Progress in Inertial Fusion Energy Modelling at DENIM

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Abstract. New results of the jet driven ignition target are presented, both with direct and indirect drive. This target is based on the conical guided target used in fast ignition, but use only one laser pulse. The ignition of the target is started by the impact of a jet produced in the guiding cone, instead of using charged particles generated by a other high power laser. We have shown that a laser or X-ray pulse could be used to produce a high velocity jet of several hundred of km/s by an accumulative effect, and we use these ideas to design this new kind of targets. In order to increase the efficiency of the process, we scan in the simulations different materials, cone profiles and laser intensities. ANALOP is a code developed to calculate opacities for hot plasmas, using analytical potentials including density and temperature effects. It has been recently updated to include the radiative transport into the rate equations by mean of the escape factors, and in parallel a line transport code which solve self-consistently the rate equation and radiative transfer equation in 1D planar geometry has been also developed. We have developed a comprehensive methodology to compute uncertainties on activation calculations. First we developed a sensitivity-uncertainty analysis method, providing the uncertainties of the different inventory responses functions due to the uncertainty of each of the reaction cross sections separately. Lately, we have developed and proved the excellent behaviour of a Monte Carlo-based methodology in assessing the synergetic/global effect of the complete set of cross-sections uncertainties on calculated radiological quantities. The methods have been applied to the activation analysis of the National Ignition Facility (NIF) and different IFE concepts (HYLIFE and Sombrero). Research on multiscale modelling of radiation damage in metals will be presented in comparison with "*ad hoc*" experiments. Research on SiC composite is being pursued at macroscopic level. However, results from theory and simulation to explain that physics is being slowly progressing. The systematic identification of type of stable defects is the first goal that will presented after verification of a new tight binding MD technique. The different level of knowledge between simulation and experiments will be remarked. Our research on simulation of Silica Irradiation Damage will also be presented. We also will present the role of ingestion by tritiated foods, when the most important chemical forms of tritium, elemental tritium (HT) and tritiated water (HTO) derive in special form of tritium: Organically Bound Tritium (OBT)

1. Target design and fluid dynamic simulations

A new target design for ICF has been proposed and simulated, in search for a new and simpler way to achieve ignition using fast ignition [1]. The fast ignition concepts so far designed were based in a conventional implosion scheme combined with a secondary energy drive that imparts an ultra-fast pulse of energy that ignites a spark on the compressed target, starting a burning wave that spreads to the rest of nuclear fuel. That secondary drive has been proposed to be either laser or ions, but in every case different from the primary drive of energy, which increases the complexity and costs of the needed facilities.
The new proposed design contains the main ideas of fast ignition, while using a single energy drive that produces both fuel compression and ultra-fast energy deposition on it. The

deposition of energy is produced by the impact of a hypervelocity jet onto the compressed core, converting therefore kinetic energy into thermal energy that produces a hot spot. That hypervelocity jet is produced simultaneously to the fuel compression, by the ablationally driven collapse of a conically shaped system, which absorbs energy from the same energy source that produces the fuel compression. The design (*see FIG. 1*) includes a spherical conventional target for fast ignition (that is, not a full sphere) coupled to one or two cones pointing inwards in such a way that, under the proper design, produce hypervelocity jets arriving at the center of the system in the very precise moment of highest compression and temperature of the nuclear fuel. Between fuel and the conical system, there are conical shapes facing outwards, with the mission of preventing interaction between the two mentioned zones of the target.

