\tilde{\mathbf{u}}_{\mathrm{i}}\ \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}}} + \widetilde{\mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}}\ \mathbf{u}_{\mathrm{i}}''\big|_{\mathrm{LES}}} \quad . \tag{68}
$$

Eq. (67) shows the relationship between the RANS Reynolds stress tensor (${}^{\mathrm{tur}}\mathbf{R}_{\mathrm{i}}$) and the LES subgrid stress tensor (${}^{\mathrm{SG}}\mathbf{R}_{\mathrm{i}}$). In other words, both models of turbulence (RANS vs. LES) can control each other. Indeed, the LHS of Eq. (67) is the filtered Reynolds turbulence stress given by a specific RANS model, whereas the first RHS term of Eq. (67) is the average of the subgrid stress model supplied by a LES model. The two other RHS terms in Eq. (67), ($\tilde{\mathbf{u}}_{\mathrm{i}}\tilde{\mathbf{u}}_{\mathrm{i}}$ and $\left\langle \tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}} \left\langle \tilde{\mathbf{u}}_{\mathrm{i}} \right\rangle_{\mathrm{av}}$), are known because they are modeled by the respective momentum equations (from either the LES or RANS frameworks).

Needless to say, Eq. (67) turns out to be critical for the hybrid-LES model because it makes a specific connection between the RANS subdomain (usually near a wall boundary) and LES subdomain (usually far away from a wall boundary).

5. Method of Characteristics

5.1. Introduction

We will now demonstrate that the hydrodynamic and thermodynamic model presented in §3 and based upon the demonstrations in Appendix 2 and Appendix 3 meets the necessary condition for well-posedness as an initial value problem [e.g., Sedney 1970; Lyczkowski 1978; Wendroff 1979; Lyczkowski et al., 1982; Stewart and Wendroff 1984].

A mathematical problem is said to be *well posed* as an initial value or Cauchy problem (also called a properly posed problem) if and only if

- There is a solution ("existence"),
- The solution is uniquely determined ("uniqueness"), and
- The solution smoothly and continuously depends on the initial (or previous time-step) data ("stability").

In typical time-dependent problems of this manuscript, it is necessary that all "characteristics" of a set of partial differential equations are strictly real[17]. If not (i.e., "complex characteristics"), any perturbation introduced at the initial time would grow exponentially[18].

Let us define a characteristic function within the (t,x)-plane, $\chi_{(t,x)}=0$, as "*a discontinuity of a solution which only occurs along the characteristics*"[19] [Courant 1965]. In other words, a set of variables $\mathbf{U}$ (density, velocities, energies, porosity, pressures, …) is continuous across $\chi_{(t,x)}=0$ [and possibly everywhere else in the (t,x)-plane], but the normal derivatives of $\mathbf{U}$, $\frac{\partial \mathbf{U}}{\partial n}$, taken on $\chi_{(t,x)}=0$, may present "jump" in that they may be undetermined[20].

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[17] Real characteristics in themselves are not a *sufficient* condition to guarantee well-posedness, but a *necessary* condition to be met The reason is that, for time-dependent problem, proper initial and boundary conditions must be also provided [e.g., Courant 1965; Lyczkowski et al., 1978]

[18] A time-dependent elliptical system seems to be physical nonsense because the variable "time" does not have the exact meaning of time as it is understood in this part of the Universe. Theoretically, such a time-dependent elliptical system would lead to solutions within the current time step that would depend as much as on the past data as on the future data. Because time flows into one unbounded direction (from past to future), this is clearly not acceptable.

[19] By discontinuity, we mean a "weak discontinuity" (i.e., not shock, which is a strong discontinuity) in which any variables are perfectly continuous, but normal derivatives of these variables *upon* the characteristics' function *may* be discontinuous or undetermined [Sedney 1970; Garabedian 1986].

[20] Because the normal derivative on the characteristic curve "goes out of the curve," it is commonly named the "exterior derivative," whereas the tangential derivative that lies on the curve itself is often named "interior derivative" [Sedney 1970]. This "interior/exterior" nomenclature is after Courant [1965].

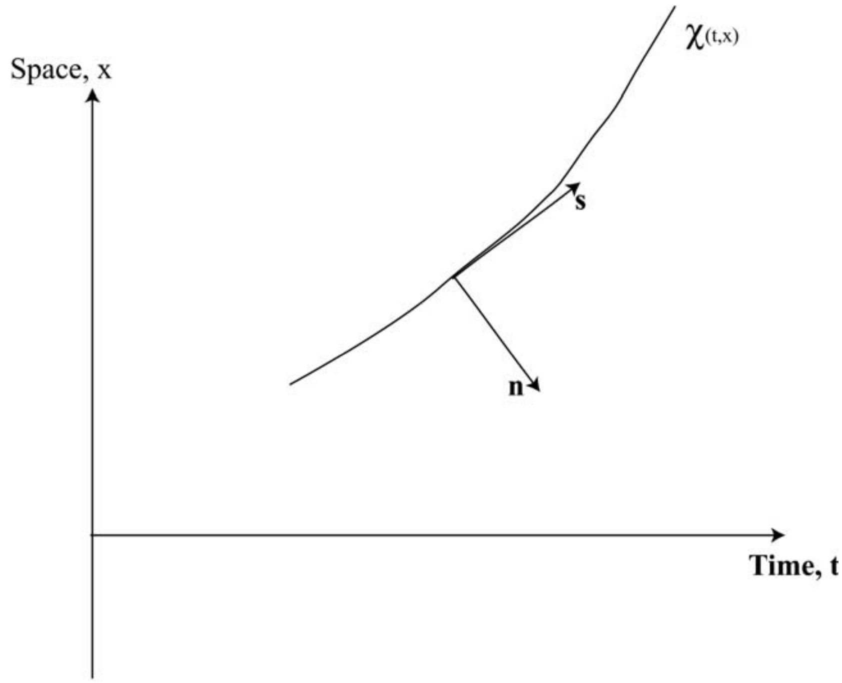

Figure 9

Characteristic curve, χ, in the (t,x)-plane with the normal and tangential (n,s) coordinates on χ.

Knowing, **U**, the vector column formed of n dependent variables (i.e., the n components of **U**), the set of PDEs (continuity, momentum, energy) seen in the previous paragraphs may be written as

$$L(\mathbf{U}) + D(\mathbf{U}) = 0 \quad , \tag{69}$$

where L(**U**) is a matrix operator that can be written in 1-D as the following:

$$L(\mathbf{U}) = A_t \frac{\partial \mathbf{U}}{\partial t} + A_x \frac{\partial \mathbf{U}}{\partial x} \quad . \tag{70}$$

A_t and A_x are n×n square matrices, and D(**U**) is a vector function of **U** but *not* of any of its derivatives.

In this one-dimensional demonstration, the characteristic functions are curves in the (t,x)-plane. On these curves, let "s" be an arc length and "n" be a unit normal to the curve (see Figure 9). By the chain rule, we have

$$\begin{cases} \dfrac{\partial \mathbf{U}}{\partial t} = \dfrac{\partial \mathbf{U}}{\partial s}\dfrac{\partial s}{\partial t} + \dfrac{\partial \mathbf{U}}{\partial n}\dfrac{\partial n}{\partial t} \\ \\ \dfrac{\partial \mathbf{U}}{\partial x} = \dfrac{\partial \mathbf{U}}{\partial s}\dfrac{\partial s}{\partial x} + \dfrac{\partial \mathbf{U}}{\partial n}\dfrac{\partial n}{\partial x} \end{cases} . \tag{71}$$

Let us cast Eq. (71) into Eq. (69), which yields the following after rearrangements:

$$\left(A_t \frac{\partial n}{\partial t} + A_x \frac{\partial n}{\partial x} \right) \frac{\partial \mathbf{U}}{\partial n} + \left(A_t \frac{\partial s}{\partial t} + A_x \frac{\partial s}{\partial x} \right) \frac{\partial \mathbf{U}}{\partial s} + D(\mathbf{U}) = 0 \quad . \tag{72}$$

In other words, we have just made a change of variables to rewrite the original time and space Eq. (71) in terms of normal and tangential variables (see Figure 9). In order to have, across the characteristic curve, a "jump" of the normal derivative of **U**, $\dfrac{\partial \mathbf{U}}{\partial n}$, (i.e., a nontrivial solution), we must have the following determinant as

$$\begin{aligned} &\mathrm{Det}\left[\!\left[A_t \frac{\partial n}{\partial t} + A_x \frac{\partial n}{\partial x} \right]\!\right] = 0 \\ &\Leftrightarrow \\ &\mathrm{Det}\left[\!\left[A_x - \lambda\, A_t \right]\!\right] = 0 \end{aligned} , \tag{73}$$

where λ is the eigenvalues of the characteristics

$$\lambda = -\frac{\dfrac{\partial n}{\partial t}}{\dfrac{\partial n}{\partial x}} = -\frac{dx}{dt} \quad , \tag{74}$$

and Eq. (73) is a characteristic equation or characteristic condition. Every characteristic curve for the system of equations, Eq. (69), is a solution of the Ordinary Differential Equation, Eq. (74), where λ is the root of the polynomial equation given by Eq. (73). A characteristic function, $\chi_{(t,x)}=0$, is therefore a privileged path of points of (weak) discontinuities moving along the direction x with time t at a velocity $\frac{dx}{dt}$. Associated with each eigenvalue, λ_1, λ_2, …, λ_n, it is possible to find at least one eigenvector[21], u_i,

$$u_i \left(A_x - \lambda_i A_t \right) = 0 \quad . \tag{75}$$

These eigenvectors are, by definition, all linearly independent with each other. Hence, if n real and distinct eigenvalues can be found, the system, Eq. (69), is *totally* hyperbolic. If all eigenvalues are real, but not necessarily distinct (nonequilibrium flows), the system is simply referred as hyperbolic [Sedney 1970].

In Appendix 6, this preceding MOC technique is applied to a single-phase compressible flow for the Euler and Navier-Stokes PDEs. Appendix 6 highlights the importance of viscous phenomena (molecular and/or turbulent) because the Euler and Navier-Stokes do not have all their characteristics in common. However, both single-phase models (inviscid vs. viscous) have real eigenvalues, hence satisfy the necessary condition required for well-posed initial-value problems [Lyczkowski et al., 1978].

In the following, we will demonstrate that the multiphase Navier-Stokes PDEs satisfy the necessary condition for well-posed initial-value problems *if and only if* viscous phenomena are included in the model. In other words, multiphase Euler PDEs are not a well-posed model as an initial value problem[22].

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[21] Which happens to be the normal derivative of **U**.

[22] We won't demonstrate that result in this manuscript, but the demonstration is rather straightforward. This result has, however, important implications because the turbulence phenomena become critical if not a necessity for the stability and uniqueness of the mathematical model.

5.2. Necessary Requirement for Well-Posed RANS and LES Systems

Let us summarize our equations in 1-D, two phases[23] (gas, g, and dispersed, s) with no phase change within the RANS and LES frameworks:

Continuity

$$\begin{cases} \dfrac{\partial \varepsilon_g \rho_g}{\partial t} + \dfrac{\partial}{\partial x} \varepsilon_g \rho_g u_g & = 0 \\ \dfrac{\partial \varepsilon_s \rho_s}{\partial t} + \dfrac{\partial}{\partial x} \varepsilon_s \rho_s u_s & = 0 \end{cases}$$

Momentum

$$\begin{cases} \dfrac{\partial \varepsilon_g \rho_g u_g}{\partial t} + \dfrac{\partial}{\partial x} \varepsilon_g \rho_g u_g u_g + \varepsilon_g \dfrac{\partial P_g}{\partial x} + \varepsilon_g \dfrac{\partial \tau_g}{\partial x} + T_g \dfrac{\partial}{\partial x} \varepsilon_g & = M + \varepsilon_g \rho_g G_g \\ \dfrac{\partial \varepsilon_s \rho_s u_s}{\partial t} + \dfrac{\partial}{\partial x} \varepsilon_s \rho_s u_s u_s + \varepsilon_s \dfrac{\partial P_g}{\partial x} + \varepsilon_s \dfrac{\partial P_s}{\partial x} + \varepsilon_s \dfrac{\partial \tau_s}{\partial x} + T_s \dfrac{\partial}{\partial x} \varepsilon_s & = -M + \varepsilon_s \rho_s G_s \end{cases}$$

Energy

$$\begin{cases} \dfrac{\partial \varepsilon_g \rho_g h_g}{\partial t} + \dfrac{\partial}{\partial x} \varepsilon_g \rho_g u_g h_g - \varepsilon_g \dfrac{dP_g}{dt} + \dfrac{\partial}{\partial x} \varepsilon_g q_g & = \varepsilon_g W_{\tau,g} + \varepsilon_g \rho_g S_g + Q \\ \dfrac{\partial \varepsilon_s \rho_s h_s}{\partial t} + \dfrac{\partial}{\partial x} \varepsilon_s \rho_s u_s h_s - \varepsilon_s \dfrac{dP_s}{dt} + \dfrac{\partial}{\partial x} \varepsilon_s q_s & = \varepsilon_s W_{\tau,s} + \varepsilon_s \rho_s S_s - Q \end{cases} \qquad (76)$$

We have dropped out the symbol referring to LES and RANS because these equations are identical in both frameworks. All terms on the RHS of Eq. (76) are scalar functions of the column vector **U**: M is a momentum transfer function, Q is a heat exchange function between phases, G is a body force, S is a heat source within a given phase, and W is a viscous dissipation function. On the LHS, all the stress terms, T, τ, and P, may involve turbulence and/or subgrid dissipation with "molecular" viscous dissipations. For instance, for the dispersed phase, the pressure, P_s, and the shear stress, τ_s, may include plastic contribution and a contribution from RANS or from LES. The term q_i represents the heat transfer by conduction within a given phase and is generally given by a Fourier law. Let us further note that in 1-D

[23] Hereafter, "s" represents any dispersed phase—in some cases, it may be compressible, in other cases, fully incompressible (it is then a true granular phase).

$$\begin{cases} T_g = P_g + \tau_g = P_g - \mu_g \dfrac{\partial u_g}{\partial x} \\ T_s = P_s + \tau_s = P_s - \mu_s \dfrac{\partial u_s}{\partial x} \end{cases} \quad , \tag{77}$$

where μ_g and μ_s are viscous functions, possibly functions of turbulence, and

$$\begin{cases} \dfrac{dP_g}{dt} = \dfrac{\partial P_g}{\partial t} + u_g \dfrac{\partial P_g}{\partial x} \\ \dfrac{dP_s}{dt} = \dfrac{\partial P_s}{\partial t} + u_s \dfrac{\partial P_s}{\partial x} \end{cases} \quad . \tag{78}$$

Last but not least, it should be recalled that our multiphase model is entirely derived from the phasic function of presence, X_i, which takes two values—1 or 0 (see §2.3). In addition, these unique binary values for X_i are ensured with the following property (written in 1-D):

$$\frac{\partial X_i}{\partial t} + u_{Int} \frac{\partial X_i}{\partial x} = 0 \quad , \tag{79}$$

where u_{Int} is the bulk velocity all the interface in the system. After averaging/filtering, Eq. (79) becomes

$$\frac{\partial \varepsilon_g}{\partial t} + \bar{u}_{Int} \frac{\partial \varepsilon_g}{\partial x} = 0 \quad . \tag{80}$$

The exact formulation of the ensemble-averaged or filtered u_{Int} is not really needed for the following demonstrations; nonetheless, Appendix 4 suggests different possibilities to approximate $\bar{u}_{Int}$ and shows that it can be written as a function of each bulk phasic velocity.

We will now demonstrate that the set of PDEs, Eq. (76), Eq. (77), and Eq. (80), meets the *necessary* condition for well-posed initial-value problems (i.e., all eigenvalues on the characteristics are real) and also that the characteristics are invariant to the chosen dependent variables' vector and Equation of State. The demonstration starts first with the most general case possible, i.e., all phase are compressible. Afterwards, we redemonstrate with a more realistic case, i.e., the dispersed phase is incompressible.

5.2.1. *General case: all phases are compressible*

We assume both phases are fully compressible with the following EOS for each phase:

Gas phase	**Dispersed phase**
$h_g = h_g(P_g, \rho_g)$	$h_s = h_s(P_s, \rho_s)$
$dh_g = \left.\dfrac{\partial h_g}{\partial P_g}\right\vert_\rho dP_g + \left.\dfrac{\partial h_g}{\partial \rho_g}\right\vert_P d\rho_g = h_{g,\rho}\, dP_g + h_{g,P}\, d\rho_g$	$dh_s = \left.\dfrac{\partial h_s}{\partial P_s}\right\vert_\rho dP_s + \left.\dfrac{\partial h_s}{\partial \rho_s}\right\vert_P d\rho_s = h_{s,\rho}\, dP_s + h_{s,P}\, d\rho_s$

Rearranging the set of Eq. (76), we now have the following:

Continuity:

$$\begin{cases} \varepsilon_g \dfrac{\partial \rho_g}{\partial t} + \rho_g \dfrac{\partial \varepsilon_g}{\partial t} + \varepsilon_g u_g \dfrac{\partial \rho_g}{\partial x} + \rho_g u_g \dfrac{\partial \varepsilon_g}{\partial x} + \rho_g \varepsilon_g \dfrac{\partial u_g}{\partial x} = 0 \\ \left(1-\varepsilon_g\right) \dfrac{\partial \rho_s}{\partial t} - \rho_s \dfrac{\partial \varepsilon_g}{\partial t} + \left(1-\varepsilon_g\right) \rho_s \dfrac{\partial u_s}{\partial x} + \left(1-\varepsilon_g\right) u_s \dfrac{\partial \rho_s}{\partial x} - \rho_s u_s \dfrac{\partial \varepsilon_g}{\partial x} = 0 \end{cases} \tag{81}$$

Momentum:

$$\begin{cases} \varepsilon_g \rho_g \dfrac{du_g}{dt} + \varepsilon_g \dfrac{\partial P_g}{\partial x} + \varepsilon_g \dfrac{\partial \tau_g}{\partial x} + T_g \dfrac{\partial \varepsilon_g}{\partial x} = M + \varepsilon_g \rho_g G_g \\ \left(1-\varepsilon_g\right) \rho_s \dfrac{du_s}{dt} + \left(1-\varepsilon_g\right) \dfrac{\partial P_g}{\partial x} + \left(1-\varepsilon_g\right) \dfrac{\partial P_s}{\partial x} + \left(1-\varepsilon_g\right) \dfrac{\partial \tau_s}{\partial x} - T_s \dfrac{\partial \varepsilon_g}{\partial x} = -M + \varepsilon_s \rho_s G_s \end{cases} \tag{82}$$

Energy:

$$\frac{\partial \varepsilon_i \rho_i h_i}{\partial t} + \frac{\partial}{\partial x} \varepsilon_i \rho_i u_i h_i - \varepsilon_i \frac{dP_i}{dt} + \frac{\partial}{\partial x} \varepsilon_i q_i = \varepsilon_i W_{\tau,i} + \varepsilon_i \rho_i S_i + Q$$

$\Leftrightarrow$

$$\varepsilon_i \rho_i \left(\frac{dh_i}{dt} \right) - \varepsilon_i \left(\frac{dP_i}{dt} \right) + q_i \frac{\partial \varepsilon_i}{\partial x} = \varepsilon_i W_{\tau,i} + \varepsilon_i \rho_i S_i + Q - \varepsilon_i \frac{\partial q_i}{\partial x}$$

$\Leftrightarrow$

$$\varepsilon_i \rho_i \left(h_{i,\rho} \frac{dP_i}{dt} + h_{i,P} \frac{d\rho_i}{dt} \right) - \varepsilon_i \left(\frac{dP_i}{dt} \right) + q_i \frac{\partial \varepsilon_i}{\partial x} = \varepsilon_i W_{\tau,i} + \varepsilon_i \rho_i S_i + Q - \varepsilon_i \frac{\partial q_i}{\partial x}$$

$\Leftrightarrow$

$$-\varepsilon_i \left(1 - \rho_i h_{i,\rho}\right) \frac{dP_i}{dt} + \varepsilon_i \rho_i h_{i,P} \frac{d\rho_i}{dt} + q_i \frac{\partial \varepsilon_i}{\partial x} = \varepsilon_i W_{\tau,i} + \varepsilon_i \rho_i S_i + Q - \varepsilon_i \frac{\partial q_i}{\partial x}$$

$\Leftrightarrow$

$$-\varepsilon_i \frac{dP_i}{dt} + \varepsilon_i \rho_i \frac{\rho_i h_{i,P}}{\left(1 - \rho_i h_{i,\rho}\right)} \frac{d\rho_i}{dt} + \frac{q_i}{\left(1 - \rho_i h_{i,\rho}\right)} \frac{\partial \varepsilon_i}{\partial x} = \frac{\varepsilon_i W_{\tau,i} + \varepsilon_i \rho_i S_i + Q - \varepsilon_i \frac{\partial q_i}{\partial x}}{\left(1 - \rho_i h_{i,\rho}\right)} \qquad (83)$$

It can be shown (Appendix 6) that the ratio, $\frac{\rho_i h_{i,P}}{1 - \rho_i h_{i,\rho}}$, is always nonzero and positive and may be related to the square of the speed of sound. To facilitate the reading and the manipulations of the following equations, let us labeled this ratio as C_i^2. The phasic energy equations can now be written as

$$\begin{cases} -\varepsilon_g \frac{dP_g}{dt} + \varepsilon_g \rho_g C_g^2 \frac{d\rho_g}{dt} + \frac{q_g C_g^2}{\varepsilon_g \rho_g h_{g,P}} \frac{\partial \varepsilon_g}{\partial x} = \frac{\varepsilon_g W_{g,i} + \varepsilon_g \rho_g S_g + Q - \varepsilon_g \frac{\partial q_g}{\partial x}}{1 - \rho_g h_{g,\rho}} \\ -\left(1 - \varepsilon_g\right) \frac{dP_s}{dt} + \left(1 - \varepsilon_g\right) \rho_s C_s^2 \frac{d\rho_s}{dt} - \frac{q_s C_s^2}{\left(1 - \varepsilon_g\right) \rho_s h_{s,P}} \frac{\partial \varepsilon_g}{\partial x} = \frac{\varepsilon_s W_{s,i} + \varepsilon_s \rho_s S_s + Q - \varepsilon_s \frac{\partial q_s}{\partial x}}{1 - \rho_s h_{s,\rho}} \end{cases} . \qquad (84)$$

It is now clear that the column vector of dependent variables must be

$$\mathbf{U} = \left(\varepsilon_g, \rho_g, \rho_s, u_g, u_s, P_g, P_s, \tau_g, \tau_s \right)^T \quad . \qquad (85)$$

The 9 dependent variables with 9 PDEs are 2 continuities [Eq. (81)], 2 momentums [Eq. (82)], 2 energies [Eq. (84)], and 2 stress equations [Eq. (77)]; the ninth PDE is Eq. (80), which is only made of known variables, ε_g and $\mathbf{u}_{Int}$, where $\mathbf{u}_{Int}$, the interfacial velocity, is a function of dependent variables, i.e., $\mathbf{u}_s$, $\mathbf{u}_g$, ε_g, ρ_s, and ρ_g (see Appendix 4).

If our set of equations meets the necessary condition for well-posed initial-value problems, we must show that this set of equations, $A_t \dfrac{\partial \mathbf{U}}{\partial t} + A_x \dfrac{\partial \mathbf{U}}{\partial x} + D(\mathbf{U}) = 0$, has only real eigenvalues. In other words, the roots of the characteristic polynomial, $\mathrm{Det}\left[\!\left[A_x - \lambda\, A_t \right]\!\right] = 0$, must all be real (i.e., $\lambda \in \mathbb{R}$). The 9×9 square matrices A_t and A_x are respectively

$$A_t = \begin{pmatrix} \rho_g & \varepsilon_g & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\rho_s & 0 & \left(1-\varepsilon_g\right) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_g\rho_g & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \left(1-\varepsilon_g\right)\rho_s & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_g\rho_g C_g^2 & 0 & 0 & 0 & -\varepsilon_g & 0 & 0 & 0 \\ 0 & 0 & \left(1-\varepsilon_g\right)\rho_s C_s^2 & 0 & 0 & 0 & -\left(1-\varepsilon_g\right) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

and

$$A_x = \begin{pmatrix} \rho_g u_g & \varepsilon_g u_g & 0 & \varepsilon_g\rho_g & 0 & 0 & 0 & 0 & 0 \\ -u_s\rho_s & 0 & \left(1-\varepsilon_g\right)u_s & 0 & \left(1-\varepsilon_g\right)\rho_s & 0 & 0 & 0 & 0 \\ P_g+\tau_g & 0 & 0 & \varepsilon_g\rho_g u_g & 0 & \varepsilon_g & 0 & \varepsilon_g & 0 \\ -P_s-\tau_s & 0 & 0 & 0 & \left(1-\varepsilon_g\right)\rho_s u_s & \left(1-\varepsilon_g\right) & \left(1-\varepsilon_g\right) & 0 & \left(1-\varepsilon_g\right) \\ \dfrac{q_g C_g^2}{h_{g,P}} & \varepsilon_g\rho_g C_g^2 u_g & 0 & 0 & 0 & -\varepsilon_g u_g & 0 & 0 & 0 \\ -\dfrac{q_s C_s^2}{h_{s,P}} & 0 & \left(1-\varepsilon_g\right)\rho_s C_s^2 u_s & 0 & 0 & 0 & -\left(1-\varepsilon_g\right)u_s & 0 & 0 \\ 0 & 0 & 0 & -\mu_g & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\mu_s & 0 & 0 & 0 & 0 \\ u_{Int} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The characteristic polynomial is as follows:

$$\det\left[\!\left[A_x - \lambda A_t \right]\!\right] = 0$$
$$\Leftrightarrow \qquad . \qquad (86)$$
$$\left(u_g - \lambda\right)^2 \left(u_s - \lambda\right)^2 \left(u_{Int} - \lambda\right) \varepsilon_g^3 \left(1 - \varepsilon_g\right)^3 \mu_s \mu_g = 0$$

All the "characteristic polynomial roots" are real: $\lambda \to \left\{u_g, u_g, u_s, u_s, u_{Int}\right\}$. Our mathematical model in both the LES and RANS realms satisfies the necessary condition for well-posed initial-value problems.

