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5.5 Development of a Transient Criticality Evaluation Method

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Abstract

In developing a transient criticality evaluation method we model, in full spatial/temporal detail, the neutron fluxes and consequent power and the evolving material properties – their flows, energies, phase changes etc. These methods are embodied in the generic method FETCH code which is based as far as possible on basic principles and is capable of use in exploring safety-related situations somewhat beyond the range of experiment. FETCH is a general geometry code capable of addressing a range of criticality issues in fissile materials. The code embodies both transient radiation transport and transient fluid dynamics. Work on powders, granular materials, porous media and solutions is reviewed. The capability for modelling transient criticality for chemical plant, waste matrices and advanced reactors is also outlined.

1. Introduction

The motivation for this research comes from the potential for criticality where fissile materials are present in industrial or environmental matrices, and from the associated need to assess the implications for the integrity of industrial plant and potential radiation impacts on the health of workers and the public. In general these matrices will be multiphase, for example bubbly solutions, wetted or suspended powders or porous media.

While simple-design criticality assessment methods may normally be applied in a conservative manner, there is a need for a generic, fundamentally-based method capable of treating spatial and temporal detail, that may be used as a reference method and be used to assist in understanding complex behaviour. It is to meet this need that the coupled neutronics/computational fluid dynamics (CFD) code FETCH (Finite Element Transient Criticality) has been developed and benchmarked against available experiments[1-3]. The code has been developed as a reference method for modelling criticality transients in fissile solutions and other multiphase matrices. The fundamental nature of the modelling means that the code may be applied to cases somewhat beyond the range of experiment - for example dilute plutonium solution transients[1]. The extensive FETCH research into transients in fissile solutions is reviewed here in order to explore the role of radiolytic gases, transient pressure fields and of free surface 'sloshing'.

Transient criticality has been the subject of active investigation in the last 20 years with encouraging results. The CRITEX code by Mather et al.[4-6] was written to simulate the four important parameters of thermal expansion, temperature, radiolytic gas release and water vapour release, using point kinetics with cylindrical tank buckling and analytical treatments of the main variables. It has been validated against the CRAC and SILENE experiments[2]. Later work led to the CHAMPAGNE treatment for high rates of reactivity addition in the presence of gas bubble formation. The related POWDER code, designed to simulate the ingress of a moderator into fissile powder, was developed following specific experiments using the SILENE reactor.

FETCH uses the two fluid Eulerian-Eulerian model for modelling granular materials and powders. Both phases (particles and fluid) are continuous and fully inter-penetrating, and are described by separated conservative equations with interaction terms representing the coupling between the phases. The model requires additional closure laws to describe the rheology of the particulate phase. These closure laws are based on the assumptions of kinetic theory for granular flows. This model is then fully coupled to neutron radiation transport with heat being typically deposited into fissile particles where appropriate.

The FETCH porous medium model is similar to the granular model, but the granular phase (porous medium) is assumed fixed or slowly moving in response to a nuclear criticality transient. Two examples problem sets are demonstrated: criticality in waste-contaminated porous matrices and transient analysis in a Pebble Bed nuclear Reactor (PBR).

2. Neutron-fluids coupled method – FETCH

The FETCH code comprises three modules; two transient three dimensional finite element modules - the neutron transport code EVENT[7] and the computational fluid dynamics (CFD)/multiphase code FLUIDITY[9], coupled through an interface module. 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 EVENT. For a given element of the finite element (FE) mesh, a cross-section set is obtained by interpolating in temperature and voidage (due to gases) 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 WIMS8A code[1] and a representative geometry. The neutronics module generates for FLUIDITY spatial distributions of fission rate (energy deposition). An adaptive time-stepping procedure allows transient features of the fields to be resolved, having characteristic time scales which can vary over many orders of magnitude.

3. Formulation

This section the formulation used in FETCH including the discretisation, the solution methods and the equations that are solved as well as the physics modelled in these equations.