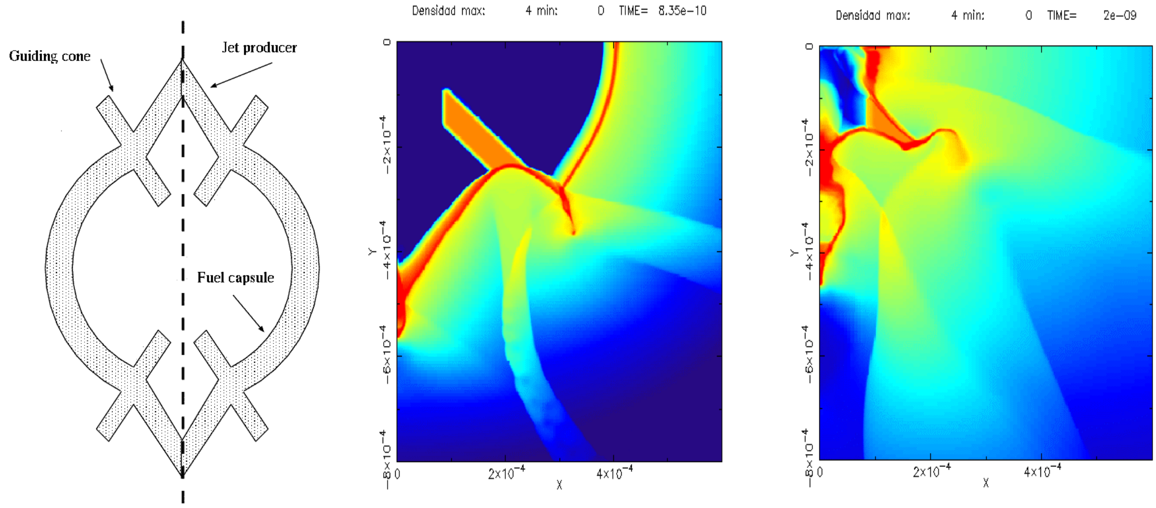

Figure 1:Schematics (a), and density plots at 835ps (b), 2000ps (c)

This design has been simulated using the ARWEN code [2] reaching to acceptable results [1]. The simulations have performed so far using one material for the whole system, showing in spite of that an appreciable temperature rise in the collision zone of the fuel core. In order to predict the propagation of the burning wave, conditions have to be established and proved to be reachable by the system in the simulations. The ARWEN code is being adapted to perform multimaterial calculations, which will show a better performance of the system. Other designs have been proposed [3] based on the idea of fast ignition by impact of high-speed matter, being the designs still in a stage of simulation and optimization of the designs.

The system has been simulated as inside of a hohlraum with an equivalent radiation temperature of 300eV, thus using indirect radiation. During the first instants, an ablation process starts, producing along the whole contour shock waves travelling inwards. These shock waves produce two different effects in both fuel shell and conical regions. On the spherical shell, and thanks to the guiding effect of the outward-facing cones, matter is compressed in a uniform way, as was first shown in [4]. At the same time, the shock waves on the conical region produce a jet that grows in time on speed and mass (figure 1b shows a density map in log scale).

Under a precise design that implies selecting angles and thickness, it was shown in [1] that an appropriate synchronisation could be achieved leading to a collision of the compressed fuel during the first stages of expansion while its core is in the most compressed state. The collision produce a hot spot in the lowest part of the compressed fuel (*FIG. 1c* shows a density maps in log scale).

2. Inertial Fusion Features In Degenerate Plasmas

Very high plasma densities can be obtained at the end of the implosion phase in Inertial Fusion targets, particularly in the so-called fast-ignition scheme, where a central hot spark is not sought at all. By properly tailoring the fuel compression stage, degenerate states can be reached. In that case, most of the relevant energy transfers mechanisms involving electrons are affected. For instance, bremsstrahlung emission is highly suppressed [5]. In fact, a low ignition-temperature regime appears at very high plasma densities, due to radiation leakage reduction [6]. Stopping power and ion-electron coulomb collisions are also changed in this case, which are important mechanisms to trigger ignition by the incoming fast jet and to launch the fusion wave from the igniting region into the colder, degenerate plasma. All these points are reviewed in a recent paper [7]. Although degenerate states would not be easy to obtain by target implosion, they present a very interesting upper limit that deserves more attention in order to complete the understanding on the different domains for Inertial Confinement Fusion. A programme F.I.N.E. (fast ignition nodal energy) has been developed. In the programme, the equations defined are valid for the degenerate and classical region, taking into account the possibility that the plasmas pass from a degenerate state to a classical state during the heating process. The results of the programme are only valid to study the possibility of ignition of plasmas in the fast ignition concept, not the burn up phase of the target. Ions have been the choice for ignitor heating until ignition conditions are reached. The optimisation of the compression phase in fast ignition inertial fusion, to obtain low temperature and high-density plasmas, can lead to a degenerate plasma. The equations that governs these plasmas are different that the classical ones. The decrease in Bremsstrahlung emission permits the decrease in ignition temperature, for high-density plasmas. This assumption has been demonstrated. The high energy needed to obtain this high density degenerate plasmas decrease the gain as compared to the results obtained in more moderated densities (see *FIG. 2).*