5.2.2. *Dusty cloud case: the dispersed phase is incompressible*

We now assume that only the gas phase is compressible with the following EOS:

Gas phase $\rho_g = \rho_g(P_g, \eta_g)$	**Dispersed phase** $\rho_s = \text{constant}$
$d\rho_g = \left.\dfrac{\partial \rho_g}{\partial P_g}\right\|_\eta dP_g + \left.\dfrac{\partial \rho_g}{\partial \eta_g}\right\|_P d\eta_g$ $= C_g^{-2} dP_g \quad + \rho_{g,P} d\eta_g$	

where η_g and C_g are the entropy and the speed of sound of the gas phase. We take note that there is no granular pressure in this specific context; hence, from thermodynamics,

$$dh_g = \left.T_g\right|_P d\eta_g + \left.\frac{1}{\rho_g}\right|_\eta dP_g \qquad \Big| \qquad dh_s = T_s d\eta_s,$$

where the symbol 'T' refers to temperature and should not be confused, in the following discussion, with the symbol for stress. Rearranging the set of Eq. (76) with this new EOS, we now have the following:

Continuity[24]:

$$\begin{cases} \varepsilon_g \dfrac{\partial \rho_g}{\partial t} + \rho_g \dfrac{\partial \varepsilon_g}{\partial t} + \varepsilon_g u_g \dfrac{\partial \rho_g}{\partial x} + \rho_g u_g \dfrac{\partial \varepsilon_g}{\partial x} + \rho_g \varepsilon_g \dfrac{\partial u_g}{\partial x} & = 0 \\ -\dfrac{\partial \varepsilon_g}{\partial t} + \left(1-\varepsilon_g\right) \dfrac{\partial u_s}{\partial x} - u_s \dfrac{\partial \varepsilon_g}{\partial x} & = 0 \end{cases} \tag{87}$$

Momentum:

$$\begin{cases} \varepsilon_g \rho_g \dfrac{du_g}{dt} + \varepsilon_g \dfrac{\partial P_g}{\partial x} + \varepsilon_g \dfrac{\partial \tau_g}{\partial x} + \left(P_g + \tau_g\right) \dfrac{\partial \varepsilon_g}{\partial x} = M + \varepsilon_g \rho_g G_g \\ \left(1-\varepsilon_g\right) \rho_s \dfrac{du_s}{dt} + \left(1-\varepsilon_g\right) \dfrac{\partial P_g}{\partial x} + \left(1-\varepsilon_g\right) \dfrac{\partial \tau_s}{\partial x} - \tau_s \dfrac{\partial \varepsilon_g}{\partial x} = -M + \varepsilon_s \rho_s G_s \end{cases} \tag{88}$$

Energy:

$$\begin{cases} \varepsilon_g \rho_g T_g \dfrac{d\eta_g}{dt} + q_g \dfrac{\partial \varepsilon_g}{\partial x} = \varepsilon_g W_{g,i} + \varepsilon_g \rho_g S_g + Q - \varepsilon_g \dfrac{\partial q_g}{\partial x} \\ \left(1-\varepsilon_g\right) \rho_s T_s \dfrac{d\eta_s}{dt} - q_s \dfrac{\partial \varepsilon_g}{\partial x} = \varepsilon_s W_{s,i} + \varepsilon_s \rho_s S_s + Q - \varepsilon_s \dfrac{\partial q_s}{\partial x} \end{cases} \tag{89}$$

With this set of PDEs, the column vector of dependent variables is

$$\mathbf{U} = \left(\varepsilon_g, \eta_g, \eta_s, u_g, u_s, P_g, \tau_g, \tau_s\right)^T \quad . \tag{90}$$

The 8 PDEs involved are 2 continuities [Eq. (87)], 2 momentums [Eq. (88)], 2 energies [Eq. (89)], and 2 stress equations [Eq. (77)]. In this case, we do not use Eq. (80). The 8×8 square matrices A_t and A_x are respectively:

[24] Interestingly enough, one can see that the void fraction (ε_g) is propagating exactly with the dispersed solid-phase velocity ($\mathbf{u}_s$) and with a dissipation rate equal to the divergence of $\mathbf{u}_s$ [Lyczkowski et al., 1982]. From Eq.(87),

$$\frac{d\varepsilon_g}{dt} = \left(1-\varepsilon_g\right) \nabla \cdot \mathbf{u}_s \quad .$$

$$
A_t = \begin{pmatrix}
\rho_g & \varepsilon_g \rho_{g,P} & 0 & 0 & 0 & \dfrac{\varepsilon_g}{C_g^2} & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \varepsilon_g \rho_g & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \left(1-\varepsilon_g\right)\rho_s & 0 & 0 & 0 \\
0 & \varepsilon_g \rho_g T_g & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \left(1-\varepsilon_g\right)\rho_s T_s & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

and

$$
A_x = \begin{pmatrix}
\rho_g u_g & \varepsilon_g \rho_{g,P} u_g & 0 & 0 & 0 & \dfrac{\varepsilon_g}{C_g^2} u_g & 0 & 0 \\
-u_s & 0 & 0 & 0 & \left(1-\varepsilon_g\right) & 0 & 0 & 0 \\
P_g + \tau_g & 0 & 0 & \varepsilon_g \rho_g u_g & 0 & \varepsilon_g & \varepsilon_g & 0 \\
-\tau_s & 0 & 0 & 0 & \left(1-\varepsilon_g\right)\rho_s u_s & \left(1-\varepsilon_g\right) & 0 & \left(1-\varepsilon_g\right) \\
q_g & \varepsilon_g \rho_g u_g T_g & 0 & 0 & 0 & 0 & 0 & 0 \\
-q_s & 0 & \left(1-\varepsilon_g\right)\rho_s u_s T_s & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\mu_g & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\mu_s & 0 & 0 & 0
\end{pmatrix}
$$

And the resulting characteristic polynomial is as follows:

$$
\begin{aligned}
&\det\left[\!\left[A_x - \lambda A_t \right]\!\right] = 0 \\
&\Leftrightarrow \\
&\left(u_g - \lambda\right)^2 \left(u_s - \lambda\right)^2 \rho_g \varepsilon_g^3 \left(1-\varepsilon_g\right)^2 \rho_s \mu_s \, \mu_g \, T_s \, T_g = 0
\end{aligned}
\qquad . \tag{91}
$$

All eigenvalues are real, $\lambda \to \left\{u_g, u_g, u_s, u_s\right\}$, and are nearly equivalent as in §5.2.1 with the exception of $\mathbf{u}_{\mathrm{Int}}$.

5.3. Characteristic Invariance

We now demonstrate that the characteristics found in §5.2.1 are invariant to the EOS used and hence to the dependent variable vector. Again, taking the general case—both phases are compressible—we may use this following EOS:

Gas phase $\rho_g = \rho_g(P_g, \eta_g)$	**Dispersed phase** $\rho_s = \rho_s(P_s, \eta_s)$
$d\rho_g = \left.\dfrac{\partial \rho_g}{\partial P_g}\right\|_{\eta} dP_g + \left.\dfrac{\partial \rho_g}{\partial \eta_g}\right\|_{P} d\eta_g = C_g^{-2} dP_g + \rho_{g,P} d\eta_g$	$d\rho_s = \left.\dfrac{\partial \rho_s}{\partial P_s}\right\|_{\eta} dP_s + \left.\dfrac{\partial \rho_s}{\partial \eta_s}\right\|_{P} d\eta_s = C_s^{-2} dP_s + \rho_{s,P} d\eta_s$

Rearranging the set of Eq. (76) with this new EOS, we now have the following:

Continuity:

$$\begin{cases} \dfrac{\varepsilon_g}{C_g^2}\dfrac{dP_g}{dt} + \varepsilon_g \rho_{g,P}\dfrac{d\eta_g}{dt} + \rho_g \dfrac{d\varepsilon_g}{dt} + \varepsilon_g \rho_g \dfrac{\partial u_g}{\partial x} = 0 \\ \dfrac{\left(1-\varepsilon_g\right)}{C_s^2}\dfrac{dP_s}{dt} + \left(1-\varepsilon_g\right)\rho_{s,P}\dfrac{d\eta_s}{dt} - \rho_s \dfrac{d\varepsilon_g}{dt} + \left(1-\varepsilon_g\right)\rho_s \dfrac{\partial u_s}{\partial x} = 0 \end{cases} \tag{92}$$

Momentum:

$$\begin{cases} \varepsilon_g \rho_g \dfrac{du_g}{dt} + \varepsilon_g \dfrac{\partial P_g}{\partial x} + \varepsilon_g \dfrac{\partial \tau_g}{\partial x} + \left(P_g + \tau_g\right)\dfrac{\partial \varepsilon_g}{\partial x} = M + \varepsilon_g \rho_g G_g \\ \left(1-\varepsilon_g\right)\rho_s \dfrac{du_s}{dt} + \left(1-\varepsilon_g\right)\dfrac{\partial P_g}{\partial x} + \left(1-\varepsilon_g\right)\dfrac{\partial P_s}{\partial x} + \left(1-\varepsilon_g\right)\dfrac{\partial \tau_s}{\partial x} - \left(P_s + \tau_s\right)\dfrac{\partial \varepsilon_g}{\partial x} = -M + \varepsilon_s \rho_s G_s \end{cases} \tag{93}$$

Energy:

$$\begin{cases} \varepsilon_g \rho_g T_g \dfrac{d\eta_g}{dt} + q_g \dfrac{\partial \varepsilon_g}{\partial x} = \varepsilon_g W_{g,i} + \varepsilon_g \rho_g S_g + Q - \varepsilon_g \dfrac{\partial q_g}{\partial x} \\ \left(1-\varepsilon_g\right)\rho_s T_s \dfrac{d\eta_s}{dt} - q_s \dfrac{\partial \varepsilon_g}{\partial x} = \varepsilon_s W_{s,i} + \varepsilon_s \rho_s S_s + Q - \varepsilon_s \dfrac{\partial q_s}{\partial x} \end{cases} \tag{94}$$

The column vector of dependent variables is [compare with Eq. (85)]

$$\mathbf{U} = \left(\varepsilon_g, \eta_g, \eta_s, u_g, u_s, P_g, P_s, \tau_g, \tau_s\right)^T \quad , \tag{95}$$

which is used with 9 PDEs: 2 continuities [Eq. (92)], 2 momentums [Eq. (93)], 2 energies [Eq. (94)], and 2 stress equations [Eq. (77)]. The ninth PDE is Eq. (80). The 9×9 square matrices A_t and A_x are respectively as follows:

$$A_t = \begin{pmatrix} \rho_g & \varepsilon_g\rho_{g,P} & 0 & 0 & 0 & \dfrac{\varepsilon_g}{C_g^2} & 0 & 0 & 0 \\ -\rho_s & 0 & \left(1-\varepsilon_g\right)\rho_{s,P} & 0 & 0 & 0 & \dfrac{\left(1-\varepsilon_g\right)}{C_s^2} & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_g\rho_g & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \left(1-\varepsilon_g\right)\rho_s & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_g\rho_g T_g & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \left(1-\varepsilon_g\right)\rho_s T_s & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

and

$$A_x = \begin{pmatrix} \rho_g u_g & \varepsilon_g u_g \rho_{g,P} & 0 & 0 & 0 & \dfrac{\varepsilon_g}{C_g^2} u_g & 0 & 0 & 0 \\ -u_s\rho_s & 0 & \left(1-\varepsilon_g\right) u_s\rho_{s,P} & 0 & \left(1-\varepsilon_g\right)\rho_s & 0 & \dfrac{\left(1-\varepsilon_g\right)}{C_s^2} u_s & 0 & 0 \\ P_g + \tau_g & 0 & 0 & \varepsilon_g\rho_g u_g & 0 & \varepsilon_g & 0 & \varepsilon_g & 0 \\ -P_s - \tau_s & 0 & 0 & 0 & \left(1-\varepsilon_g\right)\rho_s u_s & \left(1-\varepsilon_g\right) & \left(1-\varepsilon_g\right) & 0 & \left(1-\varepsilon_g\right) \\ q_g & \varepsilon_g\rho_g u_g T_g & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -q_s & 0 & \left(1-\varepsilon_g\right)\rho_s u_s T_s & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mu_g & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\mu_s & 0 & 0 & 0 & 0 \\ u_{Int} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The characteristic polynomial is as follows:

$$\det\left[\!\left[A_x - \lambda\, A_t \right]\!\right] = 0$$
$$\Leftrightarrow \qquad . \tag{96}$$
$$\left(u_g - \lambda\right)^2 \left(u_s - \lambda\right)^2 \left(u_{Int} - \lambda\right) \varepsilon_g^3 \rho_g \left(1 - \varepsilon_g\right)^3 \rho_s\, \mu_s\, \mu_g\, T_s\, T_g = 0$$

Not only are all eigenvalues real, $\lambda \to \left\{u_g, u_g, u_s, u_s, u_{Int}\right\}$, but they are exactly the same as in §5.2.1. Hence, the characteristics of our model are invariant to the choice of EOS and to the desired dependent variables.

6. LES and RANS Entropy Constraints

The second law of thermodynamics[25] states that the entropy change of a nonisolated system cannot be less than the entropy exchanged with the surrounding world[26] [Lhuillier 1996]. The entropy can be seen as the amount of disorder of a system; its internal energy directly depends on the amount of disorder, and its temperature quantifies this amount of disorder.[27] However, in a multiphase system with enormous scale differences between the constituents of the multiphase system (gas molecule sizes vs. grain-sizes), the notion of entropy is not obvious to define because the exact meaning of microscale depends on the phase under consideration (gas or granular phase). Nevertheless, the entropy condition can be used to somehow assess or, at least, shed some light on the physical soundness of a multiphase model. Indeed, the Clausius-Duhem inequality can be used as a restriction on the various constitutive laws making up the mathematical model [Ishii 1975; Arnold et al., 1990; Lhuillier 1996] and also the constitutive laws (closures) of the turbulence models (RANS or LES). From this particular perspective of closures and constitutive laws, the Clausius-Duhem inequality should be rather seen as a macroscopic (or mesoscale) entropy condition [Drew and Passman 1999] obtained either by statistical (RANS) or by filtering (LES) processes.

From Appendix 2 (RANS) and Appendix 3 (LES), the entropy condition in a multiphase system of n phases (i=1,2,..,n) may be written as

$$\hat{\rho}_i \frac{d\tilde{\eta}_i}{dt} \geq -\nabla \cdot \varepsilon_i \left(\bar{\boldsymbol{\Phi}}_i + {}^{tur/SG}\boldsymbol{\Phi}_i \right) + \hat{\rho}_i \widetilde{\Sigma_i} + {}^{\eta}H_i \quad , \tag{97}$$

where, $\boldsymbol{\Phi}_i$, the flux of entropy, has two sources: one Favre-phasic averaged/filtered ($\bar{\boldsymbol{\Phi}}_i = \overline{\left(\frac{\mathbf{q}_i}{T_i}\right)}$) and one from the turbulence/subgrid [${}^{tur/SG}\boldsymbol{\Phi}_i$, see Eq. (AII.44) for RANS or Eq. (AIII.27) for LES]; the entropy source is defined by a Favre-mass weighted relationship: $\tilde{\Sigma}_i = \widetilde{\left(\frac{S_i}{T_i}\right)}$; and the mean rate of interfacial entropy between phases, ${}^{\eta}H_i$, complies with the entropic jump condition, $\sum_{i=1}^{n} {}^{\eta}H_i \geq 0$,

---

[25] Or the Entropy law, or the Clausius-Duhem inequality.

[26] If the system is isolated, then the entropy of this system cannot decrease.

[27] This mental picture works well for the gas phase. At the molecular level, the disorder is captured by the temperature of the gas phase: the hotter the gas, the more disorder and the higher the fluctuating kinetic energy of gas molecules. For an Eulerian dispersed (solid) phase, this notion of disorder is less clear as we may have very hot grains in a perfectly idle granular deposit. In other word, there is no clear relationship between internal energy, entropy, and amount of disorder at the grain scale.

which does not necessarily vanish because an entropy production may occur at the interface [Lhuillier 1996]. At this stage, we do not need to make any distinction between filtered (LES) or ensemble-averaged (RANS) variables[28]. However, let us keep in mind that the exact definition and the meaning of each variable (averaged vs. filtered) are, of course, not the same.

Because it is universally acknowledged within the multiphase flow realm [Ishii 1975; Arnold et al., 1990; Drew and Passman 1999], we follow the main idea of Ishii [1975]. Let us assume that the fluctuating part (RANS) or the subgrid part (LES) of any constitutive variables of the internal energy is much smaller than the macroscopic change (averaged/filtered) of the variable under consideration[29]. Such an assumption holds if we consider a time interval sufficiently short (Δt<<) and, in addition for LES, a filter size sufficiently small (Δx_k<<). With this assumption in mind, let us define the phasic internal energy as a function of the macroscopic phasic density ($\overline{\rho}_i$) and entropy ($\tilde{\eta}_i$)[30]:

$$\tilde{I}_i \approx \tilde{I}_i\left(\tilde{\eta}_i, \overline{\rho}_i\right) \quad , \tag{98}$$

with

$$\begin{cases} \tilde{T}_i & \approx \dfrac{\partial \tilde{I}_i}{\partial \tilde{\eta}_i} & \text{a.} \\ \overline{P}_i & \approx \overline{\rho}_i^2 \, \dfrac{\partial \tilde{I}_i}{\partial \overline{\rho}_i} & \text{b.} \\ d\tilde{I}_i & \approx \tilde{T}_i d\tilde{\eta}_i - \overline{P}_i \, d\dfrac{1}{\overline{\rho}_i} = \tilde{T}_i d\tilde{\eta}_i + \dfrac{\overline{P}_i}{\overline{\rho}_i^2} d\overline{\rho}_i & \text{c.} \\ \dfrac{d\tilde{I}_i}{dt} & = \dfrac{\partial \tilde{I}_i}{\partial \tilde{\eta}_i}\dfrac{d\tilde{\eta}_i}{dt} + \dfrac{\partial \tilde{I}_i}{\partial \overline{\rho}_i}\dfrac{d\overline{\rho}_i}{dt} & \text{d.} \end{cases} \tag{99}$$

---

[28] We have dropped out the "bottom lower hat" for the LES variables.

[29] Hence, $P_i \approx \tilde{P}_i \approx \overline{P}_i$; $\eta_i \approx \overline{\eta}_i$; and $T_i \approx \tilde{T}_i \approx \overline{T}_i$.

[30] It could be shown that the internal energy is a much more complicated function [e.g., Bedford and Ingram 1971] if one strictly follows "the principle of equipresence" that states that "*a variable present as an independent variable in one constitutive equation should be present in all constitutive equations*" [Coleman and Mizel 1963]. Hence, Eq. (98) should be rather written as [e.g., Bedford and Ingram 1971]:

$$I_i \approx I_i\left(\rho_{i=1,..,n}, \nabla\rho_{i=1,..,n}, \mathbf{u}_i, \nabla\mathbf{u}_i, T_i, \nabla T_i, \ldots\right) \quad .$$

And, most certainly, the interfacial terms may need to be added as well. Hence, in a multiphase flow system, this principle of equipresence turns out to be very quickly unmanageable and totally inappropriate [Drew and Passman 1999]. In the following (simplified) discussion, we aim to reach an entropy condition as "usable" and "manageable" as possible within a specific mathematical model (and computer code) [e.g., Arnold et al., 1990]. Therefore, we follow the "principle of separation of components" [Drew 1971; Drew and Passman 1999] that states that "*the constitutive equation of a variable of a given component is a unique function of variables associated to that component only.*" This principle of separation of components is exactly applied in Eq. (98).

Therefore, we may rewrite Eq. (97) as the following:

$$\hat{\rho}_i \left(\tilde{T}_i \frac{d\tilde{\eta}_i}{dt} \right) \geq -\tilde{T}_i \nabla \cdot \varepsilon_i \bar{\boldsymbol{\Phi}}_i + \hat{\rho}_i \tilde{S}_i + \tilde{T}_i \, {}^{\eta}H_i \quad . \tag{100}$$

We also note that the macroscopic internal energy is (see, for instance, the demonstration in Appendix 2 with the appropriate simplifications of Appendix 5) as follows:

$$\begin{aligned}
&\frac{\partial \hat{\rho}_i \tilde{I}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{I}_i \tilde{\mathbf{u}}_i = \varepsilon_i \left(W_{\mathbf{T},i} + {}^{tur/SG}W_{\mathbf{T},i} \right) - \nabla \cdot \varepsilon_i \left(\bar{\mathbf{q}}_i + {}^{tur/SG}\mathbf{q}_i \right) + \hat{\rho}_i \tilde{S}_i + {}^{I}H_i \\
&\Leftrightarrow \\
&\hat{\rho}_i \frac{d\tilde{I}_i}{dt} \approx \varepsilon_i \left(W_{\boldsymbol{\tau},i} + {}^{tur/SG}W_{\boldsymbol{\tau},i} \right) - \varepsilon_i \overline{P_i \nabla \cdot \mathbf{u}_i} - \nabla \cdot \varepsilon_i \left(\bar{\mathbf{q}}_i + {}^{tur/SG}\mathbf{q}_i \right) + \hat{\rho}_i \tilde{S}_i + {}^{I}H_i \quad , \\
&\Leftrightarrow \\
&\hat{\rho}_i \frac{d\tilde{I}_i}{dt} \approx \varepsilon_i \left(W_{\boldsymbol{\tau},i} + {}^{tur/SG}W_{\boldsymbol{\tau},i} \right) - \varepsilon_i \bar{P}_i \nabla \cdot \tilde{\mathbf{u}}_i - \nabla \cdot \varepsilon_i \left(\bar{\mathbf{q}}_i + {}^{tur/SG}\mathbf{q}_i \right) + \hat{\rho}_i \tilde{S}_i + {}^{I}H_i
\end{aligned} \tag{101}$$

where ${}^{tur/SG}\mathbf{q}_i$ is the heat flux contribution from turbulence or from the subgrid; the mean rate of interfacial internal energy transfer between phases, ${}^{I}H_i$, that fully complies with the jump condition between all possible interfaces is $\sum_{i=1}^{n} {}^{I}H_i = 0$. In Eq. (101), we further assume that the fluctuating (RANS) or the subgrid (LES) velocity is divergenceless ($\nabla \cdot \mathbf{u}_i' \approx \nabla \cdot \mathbf{u}_i'' \approx 0$) [Besnard et al., 1992].

Taking the material derivative of the equation of state, Eq. (99)c:

$$\begin{aligned}
&\frac{d\tilde{I}_i}{dt} = \tilde{T}_i \frac{d\tilde{\eta}_i}{dt} + \frac{\bar{P}_i}{\bar{\rho}_i^2} \frac{d\bar{\rho}_i}{dt} \\
&\Leftrightarrow \\
&\frac{d\tilde{I}_i}{dt} = \tilde{T}_i \frac{d\tilde{\eta}_i}{dt} + \frac{\bar{P}_i}{\varepsilon_i \bar{\rho}_i^2} \left(R_i - \varepsilon_i \bar{\rho}_i \nabla \cdot \tilde{\mathbf{u}}_i - \bar{\rho}_i \frac{d\varepsilon_i}{dt} \right) \\
&\Leftrightarrow \\
&\hat{\rho}_i \frac{d\tilde{I}_i}{dt} = \hat{\rho}_i \left(\tilde{T}_i \frac{d\tilde{\eta}_i}{dt} \right) + \frac{\bar{P}_i}{\bar{\rho}_i} R_i - \varepsilon_i \bar{P}_i \nabla \cdot \tilde{\mathbf{u}}_i - \bar{P}_i \frac{d\varepsilon_i}{dt}
\end{aligned} \tag{102}$$

Eq. (101) and Eq. (102) into Eq. (100) gives the following:

$$
\begin{aligned}
&\hat{\rho}_i \frac{d\tilde{I}_i}{dt} - \frac{\overline{P}_i}{\overline{\rho}_i} R_i + \varepsilon_i \overline{P}_i \nabla \cdot \tilde{\mathbf{u}}_i + \overline{P}_i \frac{d\varepsilon_i}{dt} \geq -\tilde{T}_i \nabla \cdot \varepsilon_i \overline{\mathbf{\Phi}}_i + \hat{\rho}_i \tilde{S}_i + \tilde{T}_i\, {}^{\eta}H_i \\
&\Leftrightarrow \\
&\varepsilon_i \left(W_{\boldsymbol{\tau},i} + {}^{tur/SG}W_{\boldsymbol{\tau},i} \right) - \nabla \cdot \varepsilon_i \left(\overline{\mathbf{q}}_i + {}^{tur/SG}\mathbf{q}_i \right) + {}^{I}H_i - \frac{\overline{P}_i}{\overline{\rho}_i} R_i + \overline{P}_i \frac{d\varepsilon_i}{dt} \geq -\tilde{T}_i \nabla \cdot \varepsilon_i \overline{\mathbf{\Phi}}_i + \tilde{T}_i\, {}^{\eta}H_i \\
&\Leftrightarrow \\
&\varepsilon_i \left(W_{\boldsymbol{\tau},i} + {}^{tur/SG}W_{\boldsymbol{\tau},i} \right) + \frac{\varepsilon_i k_i \left(\nabla \tilde{T}_i \right)^2}{\tilde{T}_i} - \nabla \cdot \varepsilon_i\, {}^{tur/SG}\mathbf{q}_i + \left({}^{I}H_i - \tilde{T}_i\, {}^{\eta}H_i \right) - \frac{\overline{P}_i}{\overline{\rho}_i} R_i + \overline{P}_i \frac{d\varepsilon_i}{dt} \geq 0 \\
&\Leftrightarrow \\
&\varepsilon_i \left(W_{\boldsymbol{\tau},i} + {}^{tur/SG}W_{\boldsymbol{\tau},i} \right) + \frac{\varepsilon_i k_i \left(\nabla \tilde{T}_i \right)^2}{\tilde{T}_i} - \nabla \cdot \varepsilon_i\, {}^{tur/SG}\mathbf{q}_i + \left[{}^{f}H_i - \frac{\overline{P}_i}{\overline{\rho}_i} R_i + \overline{P}_i \frac{d\varepsilon_i}{dt} \right] \geq 0
\end{aligned}
\tag{103}
$$

which is the equation's aim as it clearly imposes a condition to the whole set of various closures laws. Reading from left to right, on the LHS of Eq. (103) are the following: (i) molecular shear-viscous dissipation ($W_{\tau,i}>0$); (ii) the RANS turbulent energy (${}^{tur}W_{\tau,i}>0$) or LES subgrid energy (${}^{SG}W_{\tau,i}>0$) dissipations[31]; (iii) molecular heat conduction where k_i is the phasic conduction of heat ($k_i>0$); (iv) heat conduction within a given phase by turbulent means ($-\nabla \cdot \varepsilon_i\, {}^{tur}\mathbf{q}_i$) or within the subgrid ($-\nabla \cdot \varepsilon_i\, {}^{SG}\mathbf{q}_i$); and finally, (v) between brackets, the interfacial Helmholtz free energy (${}^{f}H_i>0$), the mass exchange rate through the interface ($-R_i$); and the phasic volumetric concentration variations, $\frac{d\varepsilon_i}{dt}$, "seen" by the material, where $\frac{d\varepsilon_i}{dt} = \frac{\partial \varepsilon_i}{\partial t} + \tilde{\mathbf{u}}_i \cdot \nabla \varepsilon_i$.