3.1 Multi-phase discretisation and solution methods

A high resolution method is used in this work to achieve bounded physical meaningful solutions that are also highly accurate. The method used to limit the spatial derivatives is based on the NVD approach[8]. A second order temporarily limited time stepping method (based on the Crank Nicholson method) is used in this work to help achieve bounded solutions, e. g., positive volume fraction. To maintain consistency with the discretized continuity equation, pressure as well as volume fractions have a piecewise constant variation across each hexahedral element. For similar reasons the granular temperature equations are also discretized using the high resolution method described above. The velocities have a tri-linear variation across each element and are thus centred on the nodes of the finite element mesh. The momentum equations are discretized using a Petrov-Galerkin method by multiplying each of the momentum equations for the three velocity components by finite element basis functions and integrating the resulting pressure term by parts. A non-linear Petrov-Galerkin method is used to suppress velocity oscillations normal to the flow direction. The momentum equations are discretized in time using implicit Crank-Nicholson time stepping. A semi-implicit projection method is used to solve the coupled multiphase continuity and momentum equations, see [9]. This method treats the coupling between the phases implicitly in pressure. A mixed finite element method with a constant variation of pressure throughout each element and a bi-linear variation of velocity is used here to avoid singularities in the discretized equations.

3.2 Multi-phase modelling

In this section the approach to solving the multiphase fluid equations[9] is discussed. The three conservation equations cover mass, momentum and thermal energy. The mass equation represents the void fraction, densities and velocities of liquids in given phases and also allows the position of a free surface to be tracked. In addition to momentum transfer terms between phases, the momentum equation has terms for interfacial pressure and drag forces, virtual mass and lift[9]. Buoyancy forces evolve naturally on the appearance of temperature differences and gases in the system.

Scalar field equations cover all field variables, together with delayed neutron precursors, water vapour and when appropriate radiolytic gas concentration dissolved in liquid, and embodies interfacial exchanges between phases. Delayed neutron precursors are assumed to exist only in the fissile liquid or solid phase and are in six delayed neutron precursor group form[1]. The continuity equation for the liquid depends on an equation of state embodying the response of liquid density to pressure and temperature (via the speed of sound and the expansion coefficient respectively).

In the Two-Fluids Model, both phases are modelled as interpenetrating continua and corresponding mass, momentum, thermal energy and fluctuation energy balance equations are solved with interaction terms representing the coupling between the phases. However, in the granular flow, particles dissipate energy due to inelastic collisions, therefore, a conservative equation for the kinetic energy of the particles is introduced into overall balance. This leads to a model in which the granular temperature, as an analogy of the thermodynamic temperature in the kinetic theory of gases, is used to measure the random oscillations of particles.

Mass balance within both phases is represented by the continuity equations defined as

$$\frac{\partial}{\partial t}\left(\varepsilon_k \rho_k\right)+\frac{\partial}{\partial x_i}\left(\varepsilon_k \rho_k \upsilon_k\right)=0 \tag{1}$$

where t, x_i ε_k, ρ_k v_k are the time, spatial coordinate, volume fraction of phase k, density of phase k and velocity of phase k respectively. The first term on the left-hand side of equation (1) is related to the rate of mass accumulation per unit volume and the second term represents the net rate of convective mass flux. The momentum balance for both phases is expressed as:

$$\frac{\partial}{\partial t}\left(\varepsilon_k \rho_k \upsilon_{ki}\right)+\frac{\partial}{\partial x_j}\left(\varepsilon_k \rho_k \upsilon_{ki}\upsilon_{kj}\right)\frac{\partial}{\partial x_j}\left(\varepsilon_k \rho_k \upsilon_{ki}\upsilon_{kj}\right)=-\varepsilon_k\frac{\partial p}{\partial x_i}+\varepsilon_k \rho_k g_i+ \beta\left(\upsilon_{k'i}-\upsilon_{ki}\right)-\frac{\partial}{\partial x_i}\left(\tau_{kij}\right)-\Gamma_k \upsilon_{ki} \tag{2}$$

where p is the pressure and the first and the second terms on the right hand side represent buoyancy and gravitational forces, respectively. The third and fourth terms are, respectively, the interaction force representing the momentum transfer between the fluid and solid phases and the stress tensor. The fifth term represents the frictional force exerted by the phase k on the wall. The thermal energy equations for dispersed (e.g. solid phase) and continuum (fluid) phases are described as:

$$C_f \rho_f \varepsilon_f \frac{DT_f}{Dt}=-p_f\left(\frac{\partial}{\partial x_i}\varepsilon_f \upsilon_{gi}+\frac{\partial}{\partial x_i}\varepsilon_{si}\right)+\frac{\partial}{\partial x_i}\left(\varepsilon_f \kappa_f \frac{\partial T_f}{\partial x_i}\right)+ \frac{\partial}{\partial x_i}\left(\varepsilon_f \kappa_f \frac{\partial T_f}{\partial x_i}\right)+\alpha\left(T_s-T_f\right)+\hat{\Gamma}_{wf} \tag{3}$$

$$C_s \rho_s \varepsilon_s \frac{DT_s}{Dt}=\frac{\partial}{\partial x_i}\left(\varepsilon_s \kappa_s \frac{\partial T_s}{\partial x_i}\right)+\alpha\left(T_g-T_s\right)+\hat{\Gamma}_{ws} \tag{4}$$

where C_s is the heat capacity at constant pressure and the last three terms on the r.h.s. of these equations represent the thermal energy transferred by conduction, convection and between phase 'k' and the wall, respectively.

3.3 Multi component models

Multiphase multi-component models for the simulation of flow and transport processes in the liquid, gas and granular flows are used widely in various technical application fields. They are characterized by the flow of more than one fluid phase (e.g. water, vapours, gas) and the transport of components in the fluid phases. Many multiphase multi-component processes are strongly affected by non-isothermal effects, in particular when processes such as evaporation/condensation play a dominant role. For the description of temperature-dependent processes, transitions of components between the phases, coupled with an exchange of thermal energy, have to be taken into account in addition to the flow of the individual phases. These models are important as they allow FETCH to track the movement and evolution of a large number of materials in a criticality. Consider a system with r chemical components in the solid, liquid or gas phases and suppose the superscript h represent the component.

The volume fraction of the solid phase may be represented by: $\varepsilon_s=\sum_{h=1}^{r}\varepsilon_s^h$ where, is the component of the solid phase for example. Thus, a mass balance of each component of the solid phase may lead to $\rho_s \varepsilon_s = \sum_{h=1}^{r} \rho_s^h \varepsilon_s^h$. Therefore the continuity equation may be re-written for the solid phase as:

$$\frac{\partial}{\partial t}\left(\varepsilon_s^h \rho_s^h\right) + \frac{\partial}{\partial x_i}\left(\varepsilon_s^h \rho_s^h \upsilon_{s_i}\right) = 0 \qquad (5)$$

The multi-component flow sub-model may also be extended for the thermal energy balance expressed by equation 4. It thus may be derived from the energy conversation of each component h as:

$$C_s^h \rho_s^h \varepsilon_s^h \frac{DT_s}{Dt} = \frac{\partial}{\partial x_i}\left(\varepsilon_s^h \kappa_s^h \frac{\partial T_s}{\partial x_i}\right) + \alpha^h\left(T_f - T_s\right) + \hat{\Gamma}'_{ws} \qquad (6)$$

where, C_s^h and κ_s^h are the heat capacity and thermal conductivity of each component. By summing the set of equations represented in equation 6, it leads to equation 4, where C_s is the bulk capacity of the solid phase, $C_s \rho_s \varepsilon_s = \sum_{h=1}^{3} C_s^h \rho_s^h \varepsilon_s^h$.

