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Advances in the characterisation of reactive gas and solid mixtures under low pressure conditions

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ABSTRACT

This work describes the use of splitting methods in the analysis of reactive two-phase mixtures of gases and particles under conditions that make the source terms very stiff. In our particular case, these are low pressure, small particles, high solid concentration, and very dense solids. The gas phase is considered a perfect gas and the solid one is assumed to be incompressible. The integration of the source terms proposed seems to help tackle without difficulty the type of dust mobilisation and combustion problems studied: This consists of an implicitisation of the source term performed after the evaluation of the advection problem. Some numerical results are included; they correspond to a mobilisation of the mixture by means of shock, a mobilisation problem provoked by a rarefaction wave, and the combustion of tungsten-dust in a reacting atmosphere. An example of a 3D dust mobilisation sequence inside the vacuum vessel (VV) of the ITER (International Thermonuclear Experimental Reactor) completes this work.

1. Introduction

Gas–particle interaction is a key process nowadays in many scientific and industrial fields such as combustion, filter technology, pollutant dispersion or nuclear safety [1]. In this last field, it is especially important not only in the analysis of accident sequences in nuclear fission power plants [2], but also in fusion facilities, such as tokamaks [3], as in the ITER facility [4]. In these types of installations, neutron fluxes erode the plasma facing materials (based on carbon (C), beryllium (Be) or tungsten (W), in most cases) generating small loose particle agglomerates ranging from nanometres to millimetres, usually referred to as "dust" [5–7]. During an unlikely Loss Of Vacuum Accident (LOVA) or Ingress of Coolant Event (ICE) in the ITER, the potential dust mobilisation may degenerate into chemical reactions, hydrogen production, dust explosion and the dissemination of radioactive material out of the vacuum vessel [3,8,9]. Thus, it is of major importance to characterise pressure loads during dust mobilisation and explosion under LOVA and ICE sequences within the ITER vacuum vessel [8].

In the last decade, many models have been developed for the analysis of mixtures of gas and particles. They study the set of non-linear conservation equations for each phase with complex source terms. Most of them lie between two different approximations: EulerianEulerian (EE) [10] or EulerianLagrangian (EL) approximations. The use of an EE approach, while economical and suited to dense mixtures with two-way coupling, requires good phenomenological models, usually based on kinetic theories for granular flows [11]. Based on a finite volume approach, the authors have successfully extended several approximate Riemann solvers such as AUSM + *up* (advection upwind splitting method), Roe and van Leer Hanel solvers to analyse this sort of problem [12]. In the case of the solid phase some versions of the AUSM + or Rusanov schemes have been extended and used [13] to calculate the numerical fluxes at the interfaces.

In this context, the DUST code for 3D simulation of gas-particle interaction has been developed in close collaboration between IRSN (Institut de Radioprotection et Sret Nuclaire, France) and the Technical University of Cartagena (Spain), on the basis of the CAST3M code developed at the CEA (Commissariat lEnergie Atomique, France) [14–17]. The code permits the analysis of dust spatial distribution, remobilisation and entrainment, and explosion to be carried out in the cases of laden and high dilute mixtures. Some assumptions such as particle incompressibility and a negligible effect of pressure on the solid phase make the high dilute model quite appealing from the mathematical point of view as the systems of equations that characterise the behaviour of the phases are decoupled. The code allows multi-dimensional problems in unstructured grids to be studied. It is based on a EulerianEulerian