In the most classical way to approach turbulence [Kashiwa 2001; Dartevelle 2004], the turbulent heat flux term ($-\nabla \cdot \varepsilon_i\, {}^{tur/SG}\mathbf{q}_i$) is always positive with an eddy-viscosity model (RANS or LES):

$$
{}^{tur/SG}\mathbf{q}_i = -\frac{Cp_i}{{}^{tur/SG}Pr}\, {}^{tur/SG}\mu_i\, \nabla \tilde{T}_i \quad , \tag{104}
$$

where Cp_i is the specific heat at constant pressure, ${}^{tur/SG}Pr$ is the turbulent Prandtl number, and ${}^{tur/SG}\mu_i$ is the turbulent eddy-viscosity that must be provided by a RANS or a LES model. Therefore,

[31] As a reminder, ${}^{tur/SG}W_{\tau,i}$ is often neglected.

one can see that, with maybe the exception of the bracket term, all the terms of Eq. (103) are always positive.

Let us define, anywhere and anytime, the system as the mixture of all the phases in a CV. Therefore, for the mixture system, we must sum all terms of Eq. (103) between all the n phases [Kashiwa 2001]:

$$\sum_{i=1}^{n}\left\{\varepsilon_i\left(W_{\boldsymbol{\tau},i}+{}^{tur/SG}W_{\boldsymbol{\tau},i}\right)+\frac{\varepsilon_i k_i\left(\nabla\tilde{T}_i\right)^2}{\tilde{T}_i}-\nabla\cdot\varepsilon_i\,{}^{tur/SG}\mathbf{q}_i+\left[{}^{f}H_i-\frac{\overline{P}_i}{\overline{\rho}_i}R_i+\overline{P}_i\frac{d\varepsilon_i}{dt}\right]\right\}\geq 0 \quad (105)$$

where the bracket term in Eq. (105), $\sum_{i=1}^{n}\left[{}^{f}H_i-\frac{\overline{P}_i}{\overline{\rho}_i}R_i+\overline{P}_i\frac{d\varepsilon_i}{dt}\right]$, is, by definition, either positive or equal to zero because $\sum_{i=1}^{n}R_i=0$, $\sum_{i=1}^{n}\varepsilon_i=1$, and $\sum_{i=1}^{n}{}^{f}H_i\geq 0$.

Hence, overall (for all phases), the mixture condition of Eq. (105) is fully satisfied as required by the second law of thermodynamics.

7. Summary and Conclusions

This manuscript has developed a multiphase flow hydrodynamic and thermodynamic model within both the RANS and the LES frameworks. With the mathematical methodologies established in §2, it has been demonstrated that the basic Navier-Stokes equations are essentially the same for RANS and LES, even though the mathematical and physical meaning of these PDEs is radically different: *ensemble-averaged* (RANS) vs. *filtered* (LES) fields. Yet, because the hydrodynamic and thermodynamic PDEs share essentially the same basic "structure," they may be discretized within the same computer code with appropriate subroutines for turbulence/subgrid closures and for interfacial closures. This manuscript also demonstrates that this model meets the necessary requirement for a well-posed initial value problem and is fully consistent with the second law of thermodynamics.

The main asset of this model is its versatility with respect to the multiphase turbulence approaches; therefore, it would be possible to apply this model to different multiphase flows as seen in §1.1: gravity currents within the atmospheric boundary layer (near/at the ground) or "boundary-free" flows within the atmosphere (e.g., dusty plumes and jets). This versatility makes possible using hybrid-RANS/LES approaches to simulate dusty surges and associated buoyant co-ash clouds, or, possibly, to simulate engineering multiphase flows (e.g., in nuclear reactor, aeronautical, and automotive industries; aerosol dispersions; and atomization and sprays dynamics) with RANS near the wall-boundary and LES away from the boundary.

In a next manuscript, we will develop specific RANS turbulence and LES subgrid closures to be implemented within this current multiphase Navier-Stokes model. Afterwards, in a hopefully not too far future, the main step will be to implement the code of the whole model as presented in this manuscript with the appropriate turbulence, subgrid, and interfacial closures.

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Appendix 1: Averaging and Filtering Rules

In this manuscript,we have used

- the angular operator to signify an "ensemble-averaging or a filtering process,"
- a *horizontal bar* for a "phasic-weighted process,"
- a *tilde* for a "mass-weighted process," and
- an *upside-down hat* under a variable to indicate a "LES filtering process."

Let $\alpha(\mathbf{x},t)$ and $\beta(\mathbf{x},t)$ be some fluid property (scalar, vector, tensor) and let c be a constant. $X(\mathbf{x},t)$ is the phase indicator function. The volumetric concentration and the bulk density of the i^{th} phase are respectively:

$$\varepsilon_i = \left\langle X_i \right\rangle = \begin{cases} \displaystyle\int_{-\infty}^{\infty} X_i \; dF(X_i, \rho_i) & \text{a.} \\ \displaystyle\iiint_{\Omega} G_x(\mathbf{x}-\mathbf{x}')\, X_i \; d\mathbf{x}' & \text{b.} \end{cases}$$

$$\hat{\rho}_i = \varepsilon_i \bar{\rho}_i = \left\langle X_i \rho_i \right\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(X_i \rho_i \right) dF(X_i, \rho_i) \qquad \text{c.} \qquad \text{(AI.1)}$$

$$\underset{\smile}{\hat{\rho}}_i = \varepsilon_i \underset{\smile}{\bar{\rho}}_i = \left\langle X_i \rho_i \right\rangle = \iiint_{\Omega} G_x(\mathbf{x}-\mathbf{x}') \left(X_i \rho_i \right) d\mathbf{x}' \qquad \text{d.}$$

Favre phasic-weighted decomposition

RANS framework:	$\alpha_i = \bar{\alpha}_i + \alpha_i'$, where $\bar{\alpha}_i = \dfrac{\left\langle X_i \alpha_i \right\rangle}{\varepsilon_i} \Leftrightarrow \left\langle X_i \alpha_i \right\rangle = \varepsilon_i \bar{\alpha}_i$	(AI.2)
LES framework:	$\alpha_i = \underset{\smile}{\bar{\alpha}}_i + \underset{\smile}{\alpha}_i'$, where $\underset{\smile}{\bar{\alpha}}_i = \dfrac{\left\langle X_i \alpha_i \right\rangle}{\varepsilon_i} \Leftrightarrow \left\langle X_i \alpha_i \right\rangle = \varepsilon_i \underset{\smile}{\bar{\alpha}}_i$	(AI.3)

Favre mass-weighted decomposition

RANS framework:	$\alpha_i = \tilde{\alpha}_i + \alpha_i''$, where $\tilde{\alpha}_i = \dfrac{\left\langle X_i \rho_i \alpha_i \right\rangle}{\hat{\rho}_i} \Leftrightarrow \left\langle X_i \rho_i \alpha_i \right\rangle = \hat{\rho}_i \tilde{\alpha}_i$	(AI.4)
LES framework:	$\alpha_i = \underset{\smile}{\tilde{\alpha}}_i + \underset{\smile}{\alpha}_i''$, where $\underset{\smile}{\tilde{\alpha}}_i = \dfrac{\left\langle X_i \rho_i \alpha_i \right\rangle}{\underset{\smile}{\hat{\rho}}_i} \Leftrightarrow \left\langle X_i \rho_i \alpha_i \right\rangle = \underset{\smile}{\hat{\rho}}_i \underset{\smile}{\tilde{\alpha}}_i$	(AI.5)

Operation upon a constant

$$\overline{c} = \tilde{c} = c \tag{AI.6}$$

Average of the average (RANS only)

$$\begin{aligned}
&\overline{\overline{\alpha}}_i = \overline{\tilde{\alpha}}_i = \overline{\alpha}_i \\
&\tilde{\tilde{\alpha}}_i = \tilde{\overline{\alpha}}_i = \tilde{\alpha}_i \\
&\text{e.g.,} \\
&\overline{\overline{\alpha}}_i = \int_{-\infty}^{\infty} \overline{\alpha}_i \; dP(\alpha) = \overline{\alpha}_i \int_{-\infty}^{\infty} dP(\alpha) = \overline{\alpha}_i
\end{aligned} \tag{AI.7}$$

(Note that, in LES, $\overline{\overline{\underset{\smile}{\alpha}}}_i \neq \overline{\underset{\smile}{\alpha}}_i$.)

Average of the fluctuating part (RANS only)

$$\begin{aligned}
&\overline{\alpha_i'} = \widetilde{\alpha_i''} = 0 \\
&\text{e.g.,} \\
&\alpha_i' = \alpha_i - \overline{\alpha}_i \\
&\overline{\alpha_i'} = \overline{\alpha_i - \overline{\alpha}_i} = \overline{\alpha}_i - \overline{\overline{\alpha}}_i = 0
\end{aligned} \tag{AI.8}$$

(Note that, in LES, $\overline{\underset{\smile}{\alpha}_i'} \neq \widetilde{\underset{\smile}{\alpha}_i''} \neq 0$.)

Operation upon time derivative (RANS and LES)

$$\left\langle \frac{\partial \alpha_i}{\partial t} \right\rangle = \frac{\partial \left\langle \alpha_i \right\rangle}{\partial t} \tag{AI.9}$$

bcause within RANS,

$$\left\langle \frac{\partial \alpha_i}{\partial t} \right\rangle = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} \alpha_i\,(\mathbf{x}, t)\ dP(\alpha_i)$$

$$= \frac{\partial}{\partial t}\left[\int_{-\infty}^{\infty} \alpha_i\,(\mathbf{x}, t)\ dP(\alpha_i) \right] \quad ,$$

$$= \frac{\partial \left\langle \alpha_i \right\rangle}{\partial t}$$

and within LES (spatial filter),

$$\left\langle \frac{\partial \alpha_i}{\partial t} \right\rangle = \iiint_{\Omega} G_x\,(\boldsymbol{\xi}) \frac{\partial}{\partial t} \alpha_i\,(\mathbf{x}', t)\ d\mathbf{x}'$$

$$= \frac{\partial}{\partial t}\left[\iiint_{\Omega} G_x\,(\boldsymbol{\xi})\,\alpha_i\,(\mathbf{x}', t)\ d\mathbf{x}' \right] \quad .$$

$$= \frac{\partial \left\langle \alpha_i \right\rangle}{\partial t}$$

Operation upon space derivative (gradient or divergence) is as follows:

$$\left\langle \frac{\partial \alpha}{\partial x_i} \right\rangle = \frac{\partial \left\langle \alpha \right\rangle}{\partial x_i} \tag{AI.10}$$

because within RANS,

$$\left\langle \frac{\partial \alpha}{\partial x_i} \right\rangle = \int_{-\infty}^{\infty} \frac{\partial \alpha}{\partial x_i}\ dP(\alpha)$$

$$= \frac{\partial}{\partial x_i}\left[\int_{-\infty}^{\infty} \alpha\ dP(\alpha) \right] \quad ,$$

$$= \frac{\partial \left\langle \alpha \right\rangle}{\partial x_i}$$

and within LES (spatial filter)[32],

$$\left\langle \frac{\partial\alpha}{\partial x_i} \right\rangle = \iiint_{\Omega} G_x(\xi) \frac{\partial}{\partial x_i} \alpha_i(\mathbf{x}', t)\, d\mathbf{x}'$$
$$= \frac{\partial}{\partial x_i} \left[\iiint_{\Omega} G_x(\xi)\, \alpha_i(\mathbf{x}', t)\, d\mathbf{x}' \right] \quad .$$
$$= \frac{\partial \langle \alpha \rangle}{\partial x_i}$$

Hence,

$$\begin{aligned} \langle \nabla \cdot \boldsymbol{\alpha}_i \rangle &= \nabla \cdot \langle \boldsymbol{\alpha}_i \rangle \\ \langle \nabla \alpha_i \rangle &= \nabla \langle \alpha_i \rangle \end{aligned} \quad . \tag{AI.11}$$

From Eq. (AI.9), Eq. (AI.10), and Eq. (AI.11), the following can be inferred by chain rules:

$$\frac{\partial \langle X_i \alpha_i \rangle}{\partial t} = \left\langle X_i \frac{\partial \alpha_i}{\partial t} \right\rangle + \left\langle \alpha_i \frac{\partial X_i}{\partial t} \right\rangle \tag{AI.12}$$

$$\begin{aligned} \nabla \langle X_i \alpha_i \rangle &= \langle X_i \nabla \alpha_i \rangle + \langle \alpha_i \nabla X_i \rangle \\ \nabla \cdot \langle X_i \boldsymbol{\alpha}_i \rangle &= \langle X_i \nabla \cdot \boldsymbol{\alpha}_i \rangle + \langle \boldsymbol{\alpha}_i \cdot \nabla X_i \rangle \end{aligned} \tag{AI.13}$$

Operation upon a sum (linearity)[33]

$$\langle \alpha_i + \beta_i \rangle = \langle \alpha_i \rangle + \langle \beta_i \rangle \tag{AI.14}$$

[32] Within the LES framework, it is essential that the spatial filter size, ξ, remain constant and that the cutoff length, $\vec{\Delta}$, remain constant as well over the whole domain (or subdomains) of integration, Ω. In other words, within any domain (or subdomain) of integration, the grid size must be homogenous (see §2.6.5).
[33] In statistics (RANS framework), this is one of the fundamental properties of the expectation of a random variable.

Useful correlations (RANS only)

$$\overline{\bar{\alpha}\alpha'} = \overline{\bar{\alpha}\beta'} = 0$$

since,

$$\overline{\bar{\alpha}\beta'} = \int_{-\infty}^{\infty} \bar{\alpha}\beta' \, dP(\beta') \;= \bar{\alpha}\int_{-\infty}^{\infty} \beta' \, dP(\beta') \tag{AI.15}$$

$$= \bar{\alpha}\overline{\beta'}$$

$$= 0$$

$$\overline{\rho_i \alpha_i''} \qquad = 0$$

$$\overline{\varepsilon_i \rho_i \alpha_i''} \qquad = 0$$

e.g.,

$$= \frac{\left\langle X_i \varepsilon_i \rho_i \alpha_i'' \right\rangle}{\varepsilon_i} = \left\langle X_i \rho_i \alpha_i'' \right\rangle$$

$$= \int_{-\infty}^{\infty} X_i \rho_i \alpha_i'' dP = \int_{-\infty}^{\infty} X_i \rho_i \alpha_i \, dP - \int_{-\infty}^{\infty} X_i \rho_i \tilde{\alpha}_i \, dP$$

$$= \left\langle X_i \rho_i \alpha_i \right\rangle - \tilde{\alpha}_i \left\langle X_i \rho_i \right\rangle = \left\langle X_i \rho_i \alpha_i \right\rangle - \tilde{\alpha}_i \hat{\rho}_i$$

$$= \hat{\rho}_i \left(\frac{\left\langle X_i \rho_i \alpha_i \right\rangle}{\hat{\rho}_i} - \tilde{\alpha}_i \right) = \hat{\rho}_i \left(\tilde{\alpha}_i - \tilde{\alpha}_i \right) = 0 \tag{AI.16}$$

$$\overline{\alpha\beta} \qquad = \bar{\alpha}\bar{\beta} + \overline{\alpha'\beta'}$$

since,

$$= \overline{\left(\bar{\alpha} + \alpha'\right)\left(\bar{\beta} + \beta'\right)} \tag{AI.17}$$

$$= \overline{\bar{\alpha}\bar{\beta} + \bar{\alpha}\beta' + \alpha'\bar{\beta} + \alpha'\beta'} = \overline{\bar{\alpha}\bar{\beta}} + \overline{\bar{\alpha}\beta'} + \overline{\alpha'\bar{\beta}} + \overline{\alpha'\beta'}$$

$$= \bar{\alpha}\bar{\beta} + \overline{\alpha'\beta'}$$

$$\overline{\alpha^2} = \bar{\alpha}^2 + \overline{\alpha'^2} \tag{AI.18}$$

Relations for which any operation holds[34]

$$\left\langle \alpha_i \beta_i \right\rangle \neq \left\langle \alpha_i \right\rangle \left\langle \beta_i \right\rangle \tag{AI.19}$$

$$\begin{aligned} &\overline{\hat{\rho}_i \alpha_i''} \neq 0 \\ &\text{since,} \\ &= \hat{\rho}_i \left(\overline{\alpha}_i - \tilde{\alpha}_i \right) = \hat{\rho}_i \left(\frac{\left\langle X_i \alpha_i \right\rangle}{\varepsilon_i} - \frac{\left\langle X_i \rho_i \alpha_i \right\rangle}{\hat{\rho}_i} \right) \end{aligned} \tag{AI.20}$$

and more generally, Eq. (AI.20) can be written as

$$\begin{aligned} &\overline{\overline{\beta}_i \alpha_i''} \neq 0 \\ &= \overline{\beta}_i \left(\overline{\alpha}_i - \tilde{\alpha}_i \right) \end{aligned} . \tag{AI.21}$$

For a compressible phase (both RANS and LES),

$$\begin{aligned} &\tilde{\rho}_i \neq \overline{\rho}_i \\ &\tilde{\mathbf{u}}_i \neq \overline{\mathbf{u}}_i \end{aligned} \tag{AI.22}$$

[34] Within RANS, in Eq. (AI.19), the equality cannot hold because these two random functions are not stochastically independent.

Appendix 2: Favre-Averaged Navier-Stokes Equations

1. RANS Phasic Continuity

The continuity for a single-phase system (n=i=1):

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i \, \mathbf{u}_i = 0 \tag{AII.1}$$

Because we have more than one phase, we must modify Eq. (AII.1) to account for all the possible random occupations by the different phases in the system anywhere and anytime. Let us multiply Eq. (AII.1) by the phasic function of presence (X_i, §2.3):

$$\begin{aligned} & X_i \left[\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i \mathbf{u}_i \right] = 0 \\ \Leftrightarrow \; & \frac{\partial X_i \rho_i}{\partial t} + \nabla \cdot X_i \rho_i \mathbf{u}_i = \rho_i \frac{\partial X_i}{\partial t} + \rho_i \mathbf{u}_i \cdot \nabla X_i \quad . \\ \Leftrightarrow \; & \frac{\partial X_i \rho_i}{\partial t} + \nabla \cdot X_i \rho_i \mathbf{u}_i = \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} \end{aligned} \tag{AII.2}$$

Let us average

$$\begin{aligned} & \left\langle \frac{\partial X_i \rho_i}{\partial t} + \nabla \cdot X_i \rho_i \mathbf{u}_i \right\rangle = \left\langle \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} \right\rangle \\ \Leftrightarrow \; & \frac{\partial \left\langle X_i \rho_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \mathbf{u}_i \right\rangle = R_i \end{aligned} \quad , \tag{AII.3}$$

where R_i is the mass-production or mass-destruction rate of the i^{th} phase and must be specified in a specific context; δ_{Int} is the function of presence of all the interfaces. R_i must follow the jump condition

$$\sum_{i=1}^{n} R_i = 0 \quad . \tag{AII.4}$$

Knowing that that $\left\langle X_i \rho_i \right\rangle = \hat{\rho}_i$ and that $\left\langle X_i \rho_i \mathbf{u}_i \right\rangle = \hat{\rho}_i \tilde{\mathbf{u}}_i$, Eq. (AII.3) can be rewritten as the following:

$$\frac{\partial \hat{\rho}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i = R_i \quad . \tag{AII.5}$$

2. RANS Species Continuity

If phase 'i' is made of different species, then the continuity equation for the j[th] species is simply written as the following [Besnard et al., 1992; Veynante and Poinsot 1997; Travis et al., 1998], assuming one phase only (n=i=1):

$$\frac{\partial y_j \rho_i}{\partial t} + \nabla \cdot y_j \rho_i \, \mathbf{u}_i = -\nabla \cdot \varpi \rho_i \nabla y_j + \Gamma_j \quad , \tag{AII.6}$$

where y_j is the mass fraction of the j[th] species; ϖ is the molecular diffusion coefficient of species j in the mixture; and Γ_i is the mass source or sink rate because chemical or physical processes between species. Global conservation upon all m species of phase i imposes that $\sum_{j=1}^{m} y_j = 1$.

Let us account for n phases in the system by multiplying Eq. (AII.6) by the phasic function of presence (X_i, §2.3):

$$\begin{aligned}
& X_i \left[\frac{\partial y_j \rho_i}{\partial t} + \nabla \cdot y_j \rho_i \, \mathbf{u}_i \right] = X_i \left[-\nabla \cdot \varpi \rho_i \nabla y_j + \Gamma_j \right] \\
\Leftrightarrow\ & \frac{\partial X_i y_j \rho_i}{\partial t} + \nabla \cdot X_i y_j \rho_i \, \mathbf{u}_i = -\nabla \cdot \varpi X_i \rho_i \nabla y_j + X_i \Gamma_j \\
& \qquad + \left[y_j \rho_i \frac{\partial X_i}{\partial t} + y_j \rho_i \mathbf{u}_i \cdot \nabla X_i + \varpi \rho_i \nabla y_j \cdot \nabla X_i \right] \quad . \\
\Leftrightarrow\ & \frac{\partial X_i y_j \rho_i}{\partial t} + \nabla \cdot X_i y_j \rho_i \, \mathbf{u}_i = -\nabla \cdot \varpi X_i \rho_i \nabla y_j + X_i \Gamma_j \\
& \qquad + \left[y_j \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} - \varpi \rho_i \nabla y_j \cdot \mathbf{n}_i \delta_{Int} \right]
\end{aligned} \tag{AII.7}$$

Let us average Eq. (AII.7) as follows:

$$\left\langle \frac{\partial X_i y_j \rho_i}{\partial t} + \nabla \cdot X_i y_j \rho_i \ \mathbf{u}_i \right\rangle = \left\langle -\nabla \cdot \varpi X_i \rho_i \nabla y_j + X_i \Gamma_j \right\rangle$$

$$+ \left\langle \left[y_j \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} - \varpi \rho_i \nabla y_j \cdot \mathbf{n}_i \delta_{Int} \right] \right\rangle \quad . \qquad \text{(AII.8)}$$

$\Leftrightarrow$

$$\frac{\partial \left\langle X_i y_j \rho_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i y_j \ \mathbf{u}_i \right\rangle = -\nabla \cdot \left\langle \varpi X_i \rho_i \nabla y_j \right\rangle + \left\langle X_i \Gamma_j \right\rangle + C_{i,j}$$

The mean interfacial species mass transfer rate ($C_{i,j}$) must be specified in a specific context. However, it clearly has two contributions: one from the mass transfer between phases as described in Eq. (AII.3) (i.e., R_i) and one describing the "diffusion" of the interface belonging to species j of the ith phase:

$$C_{i,j} = \left\langle \left[y_j \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \varpi \rho_i \nabla y_j \right] \cdot \mathbf{n}_i \delta_{Int} \right\rangle \quad . \qquad \text{(AII.9)}$$

Very often the molecular diffusion term is simply neglected [Symlal et al., 1993], and this neglect is even more justified if the flow is at high Reynolds number [Veynante and Poinsot 1997].