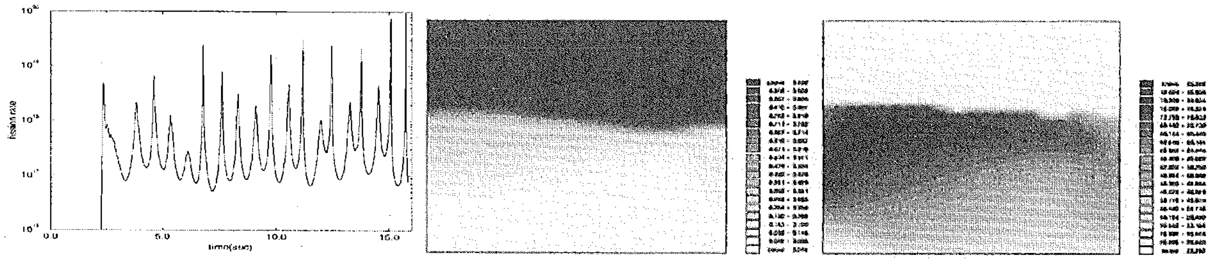

Fig 1. Fission rate verses time (sec) for a simulation of the CRAC 43 experiment - the liquid inflow rate of 1440 l/h through a small pip at the bottom of the vessel (bottom left of diagrams) provides the ramp reactivity insertion -200 g/l concentration 93 % enrichment. The central axis is on the left of the picture.

4. Applications

In this section we demonstrate FETCH for a wide range of applications.

Fissile solutions: Rapid transients in fissile solutions are typically characterised by the production of radiolytic gases and if energetic enough boiling. For example, an axi-symmetric simulation of a fissile solution experiment conducted by IPSN-Valduc, France called CRAC 43 was performed (see Fig. 1). This has a constant uranyl nitrate solution inflow rate of 1440 l/h and as a result is characterised by a series of fission spikes (Fig1 – left) which are related to the frequency of free surface sloshing and rate of rise of radiolytic gases bubbles out of the system. The central figure in Fig. 1 shows the solution volume fraction, the radiolytic gas bubbles near the surface and the free surface motion. The figure on the right of Fig. 1 shows the corresponding temperature distribution at 4.6 s into this transient and has a maximum temperature of some 60 Deg C. The radiolytic gas production models have been carefully validated against TRACY as well as SILENE experiments. See Fig. 2 (left) for a simulated solution volume fraction distribution for one of the more energetic transient experiments. The motivation of these experiments and simulations to achieve an understanding of criticality events such as the Toki-Mura incident – see right most two figures for a simulated solution volume fraction distribution just after the initial fission pulse when the mass of radiolytic gases are rises to the free surface and the temperature distribution at steady state. The rising radiolytic gas bubbles perturb the free surface (sloshing) and results in oscillations in the fission rate (Fig. 3 - right). Notice also the rapid variation of the pressure at a detector in the solution just after the first pulse. This is due to the rapid expansion and contraction of the mass of radiolytic gas bubbles in the solution. In addition, FETCH has been able to explore the dynamics of dilute Plutonium solutions with an overall positive temperature coefficient and has discovered a surprisingly benign behaviour.

