Modelling Transient 3D Multi-phase Criticality in Fluidised Granular Materials - The FETCH Code
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The development and application of a generic model for modelling criticality in fluidised granular materials is described within the Finite Element Transient Criticality (FETCH) code - which models criticality transients in spatial and temporal detail from fundamental principles, as far as is currently possible. The neutronics model in FETCH solves the neutron transport in full phase space with a spherical harmonics angle of travel representation, multi-group in neutron energy, Crank Nicholson based in time stepping, and finite elements in space. The fluids representation coupled with the neutronics model is a two-fluid-granular-temperature model, also finite element based. A separate fluid phase is used to represent the liquid/vapour/gas and the solid fuel particle phases, respectively. Particle-particle, particle-wall interactions are modelled using a kinetic theory approach based on an analogy between the motion of gas molecules subject to binary collisions and granular flows. This model has been extensively validated by comparison with fluidised bed experimental results. Gas-fluidised beds involve particles that are often extremely agitated (measured by granular temperature) and can thus be viewed as a particularly demanding application of the two-fluid model. Liquid fluidised systems are of criticality interest, but these can become demanding with the production of gases (e.g. radiolytic and water vapour) and large fluid/particle velocities in energetic transients. We present results from a test transient model in which fissile material (239Pu) is presented as spherical granules subsiding in water, located in a tank initially at constant temperature and at two alternative over-pressures in order to verify the theoretical model implemented in FETCH.

KEYWORDS: Criticality, multi-phase; granular materials; coupled models; fluidised bed reactors.

1. Introduction

Imperial College has developed a 3D modelling capability in its FETCH code to solve nuclear criticality problems in fluidised granular materials. FETCH has already been validated against transient criticality experiments in multi-phase solutions. We present a summary of the basis and applications of the new fluidised granular criticality model, in particular the fluids model, which has recently been implemented in FETCH. It has been found that the multi-fluid approach to modelling of granular materials is often the only feasible approach. The alternative 'Discrete Element Method' may not treat sufficient numbers of particles and for sufficient long time periods and therefore it may not present a feasible option.

The granular criticality model implemented within FETCH is proving to be particularly flexible and useful as demonstrated by its application to a range of problems from, modelling new nuclear reactors whose fuel is in granular form, modelling pebble bed nuclear reactors, to modelling the ingress of powder into moderating water and the study of collapse of granular material in water. The latter two scenarios may involve the production of steam along with an increase in pressurisation of the system. Modelling of pressure is particularly important as this can provide useful information about the integrity of containers of nuclear waste with traces of fissile materials.

The aim of this paper is to present a summary of the basis and applications of the fluidised granular criticality model. In particular a representative test transient model has been set up to verify the theoretical model implemented. We have explored criticality transients due to solid granules taking into account their surroundings in a coupled neutronics/two-fluids model.

The neutronics part of the granular fluidised transient criticality models is based on the solution of seven-dimensional space using the second-order even parity form of the transport equation. A six-energy group scheme was used in transient calculations, which were derived from the cell code WM5 using the 69 group library, taking into account resonant self-shielding and particle (granules) spatial effects including neutronics properties of its surroundings. A set of cross sections were generated for various temperatures and these are used to obtain, using a temperature interpolation procedure, the local cross section for each element of the finite element spatial mesh.

In the two-fluid models (TFM) presented, both phases have been represented with separate density, temperature and velocity fields. The interaction terms have been used to represent the coupling between phases.

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The TFM requires additional closure laws to describe the rheology of the particulate phase, which are based on the assumptions of kinetic theory of granular flows. To avoid empirical correlations being used for the rheology of the granular phase, in the proposed model the solid viscosity and the normal stress are derived using an analogy between the particle-collision during the granular flows and the gas kinetic theory. Hence, the concept of granular temperature as a measure of the agitation of particles was introduced. The granular temperature is therefore, a link between the kinetic theory and conventional fluid mechanics. The set of TFM conservation equations that describes the gas-solid flow and additional closure laws are given in Pain et al., where more detailed information is available. In this paper, we describe the granular fluids model developed, some of the approximations made and present results from a test transient criticality study.