$C_{i,j}$ fully complies with the mean jump condition at the interfaces between species of a given phase and all other phases:

$$\sum_{i=1}^{n} \sum_{j=1}^{m} C_{i,j} = 0 \quad . \qquad \text{(AII.10)}$$

Let us take the Favre mass-weighted ensemble average of velocity and species mass fraction and decompose these into mean and fluctuating parts:

$$\frac{\partial \left\langle X_i y_j \rho_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \left(\tilde{y}_j + y_j''\right)\left(\tilde{\mathbf{u}}_i + \mathbf{u}_i''\right)\right\rangle = -\nabla \cdot \left\langle \varpi X_i \rho_i \nabla y_j \right\rangle + \left\langle X_i \Gamma_j \right\rangle + C_{i,j}$$

$$\Leftrightarrow$$

$$\begin{aligned} &\frac{\partial \hat{\rho}_i \tilde{y}_j}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \tilde{y}_j \tilde{\mathbf{u}}_i \right\rangle + \nabla \cdot \left\langle X_i \rho_i \tilde{y}_j \mathbf{u}_i'' \right\rangle + \nabla \cdot \left\langle X_i \rho_i \tilde{y}_j \mathbf{u}_i'' \right\rangle + \nabla \cdot \left\langle X_i \rho_i y_j'' \mathbf{u}_i'' \right\rangle \\ &\qquad = -\nabla \cdot \varpi \hat{\rho}_i \nabla \tilde{y}_j + \varepsilon_i \overline{\Gamma}_j + C_{i,j} \end{aligned} \quad , \qquad \text{(AII.11)}$$

$$\Leftrightarrow$$

$$\frac{\partial \hat{\rho}_i \tilde{y}_j}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{y}_j \tilde{\mathbf{u}}_i = -\nabla \cdot \varpi \hat{\rho}_i \nabla \tilde{y}_j - \nabla \cdot \hat{\rho}_i \widetilde{y_j'' \mathbf{u}_i''} + \varepsilon_i \overline{\Gamma}_j + C_{i,j}$$

$$\Leftrightarrow$$

$$\frac{\partial \hat{\rho}_i \tilde{y}_j}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{y}_j \tilde{\mathbf{u}}_i = -\nabla \cdot \hat{\rho}_i \left(\mathbf{y}_j + {}^{tur}\mathbf{y}_j\right) + \varepsilon_i \overline{\Gamma}_j + C_{i,j}$$

where the species' mass fraction fluxes have two contributions: one from the averaged mean flux (i.e., $\mathbf{y}_j$) and one from turbulence (i.e., ${}^{tur}\mathbf{y}_j$):

$$\begin{aligned} \mathbf{y}_j &= \varpi \nabla \tilde{y}_j \\ {}^{tur}\mathbf{y}_j &= \widetilde{y_j'' \mathbf{u}_i''} \end{aligned} \qquad \text{(AII.12)}$$

3. RANS Momentum

Let us start with the momentum equation of a single-phase (n=i=1),

$$\frac{\partial \rho_i \mathbf{u}_i}{\partial t} + \nabla \cdot \rho_i \mathbf{u}_i \mathbf{u}_i = -\nabla P_i - \nabla \cdot \boldsymbol{\tau}_i + \rho_i \mathbf{G}_i \quad , \qquad \text{(AII.13)}$$

where P_i is a thermodynamic isotropic pressure; τ_i is a viscous symmetric stress tensor (that can be broken into a spherical and deviatoric parts); and $\mathbf{G}_i$ represents the body force contribution (e.g., gravity). We have used the dyadic notation so that $\mathbf{u}_i\mathbf{u}_i$ is a second order tensor. Let us combine P_i and τ_i:

$$\mathbf{T}_i = P_i \mathbf{I} + \boldsymbol{\tau}_i \quad , \qquad \text{(AII.14)}$$

where the viscous stress tensor $\boldsymbol{\tau}_i$ is defined in Appendix 7 (as a reminder, compression and its rate are taken as positive). Let us account the presence of all n phases in the system in multiplying Eq. (AII.13) by the phasic function of presence (X_i, §2.3):

$$\begin{aligned}
& X_i\left[\frac{\partial \rho_i \mathbf{u}_i}{\partial t}+\nabla\cdot\rho_i \mathbf{u}_i \mathbf{u}_i=-\nabla\cdot\mathbf{T}_i+\rho_i \mathbf{G}_i\right] \\
\Leftrightarrow & \frac{\partial X_i \rho_i \mathbf{u}_i}{\partial t}+\nabla\cdot X_i \rho_i \mathbf{u}_i \mathbf{u}_i=-\nabla\cdot X_i \mathbf{T}_i+X_i \rho_i \mathbf{G}_i+\left[\rho_i \mathbf{u}_i \frac{\partial X_i}{\partial t}+\left(\mathbf{T}_i+\rho_i \mathbf{u}_i \mathbf{u}_i\right)\cdot\nabla X_i\right] \quad . \\
\Leftrightarrow & \frac{\partial X_i \rho_i \mathbf{u}_i}{\partial t}+\nabla\cdot X_i \rho_i \mathbf{u}_i \mathbf{u}_i=-\nabla\cdot X_i \mathbf{T}_i+X_i \rho_i \mathbf{G}_i+\left[\rho_i \mathbf{u}_i\left(\mathbf{u}_{Int}-\mathbf{u}_i\right)\cdot\mathbf{n}_i \delta_{Int}-\mathbf{T}_i\cdot\mathbf{n}_i \delta_{Int}\right]
\end{aligned} \tag{AII.15}$$

Let us average Eq. (AII.15):

$$\begin{aligned}
& \left\langle\frac{\partial X_i \rho_i \mathbf{u}_i}{\partial t}+\nabla\cdot X_i \rho_i \mathbf{u}_i \mathbf{u}_i\right\rangle=\left\langle-\nabla\cdot X_i \mathbf{T}_i+X_i \rho_i \mathbf{G}_i+\left[\rho_i \mathbf{u}_i\left(\mathbf{u}_{Int}-\mathbf{u}_i\right)-\mathbf{T}_i\right]\cdot\mathbf{n}_i \delta_{Int}\right\rangle \\
\Leftrightarrow & \frac{\partial\left\langle X_i \rho_i \mathbf{u}_i\right\rangle}{\partial t}+\nabla\cdot\left\langle X_i \rho_i \mathbf{u}_i \mathbf{u}_i\right\rangle=-\nabla\cdot\left\langle X_i \mathbf{T}_i\right\rangle+\left\langle X_i \rho_i \mathbf{G}_i\right\rangle+\left\langle\left[\rho_i \mathbf{u}_i\left(\mathbf{u}_{Int}-\mathbf{u}_i\right)-\mathbf{T}_i\right]\cdot\mathbf{n}_i \delta_{Int}\right\rangle \\
\Leftrightarrow & \frac{\partial\left\langle X_i \rho_i \mathbf{u}_i\right\rangle}{\partial t}+\nabla\cdot\left\langle X_i \rho_i \mathbf{u}_i \mathbf{u}_i\right\rangle=-\nabla\cdot\left\langle X_i \mathbf{T}_i\right\rangle+\left\langle X_i \rho_i \mathbf{G}_i\right\rangle+\mathbf{M}_i
\end{aligned} \tag{AII.16}$$

The mean interfacial momentum transfer rate between phases ($\mathbf{M}_i$) must be specified in a specific context. It has two contributions as expected: one from the mass transfer between phases as described in Eq. (AII.3) (i.e., R_i) and one from the interfacial forces at the interfaces (e.g., drag force, added mass forces, …):

$$\mathbf{M}_i=\left\langle\left[\rho_i \mathbf{u}_i\left(\mathbf{u}_{Int}-\mathbf{u}_i\right)-\mathbf{T}_i\right]\cdot\mathbf{n}_i \delta_{Int}\right\rangle \quad . \tag{AII.17}$$

$\mathbf{M}_i$ fully complies with the mean jump condition derived from the local balance momentum at the interfaces between phases,

$$\sum_{i=1}^{n}\mathbf{M}_i=0 \quad , \tag{AII.18}$$

where we have neglected all surface tension effects between phases [Ishii 1975; Ishii and Mishima 1984; Lhuillier 1996].

Let us take Favre mass-weighted ensemble average of velocity, decompose it into a mean and fluctuating part, and subsequently develop Eq. (AII.16):

$$
\begin{aligned}
&\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \left(\tilde{\mathbf{u}}_i + \mathbf{u}_i'' \right)\left(\tilde{\mathbf{u}}_i + \mathbf{u}_i'' \right) \right\rangle = -\nabla \cdot \left\langle X_i \mathbf{T}_i \right\rangle + \left\langle X_i \rho_i \mathbf{G}_i \right\rangle + \mathbf{M}_i \\
\Leftrightarrow\ &\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i \right\rangle + 2\nabla \cdot \left\langle X_i \rho_i \tilde{\mathbf{u}}_i \mathbf{u}_i'' \right\rangle + \nabla \cdot \left\langle X_i \rho_i \mathbf{u}_i'' \mathbf{u}_i'' \right\rangle = -\nabla \cdot \varepsilon_i \overline{\mathbf{T}}_i + \hat{\rho}_i \tilde{\mathbf{G}}_i + \mathbf{M}_i \\
\Leftrightarrow\ &\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \widetilde{\tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i} + 2\nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i \widetilde{\mathbf{u}_i''} + \nabla \cdot \left\langle X_i \rho_i \mathbf{u}_i'' \mathbf{u}_i'' \right\rangle = -\nabla \cdot \varepsilon_i \overline{\mathbf{T}}_i + \hat{\rho}_i \tilde{\mathbf{G}}_i + \mathbf{M}_i \\
\Leftrightarrow\ &\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i + \quad 0 \quad + \nabla \cdot \varepsilon_i \overline{\rho}_i \widetilde{\mathbf{u}_i'' \mathbf{u}_i''} = -\nabla \cdot \varepsilon_i \overline{\mathbf{T}}_i + \hat{\rho}_i \tilde{\mathbf{G}}_i + \mathbf{M}_i \\
\Leftrightarrow\ &\frac{\partial \hat{\rho}_i \tilde{\mathbf{u}}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i = -\nabla \cdot \varepsilon_i \left(\overline{\mathbf{T}}_i + {}^{tur}\mathbf{T}_i \right) + \hat{\rho}_i \tilde{\mathbf{G}}_i + \mathbf{M}_i
\end{aligned}
\tag{AII.19}
$$

where the RANS Reynolds stress is clearly defined from Eq. (AII.19) as

$$
{}^{tur}\mathbf{T}_i = \overline{\rho}_i \widetilde{\mathbf{u}_i'' \mathbf{u}_i''} \quad . \tag{AII.20}
$$

See Appendix 5 for further discussions on the term $\overline{\mathbf{T}}_i$.

4. RANS Energy

Let us write first the energy balance for a pure single phase (n=i=1) [Bird et al., 1960],

$$
\frac{\partial \rho_i E_i}{\partial t} + \nabla \cdot \rho_i E_i \mathbf{u}_i = -\nabla \cdot \left(\mathbf{T}_i \cdot \mathbf{u}_i \right) - \nabla \cdot \mathbf{q}_i + \rho_i S_i + \rho_i \mathbf{G}_i \cdot \mathbf{u}_i \quad , \tag{AII.21}
$$

where E_i is the total energy per unit of mass; the first term on the RHS represents the total work done by all the surface forces (viscous and pressure); $\mathbf{q}_i$ is the heat conduction flux vector that follows a classical Fourier law; $\rho_i S_i$ represents a source contribution involving, for instance, radiation; and the last term is the work done by the body forces (e.g., gravity). The total energy is defined as

$$E_i = I_i + \frac{u_i^2}{2} \quad , \tag{AII.22}$$

where I_i is the internal energy per unit of mass of the phase under consideration; the second term of Eq. (AII.22) is the kinetic energy of phase i.

The total stress tensor, $\mathbf{T}_i$ and the viscous stress tensor, τ_i, (see also Appendix 7) are

$$\begin{cases} \mathbf{T}_i = P_i\ \mathbf{I} + \boldsymbol{\tau}_i \\ \boldsymbol{\tau}_i = 2\,\mu_i\ \overset{\circ}{\overline{\overline{\mathbf{D}}}}_i - {}^b\mu_i \nabla\cdot\mathbf{u}_i\ \mathbf{I} \quad = 2\,\mu_i \left[\mathbf{D}_i + \frac{1}{3}\left(\nabla\cdot\mathbf{u}_i\right)\mathbf{I} \right] - {}^b\mu_i \nabla\cdot\mathbf{u}_i\ \mathbf{I} \\ \qquad\qquad\qquad\qquad\qquad\quad = \mu_i \left[-\left(\nabla\mathbf{u}_i + \nabla\mathbf{u}_i^{\,T}\right) + \frac{2}{3}\left(\nabla\cdot\mathbf{u}_i\right)\mathbf{I} \right] - {}^b\mu_i \nabla\cdot\mathbf{u}_i\ \mathbf{I} \end{cases} \quad , \tag{AII.23}$$

where μ_i and ${}^b\mu_i$ are the shear and volumetric viscosities; $\mathbf{D}_i$ is the rate-of-strain tensor and $\overset{\circ}{\overline{\overline{\mathbf{D}}}}_i$ is its deviator; and $\mathbf{I}$ is the unit tensor. From Eq. (AII.23), we define rate-of-strain positive in compression.

Let us account the presence of n different phases in the system (i=1,2,…, n) in multiplying Eq. (AII.21) by the phasic function of presence (X_i, §2.3):

$$X_i \left[\frac{\partial \rho_i\ E_i}{\partial t} + \nabla\cdot\rho_i\ E_i\ \mathbf{u}_i \right] = X_i \left[-\nabla\cdot\left(\mathbf{u}_i\cdot\mathbf{T}_i\right) - \nabla\cdot\mathbf{q}_i + \rho_i\ S_i + \rho_i\ \mathbf{G}_i\cdot\mathbf{u}_i \right]$$

$\Leftrightarrow$

$$\begin{aligned} \frac{\partial X_i\rho_i\ E_i}{\partial t} + \nabla\cdot X_i\rho_i\ E_i\ \mathbf{u}_i &= -\nabla\cdot X_i\left(\mathbf{u}_i\cdot\mathbf{T}_i\right) - \nabla\cdot X_i\mathbf{q}_i + X_i\rho_i\ S_i + X_i\rho_i\ \mathbf{G}_i\cdot\mathbf{u}_i \\ &+ \left[\rho_i\ E_i \frac{\partial X_i}{\partial t} + \rho_i\ E_i\ \mathbf{u}_i\cdot\nabla X_i + \mathbf{q}_i\cdot\nabla X_i + \left(\mathbf{u}_i\cdot\mathbf{T}_i\right)\cdot\nabla X_i \right] \quad . \end{aligned} \tag{AII.24}$$

$\Leftrightarrow$

$$\begin{aligned} \frac{\partial X_i\rho_i\ E_i}{\partial t} + \nabla\cdot X_i\rho_i\ E_i\ \mathbf{u}_i &= -\nabla\cdot X_i\left(\mathbf{u}_i\cdot\mathbf{T}_i\right) - \nabla\cdot X_i\mathbf{q}_i + X_i\rho_i\ S_i + X_i\rho_i\ \mathbf{G}_i\cdot\mathbf{u}_i \\ &+ \left[\rho_i\ E_i\left(\mathbf{u}_{Int} - \mathbf{u}_i\right)\cdot\mathbf{n}_i\delta_{Int} - \left(\mathbf{q}_i + \mathbf{u}_i\cdot\mathbf{T}_i\right)\cdot\mathbf{n}_i\delta_{Int} \right] \end{aligned}$$

This equation can be rearranged in terms of the internal energy, I_i. To do so, let us "dot multiply" the momentum equation, Eq. (AII.13), by $\mathbf{u}_i$ to obtain the equation of mechanical energy only as follows:

$$X_i \left[\frac{\partial \rho_i \frac{u_i^2}{2}}{\partial t} + \nabla \cdot \rho_i \frac{u_i^2}{2} \mathbf{u}_i = -\mathbf{u}_i \cdot \nabla \cdot \mathbf{T}_i + \rho_i \mathbf{G}_i \cdot \mathbf{u}_i \right]$$

$\Leftrightarrow$

$$\frac{\partial X_i \rho_i \frac{u_i^2}{2}}{\partial t} + \nabla \cdot X_i \rho_i \frac{u_i^2}{2} \mathbf{u}_i = -\mathbf{u}_i \cdot \nabla \cdot X_i \mathbf{T}_i + X_i \rho_i \mathbf{G}_i \cdot \mathbf{u}_i + \left[\rho_i \frac{u_i^2}{2} \frac{\partial X_i}{\partial t} + \left(\mathbf{u}_i \cdot \mathbf{T}_i + \rho_i \frac{u_i^2}{2} \mathbf{u}_i \right) \cdot \nabla X_i \right]$$

$\Leftrightarrow$

$$\frac{\partial X_i \rho_i \frac{u_i^2}{2}}{\partial t} + \nabla \cdot X_i \rho_i \frac{u_i^2}{2} \mathbf{u}_i = -\mathbf{u}_i \cdot \nabla \cdot X_i \mathbf{T}_i + X_i \rho_i \mathbf{G}_i \cdot \mathbf{u}_i + \left[\rho_i \frac{u_i^2}{2} \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} - \left(\mathbf{u}_i \cdot \mathbf{T}_i \right) \cdot \mathbf{n}_i \delta_{Int} \right] \tag{AII.25}$$

And subtracting this Eq. (AII.25) from Eq. (AII.24), we obtain, after simplifications,

$$\frac{\partial X_i \rho_i I_i}{\partial t} + \nabla \cdot X_i \rho_i I_i \mathbf{u}_i = X_i W_{\mathbf{T},i} - \nabla \cdot X_i \mathbf{q}_i + X_i \rho_i S_i + \left[\rho_i I_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} - \mathbf{q}_i \cdot \mathbf{n}_i \delta_{Int} \right] \quad , \tag{AII.26}$$

where $W_{\mathbf{T},i}$ $(= -\mathbf{T}_i : \nabla \mathbf{u}_i)$ represents the reversible and irreversible work done by all the surface forces upon the internal energy. Let us average Eq. (AII.26) in the following:

$$\left\langle \frac{\partial X_i \rho_i I_i}{\partial t} + \nabla \cdot X_i \rho_i I_i \mathbf{u}_i \right\rangle = \left\langle X_i W_{\mathbf{T},i} - \nabla \cdot X_i \mathbf{q}_i + X_i \rho_i S_i \right\rangle + \left\langle \left[\rho_i I_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} - \mathbf{q}_i \cdot \mathbf{n}_i \delta_{Int} \right] \right\rangle$$

$\Leftrightarrow$ (AII.27)

$$\frac{\partial \left\langle X_i \rho_i I_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i I_i \mathbf{u}_i \right\rangle = \left\langle X_i W_{\mathbf{T},i} \right\rangle - \nabla \cdot \left\langle X_i \mathbf{q}_i \right\rangle + \left\langle X_i \rho_i S_i \right\rangle + {}^{I}H_i$$

where ${}^{I}H_i$ is the mean rate of interfacial heat transfer between phases and must be defined within a specific context for a specific phase,

$$ {}^{I}H_i = \left\langle \left[\rho_i \, I_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \mathbf{q}_i \right] \cdot \mathbf{n}_i \delta_{Int} \right\rangle \quad , \tag{AII.28} $$

where the first RHS term represents heat source or sink from mass transfer at the interfaces between phases [see Eq. (AII.3)]; the second term is the heat flux exchange at the interfaces between phases. ${}^{I}H_i$ must fully comply with the jump condition between all possible interfaces,

$$ \sum_{i=1}^{n} {}^{I}H_i = 0 \quad , \tag{AII.29} $$

where we have neglected all interfacial energy source between phases [Ishii 1975; Ishii and Mishima 1984; Lhuillier 1996].

Let us take the Favre phasic-weighted ensemble average and mass-weighted average of velocity. Then, let us decompose these into a mean and fluctuating part and subsequently develop Eq. (AII.27) as follows:

$$ \begin{aligned} & \frac{\partial \left\langle X_i \rho_i I_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i I_i \mathbf{u}_i \right\rangle = \left\langle X_i W_{\mathbf{T},i} \right\rangle - \nabla \cdot \left\langle X_i \mathbf{q}_i \right\rangle + \left\langle X_i \rho_i S_i \right\rangle + {}^{I}H_i \\ & \Leftrightarrow \\ & \frac{\partial \left\langle X_i \rho_i I_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \left(\tilde{I}_i + I_i'' \right) \left(\tilde{\mathbf{u}}_i + \mathbf{u}_i'' \right) \right\rangle = \varepsilon_i \overline{- \mathbf{T}_i : \nabla \mathbf{u}_i} - \nabla \cdot \varepsilon_i \overline{\mathbf{q}}_i + \hat{\rho}_i \tilde{S}_i + {}^{I}H_i \\ & \Leftrightarrow \\ & \frac{\partial \hat{\rho}_i \tilde{I}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{I}_i \tilde{\mathbf{u}}_i + \nabla \cdot \left\langle X_i \rho_i I_i'' \mathbf{u}_i'' \right\rangle = \varepsilon_i \left(- \overline{\boldsymbol{\tau}}_i : \nabla \overline{\mathbf{u}}_i - \overline{P}_i \nabla \cdot \overline{\mathbf{u}}_i - \overline{\boldsymbol{\tau}_i' : \nabla \mathbf{u}_i'} - \overline{P_i' \nabla \cdot \mathbf{u}_i'} \right) - \nabla \cdot \varepsilon_i \overline{\mathbf{q}}_i + \hat{\rho}_i \tilde{S}_i + {}^{I}H_i \\ & \Leftrightarrow \\ & \frac{\partial \hat{\rho}_i \tilde{I}_i}{\partial t} + \nabla \cdot \hat{\rho}_i \tilde{I}_i \tilde{\mathbf{u}}_i = \varepsilon_i \left(W_{\mathbf{T},i} + {}^{tur}W_{\mathbf{T},i} \right) - \nabla \cdot \varepsilon_i \left(\overline{\mathbf{q}}_i + {}^{tur}\mathbf{q}_i \right) + \hat{\rho}_i \tilde{S}_i + {}^{I}H_i \end{aligned} \tag{AII.30} $$

where the surface force works have ensemble-averaged and fluctuating (from turbulence) contributions (see also demonstration in Appendix 5):

$$ \begin{aligned} W_{\mathbf{T},i} &= - \overline{\boldsymbol{\tau}}_i : \nabla \overline{\mathbf{u}}_i - \overline{P}_i \nabla \cdot \overline{\mathbf{u}}_i \\ {}^{tur}W_{\mathbf{T},i} &= \overline{- \boldsymbol{\tau}_i' : \nabla \mathbf{u}_i'} - \overline{P_i' \nabla \cdot \mathbf{u}_i'} \end{aligned} \quad . \tag{AII.31} $$

Idem for the heat flux:

$$\begin{aligned} \overline{\mathbf{q}}_i &= -k_i \nabla \overline{T}_i \\ {}^{tur}\mathbf{q}_i &= \overline{\rho_i I_i'' \mathbf{u}_i''} = \overline{\rho}_i \widetilde{I_i'' \mathbf{u}_i''} \end{aligned} \quad , \tag{AII.32}$$

where k_i is the molecular (not affected by turbulence) thermal conductivity coefficient of phase i. Eq. (AII.31) is particularly difficult because it involves two new unknowns in this system: the Favre phasic-weighted averaged and fluctuating parts of the velocity ($\overline{\mathbf{u}}_i$ and $\mathbf{u}_i'$) instead of the Favre mass-weighted components [$\tilde{\mathbf{u}}_i$ and $\mathbf{u}_i''$ as in Eq. (AII.19) and Eq. (AII.20)]. For a detailed discussion on $W_{\mathbf{T},i}$ and ${}^{tur}W_{\mathbf{T},i}$ and possible approximations, see Appendix 5.

For many engineering purposes, it is much more practical to have the energy equations in terms of the enthalpy instead of the internal energy. The enthalpy, h_i, of a single phase i (n=i=1) is as follows:

$$h_i = I_i + \frac{P_i}{\rho_i} \quad . \tag{AII.33}$$

Let us take the material derivative of h_i

$$\begin{aligned} \frac{dh_i}{dt} &= \frac{dI_i}{dt} + \frac{d}{dt}\left(\frac{P_i}{\rho_i}\right) \\ \Leftrightarrow & \\ \frac{dh_i}{dt} &= \frac{dI_i}{dt} + P_i \frac{d \, {}^1\!/\!_{\rho_i}}{dt} + \frac{1}{\rho_i}\frac{dP_i}{dt} \end{aligned} \quad . \tag{AII.34}$$

Using the continuity equation of a single phase, Eq. (AII.1), we know that

$$\frac{d \, {}^1\!/\!_{\rho_i}}{dt} = -\frac{1}{\rho_i^2}\frac{d\rho_i}{dt} = \frac{1}{\rho_i}\nabla \cdot \mathbf{u}_i \quad . \tag{AII.35}$$

Let us recall that we have not yet averaged anything and we still only see one phase in the system. From Eq. (AII.26), we may deduce the equation of internal energy of only one phase in the system (n=i=1),

$$
\begin{aligned}
&\frac{\partial \rho_i I_i}{\partial t} + \nabla\cdot\rho_i I_i \mathbf{u}_i = -\mathbf{T}_i : \nabla\mathbf{u}_i - \nabla\cdot\mathbf{q}_i + \rho_i S_i \\
&\Leftrightarrow \\
&\frac{d\rho_i I_i}{dt} + \rho_i I_i \nabla\cdot\mathbf{u}_i = -\mathbf{T}_i : \nabla\mathbf{u}_i - \nabla\cdot\mathbf{q}_i + \rho_i S_i
\end{aligned}
\quad , \qquad \text{(AII.36)}
$$

where $-\mathbf{T}_i : \nabla\mathbf{u}_i = -P_i \nabla\cdot\mathbf{u}_i - \boldsymbol{\tau}_i : \nabla\mathbf{u}_i$. Substituting Eq. (AII.35) into Eq. (AII.34), multiplying the latter by ρ_i, and applying the chain rules yields the following:

$$
\frac{d\rho_i h_i}{dt} = \frac{d\rho_i I_i}{dt} + \frac{dP_i}{dt} \quad . \qquad \text{(AII.37)}
$$

Substituting Eq. (AII.36) into Eq. (AII.37) yields the following:

$$
\begin{aligned}
&\frac{d\rho_i h_i}{dt} = -\rho_i I_i \nabla\cdot\mathbf{u}_i - \mathbf{T}_i : \nabla\mathbf{u}_i - \nabla\cdot\mathbf{q}_i + \rho_i S_i + \frac{dP_i}{dt} \\
&\Leftrightarrow \\
&\frac{d\rho_i h_i}{dt} = -\rho_i \left(h_i - \frac{P_i}{\rho_i} \right) \nabla\cdot\mathbf{u}_i - \mathbf{T}_i : \nabla\mathbf{u}_i - \nabla\cdot\mathbf{q}_i + \rho_i S_i + \frac{dP_i}{dt} \\
&\Leftrightarrow \\
&\frac{\partial \rho_i h_i}{\partial t} + \nabla\cdot\rho_i h_i \mathbf{u}_i = P_i \nabla\cdot\mathbf{u}_i - \mathbf{T}_i : \nabla\mathbf{u}_i - \nabla\cdot\mathbf{q}_i + \rho_i S_i + \frac{dP_i}{dt} \\
&\Leftrightarrow \\
&\frac{\partial \rho_i h_i}{\partial t} + \nabla\cdot\rho_i h_i \mathbf{u}_i = -\boldsymbol{\tau}_i : \nabla\mathbf{u}_i - \nabla\cdot\mathbf{q}_i + \rho_i S_i + \frac{dP_i}{dt}
\end{aligned}
\quad . \qquad \text{(AII.38)}
$$

Let us account the presence of all n phases in the system in multiplying Eq. (AII.38) by the phasic function of presence (X_i). After development and rearranging all the terms, we have

$$\frac{\partial\left\langle X_i\rho_i h_i\right\rangle}{\partial t}+\nabla\cdot\left\langle X_i\rho_i h_i\mathbf{u}_i\right\rangle=\left\langle -X_i\boldsymbol{\tau}_i:\nabla\mathbf{u}_i\right\rangle-\nabla\cdot\left\langle X_i\mathbf{q}_i\right\rangle+\left\langle X_i\frac{dP_i}{dt}\right\rangle+\left\langle X_i\rho_i S_i\right\rangle$$

$$+\left\langle\left[\rho_i h_i\left(\mathbf{u}_{Int}-\mathbf{u}_i\right)\cdot\mathbf{n}_i\delta_{Int}-\mathbf{q}_i\cdot\mathbf{n}_i\delta_{Int}\right]\right\rangle$$

$$\Leftrightarrow$$

$$\frac{\partial\hat{\rho}_i\tilde{h}_i}{\partial t}+\nabla\cdot\left\langle X_i\rho_i\left(\tilde{h}_i+h_i''\right)\left(\tilde{\mathbf{u}}_i+\mathbf{u}_i''\right)\right\rangle=\left\langle -X_i\boldsymbol{\tau}_i:\nabla\mathbf{u}_i\right\rangle-\nabla\cdot\varepsilon_i\overline{\mathbf{q}}_i+\varepsilon_i\frac{d\overline{P}_i}{dt}+\hat{\rho}_i\tilde{S}_i+{}^{h}H_i \quad , \qquad \text{(AII.39)}$$

$$\Leftrightarrow$$

$$\frac{\partial\hat{\rho}_i\tilde{h}_i}{\partial t}+\nabla\cdot\hat{\rho}_i\tilde{h}_i\tilde{\mathbf{u}}_i=\varepsilon_i\left(W_{\boldsymbol{\tau},i}+{}^{tur}W_{\boldsymbol{\tau},i}\right)-\nabla\cdot\varepsilon_i\left(\overline{\mathbf{q}}_i+{}^{tur}\mathbf{q}_i\right)+\varepsilon_i\frac{d\overline{P}_i}{dt}+\hat{\rho}_i\tilde{S}_i+{}^{h}H_i$$

where ${}^{h}H_i$ is the mean rate of interfacial heat transfer between phases for the enthalpy equation and must be defined within a specific context for a specific phase. As usual, ${}^{h}H_i$ must comply with the jump condition (i.e., $\sum_{i=1}^{n}{}^{h}H_i=0$). The contributions of turbulence in the enthalpy equations from viscous dissipation and heat transfer are respectively defined in Eq. (AII.31) and Eq. (AII.32).