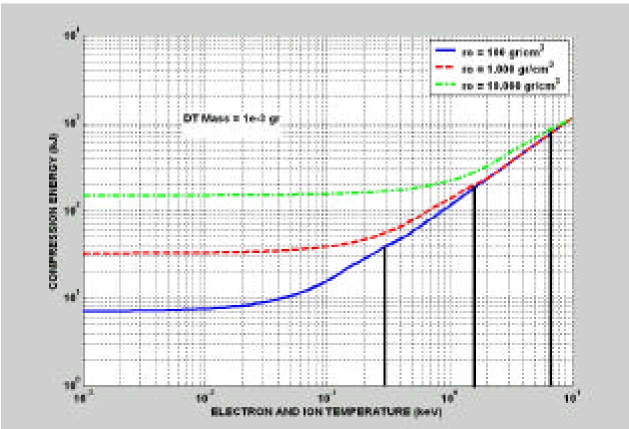

Figure 2.- Electron Compression (kJ) vs. Electron and ion temperature for three different densities of compression from 100 (lower) to 10. 000 g.cm^{-3} (upper)

3. Atomic Physics

Optical properties of plasmas are a powerful tool for plasma diagnosis. As it is known, optical properties depend strongly on the level populations into the plasma, both for plasmas at LTE and NLTE conditions. Up to now the model proposed by us, ANALOP code [8], was only able to model optically thin plasmas, i.e. assuming that the self-absorption is negligible. For optically thick plasmas the rate equations and the radiation transfer equation are coupled and

they should be resolved in a simultaneous way, since under these conditions the self-absorption of the radiation in the plasma influences considerably in the level populations.
Recently, we have proposed two different models in order to provide level populations for this kind of plasmas. The first one is based on the solution of the radiation transfer equation (LTNEP code) and the second one is based on the escape factor formalism (M3R-EF code).
In the LTNEP model, a 1D plasma divided into N cells is considered, having each cell different density and temperature. The profiles of density and temperature are provided by hydrodynamics calculations as input of the model. Then, the atomic kinetics and the radiation transfer equation are solved self-consistently for the whole plasma. The rates equations are solved in the Collisional-Radiative Steady State (CRSS) model and the atomic processes included are the following: spontaneous emission, resonant emission and stimulated emission, photoionization and radiative recombination, collisional excitation and dexexcitation, collisional ionization and 3-body recombination and dielectronic recombination.
The other model, M3R-EF code, introduces the reabsorption of the radiation through the escape factor formulism. The escape factor q denotes the mean probability that a photon emitted anywhere in the source travels directly to the surface of the source in any direction and escapes. In this work we have assumed a uniform distribution of emitting atoms and isotropic emission and a slab geometry [9]. The rate equations are also solved in the CRSS model including the same atomic processes but the resonant emission and photoionization.
In both codes, the atomic data required for the calculations are provided as an input file and the Stark profile is calculated by the Code Pim Pam Poum [10]. Then, the source function is obtained from the calculated line opacity and the bound-free opacity is provided by hydrogenic formulas. Finally, the specific intensity is determined solving the transfer equation with the known source function.
With these two models we have studied uniform aluminium plasmas, which length of 100 μm, for a fixed electronic density (10^{23} cm^{-3}) and several temperatures (from 200 to500 eV). It has been seen that for these plasmas the self-absorption must be included because it introduces relevant changes in the level populations. For example, for the Lyman series we obtain that the ratio of the level populations calculated assuming optically thick and thin plasma, P_{thick} / P_{thin}, is equal to 10 for the ground states and 10^2 for the excited states while for the Helium series is equal to 1 and 10, respectively. Taking into account the results of the ratios of populations shown before and according with the relations between the populations and the source function we obtain that source function for optically thick plasmas is ten times greater than for the optically thin ones. We have also verified that the escape factor formulism is a good alternative to those methods based on the resolution of the rate equations coupled to the radiation transport equation for uniform plasmas since LTNEP and M3R-EF codes provide similar results.