2. The Two-Fluid Granular Model
2.1 Governing Equations

The governing equations solved here are the two fluid equations with separate phases for the gas and the particle (solid) phases. In each phase, conservation equations for continuity, namely mass, momentum, energy and volume fraction are solved, which are coupled to suitable equations of state - ideal gas for the gas phase, and incompressible for the particle phase. In the solid phase, the particle-particle interactions are modelled using a kinetic theory based on the granular temperature, which represents the width of the Maxwellian distribution of particle velocities. Solid particles representing the fissile material are associated with the solid phase and its neutronics properties, like delayed neutron precursor concentrations, are advected with the solid particle phase. The liquid phase (water and gas) are treated together.

The continuity equations for phase k, where k=g denotes liquid/gas phases and k=s denotes solid particles are:

\[
\frac{\partial}{\partial t} \left( \rho_k \right) + \frac{\partial}{\partial x_j} \left( \rho_k v_{ki} \right) = 0
\]  

(1)

Where \( \rho_k \) and \( v_k \) are the density and volume fraction of phase k, \( v_{ki} \) is the velocity of phase k in the i\textsuperscript{th} direction, t is the time and \( x_i \) is the spatial coordinate in the i\textsuperscript{th} direction. The first term on the left-hand side of equation (1) which is written for k=liquid and k=liquid/gas phases are related to the rate of mass accumulation per unit volume and the second term represents the net rate of convective mass flux. In the formulations presented here mass and heat generation due to chemical reactions and radiative heat transfer are neglected. The corresponding momentum equation is for again k=gas and k=liquid/gas phases:

\[
\frac{\partial}{\partial t} \left( \rho_k \right) + \frac{\partial}{\partial x_j} \left( \rho_k v_{ki} v_{kj} \right) = F_{kj} - \frac{\partial}{\partial x_j} \left( \sigma_{kj} \right)
\]

(2)

In equation (2), the first and second terms are related to buoyancy and gravitational forces and \( \rho_k \) is the component of gravity in the i\textsuperscript{th} direction, \( \varepsilon_k \) denotes the opposite phase, \( \rho_s \) is the shared pressure and \( \beta \) is the friction coefficient and is obtained from a modified form of the Ergun equation. The wall-particle boundary conditions are applied as described in reference 3. The third and fourth terms are, respectively, the interaction force representing the momentum transfer between the fluid and the solid phases and the stress tensor. The last term represents the frictional force exerted by the phase k on the wall.

The thermal energy equations are described as:

\[
\frac{\partial}{\partial t} \left( C_f \rho_f T_f \right) = -p_f \left[ \frac{\partial}{\partial x_i} (\varepsilon_f v_{fi}) + \frac{\partial}{\partial x_i} (\varepsilon_s v_{si}) \right]
\]

\[+ \frac{\partial}{\partial x_i} (\varepsilon_f \frac{\sigma_f}{\partial x_i}) + \alpha(T_s - T_f) + \Omega_{wf}
\]

(3)

The last three terms in the right hand side of equations number (3) represent the thermal energy transferred by conduction, convection and between phase k and the wall respectively.

We have defined the solid fluctuation energy equation for smooth slightly inelastic and spherical particles representing the granules as:
2.2.2 Fluid Phase Density

The density of the water-steam system was obtained through an empirical equation of state for \( 0 \leq \rho \leq 9000 \) bars and \( 273.15 \leq T \leq 1273.15 \) K. For large pressures and temperatures, a fitting curve based on a modified Redlich-Kwong equation of state was used.

2.2.3 Stress Tensor

The gas-phase turbulence has been neglected in the model used in this work. This is due to the uncertainty in the turbulence model closures and large gas phase space turbulent suppression in densely packed beds. Either a constant viscosity which equals the gas viscosity is used or a larger viscosity to act as an eddy viscosity. In densely packed beds, the solid stresses are dominated by inter-particle friction rather than by collision or fluctuation motion.