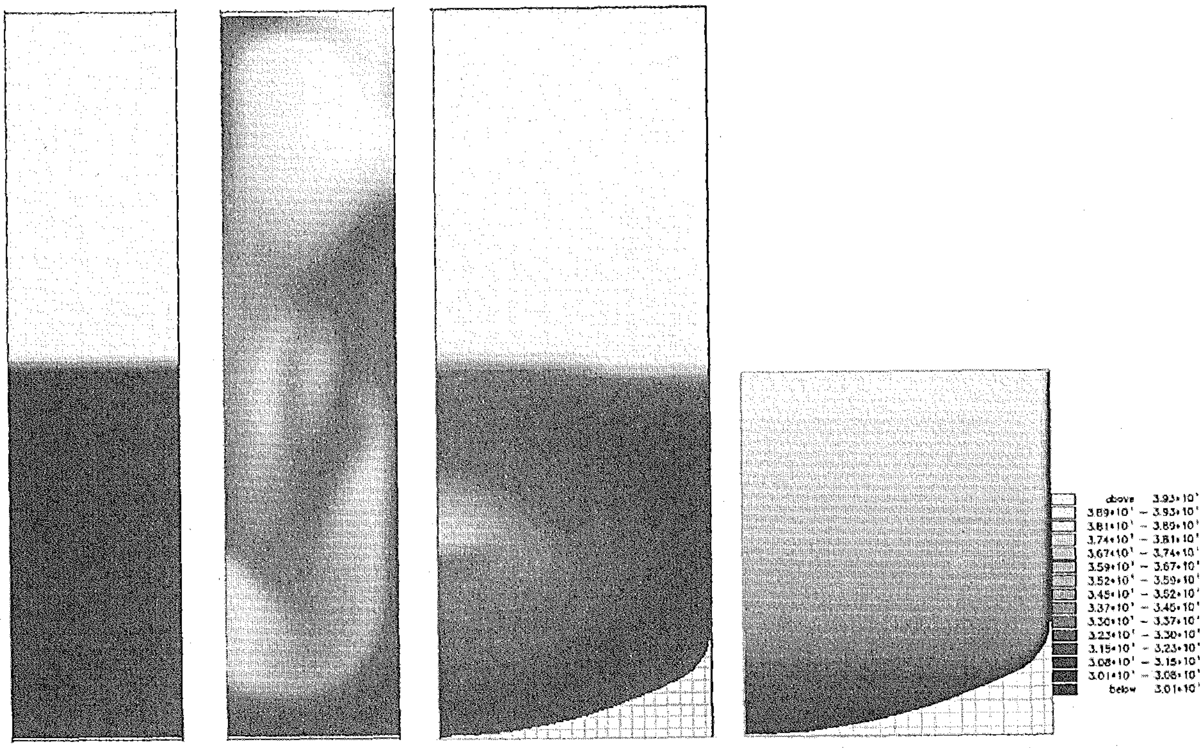

Fig 2. From left to right: Tracy simulation initial solution volume fraction and at 0.4 seconds into transient with a 2.8$ excess reactivity; solution volume fraction at 0.5 s into a simulation of the Toki-Mura simulation with a 2.5$ excess reactivity and an initial temperature of 20Deg C. and a similar simulation at steady state with the water jacket held at a constant 30 Deg C (far right).

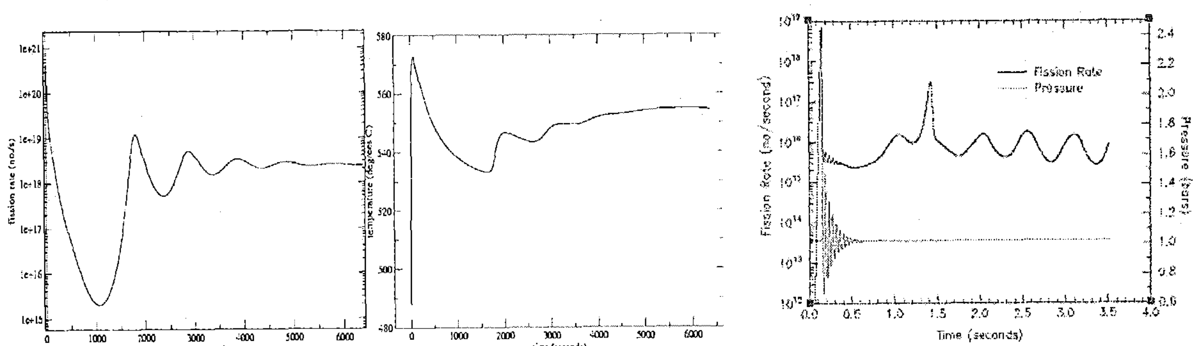

Fig. 3 A PBR reactor simulation 1st two graphs on the left. Fission rate then temperature versus time with a superficial gas inlet velocity of 440 cm/s. Far right graph; Toki-Mura simulated fission rate and pressure versus time for a 2.5 $ step simulation.