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List of symbols

c_g	gas speed of sound (m/s)
c_{pg}	specific heat of the gas phase at constant pressure (J/(kg K))
c_{pp}	specific heat of the solid phase (J/(kg K))
c_{vg}	specific heat of the gas phase at constant volume (J/(kg K))
d_p	particle diameter (m)
F	interphase forces (Pa/m)
C_d	particle drag coefficient
$e_g = \sum_{i=1}^{NGSP} Y_{g,i} \int_{T_{ref}}^{T} c_{vgi}(T)dT$	gas specific internal energy (J/kg)
$e_p = \sum_{i=1}^{NPSP} Y_{p,i} \int_{T_{ref}}^{T} c_{pp,i}(T)dT$	solid specific internal energy (J/kg)
$E_k = e_k + \frac{\lvert\vec{u}_k\rvert}{2}$	total internal energy of phase k (J/kg)
$\vec{F}_d$	gas–particle drag force (Pa/m)
$\vec{g}$	gravity (9.81 m/s^2)
$\mathcal{H}(y)$	Heavyside function
$\boldsymbol{\mathcal{H}} = [\mathbf{F}\ \mathbf{G}\ \mathbf{H}]$	convective flux tensor
h_c	convection heat transfer coefficient (W/(m^2 K))
$h_g = e_g + p/\rho_g$	gas specific enthalpy (J/kg)
$H_g = h_g + \lvert\vec{u}_g\rvert^2/2 = E_g + p/\rho_g$	gas total enthalpy (J/kg)
k_g	thermal conductivity of the gas phase (W/(m K))
m_p	mass of a particle (kg)
M_i	molar mass of species i (kg/mol)
$\hat{n}$	unit outward normal vector to the surface element dS
$n = \sigma/m_p$	number of particles per unit volume
$NGSP$	number of species in the gas phase
$NSSP$	number of species in the solid phase
p	pressure (Pa)
q	heat transferred per unit area and per unit time to the particle (W/m^2)
Q	interfacial heat exchanged (W/m^3)
Q_{ck}	heat released by gaseous of solid species (W/m^3)
Q_r	radiation heat transferred. Not considered in this study (W/m^3)
$\bar{q}$	average value of q in the surface S (W/m^2)
Q_g	interfacial heat transferred between the phases (W/m^2)
$\dot{r}_i$	molar reaction rate for species i per unit volume (mol$_i$/(m^3 s))
Re, Re_p	particle Reynolds number
R_u	universal gas constant (J/(mol K))
S	particle surface
t	time (s)
$\overline{\overline{T}}$	stress tensor (Pa)
T_s	threshold temperature (K)
T_k	temperature (K) of phase k
$\vec{u}_k$	velocity of phase k (m/s)
$\dot{v}_i$	volume rate released of species i in a reaction (l$_i$/(m^2 s))
x, y	Cartesian coordinates
X_i	molar fraction of species i
Y_i	mass fraction of species i

Greek letters

α	void fraction
γ_g	gas specific heat ratio
Γ	total mass exchange between phases (kg/(m^3 s))
μ_g	gas dynamic viscosity (Pa s)
ρ_g	gas density (kg/m^3)
$\sigma = \rho_p(1-\alpha)$	particle concentration (kg/m^3)
Ψ_S	rotation matrix
$\dot{\omega}_i$	mass reaction rate for species i per unit volume (kg$_i$/(m^{3}s))

Subscripts

c	combustion
g	gas phase
i	initial
i	summation index
k	a general index to refer to a species
m	a general index to refer to a phase
p	particles, solid phase
ref	reference
t	time derivative

finite volume approximation where the numerical fluxes at each element interface are evaluated explicitly. Second order is obtained by means of variable extrapolation (MUSCL technique).

In some cases, such as in ITER accident sequences, the type of dust mobilisation problems being analysed become very complex as they may involve very low initial pressure (of the order of 4200 Pa) and a high concentration of particles (about 120 kg/m^3) with small diameter and high density (tungsten has a density of ρ_W = 20,000 kg/m^3). Under these conditions, source terms in the system of balance equations become so stiff that a reformulation of the finite volume is needed. The use of splitting methods with an implicitisation of the source terms is proven to help circumvent these difficulties [21,44].

A system of equations for dust mobilisation and combustion problems is proposed on this paper. Some features of the system are characterised, such as its hyperbolicity and constitutive laws. Then, the numerical schemes applied for the resolution are briefly described, as well as the methodology corresponding to the splitting methods. We continue showing the different techniques studied to solve the ODE which involve the source terms. Then, a new approach is proposed for the treatment of source terms, which delivers physical solutions from the system of equations, even when the source terms become stiffer. We present this new option as an alternative in numerical calculation of problems with adverse conditions that are too demanding with conventional upwinding methods, such as thermodynamic conditions encountered in the simulation of air ingress in ITER fusion reactor. Next, some numerical results are analysed, corresponding to different benchmarks aiming to serve as a test of performance of the numerical method. To conclude, a preliminary simulation test for dust mobilisation in ITER is shown.

2. Two-phase model

2.1. System of equations for a mixture of a gas and monoparticles

This work is devoted to the study of reactive high dilute mixtures of gases and particles. Thus, the reactive Euler equations for two-phase flows are considered. The system of equations consists of two sets of conservation equations for each phase (gas and solid), formed by the equations of mass, momentum, total energy and those corresponding to the concentration of the species of each mixture. The void fraction is practically equal to one ($\alpha \approx 1$), since the mixture of gases and particles is considered as highly diluted, and pressure effect on the solid phase is negligible. So, the dynamic behaviour of the mixture is characterised by the systems of conservation equations for each phase, which are only coupled by the source terms (Eq. (1)):