4. Activation of Materials: Safety and Environmental Issues

In the field of computational modelling for S&E analysis our main contribution refers to the computational system ACAB [11] that is able to compute the inventory evolution as well as a number of related inventory response functions useful for safety and waste management assessments. The ACAB system has been used by Lawrence Livermore National Laboratory (LLNL) for the activation calculation of the National Ignition Facility (NIF) design [12] as well as for most of the activation calculations, S&E studies of the HYLIFE-II and Sombrero IFE power plants with a severe experimental testing at RTNS-II of University Berkeley [13] (see *FIG. 3*). Pulsed activation regimes can be modelled (key in inertial confinement fusion devices test/experimental facilities and power plants), and uncertainties are computed on activation calculations due to cross section uncertainties. In establishing an updated methodology for IFE safety analysis, we have also introduced time heat transfer and thermal-hydraulics calculations to obtain better estimates of radionuclide release fractions. Off-site doses and health effects are dealt with by using MACSS2 and developing an appropriate methodology to generate dose conversion factor (DCF) for a number of significant radionuclides unable to be dealt with the current MACSS2 system. We performed LOCA and LOFA analyses for the HYLIFE-II design. It was demonstrated the inherent radiological safety of HYLIFE-II design relative to the use of Flibe. Assuming typical weather conditions, total off-site doses would result below the 10-mSv limit. The dominant dose comes from the tritium in HTO form. In the Sombrero design, a severe accident consisting of a total LOFA with simultaneous LOVA was analysed. Key safety issues are the tritium retention in the C/C composite, and the oxidation of graphite with air that should be prevented. The activation products from the Xe gas in the chamber are the most contributing source to the final dose leading to 47 mSv. We also analysed the radiological consequences and the chemical toxicity effects of accidental releases associated to the use of Hg, Pb, and Be, as IFE materials under HYLIFE-II framework scenario. For those three materials, the chemical safety requirements dominate strongly over radiological considerations. Also, the role of clearance as waste management option for HYLIFE-II was explored. For the confinement building, which dominates the total volume of the waste stream, all the material could be released from regulatory control for unconditional re-use after about one year of cooling following plant-shutdown. We also explored liquid wall options for tritium-lean fast ignition IFE power plants. Many single, binary, and ternary molten-salts were evaluated for their S&E characteristics, as well as for the required pumping power. In analysing the impact of cross section uncertainties on the contact dose rate from the activated concrete-gunite outer shell of the NIF reaction chamber, it is shown that current cross sections allows a reasonably confidence in the results. Regarding IFE, uncertainties in the prediction of the neutron induced long-lived activity in all the natural elements shown that for the HYLIFE vessel a significant error is estimated in the activation of several elements, while the estimated errors in the Sombrero case are much less important.

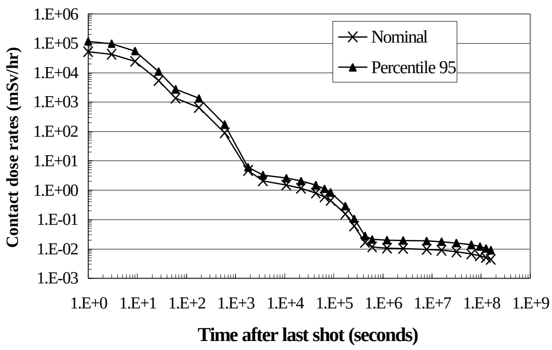

Figure 3.- Nominal (without uncertainties) and 95% confidence interval in the contact dose rate from the activated NIF gunite shielding after thirty years of operation

5. Radiation Damage of Fusion Materials

Ferritic-Martensitic Steels (in their more advanced type using experimentally testing Oxide Dispersion Strength, ODS, technique), Composites namely based in SiC, and Vanadium alloys are those materials presently under discussion as structural materials, together with C, Be, W, as first wall materials and some ceramics (silica, alumina) as optics and insulators elements. A systematic experimental program is partially pursued in different countries to assess their performance under the specific conditions they will be working on. It is very certain that a large and new irradiation facility is critically needed, and International Fusion Materials Irradiation Facility (IFMIF) will cover such role. In the present time also Multiscale Modelling (MM) is getting a large role in obtaining predictive characteristic and defining the needed experiments. A common methodology work appears for fusion programs but also for other nuclear systems such as fission (advanced Fission Reactors/Generation IV and Accelerator Driven Systems for Transmutation) with coincidences in some of the analysed materials. Key value has the validation of MM against specific experiments step by step at the microscopic and macroscopic levels and real understanding of damage processes, and effects of alloying and impurities elements. Microscopic parameters (using Molecular Dynamics, MD, DENIM models), which identify the effect of irradiation through new defects formation and diffusion, are being generated for some specific metallic materials (Fe, binary alloys FeCr, FeCu, V...) and their diffusion conducted by MonteCarlo [14]. Next step is being their interaction with dislocations (Dislocation Dynamics) and study of nucleation in the presence of He. That effect of He in FeCr alloys is certainly critical. We also derive macroscopic magnitudes using small-scale MM models in short simulation times by using MD defect-dislocation studies under stress [15]. We modelled pulse radiation damage, and we progress in the microscopic validation of Multiscale Modelling with experiments using pure and ultra-high pure Fe (effect of impurities) through a National Simulation-Experimental Program using ion irradiation [14]. Our work is also being concentrated in two IFE key materials (SiO_2/optics, SiC/low activation advance material). A MD *tight binding* scheme has been fully developed for β-SiC to understand the microscopic phenomena of the native defects and its diffusion at different temperatures. We reach an extraordinary good agreement among our calculated defects energetic and those results obtained using sophisticated and expensive method such as *ab-initio* at 2000K. We observe that β-SiC crystal remains perfect with its typical cubic structure at that temperature, and we have shown that the carbon atoms do not diffuse into the crystal. Self-interstitial silicon atom prefers the relation with atoms of the same specie due to the effect that the repulsive force of the silicon atoms is larger than the repulsive forces of the carbon atoms [16]. MD is also being used to study the defects produced in fused silica by energetic atoms, neutron and gamma irradiation. We determine the structure factor, the bond angle distribution, co-ordination and ring statistics, and we conclude very good agreement with measurement of generation of fused silica glass [17], (see *FIG. 4*). Threshold displacement energies have been computed as a function of the direction of movement of PKA, and cascades of 5 keV are being actually extended to 10 keV. Two modelling-experimental programs have been started with CIEMAT for Silica analysis, which will be extended in the future to Alumina as first wall and ceramics insulators.