2.2.4 Solid Phase Pressure

The solid phase pressure, \( p_s \), represents the solid-phase normal forces due to particle-particle interactions and can be written in two parts representing (1) a kinetic and (2) collisional contributions:

\[
p_s = \varepsilon_9 \rho_s \theta + 2 \varepsilon_{sp} \rho_s \theta (1 + e_{pp})
\]

In (6), \( \varepsilon_9 \) is the radial distribution function and \( e_{pp} \) is the particle collision coefficient. The kinetic part is expressed by the first term on the right hand side of the equation by the shear stress caused by the flow of granules (or particles). The second term is the collision contribution due to the momentum transferred between particle collisions.

2.2.5 Solid Phase Shear Viscosity

Several empirical correlations were developed to calculate the solid shear viscosity, \( \xi \), most of them are suitable for densely packed beds, however they differ in dilute regions. We have used the relationship reported by van Wachem.

2.2.6 Solid Phase Bulk Viscosity

The solid bulk viscosity can be defined as the resistance of the particle suspension against compression. This relationship has been taken from Lun et al.

2.2.7 Inter-phase Heat Transfer

The inter-phase heat transfer is defined as the temperature gradient between theoretical fluid-layer along the surface and the surface itself. We have used the

\[
\frac{3}{2} \left[ \frac{\partial}{\partial t} (\varepsilon_s \rho_s \theta) + \frac{\partial}{\partial x_j} (\varepsilon_s \rho_s v_j \theta) \right] = \frac{\partial v_{si}}{\partial x_j} - \frac{\partial q_f}{\partial x_j} - \gamma - 3 \beta \theta
\]

Where the granular temperature \( \theta \) is expressed as:

\[
\frac{3}{2} \theta = \frac{1}{2} \left< v^2 \right>
\]

The second, third and fourth terms on the right hand side of the equation (4) represent the diffusive flux of granular energy, the rate of granular energy dissipation due to inelastic collisions, and the transfer of granular energy between the fluid and solid phases. The granular temperature, \( \theta \), is proportional to the 'granular energy' of the continuum, defined as the specific kinetic energy of the random fluctuation component of the particle velocity. Here, \( \varepsilon \) is the average of the sum of the fluctuating granular particle velocity components.

2.2 Constitutive Equations and Empirical Correlations

The conservative equations described in the previous section comprise a number of variables that are defined by specific functions. These functions are established either by fundamental equations or by empirical or experimental correlations. In this section, we briefly describe them below. Interested reader should consult reference 3 for more detailed information.

2.2.1 Drag Coefficient

The momentum transfer between the fluid and solid phases, \( \beta \), is usually obtained experimentally from pressure drop correlations and there are several correlations available in the literature, acquired from fixed or fluidised beds operating with either gas-liquid, gas-solid, or solid-liquid systems. Many of these correlations are valid for a wide range of granular diameter and porosity. In the present work, we have used a hybrid equation that applies to the Gidaspow's correlation for a range of porosity, and a swarm-corrected single particle drag law for volume fractions less than 0.2, as suggested by Pain et al.
volumetric inter-phase heat transfer coefficient to represent uniformly sized granules. The fluid/particle heat transfer coefficient was represented by Gunn and used in this work. His expression represents the Nusselt number as a function of the local flow dynamics, represented by the granular Reynolds number. The thermo physical properties of the fluid phase are expressed by the Prandtl number. This model is accurate for the large volumetric heat transfer coefficients as the temperature differences between the phases remain small.

2.2.8 Thermal Conductivities

The conductive mechanism is concerned with the thermal diffusion through a phase. In the fluid phase, the conduction is a function of the thermo-physical properties, whereas in the solid phase, the inter-particle collisions and granular bulk formation provide an additional effect. We have used the correlation suggested by Hunt to represent thermal conductivities.

3. Neutronics

The Boltzmann neutron transport equation is solved using finite elements in space, spherical harmonics ($P_N$) in angle, multi-group in energy and implicit two level time discretization methods. These methods have been applied using the second-order even-parity variational principle in the EVENT computer code. Its lowest mode of angular resolution is equivalent to diffusion theory.