5. RANS Entropy

Let us write the entropy condition for a pure single phase (n=i=1) [Aris 1962; Ishii 1975] as

$$\frac{\partial\rho_i\eta_i}{\partial t}+\nabla\cdot\rho_i\eta_i\mathbf{u}_i+\nabla\cdot\frac{\mathbf{q}_i}{T_i}-\frac{\rho_i S_i}{T_i}\geq 0 \quad , \qquad \text{(AII.40)}$$

where η_i is the specific entropy (entropy per unit of mass); $\mathbf{q}_i$ is the heat conduction flux vector that follows a classical Fourier law; S_i represents various heat sources per unit of mass (e.g., radiation); and ρ_i and T_i are the density and temperature of phase i. Hence, $\frac{\mathbf{q}_i}{T_i}$ is the entropy flux, and $\frac{S_i}{T_i}$ is any source of entropy.

Let us account the presence of n different phases in the system (i=1,…, n) in multiplying Eq. (AII.40) by the phasic function of presence (X_i):

$$\frac{\partial X_i\rho_i\eta_i}{\partial t}-\rho_i\eta_i\frac{\partial X_i}{\partial t}+\nabla\cdot X_i\rho_i\eta_i\mathbf{u}_i-\rho_i\eta_i\mathbf{u}_i\cdot\nabla X_i\geq-\nabla\cdot\frac{X_i\mathbf{q}_i}{T_i}+\frac{\mathbf{q}_i}{T_i}\cdot\nabla X_i+\frac{X_i\rho_iS_i}{T_i}$$

$\Leftrightarrow$

$$\frac{\partial X_i\rho_i\eta_i}{\partial t}+\nabla\cdot X_i\rho_i\eta_i\mathbf{u}_i\geq-\nabla\cdot\frac{X_i\mathbf{q}_i}{T_i}+\frac{X_i\rho_iS_i}{T_i}+\left[\rho_i\eta_i\frac{\partial X_i}{\partial t}+\rho_i\eta_i\mathbf{u}_i\cdot\nabla X_i+\frac{\mathbf{q}_i}{T_i}\cdot\nabla X_i\right] \quad . \qquad \text{(AII.41)}$$

$\Leftrightarrow$

$$\frac{\partial X_i\rho_i\eta_i}{\partial t}+\nabla\cdot X_i\rho_i\eta_i\mathbf{u}_i\geq-\nabla\cdot\frac{X_i\mathbf{q}_i}{T_i}+\frac{X_i\rho_iS_i}{T_i}+\left[\rho_i\eta_i\left(\mathbf{u}_{Int}-\mathbf{u}_i\right)\cdot\mathbf{n}_i\delta_{Int}-\frac{\mathbf{q}_i}{T_i}\cdot\mathbf{n}_i\delta_{Int}\right]$$

Let us average Eq. (AII.41)

$$\frac{\partial\left\langle X_i\rho_i\eta_i\right\rangle}{\partial t}+\nabla\cdot\left\langle X_i\rho_i\eta_i\mathbf{u}_i\right\rangle\geq-\nabla\cdot\left\langle X_i\frac{\mathbf{q}_i}{T_i}\right\rangle+\left\langle X_i\frac{\rho_iS_i}{T_i}\right\rangle+{}^{\eta}H_i \quad , \qquad \text{(AII.42)}$$

where ${}^{\eta}H_i$ is the mean rate of interfacial entropy between phases

$${}^{\eta}H_i=\left\langle\left[\rho_i\eta_i\left(\mathbf{u}_{Int}-\mathbf{u}_i\right)-\frac{\mathbf{q}_i}{T_i}\right]\cdot\mathbf{n}_i\delta_{Int}\right\rangle \quad , \qquad \text{(AII.43)}$$

which complies with the entropic jump condition between all phases in the system [Lhuillier 1996]—i.e., $\sum_{i=1}^{n}{}^{\eta}H_i\geq 0$ (it may be possible to have some entropy production at the interface).

Let us take the classical Favre decompositions of mean and fluctuating part in Eq. (AII.42) and use all the averaging rules of Appendix 1 in the following:

$$\frac{\partial\left\langle X_i\rho_i\eta_i\right\rangle}{\partial t}+\nabla\cdot\left\langle X_i\rho_i\left(\tilde{\eta}_i+\eta_i''\right)\left(\tilde{\mathbf{u}}_i+\mathbf{u}_i''\right)\right\rangle\geq-\nabla\cdot\left\langle X_i\frac{\mathbf{q}_i}{T_i}\right\rangle+\left\langle X_i\rho_i\frac{S_i}{T_i}\right\rangle+{}^{\eta}H_i$$

$\Leftrightarrow$

$$\frac{\partial\hat{\rho}_i\tilde{\eta}_i}{\partial t}+\nabla\cdot\hat{\rho}_i\tilde{\eta}_i\tilde{\mathbf{u}}_i\geq-\nabla\cdot\varepsilon_i\left[\overline{\left(\frac{\mathbf{q}_i}{T_i}\right)}+\overline{\rho_i\eta_i''\mathbf{u}_i''}\right]+\hat{\rho}_i\widetilde{\left(\frac{S_i}{T_i}\right)}+{}^{\eta}H_i \quad , \qquad \text{(AII.44)}$$

$\Leftrightarrow$

$$\frac{\partial\hat{\rho}_i\tilde{\eta}_i}{\partial t}+\nabla\cdot\hat{\rho}_i\tilde{\eta}_i\tilde{\mathbf{u}}_i\geq-\nabla\cdot\varepsilon_i\left(\bar{\boldsymbol{\Phi}}_i+{}^{tur}\boldsymbol{\Phi}_i\right)+\hat{\rho}_i\tilde{\Sigma}_i+{}^{\eta}H_i$$

where the flux of entropy has two sources, one Favre-phasic averaged ($\bar{\boldsymbol{\Phi}}_i = \overline{\left(\frac{\mathbf{q}_i}{T_i}\right)}$) and one from turbulence ($^{tur}\boldsymbol{\Phi}_i = \overline{\rho_i \eta_i'' \mathbf{u}_i''}$), whereas the entropy source is defined by a Favre mass-weighted-averaged relationship: $\tilde{\Sigma}_i = \widetilde{\left(\frac{S_i}{T_i}\right)}$. Eq. (AII.44) may also be expressed as

$$\hat{\rho}_i \frac{d\tilde{\eta}_i}{dt} \geq -\nabla \cdot \varepsilon_i \left(\bar{\boldsymbol{\Phi}}_i + {}^{tur}\boldsymbol{\Phi}_i\right) + \hat{\rho}_i \tilde{\Sigma}_i + {}^{\eta}H_i \quad . \tag{AII.45}$$

Appendix 3: Favre Filtered Navier-Stokes Equations

1. LES Phasic Continuity

From Eq. (AII.3) in Appendix 2, we know

$$\frac{\partial \left\langle X_i \rho_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \mathbf{u}_i \right\rangle = R_i \quad , \tag{AIII.1}$$

where R_i is the mass production or destruction rate of the ith phase (source or sink) and must be specified in a specific context (see §2.3),

$$R_i = \left\langle \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} \right\rangle \quad , \tag{AIII.2}$$

and R_i must follow the jump condition between all n phases: $\sum_{i=1}^{n} R_i = 0$.

Using the filtering definitions of §2.6 and §2.7, Eq. (AIII.1) becomes

$$\frac{\partial \underset{\smile}{\hat{\rho}}_i}{\partial t} + \nabla \cdot \underset{\smile}{\hat{\rho}}_i \underset{\smile}{\tilde{\mathbf{u}}}_i = R_i \quad . \tag{AIII.3}$$

2. LES Species Continuity

From Eq. (AII.8) in Appendix 2,

$$\frac{\partial \left\langle X_i y_j \rho_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i y_j \mathbf{u}_i \right\rangle = -\nabla \cdot \left\langle \varpi_j X_i \rho_i \nabla y_j \right\rangle + \left\langle X_i \Gamma_j \right\rangle + C_{i,j} \quad , \tag{AIII.4}$$

where y_j is the species mass fraction; ϖ_j is the molecular diffusion coefficient of species j in the whole mixture; Γ_j is the mass source or sink rate because chemical or physical processes between species; and $C_{i,j}$ is the mean interfacial species mass transfer rate and has two contributions: one from the mass transfer between phases [R_i in Eq. (AIII.2)] and one describing the "diffusion" of the interface belonging to species j within the mixture

$$C_{i,j} = \left\langle \left[y_j \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} - \varpi_j \rho_i \nabla y_j \cdot \mathbf{n}_i \delta_{Int} \right] \right\rangle \quad . \tag{AIII.5}$$

$C_{i,j}$ must comply with the mean jump condition at the interfaces between species of a given phase and all other phases:

$$\sum_{i=1}^{n} \sum_{j=1}^{m} C_{i,j} = 0 \quad . \tag{AIII.6}$$

Of course, global conservation upon all m species of phase i imposes that $\sum_{j=1}^{m} y_j = 1$. Using the averaging-filtering definitions of §2.6, Eq. (AIII.4) becomes

$$\begin{aligned}
&\frac{\partial \left\langle X_i y_j \rho_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \left(\underset{\smile}{\tilde{y}}_j + \underset{\smile}{y}_j'' \right) \left(\underset{\smile}{\tilde{\mathbf{u}}}_i + \underset{\smile}{\mathbf{u}}_i'' \right) \right\rangle = -\nabla \cdot \left\langle \varpi_j X_i \rho_i \nabla y_j \right\rangle + \left\langle X_i \Gamma_j \right\rangle + C_{i,j} \\
&\Leftrightarrow \\
&\frac{\partial \underset{\smile}{\hat{\rho}}_i \underset{\smile}{\tilde{y}}_j}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \underset{\smile}{\tilde{y}}_j \underset{\smile}{\tilde{\mathbf{u}}}_i \right\rangle + \nabla \cdot \left\langle X_i \rho_i \underset{\smile}{\tilde{y}}_j \underset{\smile}{\mathbf{u}}_i'' \right\rangle + \nabla \cdot \left\langle X_i \rho_i \underset{\smile}{y}_j'' \underset{\smile}{\tilde{\mathbf{u}}}_i \right\rangle + \nabla \cdot \left\langle X_i \rho_i \underset{\smile}{y}_j'' \underset{\smile}{\mathbf{u}}_i'' \right\rangle \\
&\qquad\qquad = -\nabla \cdot \varpi_j \underset{\smile}{\hat{\rho}}_i \nabla \underset{\smile}{\tilde{y}}_j + \varepsilon_i \underset{\smile}{\overline{\Gamma}}_j + C_{i,j} \qquad . \qquad \text{(AIII.7)} \\
&\Leftrightarrow \\
&\frac{\partial \underset{\smile}{\hat{\rho}}_i \underset{\smile}{\tilde{y}}_j}{\partial t} + \nabla \cdot \underset{\smile}{\hat{\rho}}_i \widetilde{\underset{\smile}{\tilde{y}}_j \underset{\smile}{\tilde{\mathbf{u}}}_i} + \nabla \cdot \underset{\smile}{\hat{\rho}}_i \widetilde{\underset{\smile}{\tilde{y}}_j \underset{\smile}{\mathbf{u}}_i''} + \nabla \cdot \underset{\smile}{\hat{\rho}}_i \widetilde{\underset{\smile}{y}_j'' \underset{\smile}{\tilde{\mathbf{u}}}_i} + \nabla \cdot \underset{\smile}{\hat{\rho}}_i \widetilde{\underset{\smile}{y}_j'' \underset{\smile}{\mathbf{u}}_i''} \\
&\qquad\qquad = -\nabla \cdot \varpi_j \underset{\smile}{\hat{\rho}}_i \nabla \underset{\smile}{\tilde{y}}_j + \varepsilon_i \underset{\smile}{\overline{\Gamma}}_j + C_{i,j}
\end{aligned}$$

Let us decompose the first convective momentum flux term with the following LES "trick":

$$\nabla \cdot \underset{\smile}{\hat{\rho}}_i \widetilde{\underset{\smile}{\tilde{y}}_j \underset{\smile}{\tilde{\mathbf{u}}}_i} = \nabla \cdot \underset{\smile}{\hat{\rho}}_i \widetilde{\underset{\smile}{\tilde{y}}_j \underset{\smile}{\tilde{\mathbf{u}}}_i} + \nabla \cdot \underset{\smile}{\hat{\rho}}_i \underset{\smile}{\tilde{y}}_j \underset{\smile}{\tilde{\mathbf{u}}}_i - \nabla \cdot \underset{\smile}{\hat{\rho}}_i \underset{\smile}{\tilde{y}}_j \underset{\smile}{\tilde{\mathbf{u}}}_i \quad . \tag{AIII.8}$$

And rewriting Eq. (AIII.7) with Eq. (AIII.8), we have

$$
\begin{aligned}
&\frac{\partial \underset{\smile}{\hat{\rho}_i}\,\underset{\smile}{\tilde{y}_j}}{\partial t} + \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\widetilde{\underset{\smile}{\tilde{y}_j}\underset{\smile}{\tilde{\mathbf{u}}_i}} + \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\underset{\smile}{\tilde{y}_j}\underset{\smile}{\tilde{\mathbf{u}}_i} - \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\underset{\smile}{\tilde{y}_j}\underset{\smile}{\tilde{\mathbf{u}}_i} + \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\widetilde{\underset{\smile}{\tilde{y}_j}\underset{\smile}{\mathbf{u}_i''}} + \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\widetilde{\underset{\smile}{y_j''}\underset{\smile}{\tilde{\mathbf{u}}_i}} + \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\widetilde{\underset{\smile}{y_j''}\underset{\smile}{\mathbf{u}_i''}} \\
&\qquad\qquad = -\nabla\cdot\varpi_j\underset{\smile}{\hat{\rho}_i}\nabla\underset{\smile}{\tilde{y}_j} + \varepsilon_i\underset{\smile}{\overline{\Gamma}_j} + C_{i,j}
\end{aligned}
$$

$\Leftrightarrow$

$$
\begin{aligned}
\frac{\partial \underset{\smile}{\hat{\rho}_i}\,\underset{\smile}{\tilde{y}_j}}{\partial t} + \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\underset{\smile}{\tilde{y}_j}\underset{\smile}{\tilde{\mathbf{u}}_i} &= -\nabla\cdot\varpi\underset{\smile}{\hat{\rho}_i}\nabla\underset{\smile}{\tilde{y}_j} + \varepsilon_i\underset{\smile}{\overline{\Gamma}_j} + C_{i,j} \\
&\quad -\left[\left(\nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\widetilde{\underset{\smile}{\tilde{y}_j}\underset{\smile}{\tilde{\mathbf{u}}_i}} - \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\underset{\smile}{\tilde{y}_j}\underset{\smile}{\tilde{\mathbf{u}}_i}\right) + \left(\nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\widetilde{\underset{\smile}{\tilde{y}_j}\underset{\smile}{\mathbf{u}_i''}} + \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\widetilde{\underset{\smile}{y_j''}\underset{\smile}{\tilde{\mathbf{u}}_i}}\right) + \left(\nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\widetilde{\underset{\smile}{y_j''}\underset{\smile}{\mathbf{u}_i''}}\right)\right]
\end{aligned}
\tag{AIII.9}
$$

$\Leftrightarrow$

$$
\frac{\partial \underset{\smile}{\hat{\rho}_i}\,\underset{\smile}{\tilde{y}_j}}{\partial t} + \nabla\cdot\underset{\smile}{\hat{\rho}_i}\,\underset{\smile}{\tilde{y}_j}\underset{\smile}{\tilde{\mathbf{u}}_i} = -\nabla\cdot\underset{\smile}{\hat{\rho}_i}\left(\mathbf{y}_j + {}^{SG}\mathbf{y}_j\right) + \varepsilon_i\underset{\smile}{\overline{\Gamma}_j} + C_{i,j}
$$

where the species mass fraction fluxes has two contributions—one from the resolved large-scale flux (i.e., $\mathbf{y}_j$) and one from the "subgrid" (i.e., ${}^{SG}\mathbf{y}_j$)—

$$
\begin{aligned}
\mathbf{y}_j &= \varpi_j\nabla\underset{\smile}{\tilde{y}_j} \\
{}^{SG}\mathbf{y}_j &= \left[\left(\widetilde{\underset{\smile}{\tilde{y}_j}\,\underset{\smile}{\tilde{\mathbf{u}}_i}} - \underset{\smile}{\tilde{y}_j}\,\underset{\smile}{\tilde{\mathbf{u}}_i}\right) + \left(\widetilde{\underset{\smile}{\tilde{y}_j}\,\underset{\smile}{\mathbf{u}_i''}} + \widetilde{\underset{\smile}{y_j''}\,\underset{\smile}{\tilde{\mathbf{u}}_i}}\right) + \left(\widetilde{\underset{\smile}{y_j''}\,\underset{\smile}{\mathbf{u}_i''}}\right)\right] \quad , \\
&= \quad {}^{L}\mathbf{y}_j + \quad {}^{C}\mathbf{y}_j + \quad {}^{R}\mathbf{y}_j
\end{aligned}
\tag{AIII.10}
$$

where between brackets, it can be recognized three contributions from the Leonard terms (${}^{L}\mathbf{y}_j$), the Cross-terms (${}^{C}\mathbf{y}_j$), and the Reynolds (${}^{R}\mathbf{y}_j$). Obviously, once a filter is specified, it is easy to calculate the Leonard-term, while the Cross-term and Reynolds-term need to be modeled. Let us note that, strictly speaking, ${}^{L}\mathbf{y}_j$ is not from the subgrid as it entirely made of known and filtered large-scale quantities.

3. LES Momentum

From Eq. (AII.16) in Appendix 2, we have

$$
\frac{\partial\left\langle X_i\rho_i\mathbf{u}_i\right\rangle}{\partial t} + \nabla\cdot\left\langle X_i\rho_i\mathbf{u}_i\mathbf{u}_i\right\rangle = -\nabla\cdot\left\langle X_i\mathbf{T}_i\right\rangle + \left\langle X_i\rho_i\mathbf{G}_i\right\rangle + \mathbf{M}_i \quad , \tag{AIII.11}
$$

where $\mathbf{T}_i$ is the stress tensor; $\mathbf{G}_i$ represents the body force contribution (e.g., gravity); and $\mathbf{M}_i$ is the interfacial momentum transfer rate between phases, which is defined as

$$\mathbf{M}_i = \left\langle \left[\rho_i \mathbf{u}_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \mathbf{T}_i \right] \cdot \mathbf{n}_i \, \delta_{Int} \right\rangle \quad , \tag{AIII.12}$$

complying with the jump condition between phases—$\sum_{i=1}^{n} \mathbf{M}_i = 0$ (all surface tension forces are assumed to be negligible).

Using the filtering definitions of §2.6 and §2.7, Eq. (AIII.11) becomes

$$\begin{aligned}
&\frac{\partial \left\langle X_i \rho_i \mathbf{u}_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \mathbf{u}_i \mathbf{u}_i \right\rangle && = -\nabla \cdot \left\langle X_i \mathbf{T}_i \right\rangle + \left\langle X_i \rho_i \mathbf{G}_i \right\rangle + \mathbf{M}_i \\
\Leftrightarrow\ &\frac{\partial \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \left(\underset{\smile}{\tilde{\mathbf{u}}_i} + \underset{\smile}{\mathbf{u}_i''} \right) \left(\underset{\smile}{\tilde{\mathbf{u}}_i} + \underset{\smile}{\mathbf{u}_i''} \right) \right\rangle && = -\nabla \cdot \left\langle X_i \mathbf{T}_i \right\rangle + \left\langle X_i \rho_i \mathbf{G}_i \right\rangle + \mathbf{M}_i \\
\Leftrightarrow\ &\frac{\partial \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} \right\rangle + 2 \nabla \cdot \left\langle X_i \rho_i \underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\mathbf{u}_i''} \right\rangle + \nabla \cdot \left\langle X_i \rho_i \underset{\smile}{\mathbf{u}_i''} \underset{\smile}{\mathbf{u}_i''} \right\rangle && = -\nabla \cdot \left\langle X_i \mathbf{T}_i \right\rangle + \left\langle X_i \rho_i \mathbf{G}_i \right\rangle + \mathbf{M}_i \\
\Leftrightarrow\ &\frac{\partial \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}}{\partial t} + \nabla \cdot \underset{\smile}{\hat{\rho}_i} \, \widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}} + 2 \nabla \cdot \underset{\smile}{\hat{\rho}_i} \, \widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\mathbf{u}_i''}} + \nabla \cdot \underset{\smile}{\hat{\rho}_i} \, \widetilde{\underset{\smile}{\mathbf{u}_i''} \underset{\smile}{\mathbf{u}_i''}} && = -\nabla \cdot \varepsilon_i \underset{\smile}{\overline{\mathbf{T}}_i} + \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{G}}_i} + \mathbf{M}_i
\end{aligned} \tag{AIII.13}$$

Let us decompose the first convective momentum flux term with the following LES "trick":

$$\nabla \cdot \underset{\smile}{\hat{\rho}_i} \, \widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}} = \nabla \cdot \underset{\smile}{\hat{\rho}_i} \, \widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}} + \nabla \cdot \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} - \nabla \cdot \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} \quad . \tag{AIII.14}$$

And rewriting Eq. (AIII.13) with Eq. (AIII.14), we have

$$\begin{aligned}
\Leftrightarrow\ &\frac{\partial \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}}{\partial t} + \nabla \cdot \underset{\smile}{\hat{\rho}_i} \, \widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}} + \nabla \cdot \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} - \nabla \cdot \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} + 2 \nabla \cdot \underset{\smile}{\hat{\rho}_i} \, \widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\mathbf{u}_i''}} + \nabla \cdot \underset{\smile}{\hat{\rho}_i} \, \widetilde{\underset{\smile}{\mathbf{u}_i''} \underset{\smile}{\mathbf{u}_i''}} \\
&\qquad\qquad = -\nabla \cdot \varepsilon_i \underset{\smile}{\overline{\mathbf{T}}_i} + \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{G}}_i} + \mathbf{M}_i \quad , \\
\Leftrightarrow\ & \\
&\frac{\partial \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i}}{\partial t} + \nabla \cdot \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} \underset{\smile}{\tilde{\mathbf{u}}_i} = -\nabla \cdot \varepsilon_i \left(\underset{\smile}{\overline{\mathbf{T}}_i} + {}^{SG}\underset{\smile}{\mathbf{T}_i} \right) + \underset{\smile}{\hat{\rho}_i} \underset{\smile}{\tilde{\mathbf{G}}_i} + \mathbf{M}_i
\end{aligned} \tag{AIII.15}$$

where ${}^{SG}\mathbf{T}_i$ is the "subgrid" stress tensor

$$
\begin{aligned}
{}^{SG}\underset{\smile}{\mathbf{T}}_i &= \left[\underset{\smile}{\bar{\rho}_i}\,\widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i}\underset{\smile}{\tilde{\mathbf{u}}_i}} - \underset{\smile}{\bar{\rho}_i}\,\underset{\smile}{\tilde{\mathbf{u}}_i}\underset{\smile}{\tilde{\mathbf{u}}_i}\right] + \left[\underset{\smile}{\bar{\rho}_i}\,\widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i}\underset{\smile}{\mathbf{u}_i''}} + \underset{\smile}{\bar{\rho}_i}\,\widetilde{\underset{\smile}{\tilde{\mathbf{u}}_i}\underset{\smile}{\mathbf{u}_i''}}\right] + \left[\underset{\smile}{\bar{\rho}_i}\,\widetilde{\underset{\smile}{\mathbf{u}_i''}\underset{\smile}{\mathbf{u}_i''}}\right] \\
&= \qquad {}^{L}\underset{\smile}{\mathbf{T}}_i \qquad + \qquad {}^{C}\underset{\smile}{\mathbf{T}}_i \qquad + \qquad {}^{R}\underset{\smile}{\mathbf{T}}_i
\end{aligned} \qquad . \tag{AIII.16}
$$

These three tensors are known as the Leonard stress (${}^{L}\mathbf{T}_i$), Cross-term stress (${}^{C}\mathbf{T}_i$), and the subgrid Reynolds stress (${}^{R}\mathbf{T}_i$). The Leonard stress terms are made only of filtered (hence known) components and do not need to be modeled. *Sensus stricto*, the Leonard stress term does not result from the subgrid. Although this decomposition is a natural result of the preceding demonstration, it is nevertheless rarely done, as it is difficult to model these three terms separately. And usually a Smagorinsky approach is used to model the whole term ${}^{SG}\mathbf{T}_i$. in (implicitly) assuming that the only term that dominates is ${}^{R}\mathbf{T}_i$ (for instance, in assuming that filtering would give similar results to ensemble averaging, it then becomes that ${}^{L}\mathbf{T}_i + {}^{C}\mathbf{T}_i \approx 0$). See Appendix 5 for a discussion on $\bar{\underset{\smile}{\mathbf{T}}}_i$.