Granular and porous media: A BPR is a good example of criticality in a porous media. The FETCH axi-symmetric model of the PBR has an inner domain (shown in the model Fig. 2) comprising of 6 cm diameter pebbles. Fissile pebbles are placed in the outer annular PBR region to a radius of 1.85m and in the inner cylinder region (radius of 1m) there are graphite pebbles. The bed height is 11m and it is surrounded by graphite (top, bottom and sides) and control rods at the sides. Helium gas at 60 bars and 755 K is pumped from the top of the domain shown in the figure and exits from the bottom. The helium gas takes a convoluted path through the pebbles enhancing its effective gas diffusivity in the thermal energy equation above; see the temperature distribution in Fig 4. This temperature distribution distorts the power profile as shown in the figure. The nuclear fluidised bed whose particle volume fraction distribution is shown in Fig 4 (far left) has a similar geometry to the PBR but with a smaller 1.3 m diameter inner core in which TRISO particles are fluidised by helium at 60 bars pressure. The resulting fission rate is quite noisy with fluctuations on a time scale of 0.1 s but the temperature of the bed is remarkably steady. This is in contrast to the slowly varying and predictable fission rate of the PBR, see Fig. 3 - see also its maximum temperature versus time. The final simulation is a simulation of a criticality of a dilute plutonium concentration attached to a porous media. The resulting transient fractures the porous media and turns into granules. The resulting fission rates and pressures are shown in Fig. 4 (far right) for two simulations; one with an over pressure of 1 bar and the second with an over pressure of 60 bars.

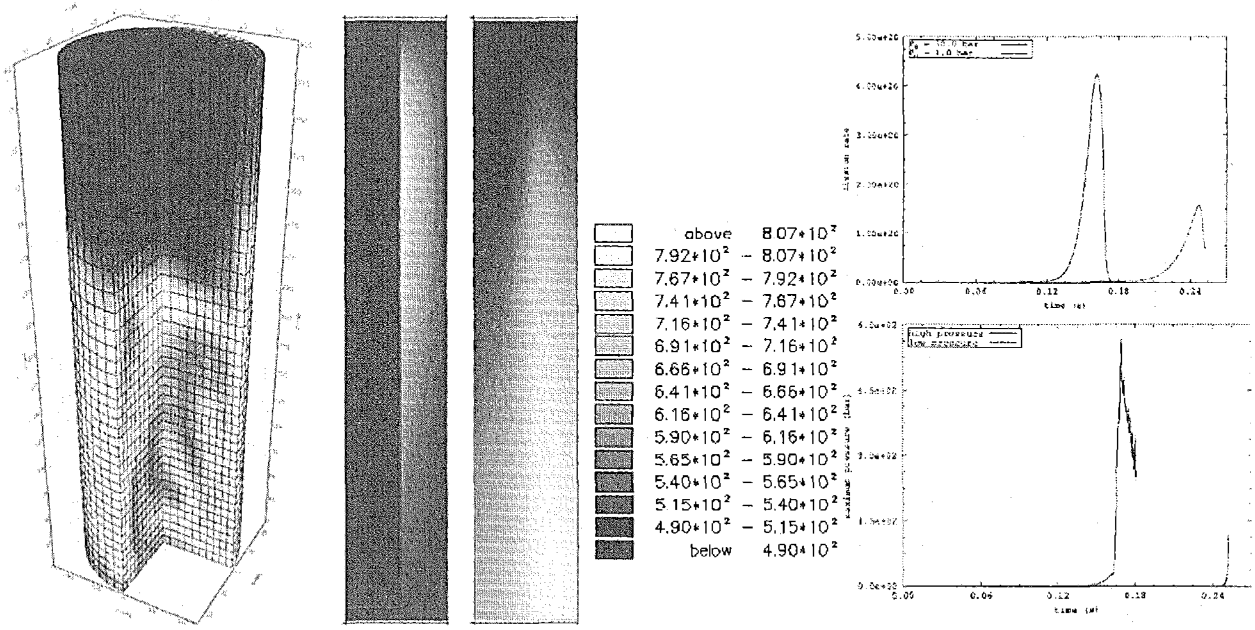

Fig. 4 Far left is a particle volume fraction distribution of a nuclear fluidised bed reactor. The inner cavity is shown with a quarter of the domain removed so that the inside of the reactor can be seen- white represents particle concentrations near maximum packing and black zero particle concentration. The next two diagrams are the power and temperature distributions of a PBR. Graphs on the far right show the maximum temperature of the 60 bar over pressure simulation and 1 bar over pressure simulations in a porous media initially at room temperature. The maximum temperatures of these simulations are 1600 Deg C and 800 Deg C respectively. Similarly, the maximum pressures are 550 bar and 120 bar respectively.

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