At each time-step the interface module organizes the feedback from FLUIDITY of spatial temperature, density and delayed neutron precursor distributions into the EVENT neutronics module and also, in the light of these fields, updates the spatial distribution of multi-group neutron cross-sections. For a given element of the finite element (FE) mesh, a cross-section set is obtained by interpolating in temperature and gas content a cross-section data-base. This database has been group-condensed taking into account resonance self shielding and thermal temperature effects, into six groups using the WIMS code and a representative geometry. The neutronics module generates, for FLUIDITY, spatial distributions of fission-power and delayed neutron generation rates.

Material cross sections are generated as follows using the lattice cell code WIMS8A. First the cross sections were self-shielded using the equivalence theory method in WHEAD (part of WIMS) which relates the heterogeneous problem to an equivalent homogeneous model. A subgroup resonance calculation was then performed using the WPROC (part of WIMS) collision probability routine which calculates collision probabilities using a synthetic approximation for a system of spherical grains packed in annular geometry. Group cross sections were then obtained for temperatures ranging from 550K to 2000K by condensing to six groups the standard WIMS 69 group library.

4. Results

4.1 Test Problem Description

A test case has been set up to illustrate the application of the coupled neutronics - granular two-fluid model in FETCH. The test case is a cylindrical 'tank' bounded by a solid material which does not interact neutronically. Fissile material in solid granules is allowed to collapse under gravity in the water until criticality is achieved somewhat above the 'fully' collapse condition with the conditions chosen the initial temperature feedback of reactivity will be positive.

4.1.1 Geometry and Materials

The cylinder has a radius of 20.0 cm and the a total height of 200cm and is filled with water. The Pu-239 concentration in granules is chosen so that in the idealised fully slumped condition the excess reactivity would be 25. The initial temperature is taken to be 40.0 degrees C. The tank is open at the top (fluids are allowed to escape freely). The spherical granular particles of uniform diameter 2.5 cm are represented as a homogeneous mixture of Pu-239 fissile isotope in SiO$_2$ - representing a medium which does not interact neutronically.

![Fig. 1 Schematic of the geometrical model showing the cylindrical tank and the volume fraction (right) solid temperature contours (left) after the transient took place (0.2s) and for 60 bars over-pressure. Also shown is the inner and outer boundaries of the solid material](image-url)
4.2 FETCH Predictions

Transients have been initiated at two over pressures of 1 bar and 60 bars to illustrate the initial effect over-pressure in suppressing boiling.

Fig. 2 Variation with time of fission rate in the FETCH model for 60 bar and 1 bar over-pressure.

In Figs. 2-5 we show results, obtained from the two numerical simulations, presenting fission rate, maximum pressure and solid and gas phase temperatures, respectively. As the system becomes super-critical, the release of energy \((t > 0.10 \text{ s})\) raises the particle temperature, which rapidly vaporises water, and so increases sharply the maximum gas pressure.

The simulation performed with the larger over pressure, i.e., 60 bars, has a larger yield and temperature. This is mainly due to negative feedback effect associated with the production of steam occurring at a higher temperature at the larger over pressure. The main factor in reaching a subcritical state is the production of steam further which increases the neutron leakage out of the system. The transients will subsequently self-stabilise at a critical state where heat, production and loses are in balance.

Fig. 3. Maximum deviation of pressure from hydrostatic pressure in the FETCH model versus time for 60 bar and 1 bar over-pressure.

In Table 1 below we summarise the maximum values of the important parameters calculated:

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5. Conclusions

A numerical model of two-fluid granular equations have been developed and coupled with the time-dependent finite element neutronics code to study criticality transients in two-fluids systems containing granular (solid) materials. The whole methodology is implemented in the FETCH code. The model has the capability to address problems in waste management in chemical plant (e.g. spillage or collapse of granular materials) and also in investigating new reactor concepts such as fluidised bed reactors.

We have demonstrated the application of the numerical model coded in FETCH using a test case, which represents the collapse under gravity of fissile granular material in a tank containing water.

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