4. LES Energy

From Eq. (AII.39) in Appendix 2, we have the conservation of the enthalpy of the i^{th} phase in a system of n phases

$$
\frac{\partial \left\langle X_i \rho_i h_i \right\rangle}{\partial t} + \nabla\cdot\left\langle X_i \rho_i h_i \mathbf{u}_i \right\rangle = \left\langle X_i \left(-\boldsymbol{\tau}_i : \nabla \mathbf{u}_i\right)\right\rangle - \nabla\cdot\left\langle X_i \mathbf{q}_i \right\rangle + \left\langle X_i \frac{dP_i}{dt}\right\rangle + \left\langle X_i \rho_i\, S_i \right\rangle + {}^{h}H_i \ , \tag{AIII.17}
$$

where ${}^{h}H_i$ is the rate of interfacial heat transfer between phases encompassing all contribution from mass flux exchange and heat flux exchange at the interfaces between phases. It is defined as

$$
{}^{h}H_i = \left\langle \left[\rho_i\, h_i \left(\mathbf{u}_{Int} - \mathbf{u}_i\right) - \mathbf{q}_i\right]\cdot \mathbf{n}_i \delta_{Int}\right\rangle \qquad , \tag{AIII.18}
$$

complying with the jump condition between all phases in the system—i.e., $\sum_{i=1}^{n} {}^{h}H_i = 0$. In Eq. (AIII.17), the first RHS term represents the irreversible work done by the surface forces (viscous dissipation), $\boldsymbol{\tau}_i$ is the viscous stress tensor, $\mathbf{q}_i$ is the heat conduction flux vector (following a Fourier's law), and S_i represents any enthalpy sources.

Using the filtering definitions of §2.6 and §2.7, Eq. (AIII.17) becomes

$$\frac{\partial \left\langle X_i\rho_i h_i\right\rangle}{\partial t} + \nabla\cdot\left\langle X_i\rho_i\left(\underset{\smile}{\tilde{h}}_i + \underset{\smile}{h}_i''\right)\left(\underset{\smile}{\tilde{\mathbf{u}}}_i + \underset{\smile}{\mathbf{u}}_i''\right)\right\rangle = \left\langle -X_i\boldsymbol{\tau}_i:\nabla\mathbf{u}_i\right\rangle - \nabla\cdot\left\langle X_i\mathbf{q}_i\right\rangle + \left\langle X_i\frac{dP_i}{dt}\right\rangle + \left\langle X_i\rho_i S_i\right\rangle + {}^{h}H_i$$

$\Leftrightarrow$

$$\frac{\partial \underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{h}}_i}{\partial t} + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{\tilde{h}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i} + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{\tilde{h}}_i\underset{\smile}{\mathbf{u}}_i''} + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{h}_i''\underset{\smile}{\tilde{\mathbf{u}}}_i}{}_i + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{h}_i''\underset{\smile}{\mathbf{u}}_i''} = \varepsilon_i\overline{-\boldsymbol{\tau}_i:\nabla\mathbf{u}_i} - \nabla\cdot\varepsilon_i\underset{\smile}{\bar{\mathbf{q}}}_i + \underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{S}}_i + \varepsilon_i\frac{d\underset{\smile}{\bar{P}}_i}{dt} + {}^{h}H_i$$

(AIII.19)

Knowing that

$$\nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{\tilde{h}}_i\,\underset{\smile}{\tilde{\mathbf{u}}}_i} = \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{\tilde{h}}_i\,\underset{\smile}{\tilde{\mathbf{u}}}_i} - \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\underset{\smile}{\tilde{h}}_i\,\underset{\smile}{\tilde{\mathbf{u}}}_i + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\underset{\smile}{\tilde{h}}_i\,\underset{\smile}{\tilde{\mathbf{u}}}_i \quad , \qquad \text{(AIII.20)}$$

Eq. (AIII.20) in Eq. (AIII.19) yields the following:

$$\begin{aligned}&\frac{\partial \underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{h}}_i}{\partial t} + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{\tilde{h}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i} + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{h}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i - \nabla\cdot\underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{h}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{\tilde{h}}_i\underset{\smile}{\mathbf{u}}_i''} + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{h}_i''\underset{\smile}{\tilde{\mathbf{u}}}_i}{}_i + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\,\widetilde{\underset{\smile}{h}_i''\underset{\smile}{\mathbf{u}}_i''}\\ &\qquad = \varepsilon_i\overline{\boldsymbol{\tau}_i:\nabla\mathbf{u}_i} - \nabla\cdot\varepsilon_i\underset{\smile}{\bar{\mathbf{q}}}_i + \underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{S}}_i + \varepsilon_i\frac{d\underset{\smile}{\bar{P}}_i}{dt} + {}^{h}H_i \quad , \qquad \text{(AIII.21)}\end{aligned}$$

$\Leftrightarrow$

$$\frac{\partial \underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{h}}_i}{\partial t} + \nabla\cdot\underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{h}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i = \varepsilon_i\left(\underset{\smile}{W}_{\boldsymbol{\tau},i} + {}^{SG}\underset{\smile}{W}_{\boldsymbol{\tau},i}\right) - \nabla\cdot\varepsilon_i\left(\underset{\smile}{\bar{\mathbf{q}}}_i + {}^{SG}\underset{\smile}{\mathbf{q}}_i\right) + \underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{S}}_i + \varepsilon_i\frac{d\underset{\smile}{\bar{P}}_i}{dt} + {}^{h}H_i$$

where the viscous dissipation has a filtered and a “subgrid” contribution (see demonstration in Appendix 5):

$$\begin{aligned}\underset{\smile}{W}_{\boldsymbol{\tau},i} &= -\underset{\smile}{\tilde{\boldsymbol{\tau}}}_i:\nabla\underset{\smile}{\tilde{\mathbf{u}}}_i\\ {}^{SG}W_{\boldsymbol{\tau},i} &= -\left\{\left[\overline{\underset{\smile}{\tilde{\boldsymbol{\tau}}}_i:\nabla\underset{\smile}{\tilde{\mathbf{u}}}_i} - \underset{\smile}{\tilde{\boldsymbol{\tau}}}_i:\nabla\underset{\smile}{\tilde{\mathbf{u}}}_i\right] + \left[\overline{\boldsymbol{\tau}_i'':\nabla\underset{\smile}{\tilde{\mathbf{u}}}_i} + \overline{\tilde{\boldsymbol{\tau}}:\nabla\underset{\smile}{\mathbf{u}}_i''}\right] + \left[\overline{\underset{\smile}{\boldsymbol{\tau}}_i'':\nabla\underset{\smile}{\mathbf{u}}_i''}\right]\right\} \quad . \qquad \text{(AIII.22)}\\ &= \qquad {}^{L}W_i \qquad + \qquad {}^{C}W_i \qquad + \qquad {}^{R}W_i\end{aligned}$$

And, in the same vein, the heat flux is

$$\begin{aligned}\underset{\smile}{\bar{\mathbf{q}}}_i &= -k_i\nabla\underset{\smile}{\bar{T}}_i\\ {}^{SG}\underset{\smile}{\mathbf{q}}_i &= \left[\underset{\smile}{\bar{\rho}}_i\,\widetilde{\underset{\smile}{\tilde{h}}_i\,\underset{\smile}{\tilde{\mathbf{u}}}_i} - \underset{\smile}{\bar{\rho}}_i\,\underset{\smile}{\tilde{h}}_i\,\underset{\smile}{\tilde{\mathbf{u}}}_i\right] + \left[\underset{\smile}{\bar{\rho}}_i\,\widetilde{\underset{\smile}{\tilde{h}}_i\,\underset{\smile}{\mathbf{u}}_i''} + \underset{\smile}{\bar{\rho}}_i\,\widetilde{\underset{\smile}{h}_i''\,\underset{\smile}{\tilde{\mathbf{u}}}_i}\right] + \left[\underset{\smile}{\bar{\rho}}_i\,\widetilde{\underset{\smile}{h}_i''\,\underset{\smile}{\mathbf{u}}_i''}\right] \quad , \qquad \text{(AIII.23)}\\ &= \qquad {}^{L}\underset{\smile}{\mathbf{q}}_i \qquad + \qquad {}^{C}\underset{\smile}{\mathbf{q}}_i \qquad + \qquad {}^{R}\underset{\smile}{\mathbf{q}}_i\end{aligned}$$

where k_i is the molecular (not affected by turbulence) thermal conductivity coefficient of phase i. In both Eq. (AIII.22) and Eq. (AIII.23), we can recognize a contribution from the Leonard-term, the Cross-terms, and the Reynolds-terms. Unlike the Leonard-terms, the Cross-terms and the Reynolds-terms are strictly speaking from the subgrid and therefore must be modeled.

As for the RANS case, Eq. (AIII.21) and Eq. (AIII.22) are particularly complicated because they involve two new unknowns in this system: the Favre phasic-weighted filtered and fluctuating parts of the velocity ($\bar{\mathbf{u}}_{\smile i}$ and $\mathbf{u}'_{\smile i}$) instead of the Favre mass-weighted components [$\tilde{\mathbf{u}}_{\smile i}$ and $\mathbf{u}''_{\smile i}$ as in Eq. (AIII.15) and Eq. (AIII.16)]. Therefore, ${}^{SG}W_{\tau,i}$ is very often neglected or seen as negligible relative to the heat conduction, the convective transport of heat, and heat transfer between phase. For a detailed discussion on $\underset{\smile}{W}_{\boldsymbol{\tau},i}$ and ${}^{SG}W_{\tau,i}$ and possible approximations, see Appendix 5.

5. LES Entropy

From Eq. (AII.42) in Appendix 2, the entropy balance inequality of the i^{th} phase in a system of n phases is

$$\frac{\partial \left\langle X_i \rho_i \eta_i \right\rangle}{\partial t} + \nabla \cdot \left\langle X_i \rho_i \eta_i \mathbf{u}_i \right\rangle \geq -\nabla \cdot \left\langle X_i \frac{\mathbf{q}_i}{T_i} \right\rangle + \left\langle X_i \frac{\rho_i S_i}{T_i} \right\rangle + {}^{\eta}H_i \quad , \tag{AIII.24}$$

where η_i is the entropy; $\frac{\mathbf{q}_i}{T_i}$ is the entropy flux ($\mathbf{q}_i$ is the heat conduction flux vector and T_i is the temperature); $\frac{\rho_i S_i}{T_i}$ is any source of entropy (S_i represents some heat sources), and ${}^{\eta}H_i$ is the mean rate of interfacial entropy between phases,

$${}^{\eta}H_i = \left\langle \left[\rho_i \eta_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \frac{\mathbf{q}_i}{T_i} \right] \cdot \mathbf{n}_i \delta_{Int} \right\rangle \quad , \tag{AIII.25}$$

where $\mathbf{u}_{Int}$ is the bulk velocity of all interfaces and $\mathbf{u}_i$ is the bulk velocity of phase i. ${}^{\eta}H_i$ complies with the jump condition between all phases in the system—i.e., $\sum_{i=1}^{n} {}^{\eta}H_i \geq 0$. Using the filtering definitions of §2.6 and §2.7, Eq. (AIII.24) becomes

$$\frac{\partial\left\langle X_i\rho_i\eta_i\right\rangle}{\partial t}+\nabla\cdot\left\langle X_i\rho_i\left(\underset{\smile}{\tilde{\eta}}_i+\underset{\smile}{\eta}_i''\right)\left(\underset{\smile}{\tilde{\mathbf{u}}}_i+\underset{\smile}{\mathbf{u}}_i''\right)\right\rangle\ge-\nabla\cdot\left\langle X_i\,\frac{\mathbf{q}_i}{T_i}\right\rangle+\left\langle X_i\,\frac{\rho_i S_i}{T_i}\right\rangle+{}^{\eta}H_i$$

$$\Leftrightarrow$$

$$\frac{\partial\underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{\eta}}_i}{\partial t}+\nabla\cdot\underset{\smile}{\hat{\rho}}_i\widetilde{\underset{\smile}{\tilde{\eta}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i}+\nabla\cdot\underset{\smile}{\hat{\rho}}_i\widetilde{\underset{\smile}{\tilde{\eta}}_i\underset{\smile}{\mathbf{u}}_i''}+\nabla\cdot\underset{\smile}{\hat{\rho}}_i\widetilde{\underset{\smile}{\eta}_i''\underset{\smile}{\tilde{\mathbf{u}}}_i}_{i}+\nabla\cdot\underset{\smile}{\hat{\rho}}_i\widetilde{\underset{\smile}{\eta}_i''\underset{\smile}{\mathbf{u}}_i''}\ge-\nabla\cdot\varepsilon_i\overline{\left(\frac{\mathbf{q}_i}{T_i}\right)}+\underset{\smile}{\hat{\rho}}_i\widetilde{\left(\frac{S_i}{T_i}\right)}+{}^{\eta}H_i \qquad \text{(AIII.26)}$$

$$\Leftrightarrow$$

$$\frac{\partial\underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{\eta}}_i}{\partial t}+\nabla\cdot\underset{\smile}{\hat{\rho}}_i\underset{\smile}{\tilde{\eta}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i\ge-\nabla\cdot\varepsilon_i\left(\underset{\smile}{\bar{\boldsymbol{\Phi}}}_i+{}^{SG}\underset{\smile}{\boldsymbol{\Phi}}_i\right)+\underset{\smile}{\hat{\rho}}_i\widetilde{\underset{\smile}{\Sigma}_i}+{}^{\eta}H_i$$

where the flux of entropy has two sources, one from the known filtered part ($\underset{\smile}{\bar{\boldsymbol{\Phi}}}_i$) and one from the subgrid (${}^{SG}\underset{\smile}{\boldsymbol{\Phi}}_i$):

$$\begin{aligned}\underset{\smile}{\boldsymbol{\Phi}}_i &= \overline{\left(\frac{\mathbf{q}_i}{T_i}\right)}\\ {}^{SG}\underset{\smile}{\boldsymbol{\Phi}}_i &= \left[\bar{\underset{\smile}{\rho}}_i\widetilde{\underset{\smile}{\tilde{\eta}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i}-\bar{\underset{\smile}{\rho}}_i\underset{\smile}{\tilde{\eta}}_i\underset{\smile}{\tilde{\mathbf{u}}}_i\right]+\left[\bar{\underset{\smile}{\rho}}_i\widetilde{\underset{\smile}{\tilde{\eta}}_i\underset{\smile}{\mathbf{u}}_i''}+\bar{\underset{\smile}{\rho}}_i\widetilde{\underset{\smile}{\eta}_i''\underset{\smile}{\tilde{\mathbf{u}}}_i}\right]+\left[\bar{\underset{\smile}{\rho}}_i\widetilde{\underset{\smile}{\eta}_i''\underset{\smile}{\mathbf{u}}_i''}\right]\quad ,\\ &= \qquad {}^{L}\underset{\smile}{\boldsymbol{\Phi}}_i \qquad + \qquad {}^{C}\underset{\smile}{\boldsymbol{\Phi}}_i \qquad + \qquad {}^{R}\underset{\smile}{\boldsymbol{\Phi}}_i\end{aligned} \qquad \text{(AIII.27)}$$

while the entropy source is simply defined by a filtered Favre mass-weighted-relationship: $\underset{\smile}{\tilde{\Sigma}}_i=\widetilde{\left(\frac{S_i}{T_i}\right)}$. In Eq. (AIII.27) we can recognize in the entropy flux a contribution from the Leonard-, Cross-, and Reynolds-terms.

Eq. (AIII.26) may also be expressed as

$$\underset{\smile}{\hat{\rho}}_i\,\frac{d\underset{\smile}{\tilde{\eta}}_i}{dt}\ge-\nabla\cdot\varepsilon_i\left(\underset{\smile}{\bar{\boldsymbol{\Phi}}}_i+{}^{SG}\underset{\smile}{\boldsymbol{\Phi}}_i\right)+\underset{\smile}{\hat{\rho}}_i\widetilde{\underset{\smile}{\Sigma}_i}+{}^{\eta}H_i\quad . \qquad \text{(AIII.28)}$$

Appendix 4: RANS and LES Interfacial Closures

When averaging or filtering the Navier-Stokes equations from a single phase towards a multiphase system, different supplementary terms arise describing mass, momentum, and energy transfers at the interface between the phases. Those terms are highly important because they couple all the phases, and, in the energy equations, if they are disregarded, the second law of thermodynamics may not be fulfilled.

The mean interfacial terms between phases are

Rate of interfacial phasic mass transfer	$R_i = \left\langle \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} \right\rangle$
Rate of interfacial species mass transfer	$C_{i,j} = \left\langle \left[y_j \rho_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \varpi_j \rho_i \nabla y_j \right] \cdot \mathbf{n}_i \delta_{Int} \right\rangle$
Rate of interfacial momentum transfer	$\mathbf{M}_i = \left\langle \left[\rho_i \mathbf{u}_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \mathbf{T}_i \right] \cdot \mathbf{n}_i \delta_{Int} \right\rangle$
Rate of interfacial internal energy transfer	${}^{I}H_i = \left\langle \left[\rho_i I_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \mathbf{q}_i \right] \cdot \mathbf{n}_i \delta_{Int} \right\rangle$
Rate of interfacial enthalpy transfer	${}^{h}H_i = \left\langle \left[\rho_i h_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \mathbf{q}_i \right] \cdot \mathbf{n}_i \delta_{Int} \right\rangle$
Rate of interfacial entropy transfer	${}^{\eta}H_i = \left\langle \left[\rho_i \eta_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) - \frac{\mathbf{q}_i}{T_i} \right] \cdot \mathbf{n}_i \delta_{Int} \right\rangle$

where $\mathbf{u}_{Int}$ is the velocity of all the interfaces between all phases making up the multiphase system and $\mathbf{u}_i$ is the bulk velocity of phase i. The jump condition imposes on any interfacial term between all n phases and between all m species that $\sum_{i=1}^{n} R_i = \sum_{i=1}^{n} M_i = \sum_{i=1}^{n} {}^{I}H_i = \sum_{i=1}^{n} {}^{h}H_i = 0$, $\sum_{i=1}^{n} \sum_{j=1}^{m} C_{i,j} = 0$, and $\sum_{i=1}^{n} {}^{\eta}H_i \geq 0$. In other words, in a system of two phases (e.g., gas and solid) with no mass transfer between species and phase, we must have

$$\begin{aligned} \mathbf{M}_g &= -\mathbf{M}_s \\ {}^{I}H_g &= -{}^{I}H_s \quad . \\ {}^{h}H_g &= -{}^{h}H_s \end{aligned} \tag{AIV.1}$$

Usually, R_i does not pose any major problems but must carefully be set in a specific situation (condensation, sublimation, magmatic "fragmentation," so forth). Most of the time, $C_{i,j}$ is taken as simply equal to $\sim \tilde{y}_j R_i$ (the contribution of the "diffusion" of the species interface is assumed to be unimportant, see Syamlal et al. [1993] and Veynante and Poinsot [1997]).

The momentum transfer, $\mathbf{M}_i$, has two parts; one comes from the mass transfer between phases, which, for instance, between the ith phase and all other phases, can be easily modeled as

$$\left\langle \rho_i \mathbf{u}_i \left(\mathbf{u}_{Int} - \mathbf{u}_i \right) \cdot \mathbf{n}_i \delta_{Int} \right\rangle \approx \overline{\mathbf{u}}_{Int} R_i \quad , \qquad \text{(AIV.2)}$$

where $\overline{\mathbf{u}}_{Int}$ is the bulk averaged/filtered velocity of all the interfaces in the system.

In a flow where all the phases are *all well mixed* [35], the bulk interfacial velocity can be approached with either a center-of-mass velocity [Saurel and Abgrall 1999] or a center-of-volume velocity [Delhaye and Boure 1982] as follows:

$$\begin{aligned} &\overline{\mathbf{u}}_{Int} \approx \frac{\sum_{i=1}^{n} \varepsilon_i \overline{\rho}_i \, \tilde{\mathbf{u}}_i}{\sum_{i=1}^{n} \varepsilon_i \overline{\rho}_i} && \text{a.} \\ &\overline{\mathbf{u}}_{Int} \approx \sum_{i=1}^{n} \varepsilon_i \, \tilde{\mathbf{u}}_i && \text{b.} \end{aligned} \qquad . \qquad \text{(AIV.3)}$$

If, in addition to the previous assumption, there is an *instantaneous microscopic velocity equilibration* between the interface and the phase itself, we may also assume that $\overline{\mathbf{u}}_{Int} \approx \tilde{\mathbf{u}}_i$, so that Eq. (AIV.2) becomes $\overline{\mathbf{u}}_{Int} R_i \approx \tilde{\mathbf{u}}_i R_i$. This second assumption, although more drastic, is certainly the most common and *by far* the most practical in engineering literatures [e.g., Lee and Lyczkowski 2000] and in code developments (e.g., MFIX codes, version of 2004). A variation of this approach is to systematically make the bulk interfacial velocity equal to the velocity of the least compressible phase [Baer and Nunziato 1986]—i.e., in a dusty cloud, this would be $\overline{\mathbf{u}}_{Int} R_i \approx \tilde{\mathbf{u}}_s R_i$.

[35] In a strongly stratified and separate flow, it may be possible that some phases may never been in contact with each other; if so, it may necessary instead to track each velocity interface separately ($\mathbf{u}_{Int,i}$) instead of an unique bulk interfacial velocity ($\mathbf{u}_{Int}$). These stratified multiphase flows are not the objective of this manuscript.

The second contribution in $\mathbf{M}_i$, $\left\langle -\mathbf{T}_i \cdot \mathbf{n}_i \delta_{Int} \right\rangle$, represents the phase interaction force induced by the local perturbation (at the interface) of the fluid flow from the particle influence. This interfacial force is clearly related to the drag. Following Drew and Passman [1999], let us rewrite the total stress $\mathbf{T}_i$ in $\mathbf{M}_i$ as

$$\begin{aligned} \left\langle -\mathbf{T}_i \cdot \mathbf{n}_i \delta_{Int} \right\rangle &= \left\langle \mathbf{T}_i \cdot \nabla X_i \right\rangle \\ &= \left\langle P_i \nabla X_i \right\rangle + \left\langle \boldsymbol{\tau}_i \cdot \nabla X_i \right\rangle \end{aligned} , \qquad \text{(AIV.4)}$$

where P_i and $\boldsymbol{\tau}_i$ are the total (bulk) pressure and shear stress contributions of phase i. Among these normal and shear stresses, there are specific stress contributions of the interface between *phase i and all the other phases*

$$\begin{cases} P_{Int,i} = \dfrac{\left\langle P_i \left(\nabla X_i \cdot \mathbf{n}_i \right) \right\rangle}{A_i} \\ \boldsymbol{\tau}_{Int,i} = \dfrac{\left\langle \boldsymbol{\tau}_i \left(\nabla X_i \cdot \mathbf{n}_i \right) \right\rangle}{A_i} \end{cases} , \qquad \text{(AIV.5)}$$

where A_i can be interpreted as the volumetric concentration of interfacial area between phase i and all other phases [see §2.3, Eq. (4)]. $P_{Int,i}$ and $\boldsymbol{\tau}_{Int,i}$ are the interfacial pressure and the interfacial shear stress between phase i and all the other phases. Before developing any further, we must recall that the angular brackets have two different meanings: ensemble averaging within the RANS framework and filtering within the LES framework; hence,

RANS framework	**LES framework**
$\left\langle P_{Int,i} \right\rangle = P_{Int,i}$ $\left\langle \boldsymbol{\tau}_{Int,i} \right\rangle = \boldsymbol{\tau}_{Int,i}$	$\left\langle P_{Int,i} \right\rangle \neq P_{Int,i}$ $\left\langle \boldsymbol{\tau}_{Int,i} \right\rangle \neq \boldsymbol{\tau}_{Int,i}$

Because we aim to produce similar multiphase Navier-Stokes within RANS and LES frameworks, we must proceed with some care and in a different manner than what is usually achieved in the common literature [e.g., Drew and Passman 1999; van Wachem et al., 2001].