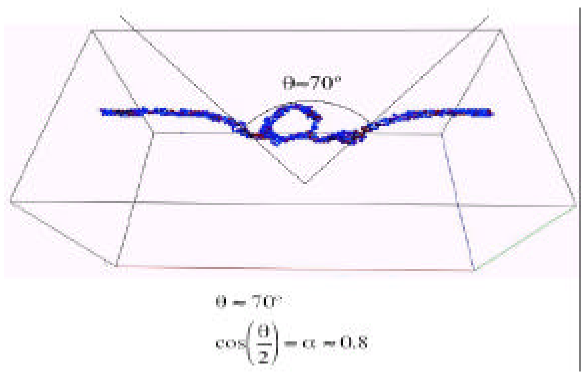

Figure 4.- Molecular Dynamic last temporal view before dislocation overpass defect loop [100] with an angle of q = 70°, which is the critical to estimate the resistance of such obstacle, conducting to determine stress-strain characteristics of the material.

6. Tritium atmospheric diffusion and Environmental Pathways to human chain

A large and completely new work has been performed in the analysis of consequences of tritium release according with expected source emission from IFE Conceptual Reactors and others nuclear systems [18]. Key aspect here is to consider all chemical forms of tritium (HT and HTO) and their conversion to Organically Bound Tritium (OBT) with soil processes and consequences of re-emission to atmosphere. We report several important conclusions for the primary and, namely, secondary phases of tritium transport in the environment with final consideration of different time-dependent phases in dosimetry. Our new approach allows a more realistic simulation, and significant more restrictive limit in tritium handling as classically assumed in conceptual systems. This methodology has been successfully used in the work performed for establishing Vandellós site for ITER (Contract under EFDA). The whole study of secondary phase drives to the conclusion that the behaviour of the tritium should be simulated using two well-differentiated studies: deterministic and probabilistic. Deterministic calculations are based on a fixed meteorological data given "a priori ", where the speed and directionality of the wind, class of atmospheric stability and rain intensity, as well as the boundary conditions of the means that surround to the atmospheric discharge (soil type, humidity of the air, temperature and solar intensity) are given. The probabilistic study is based on measured real meteorological analysis every hour, and the probability that individuals can present dose for internal irradiation of the tritium is considered. Our conclusion is that these probabilistic studies provide the real dynamics of the processes, which are different from deterministic case. The effect of formation of OBT is concluded of key importance.

Acknowledgements

Work performed under the Spanish National Programme on Thermonuclear Fusion Projects FTN2001-3886-C02-01 and FTN2001-3886-C02-02, the European Union keep-in-touch Program on IFE, and EFDA Tasks in Multiscale Modeling for Fusion (2003, 2004). A large collaboration exists on IFE activities with Lawrence Livermore National Laboratory and University of Berkeley (USA), SCK-CEN Mol (Belgium), Edf and CEA (France), University of Cagliari (Italy). This work has also performed under collaboration with CIEMAT in CSN/UNESA VENUS-II (2000-2003), and REVE Spanish Project (2004-2007).

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