In the total stress acting on a given phase [Eq. (AIV.4)], there must be a contribution of the stress at the interface and the total stress minus the interfacial stress:

$$\begin{aligned}
\left\langle \mathbf{T}_i \cdot \nabla X_i \right\rangle &= +\left\langle P_i \nabla X_i \right\rangle + \left\langle \boldsymbol{\tau}_i \cdot \nabla X_i \right\rangle \\
&= +\left\langle \left(P_{Int,i} + P_i - P_{Int,i} \right) \nabla X_i \right\rangle + \left\langle \left(\boldsymbol{\tau}_{Int,i} + \boldsymbol{\tau}_i - \boldsymbol{\tau}_{Int,i} \right) \cdot \nabla X_i \right\rangle \\
&= +\left\langle P_{Int,i} \nabla X_i \right\rangle + \left\langle \left(P_i - P_{Int,i} \right) \nabla X_i \right\rangle + \left\langle \boldsymbol{\tau}_{Int,i} \cdot \nabla X_i \right\rangle + \left\langle \left(\boldsymbol{\tau}_i - \boldsymbol{\tau}_{Int,i} \right) \cdot \nabla X_i \right\rangle \\
&= +\left\langle P_{Int,i} \nabla X_i \right\rangle + \left\langle \boldsymbol{\tau}_{Int,i} \cdot \nabla X_i \right\rangle + \left\langle \left[\left(P_i - P_{Int,i} \right) \mathbf{I} + \left(\boldsymbol{\tau}_i - \boldsymbol{\tau}_{Int,i} \right) \right] \cdot \nabla X_i \right\rangle \\
&= +\left\langle P_{Int,i} \nabla X_i \right\rangle + \left\langle \boldsymbol{\tau}_{Int,i} \cdot \nabla X_i \right\rangle + \left\langle \mathbf{T}_i^{drag} \cdot \nabla X_i \right\rangle \\
&= +\left\langle P_{Int,i} \nabla X_i \right\rangle + \left\langle \boldsymbol{\tau}_{Int,i} \cdot \nabla X_i \right\rangle + \mathbf{M}_i^{drag}
\end{aligned} \quad , \qquad \text{(AIV.6)}$$

where $\mathbf{T}_i^{drag}$ is the stress tensor specifically associated to the drag between the phases where (P_i-$P_{Int,i}$) is named the “form drag” and (τ_i-$\tau_{Int,i}$) the “skin drag” by Ishii [1975]. Usually, the whole term, $\mathbf{M}_i^{drag}$ in Eq. (AIV.6), is written as a sum of all forces associated with drag force, added mass force, lift (transverse) force, Basset (history) force, … [Viollet et al., 1992; Enwald et al., 1996; Simonin 1996; Drew and Passman 1999]. With appropriate integration (ensemble average or filtering), Eq. (AIV.6) can be rewritten as

$$\left\langle \mathbf{T}_i \cdot \nabla X_i \right\rangle = +\overline{P}_{Int,i} \nabla \varepsilon_i + \overline{\boldsymbol{\tau}}_{Int,i} \cdot \nabla \varepsilon_i + \mathbf{M}_i^{drag} \quad . \qquad \text{(AIV.7)}$$

If we assume that the particles are much heavier than the carrier phase ($\rho_s >> \rho_g$), $\mathbf{M}_i^{drag}$ can be written as the drag force’s only contribution [Simonin 1996].

As examples in a two-phase flow (other forms are also possible),

Within the RANS framework only, in a two-phase flow system with a gaseous carrier phase, the drag between the gas and the dispersed granular phases can be expressed as

$$\begin{aligned}
&\mathbf{M}_g^{drag} = -\mathbf{M}_s^{drag} \approx K \, \Delta \mathbf{U} \\
&\Delta \mathbf{U} = \tilde{\mathbf{u}}_s - \tilde{\mathbf{u}}_g - \mathbf{u}_{drift}
\end{aligned} \quad , \qquad \text{(AIV.8)}$$

where $\Delta\mathbf{U}$ is the mean relative velocity between the gas phase and the solid phase minus the drift velocity ($\mathbf{u}_{drift}$). In Eq. (AIV.8), we have neglected the influence of the drag function (K and C_d) fluctuation along particle trajectories [Viollet et al., 1992].

Drag for dilute suspension ($\varepsilon_g > 0.8$)	Drag for concentrated suspension ($\varepsilon_g \leq 0.8$)
$K \approx \frac{3}{4}\varepsilon_s C_d \frac{\hat{\rho}_g \left\langle \left\| \mathbf{u}_s - \mathbf{u}_g \right\| \right\rangle}{d_s} \varepsilon_g^{-2.65}$	$K \approx \varepsilon_s \left[150 \frac{\varepsilon_s}{\varepsilon_g} \frac{\mu_g}{d_s^2} + \frac{7}{4} C_d \rho_g \frac{\left\langle \left\| \mathbf{u}_s - \mathbf{u}_g \right\| \right\rangle}{d_s} \right]$

$$C_d = \frac{24}{Re_s}\left[1 + 0.15\, Re_s^{0.687}\right] \qquad \text{for } Re_s < 1000$$

$$C_d = 0.44 \qquad \text{for } Re_s \geq 1000 \quad , \tag{AIV.9}$$

$$Re_s = \frac{\hat{\rho}_g d_s \left\langle \left| \mathbf{u}_s - \mathbf{u}_g \right| \right\rangle}{\mu_g}$$

where C_d and Re_s are the mean drag coefficient and the mean particle Reynolds number [Peirano et al., 2001]; d_s is the grain diameter; and μ_g is the molecular viscosity of the carrier phase. The drift velocity accounts for the dispersion effect from the particle transport by the fluid turbulence; hence, it represents the correlation between turbulence in the gas phase and the spatial distribution of the particles. If we assume an homogenous isotropic turbulence of the gas phase,

$$\mathbf{u}_{drift} = \frac{{}^{int}t_{gs}\, k_{12}}{3}\left(\frac{1}{\varepsilon_g}\nabla\varepsilon_g - \frac{1}{\varepsilon_s}\nabla\varepsilon_s \right) \quad , \tag{AIV.10}$$

where ${}^{int}t_{gs}$ and k_{12} are respectively the fluid-particle turbulent characteristic time and the trace of the covariance tensor between the turbulent velocity fluctuations of the two phases:

$$
{}^{int}t_{gs} = \frac{{}^{turn}t_g}{\sqrt{1 + 6C_\beta \dfrac{\left|\left\langle \mathbf{u}_s - \mathbf{u}_g \right\rangle\right|^2}{k_1}}}
$$

$$
k_{12} = \left\langle \mathbf{u}_s'' \cdot \mathbf{u}_g'' \right\rangle \qquad , \qquad \text{(AIV.11)}
$$

where,

$$
{}^{turn}t_g = \frac{1}{\beta_1}\frac{k_1}{\varepsilon_1}
$$

where ${}^{turn}t_g$ is the eddy turnover time; k_1 and ε_1 are the turbulent kinetic energy of the gas phase and its dissipation rate respectively. C_β and β_1 are constants that may depend on the directions within the flow (stream-wise or span-wise) [Fevrier and Simonin 2000].

In the previous equations, the quantity, $\left\langle \left| \mathbf{u}_s - \mathbf{u}_g \right| \right\rangle$, represents the local instantaneous relative velocity between particles with velocity ($\mathbf{u}_s$) and the surrounding carrier fluid velocity ($\mathbf{u}_g$) undisturbed by the presence of the particles at that particle position but possibly "influenced" by turbulence [Enwald and Almstedt 1999]:

$$
\left\langle \left| \mathbf{u}_s - \mathbf{u}_g \right| \right\rangle \approx \sqrt{\left(\Delta \mathbf{U}_i\right)^2 + 2\left(k_1 + k_2 + k_{12}\right)} \qquad , \qquad \text{(AIV.12)}
$$

where k_2 is the turbulent kinetic energy of the solid phase that is related to the granular temperature, Θ, by $k_2 = \frac{1}{2}\left\langle \mathbf{u}_s'' \cdot \mathbf{u}_s'' \right\rangle = \frac{3}{2}\Theta$.

Within the LES two-interpenetrated fluids framework, interfacial closures are much less well known. Naturally, the interfacial transfer closures must be expressed in terms of the resolved (filtered and known) quantities. However, one would assume that there would be some contributions from the unresolved subgrid scales, which are unknown both theoretically and experimentally. Therefore, a simpler approach must be taken in which all subgrid contributions to the interfacial terms are assumed to be negligible [we have in a way taken a similar approach in Eq. (AIV.8)].

If we assume that the particles are much heavier than the carrier phase ($\rho_s >> \rho_g$), $\mathbf{M}_i^{drag}$ in Eq. (AIV.6) can be simply written as a drag-force-only contribution [Simonin 1996]. In a two-phase flow system with a gaseous carrier phase, the drag between the gas and the solid dispersed phase is

$$\begin{aligned} &\mathbf{M}_g^{drag} = -\mathbf{M}_s^{drag} \approx K\,\Delta\mathbf{U} \\ &\Delta\mathbf{U} = \tilde{\mathbf{u}}_s - \tilde{\mathbf{u}}_g \end{aligned} \quad , \tag{AIV.13}$$

where K is a resolved (filtered) drag function given by

Drag for dilute suspension ($\varepsilon_g > 0.8$)	**Drag for concentrated suspension ($\varepsilon_g \le 0.8$)**
$K \approx \frac{3}{4}\varepsilon_s C_d \frac{\hat{\rho}_g \left\lvert \tilde{\mathbf{u}}_s - \tilde{\mathbf{u}}_g \right\rvert}{d_s} \varepsilon_g^{-2.65}$	$K \approx \varepsilon_s \left[150 \frac{\varepsilon_s}{\varepsilon_g} \frac{\mu_g}{d_s^2} + \frac{7}{4} C_d\, \rho_g \frac{\left\lvert \tilde{\mathbf{u}}_s - \tilde{\mathbf{u}}_g \right\rvert}{d_s} \right]$

$$\begin{aligned} &C_d = \frac{24}{Re_s}\left[1 + 0.15\,Re_s^{0.687}\right] && \text{for } Re_s < 1000 \\ &C_d = 0.44 && \text{for } Re_s \ge 1000 \quad , \\ &Re_s = \frac{\hat{\rho}_g d_s \left\lvert \tilde{\mathbf{u}}_s - \tilde{\mathbf{u}}_g \right\rvert}{\mu_g} \end{aligned} \tag{AIV.14}$$

where d_s is the grain diameter; μ_g is the molecular viscosity of the carrier phase; and C_d and Re_s are the drag coefficient and the particle Reynolds number.

Finally, the internal energy/enthalpy flux exchange at the interface, $-\left\langle \mathbf{q}_i \cdot \mathbf{n}_i \delta_{Int} \right\rangle$, can be similarly modeled with the following:

$$\begin{aligned} \left\langle -\mathbf{q}_i \cdot \mathbf{n}_i \delta_{Int} \right\rangle &= +\left\langle \mathbf{q}_i \cdot \nabla X_i \right\rangle \\ &= +\left\langle \left(\mathbf{q}_{Int} + \mathbf{q}_i - \mathbf{q}_{Int} \right) \cdot \nabla X_i \right\rangle \\ &= +\left\langle \mathbf{q}_{Int} \cdot \nabla X_i \right\rangle + \left\langle \left(\mathbf{q}_i - \mathbf{q}_{Int} \right) \cdot \nabla X_i \right\rangle \end{aligned} \quad . \tag{AIV.15}$$

For the same reasons as the momentum interfacial terms, in a well-coupled phasic flow, we may neglected the interfacial heat transfer (unless there is a strong interface between phases as in separated and stratified flows):

$$\left\langle \mathbf{q}_i \cdot \nabla X_i \right\rangle \approx \left\langle \left(\mathbf{q}_i - \mathbf{q}_{Int} \right) \cdot \nabla X_i \right\rangle \quad . \tag{AIV.16}$$

In other words, the interfacial heat transfer can be simply expressed as the heat transfer between phases at the interface between them. Hence, as an example, *within the RANS and LES frameworks,* in a two-phase flow system with a gaseous carrier phase, Eq. (AIV.16) can be expressed as

$$\begin{aligned}
&{}^{h}H_i \approx \tilde{h}_i R_i + \left\langle \left(\mathbf{q}_i - \mathbf{q}_{i,Int} \right) \cdot \nabla X_i \right\rangle \approx \tilde{h}_i R_i + Q\left(T_s - T_g \right) \\
&\text{where,} \\
&Q \approx \frac{6\,\varepsilon_s k_g}{d_s^2}\,Nu \\
&Nu \approx \left(7 - 10\,\varepsilon_g + 5\,\varepsilon_g^2 \right)\left(1 + \frac{7}{10} Re_s^{7/10}\, Pr^{1/3} \right) + \left(1.33 - 2.4\,\varepsilon_g + 1.2\,\varepsilon_g^2 \right) Re_s^{7/10}\, Pr^{1/3} \quad , \\
&Pr \approx \frac{C_{pg}\mu_g}{k_g} \\
&k_g \approx 418.3925\times 10^{-10} \left(60054 + 1846\,\tilde{T}_g + 2\times 10^{-6}\,\tilde{T}_g^2 \right) \qquad [\text{J/s.m.K}]
\end{aligned} \tag{AIV.17}$$

where the mean Re number would be calculated by Eq. (AIV.9) within the RANS framework and by Eq. (AIV.14) within the LES framework. As in the interfacial momentum transfer, we have neglected any contributions from fluid characteristic fluctuation along particle trajectories or any subgrid contribution to the filtered resolved Q, Nu, and Pr quantities.

Appendix 5: RANS and LES Stress and Work

In the energy equations, the work of the surfaces forces, $-\left\langle X_i \mathbf{T}_i : \nabla \mathbf{u}_i \right\rangle$, and, in the momentum equations, the acceleration from the surface forces, $-\left\langle \nabla \cdot X_i \mathbf{T}_i \right\rangle$, are problematic in the RANS and LES frameworks of this manuscript. The problem is that these terms require the knowledge of two averaged or two filtered velocities (i.e., $\bar{\mathbf{u}}$ or $\tilde{\mathbf{u}}$). Ideally, one would not want to have within the same mathematical model a variable ($\mathbf{u}$ or P) from a Favre phasic-weighted decomposition (i.e., $\bar{\mathbf{u}}$, $\overline{\mathrm{P}}$) and, at the same time, from a Favre mass-weighted decomposition (i.e., $\tilde{\mathbf{u}}$, $\tilde{\mathrm{P}}$). Indeed, let us recall that, for a fully compressible flow in both LES and RANS,

$$\overline{\mathrm{P}''} = \overline{\mathrm{P} - \tilde{\mathrm{P}}} = \begin{cases} \overline{\mathrm{P}} - \tilde{\mathrm{P}} \neq 0 & \text{RANS} \\ \overline{\mathrm{P}} - \overline{\tilde{\mathrm{P}}} \neq 0 & \text{LES} \end{cases} . \qquad \text{(AV.1)}$$
$$\text{idem, } \overline{\mathbf{u}''} = \overline{\mathbf{u} - \tilde{\mathbf{u}}} \neq 0$$

In the following, and in this entire manuscript, we assume that the shear viscosity (μ) and bulk viscosity (${}^b\mu$) act as constants with regard to the LES and RANS integration (filtering or ensemble averaging)[36]:

$$\begin{aligned} \bar{\mu} &\approx \tilde{\mu} \approx \mu \\ \overline{{}^b\mu} &\approx \widetilde{{}^b\mu} \approx {}^b\mu \end{aligned} \qquad \text{(AV.2)}$$

Now, let us examine the acceleration resulting from the viscous forces and the work of the surfaces forces:

$$\begin{aligned} -\left\langle \nabla \cdot X_i \mathbf{T}_i \right\rangle &= -\left\langle \nabla X_i P_i \right\rangle - \left\langle \nabla \cdot X_i \boldsymbol{\tau}_i \right\rangle \\ &= -\left\langle \nabla X_i P_i \right\rangle - \left\langle X_i \mu_i \left(\nabla \mathbf{u}_i + \nabla \mathbf{u}_i^{\mathrm{T}} \right) \right\rangle - \left\langle X_i \lambda_i \nabla \cdot \mathbf{u}_i \mathbf{I} \right\rangle \\ & \qquad , \\ -\left\langle X_i \mathbf{T}_i : \nabla \mathbf{u}_i \right\rangle &= -\left\langle X_i P_i \nabla \cdot \mathbf{u}_i \right\rangle - \left\langle X_i \boldsymbol{\tau}_i : \nabla \mathbf{u}_i \right\rangle \\ &= -\left\langle X_i P_i \nabla \cdot \mathbf{u}_i \right\rangle - \left\langle X_i \nabla \cdot \boldsymbol{\tau}_i \cdot \mathbf{u}_i \right\rangle + \left\langle X_i \mathbf{u}_i \cdot \nabla \cdot \boldsymbol{\tau}_i \right\rangle \end{aligned} \qquad \text{(AV.3)}$$

[36] This is a "universal" and reasonable assumption, which also applies to the specific heats (Cp or C_v), the species diffusion coefficients (v_j), and the thermal conductivity coefficients (k_i).

where μ_i and λ_i are the shear and the second coefficients of viscosity (see Appendix 8).

We must decompose P_i and τ_i into a fluctuating and an averaged part (RANS) or into a subgrid and a filtered part (LES). It would make sense to use the Favre mass-weighted decomposition of velocities ($\mathbf{u}_i = \tilde{\mathbf{u}}_i + \mathbf{u}_i''$), because $\tilde{\mathbf{u}}_i$ is solved in the momentum equations in both the RANS and LES frameworks. However, in Eq. (AV.3), the operator $\langle\ \rangle$ represents a Favre phasic-weighted averaging/ filtering (e.g., $\mathbf{u}_i = \overline{\mathbf{u}}_i + \mathbf{u}_i'$; see §2.7). Therefore, one way or another, we have supplementary unknowns depending on how we expand Eq. (AV.3), $\overline{\mathbf{u}_i''}$ or $\overline{\mathbf{u}}_i$, which would require further assumptions and equations to solve these supplementary unknowns (possible within the RANS realm, but, within the monophase- and multiphase-LES, no solution has ever been proposed). The task may be considerably simplified in assuming [Gatski 1997] the following:

$$
\begin{aligned}
&-\left\langle \nabla\cdot X_i\mathbf{T}_i\right\rangle = -\nabla\varepsilon_i\overline{\mathbf{T}}_i \approx -\nabla\varepsilon_i\overline{P}_i - \nabla\cdot\left[\varepsilon_i\mu_i\left(\nabla\tilde{\mathbf{u}}_i + \nabla\tilde{\mathbf{u}}_i^{T}\right)\right] - \nabla\cdot\left[\varepsilon_i\lambda_i\nabla\cdot\tilde{\mathbf{u}}_i\mathbf{I}\right] && \text{a.}\\
&-\left\langle X_i\mathbf{T}_i : \nabla\mathbf{u}_i\right\rangle = -\varepsilon_i\,\overline{\mathbf{T}_i : \nabla\mathbf{u}_i} \approx -\varepsilon_i\,\overline{P}_i\nabla\cdot\tilde{\mathbf{u}}_i - \varepsilon_i\,\tilde{\boldsymbol{\tau}}_i : \nabla\tilde{\mathbf{u}}_i && \text{(AV.4)}\\
&\qquad\approx -\varepsilon_i\,\overline{P}_i\nabla\cdot\tilde{\mathbf{u}}_i - \varepsilon_i\,\nabla\cdot\tilde{\boldsymbol{\tau}}_i\cdot\tilde{\mathbf{u}}_i + \varepsilon_i\,\tilde{\mathbf{u}}_i\cdot\nabla\cdot\tilde{\boldsymbol{\tau}}_i && \text{b.}
\end{aligned}
$$

These kinds of approximations are common in atmospherical science within both LES and RANS. However, the justification is not exactly the same:

—Within the RANS realm, this assumption can be justified if $\tilde{\mathbf{u}}_i \approx \overline{\mathbf{u}}_i$. In other words,

$$
\begin{aligned}
\tilde{\mathbf{u}}_i &\approx \overline{\mathbf{u}}_i\\
\frac{\left\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\,\mathbf{u}_i(\mathbf{x},t)\right\rangle}{\left\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\right\rangle} &\approx \frac{\left\langle X_i(\mathbf{x},t)\,\mathbf{u}_i(\mathbf{x},t)\right\rangle}{\left\langle X_i(\mathbf{x},t)\right\rangle}\\
\frac{\left\langle X_i(\mathbf{x},t)\,\rho_i(\mathbf{x},t)\,\mathbf{u}_i(\mathbf{x},t)\right\rangle}{\varepsilon_i\,\overline{\rho}_i} &\approx \frac{\left\langle X_i(\mathbf{x},t)\,\mathbf{u}_i(\mathbf{x},t)\right\rangle}{\varepsilon_i}\quad. \qquad\qquad \text{(AV.5)}\\
\Rightarrow \rho_i(\mathbf{x},t) \approx \text{constant w.r.t. } \frac{d\varepsilon_i}{dt}
\end{aligned}
$$

This means that such an assumption would hold if and only if the microscopic density of a given phase acts as a constant or as a constant with respect to the phasic volumetric concentration variations. Because we aim to model buoyant dusty plumes and clouds, this assumption seems reasonable. Indeed, it has been shown [Dartevelle 2003; Dartevelle et al., 2004] that volumetric variations within the ash plume can be fairly large (several orders of magnitude), which would indicate that the variations of $\bar{\rho}_g$ (because temperature and/or pressure changes) are unimportant with respect to ε variations.

In developing Eq. (AV.4)b, we have also assumed that the contribution from the work of "turbulent surface forces" (i.e., dissipation of turbulent kinetic energy) is negligible with respect to $W_{\mathbf{T},i}$. For instance,

$$\begin{aligned}
-\left\langle X_i \mathbf{T}_i : \nabla \mathbf{u}_i \right\rangle &= -\varepsilon_i\, \overline{\mathbf{T}_i : \nabla \mathbf{u}_i} \\
&= -\varepsilon_i\, \overline{P_i \nabla \cdot \mathbf{u}_i} - \varepsilon_i\, \nabla \cdot \overline{\boldsymbol{\tau}_i \cdot \mathbf{u}_i} + \varepsilon_i\, \overline{\mathbf{u}_i \cdot \nabla \cdot \boldsymbol{\tau}_i} \\
&= -\varepsilon_i\, \overline{\left(\bar{P}_i + P_i'\right) \nabla \cdot \left(\bar{\mathbf{u}}_i + \mathbf{u}_i'\right)} - \varepsilon_i\, \nabla \cdot \overline{\left(\bar{\boldsymbol{\tau}}_i + \boldsymbol{\tau}_i'\right) \cdot \left(\bar{\mathbf{u}}_i + \mathbf{u}_i'\right)} + \varepsilon_i\, \overline{\left(\bar{\mathbf{u}}_i + \mathbf{u}_i'\right) \nabla \cdot \left(\bar{\boldsymbol{\tau}}_i + \boldsymbol{\tau}_i'\right)} \\
&= -\varepsilon_i\, \overline{\bar{P}_i \nabla \cdot \bar{\mathbf{u}}_i} - \varepsilon_i\, \overline{\bar{P}_i \nabla \cdot \mathbf{u}_i'} - \varepsilon_i\, \overline{P_i' \nabla \cdot \bar{\mathbf{u}}_i} - \varepsilon_i\, \overline{P_i' \nabla \cdot \mathbf{u}_i'} \\
&\qquad -\varepsilon_i\, \overline{\bar{\boldsymbol{\tau}}_i : \nabla \bar{\mathbf{u}}_i} - \varepsilon_i\, \overline{\bar{\boldsymbol{\tau}}_i : \nabla \mathbf{u}_i'} - \varepsilon_i\, \overline{\boldsymbol{\tau}_i' : \nabla \bar{\mathbf{u}}_i} - \varepsilon_i\, \overline{\boldsymbol{\tau}_i' : \nabla \mathbf{u}_i'}
\end{aligned} \tag{AV.6}$$

This equation can be further simplified if we assume that the fluctuating velocity is divergenceless; if $\nabla \cdot \mathbf{u}_i' \approx 0$ [Besnard et al., 1992], Eq. (AV.6) becomes

$$\begin{aligned}
-\left\langle X_i \mathbf{T}_i : \nabla \mathbf{u}_i \right\rangle &= -\varepsilon_i\, \overline{\mathbf{T}_i : \nabla \mathbf{u}_i} \\
&\approx -\varepsilon_i\, \bar{P}_i \nabla \cdot \bar{\mathbf{u}}_i - \varepsilon_i\, \bar{\boldsymbol{\tau}}_i : \nabla \bar{\mathbf{u}}_i - \varepsilon_i\, \overline{\boldsymbol{\tau}_i' : \nabla \mathbf{u}_i'}
\end{aligned} \quad . \tag{AV.7}$$

Eq. (AV.7) is discussed in great detail by Besnard et al. [1992]. It can be noted that for simplifying Eq. (AV.7) into Eq. (AV.4)b, we must not only consider that $\tilde{\mathbf{u}}_i \approx \bar{\mathbf{u}}_i$ but also that the dissipation process of turbulent viscous forces ($-\varepsilon_i\, \overline{\boldsymbol{\tau}_i' : \nabla \mathbf{u}_i'}$) is negligible for the macroscopic heat generation (or at least is negligible with regard to the other form of heat generations: convection, pressure work, heat conduction, heat generation from mass transfers, and so forth).

—Of course, within the LES framework, the development of $-\left\langle X_i \mathbf{T}_i : \nabla \mathbf{u}_i \right\rangle$ is more complicated because of the presence of the Leonard- and Cross-terms, which do not vanish during the filtering process:

$$
\begin{aligned}
-\left\langle X_i \mathbf{T}_i : \nabla \mathbf{u}_i \right\rangle &= -\varepsilon_i \, \overline{\mathbf{T}_i : \nabla \mathbf{u}_i} \\
&= -\varepsilon_i \, \overline{P_i \nabla \cdot \mathbf{u}_i} - \varepsilon_i \, \nabla \cdot \overline{\boldsymbol{\tau}_i \cdot \mathbf{u}_i} + \varepsilon_i \, \overline{\mathbf{u}_i \cdot \nabla \cdot \boldsymbol{\tau}_i} \\
&= -\varepsilon_i \, \overline{\left(\utilde{\overline{P}}_i + \utilde{P}_i' \right) \nabla \cdot \left(\utilde{\tilde{\mathbf{u}}}_i + \utilde{\mathbf{u}}_i'' \right)} - \varepsilon_i \, \nabla \cdot \overline{\left(\utilde{\tilde{\boldsymbol{\tau}}}_i + \utilde{\boldsymbol{\tau}}_i'' \right) \cdot \left(\utilde{\tilde{\mathbf{u}}}_i + \utilde{\mathbf{u}}_i'' \right)} + \varepsilon_i \, \overline{\left(\utilde{\tilde{\mathbf{u}}}_i + \utilde{\mathbf{u}}_i'' \right) \nabla \cdot \left(\utilde{\tilde{\boldsymbol{\tau}}}_i + \utilde{\boldsymbol{\tau}}_i'' \right)} \qquad \text{(AV.8)} \\
&= -\varepsilon_i \, \overline{\utilde{\overline{P}}_i \nabla \cdot \utilde{\tilde{\mathbf{u}}}_i} - \varepsilon_i \, \overline{\utilde{\overline{P}}_i \nabla \cdot \utilde{\mathbf{u}}_i''} - \varepsilon_i \, \overline{\utilde{P}_i' \nabla \cdot \utilde{\tilde{\mathbf{u}}}_i} - \varepsilon_i \, \overline{\utilde{P}_i' \nabla \cdot \utilde{\mathbf{u}}_i''} \\
&\quad -\varepsilon_i \, \overline{\utilde{\tilde{\boldsymbol{\tau}}}_i : \nabla \utilde{\tilde{\mathbf{u}}}_i} - \varepsilon_i \, \overline{\utilde{\tilde{\boldsymbol{\tau}}}_i : \nabla \utilde{\mathbf{u}}_i''} - \varepsilon_i \, \overline{\utilde{\boldsymbol{\tau}}_i'' : \nabla \utilde{\tilde{\mathbf{u}}}_i} - \varepsilon_i \, \overline{\utilde{\boldsymbol{\tau}}_i'' : \nabla \utilde{\mathbf{u}}_i''}
\end{aligned}
$$

where a phasic-weighted decomposition has been used for the pressure and a mass-weighted decomposition for the velocity vector (and therefore for the tensor $\boldsymbol{\tau}$)[37]. Using the traditional LES "trick,"

$$
\begin{aligned}
\overline{\utilde{\overline{P}}_i \nabla \cdot \utilde{\tilde{\mathbf{u}}}_i} &= \overline{\utilde{\overline{P}}_i \nabla \cdot \utilde{\tilde{\mathbf{u}}}_i} + \utilde{\overline{P}}_i \nabla \cdot \utilde{\tilde{\mathbf{u}}}_i - \utilde{\overline{P}}_i \nabla \cdot \utilde{\tilde{\mathbf{u}}}_i \\
\overline{\utilde{\tilde{\boldsymbol{\tau}}}_i : \nabla \utilde{\tilde{\mathbf{u}}}_i} &= \overline{\utilde{\tilde{\boldsymbol{\tau}}}_i : \nabla \utilde{\tilde{\mathbf{u}}}_i} + \utilde{\tilde{\boldsymbol{\tau}}}_i : \nabla \utilde{\tilde{\mathbf{u}}}_i - \utilde{\tilde{\boldsymbol{\tau}}}_i : \nabla \utilde{\tilde{\mathbf{u}}}_i
\end{aligned} \quad . \qquad \text{(AV.9)}
$$

Eq. (AV.9) into Eq. (AV.8) yields the following:

$$
-\left\langle X_i \mathbf{T}_i : \nabla \mathbf{u}_i \right\rangle = -\varepsilon_i \, \overline{\mathbf{T}_i : \nabla \mathbf{u}_i} \approx \varepsilon_i \left(\utilde{W}_{\mathbf{T},i} + {}^{SG}\utilde{W}_{\mathbf{T},i} \right) \quad , \qquad \text{(AV.10)}
$$

with

[37] The reason is obvious because filtering does not delete the Cross-terms and a filter variable is not constant with repect to the filtering integral: $\utilde{\overline{\overline{P}}}_i \neq \utilde{\overline{P}}_i$, $\overline{\utilde{\overline{\mathbf{u}}}_i} \neq \utilde{\overline{\mathbf{u}}}_i$ and $\overline{\utilde{P}_i' \nabla \cdot \utilde{\overline{\mathbf{u}}}_i} \neq \overline{\utilde{\overline{P}}_i \nabla \cdot \utilde{\mathbf{u}}_i'} \neq \overline{\utilde{\overline{\boldsymbol{\tau}}}_i : \nabla \utilde{\mathbf{u}}_i'} \neq \overline{\utilde{\boldsymbol{\tau}}_i' : \nabla \utilde{\overline{\mathbf{u}}}_i} \neq 0$. Hence, the Favre phasic-weighted decomposition is neither useful nor advisable.

$$\underset{\smile}{W}_{\mathbf{T},i} \quad = -\left\{ \underset{\smile}{\overline{P}}_i \nabla \cdot \underset{\smile}{\tilde{\mathbf{u}}}_i + \underset{\smile}{\tilde{\boldsymbol{\tau}}}_i : \nabla \underset{\smile}{\tilde{\mathbf{u}}}_i \right\}$$

$$\begin{aligned}
{}^{SG}\underset{\smile}{W}_{\mathbf{T},i} \quad = -\Bigg\{ & \underbrace{\left[\overline{\underset{\smile}{\overline{P}}_i \nabla \cdot \underset{\smile}{\tilde{\mathbf{u}}}_i} - \underset{\smile}{\overline{P}}_i \nabla \cdot \underset{\smile}{\tilde{\mathbf{u}}}_i + \overline{\underset{\smile}{\tilde{\boldsymbol{\tau}}}_i : \nabla \underset{\smile}{\tilde{\mathbf{u}}}_i} - \underset{\smile}{\tilde{\boldsymbol{\tau}}}_i : \nabla \underset{\smile}{\tilde{\mathbf{u}}}_i \right]}_{{}^{L}\underset{\smile}{W}_{\mathbf{T},i}} \\
& + \underbrace{\left[\overline{\underset{\smile}{\overline{P}}_i \nabla \cdot \underset{\smile}{\mathbf{u}}_i''} + \overline{\underset{\smile}{P}_i' \nabla \cdot \underset{\smile}{\tilde{\mathbf{u}}}_i} + \overline{\underset{\smile}{\boldsymbol{\tau}}_i'' : \nabla \underset{\smile}{\tilde{\mathbf{u}}}_i} + \overline{\underset{\smile}{\tilde{\boldsymbol{\tau}}} : \nabla \underset{\smile}{\mathbf{u}}_i''} \right]}_{{}^{C}\underset{\smile}{W}_{\mathbf{T},i}} \\
& + \underbrace{\left[\overline{\underset{\smile}{P}_i' \nabla \cdot \underset{\smile}{\mathbf{u}}_i''} + \overline{\underset{\smile}{\boldsymbol{\tau}}_i'' : \nabla \underset{\smile}{\mathbf{u}}_i''} \right]}_{{}^{R}\underset{\smile}{W}_{\mathbf{T},i}} \Bigg\}
\end{aligned} \qquad \text{(AV.11)}$$

where the subscripts ‘L’, ‘C’, and ‘R’ pertain to Leonard-, Cross-, and Reynolds-terms, the resolved (filtered) and the Leonard-terms are made of known quantities. It is interesting to note that so far we have made no simplification at all for the resolved pressure work and viscous dissipation. However, within the subgrid, the Leonard-, Cross-, and Reynolds-terms of the irreversible and reversible works of the surface forces are universally ignored, “hoping” that subgrid dissipation processes are unimportant and/or that once a variable has been filtered it will remain roughly constant within the subgrid (it can be seen then that the Leonard- and Cross-terms must go to zero).

Appendix 6: Method of Characteristics Applied to Single-Phase Flow

In order to highlight the results demonstrated in §5, we apply the same Method of Characteristics (MOC) to a “traditional” compressible single-phase flow.

The 1-D Euler equations for constant flow area within a pipe [Lyczkowski et al., 1982] taken from Bird et al. [1960] are

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial t} = 0 \\
&\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x}\right) + \frac{\partial P}{\partial x} = \rho G - F \qquad , \\
&\rho\left(\frac{\partial h}{\partial t} + u\frac{\partial h}{\partial x}\right) - \left(\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x}\right) = -\frac{\partial q}{\partial x} + uF
\end{aligned} \tag{AVI.1}$$

where G is body forces; F is a wall friction force per unit of volume along the x-direction; and, hence, uF represents dissipation along the wall. The equivalent 1-D Navier-Stokes (viscous) equations would read

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial t} = 0 \\
&\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x}\right) + \frac{\partial P}{\partial x} + \frac{\partial \tau}{\partial x} = \rho G \qquad , \\
&\rho\left(\frac{\partial h}{\partial t} + u\frac{\partial h}{\partial x}\right) - \left(\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x}\right) = -\frac{\partial q}{\partial x} - \tau\frac{\partial u}{\partial x}
\end{aligned} \tag{AVI.2}$$

where F and uF have been replace by a more comprehensive viscous model. In the momentum equation, F becomes the shear viscous force effects ($-\frac{\partial \tau}{\partial x}$), and, in the energy equation, uF becomes the work of these viscous forces ($-\tau\frac{\partial u}{\partial x}$). The viscous forces per unit of volume are defined as follows:

$$\tau = -\mu\frac{\partial u}{\partial x} \qquad , \tag{AVI.3}$$

where μ is some form of shear viscosity, possibly due to turbulence. Let us use the following EOS: $h = h(P,\rho)$; we therefore note that

$$\begin{aligned} dh &= \frac{\partial h}{\partial P}\, dP + \frac{\partial h}{\partial \rho}\, d\rho \\ &= h_\rho \;\; dP + h_P \;\; d\rho \end{aligned} \quad , \tag{AVI.4}$$

where h_ρ and h_P are the enthalpy at constant density and pressure respectively. Let us transform the enthalpy equations in the Euler set, Eq. (AVI.1), with w=uF or in the Navier-Stokes set, Eq. (AVI.2), with $w = -\tau \frac{\partial u}{\partial x}$:

$$\rho\left(\frac{\partial h}{\partial t} + u\,\frac{\partial h}{\partial x}\right) - \left(\frac{\partial P}{\partial t} + u\,\frac{\partial P}{\partial x}\right) = -\frac{\partial q}{\partial x} + w$$

$$\Leftrightarrow$$

$$\rho\left(h_\rho\;\frac{dP}{dt} + h_P\;\frac{d\rho}{dt}\right) - \frac{dP}{dt} = -\frac{\partial q}{\partial x} + w$$

$$\Leftrightarrow$$

$$\left(\rho h_\rho - 1\right)\frac{dP}{dt} + \rho h_P\;\frac{d\rho}{dt} = -\frac{\partial q}{\partial x} + w$$

$$\Leftrightarrow$$

$$\left(\frac{\partial P}{\partial t} + u\,\frac{\partial P}{\partial x}\right) + \frac{\rho\, h_P}{\left(\rho h_\rho - 1\right)}\left(\frac{\partial \rho}{\partial t} + u\,\frac{\partial \rho}{\partial x}\right) = \frac{-\frac{\partial q}{\partial x} + w}{\left(\rho h_\rho - 1\right)}$$

$$\Leftrightarrow$$

$$\left(\frac{\partial P}{\partial t} + u\,\frac{\partial P}{\partial x}\right) + \frac{\rho\, h_P}{\left(1 - \rho\, h_\rho\right)}\,\rho\,\frac{\partial u}{\partial x} = \frac{-\frac{\partial q}{\partial x} + w}{\left(\rho h_\rho - 1\right)} \quad , \tag{AVI.5}$$

Before getting any further, we must understand the meaning of $\frac{\rho\, h_P}{\left(1 - \rho\, h_\rho\right)}$. We note that this ratio has the units of the square of a velocity or of specific energy [m^2/s^2]. From standard thermodynamics, it is known that

$$dh \equiv h_\rho dP\Big|_\rho + h_P d\rho\Big|_P = T d\eta\Big|_P + \frac{1}{\rho} dP\Bigg|_\eta \qquad , \qquad \text{(AVI.6)}$$

where h is the specific enthalpy [m^2/s^2]; η is the specific entropy [$m^2/K\ s^2$]; h_ρ is $\frac{\partial h}{\partial P}$ [m^3/kg]; and h_P is $\frac{\partial h}{\partial \rho}$ [$m^5/kg\ s^2$]. Then,

$$\begin{aligned}
& h_\rho dP + h_P d\rho = T d\eta + \frac{1}{\rho} dP \\
& \Leftrightarrow \\
& \rho\, h_P d\rho = \rho\, T d\eta + \left(1 - \rho\, h_\rho\right) dP \qquad . \qquad \text{(AVI.7)} \\
& \Rightarrow \\
& \frac{\rho\, h_P}{\left(1 - \rho\, h_\rho\right)} = \frac{dP}{d\rho} + \frac{\rho\, T}{\left(1 - \rho\, h_\rho\right)} \frac{d\eta}{d\rho}
\end{aligned}$$

As shown by Lyczkowski et al. [1982] in the isoentropic case ($d\eta$=0), we must have

$$\frac{\partial P}{\partial \rho}\Bigg|_\eta = \frac{\rho\, h_P}{\left(1 - \rho\, h_\rho\right)} = C^2 \qquad , \qquad \text{(AVI.8)}$$

where C would be a constant material speed of sound. Of course, because of either the frictional dissipation along the wall (Euler set) or the viscous dissipation within the flow (Navier-Stokes set), the entropy and C cannot be constant (e.g., for an ideal gas, C would increase with the temperature). Nevertheless, the ratio, $\frac{\rho\, h_P}{\left(1 - \rho\, h_\rho\right)}$, is guaranteed to be nonzero and positive. To ease the following mathematical reading, let us label this ratio as C^2.

Therefore, the equations of continuity, momentum and energy, and shear stress for the Navier-Stokes model [Eq. (AVI.3)] lead to the following dependent variable vectors and characteristic analysis:

Euler set	Navier-Stokes set
$\mathbf{U} = (u, P, \rho)^T$ $A_t = \begin{pmatrix} 0 & 0 & 1 \\ \rho & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ $A_x = \begin{pmatrix} \rho & 0 & u \\ \rho u & 1 & 0 \\ C^2\rho & u & 0 \end{pmatrix}$ $\mathrm{Det}\left[\!\left[A_x - \lambda A_t \right]\!\right] = 0$ $\Leftrightarrow$ $\rho\left(u-\lambda\right)\left[\left(u-\lambda\right)^2 - C^2\right] = 0$	$\mathbf{U} = (u, P, \rho, \tau)^T$ $A_t = \begin{pmatrix} 0 & 0 & 1 & 0 \\ \rho & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ $A_x = \begin{pmatrix} \rho & 0 & u & 0 \\ \rho u & 1 & 0 & 1 \\ C^2\rho & u & 0 & 0 \\ -\mu & 0 & 0 & 0 \end{pmatrix}$ $\mathrm{Det}\left[\!\left[A_x - \lambda A_t \right]\!\right] = 0$ $\Leftrightarrow$ $\left(u-\lambda\right)^2 \mu = 0$

Characteristics:	Characteristics:
$\lambda \to \left\{u, u \pm C\right\}$	$\lambda \to \left\{u, u\right\}$

All eigenvalues along the characteristic curves are real as required for well-posedness. Interestingly enough, the full viscous Navier-Stokes model has a characteristic less than the Euler model—it does not have the speed of sound in its characteristic values. Indeed, in a way, the viscous phenomenon “damped out” instabilities propagation within the flow and explains why weak-instabilities “just” travel with the flow velocity.

These results, although obvious from the previous demonstration, seem not have been demonstrated before in the common literature.

Appendix 7: Operators, Tensors, and Invariants

Operators

$\overset{\circ}{\overline{\overline{\ }}}$		deviatoric part (traceless) of a symmetric tensor
$\circ$		spherical part (trace) of a symmetric tensor
$\tilde{\cdot}$		mean (RANS) or filtered (LES) part of a variable obtained by Favre mass-weighted decomposition
$\bar{\cdot}$		mean (RANS) or filtered (LES) part of a variable obtained by Favre phasic-weighted decomposition
$\breve{\cdot}$		obtained from or after a filtering process (LES framework)
$:$		scalar product of two tensors
$\cdot$		scalar product of two vectors
$\Vert\ \Vert$		Euclidian norm of a tensor
$\langle\ \rangle$		ensemble-average (RANS) or filtering (LES) operator
tr		trace operation of tensors
T		transposed operation of matrices
∇	1/m	gradient operator
$\nabla\cdot$	1/m	divergence operator
$\dfrac{d}{dt}=\dfrac{\partial}{\partial t}+\mathbf{u}\cdot\nabla$	1/s	material (Lagrangian) time-derivative

Tensors, invariants, and work terms

Rate-of-strain tensor:

(AVII.1) $\mathbf{D}=-\dfrac{1}{2}\left[\nabla\mathbf{u}+\nabla\mathbf{u}^{T}\right]$ 1/s

Deviator of the rate-of-strain:

(AVII.2) $\overset{\circ}{\overline{\overline{\mathbf{D}}}}=\mathbf{D}+\dfrac{1}{3}\nabla\cdot\mathbf{u}\,\mathbf{I}$ 1/s

First invariant of the rate-of-strain tensor:

(AVII.3) $I_D=\mathrm{tr}(\mathbf{D})=\sum_{i=1}^{3}D_{ii}=-\nabla\cdot\mathbf{u}$ 1/s

Second invariant of the rate-of-strain tensor:

(AVII.4) $II_D=\mathrm{tr}(\mathbf{D}\cdot\mathbf{D})=\sum_{i=1}^{3}\sum_{j=1}^{3}D_{ij}D_{ji}=D_{11}^2+D_{22}^2+D_{33}^2+2D_{12}^2+2D_{13}^2+2D_{23}^2$ $1/s^2$

Second invariant of the deviator of the stress tensor:

(AVII.5) $II_{dT}=\dfrac{\left(T_{11}-T_{22}\right)^2+\left(T_{22}-T_{33}\right)^2+\left(T_{33}-T_{11}\right)^2}{6}+T_{12}^2+T_{13}^2+T_{23}^2$ Pa^2 ($kg^2/m^2\,s^4$)

Second invariant of the deviator of the rate-of-strain tensor:

(AVII.6) $II_{dD}=\dfrac{\left(D_{11}-D_{22}\right)^2+\left(D_{22}-D_{33}\right)^2+\left(D_{33}-D_{11}\right)^2}{6}+D_{12}^2+D_{13}^2+D_{23}^2$ $1/s^2$

Total stress tensor:

(AVII.7) $\mathbf{T}=P\,\mathbf{I}+\boldsymbol{\tau}=P\,\mathbf{I}+2\,\mu\,\overset{\circ}{\overline{\overline{\mathbf{D}}}}-\mu^{b}\,\nabla\cdot\mathbf{u}\,\mathbf{I}$ Pa ($kg/m\,s^2$)

Viscous dissipation (irreversible work):

(AVII.8) $W_{\boldsymbol{\tau}}=-\boldsymbol{\tau}:\nabla\mathbf{u}=-\left(\nabla\cdot\left(\boldsymbol{\tau}\cdot\mathbf{u}\right)-\mathbf{u}\cdot\nabla\cdot\boldsymbol{\tau}\right)=2\,\mu\,II_D+\lambda\,I_D^2$ $J/m^3\,s$ ($kg/m\,s^3$)

Work of all surface forces:

(AVII.9) $W_{\mathbf{T}}=-\mathbf{T}:\nabla\mathbf{u}=-\left(P\mathbf{I}:\nabla\mathbf{u}+\boldsymbol{\tau}:\nabla\mathbf{u}\right)=-P\nabla\cdot\mathbf{u}-\nabla\cdot\left(\boldsymbol{\tau}\cdot\mathbf{u}\right)+\mathbf{u}\cdot\nabla\cdot\boldsymbol{\tau}=P\,I_D+W_{\boldsymbol{\tau}}$ $J/m^3\,s$ ($kg/m\,s^3$)

Appendix 8: Notations, Units, Constants, and Acronyms

Latin

A_i		1/m (m^2/m^3)	"volumetric concentration" of interfacial area of phase i
C_d		dimensionless	drag coefficient
C		m/s	isoentropic speed of sound
$C_{i,j}$		kg/m^3 s	rate of interfacial mass transfer between species j and all other species within phase i
Cp		J/kg K(m^2/s^2 K)	specific heat at constant pressure
Cv		J/kg K (m^2/s^2 K)	specific heat at constant volume
d		m	particle diameter
D		1/s	rate-of-strain tensor
E		J/kg (m^2/s^2)	total energy per unit of mass (internal + kinetic energy)
E_Θ		m^2/s^2	volume averaged granular fluctuating energy
G		m/s^2	body force
G		1/m s	LES space- and time-filter (kernel) function in $\Re^4$
G_x		1/m	LES space-filter (kernel) function in $\Re^3$
G_t		1/s	LES time-filter (kernel) function in $\Re$
g	(0,0,-9.80665)	m/s^2	gravity vector
${}^fH_i$		J/s m^3 (kg/m s^3)	rate of interfacial Helmholtz free energy between phase i and all other phases
${}^IH_i$		J/s m^3 (kg/m s^3)	rate of interfacial internal energy between phase i and all other phases
${}^hH_i$		J/s m^3 (kg/m s^3)	rate of interfacial enthalpy between phase i and all other phases
${}^\eta H_i$		J/K s m^3 (kg/K m s^3)	rate of interfacial entropy between phase i and all other phases
h		J/kg (m^2/s^2)	enthalpy per unit of mass
I		J/kg (m^2/s^2)	internal energy per unit of mass
I		dimensionless	unit tensor
k		W/m K (kg m/K s^3)	thermal conductibility coefficient
K		kg/m^3 s	gas-solid momentum transfer (drag) function
k_λ		1/m	wave number scale of the largest unresolved turbulent eddies
m		kg	mass of grain
M_a	28.9644	kg/kmol	molar weight of dry air
M_j		kg/kmol	molar weight of any gas species
$\mathbf{M}_i$		Pa/m (kg/m^2 s^2)	rate of interfacial momentum transfer between phase i and all other phases
M_w	18.0152	kg/kmol	molar weight of water
n		$1/m^3$	number of grains per unit of volume
Nu		dimensionless	Nusselt number
P		Pa (kg/m s^2)	pressure
P_s'		Pa (kg/m s^2)	granular pressure (usually understood as a kinetic and collisional within RANS)
${}^{mol}Pr$		dimensionless	"molecular" (not induced by turbulence) Prandtl number
${}^{tur}Pr$	0.95	dimensionless	turbulent Prandtl number
q		kg/s^3	thermal-heat flux or granular-heat flux vector
r		m	position vector
Q		W/m^3 K (kg/s^3 K)	gas-solid heat transfer function
R	8314.56	J/kmol K (kg m^2/s^2 kmol K)	universal gas constant
$\ddot{R}$		J/kg K (m^2/s^2 K)	mixture gas constant
Re		dimensionless	particle Reynolds number
R_i		kg/m^3 s	rate of interfacial mass transfer between phase i and all other phases
R		Pa m^3/kg (m^2/s^2)	specific Reynolds stress tensor (RANS or LES framework)
S		J/kg s (m^2/s^3)	rate of heat/energy supplementary source
t		s	time
T		K	temperature
T		Pa (kg/m s^2)	total stress tensor
u		m/s	velocity vector
$\mathbf{u}_{Int}$		m/s	bulk velocity vector of all the interfaces

U_x		m/s	mean mixture horizontal/radial-speed of all phases
V_y		m/s	mean mixture vertical-speed of all phases
$W_{\mathbf{T}}$		J/m^3 s (kg/m s^3)	total work done by all the surface forces
$W_{\boldsymbol{\tau}}$		J/m^3 s (kg/m s^3)	irreversible work done by the surface forces (viscous dissipation)
X_i	1 or 0	dimensionless	function of presence of the i^{th} phase
y		dimensionless	species mass fractions

Greek

Δ		m	3-D geometric mean of the computational grid-size
$\vec{\Delta}$		m	filter cutoff length
Δx_k		m	computational grid-size width in the k^{th} direction
ε		dimensionless	phasic volumetric concentration
${}^{max}\varepsilon_s$	0.64	dimensionless	maximum solid volumetric concentration
ε_E		m^2/s^3	turbulent energy cascade rate
$\boldsymbol{\Phi}$		kg/K s^3	entropy flux
γ	(6)	dimensionless	constant in the Gaussian spatial-filter
Γ		k/s m^3	source/sink of a given species
ι		s or m	generic symbol for the time- or a space-variable
$\lambda = \mu^b - \frac{2}{3}\mu$		Pa s (kg/m s)	second coefficient of viscosity
μ		Pa s (kg/m s)	shear viscosity
μ^b		Pa s (kg/m s)	bulk viscosity
η		J/kg K (m^2/s^2 K)	entropy per unit of mass
Θ		J/kg (m^2/s^2)	granular temperature
ρ		kg/m^3	microscopic weight density
$\hat{\rho}$		kg/m^3	macroscopic weight density
ρ_m		kg/m^3	mean mixture weight density between all phases
Σ		J/kg s K (m^2/K s^3)	entropy source
$\boldsymbol{\tau}$		Pa (kg/m s^2)	viscous stress tensor
τ		s	characteristic LES filter time interval
ϖ_j		m^2/s	diffusion coefficient of species j in the whole mixture
ξ		m	characteristic LES filter width
ξ_k		m	characteristic LES filter width in the k^{th} direction
Ω			computational domain/subdomain
$\partial\Omega$			domain/subdomain boundary

Subscripts-Superscripts

$'$	fluctuating (RANS) or unresolved (LES) part of a variable obtained by Favre phasic-weighted decomposition
$''$	fluctuating (RANS) or unresolved (LES) part of a variable obtained by Favre mass-weighted decomposition
a	dry air
b	bulk viscosity
c	collisional
C	Cross-terms
g	gas phase
Int	denotes an interface or all the interfaces
Int,i	denotes the interface between phase i and all the other phases
K	kinetic
L	Leonard-terms
m	mixture

mol	“molecular” (i.e., not induced by turbulence)
R	Reynolds terms
s	solid phase
t	relative to time
tur	induced by turbulence
k^{th}	some X-, Y-, Z-directions
x	X-direction (radial or horizontal) or relative to space
y	Y-direction (vertical)
w	water vapor (steam)

Acronyms

CFDlib	computational fluid dynamic library code
CV	control volume
EOS	equation of state
(G)MFIX	geophysical multiphase flow with interphase exchange
IMF	implicit multifield
LANL	Los Alamos National Laboratory
LES	large eddy simulation
LHS	left-hand side
MFIX	multiphase flow with interphase exchange
MOC	method of characteristics
NETL	National Energy Technology Laboratory
ODE	ordinary differential equation
ORNL	Oak Ridge National Laboratory
PDE	partial differential equation
RANS	Reynolds Averaged Navier-Stokes
RHS	right-hand side
SG	subgrid
SGH	subgrid heat (flux)
SGS	subgrid stress (flux)

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