RESULTS FROM POST-CLOSURE DOSE ASSESSMENT MODELS WITH "ALTERNATIVE" LEVELS OF DETAIL

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An important issue for long-timescale dose assessment is how to use site descriptive material to the assessment model over extended time periods. Assessments need to strike a balance between simple models and more complex approaches that draw more extensively on this site-specific information. This paper explores the relative merits of complex versus more stylized biosphere models in the context of a site-specific assessment.

We report on work undertaken on behalf of, and in co-operation with, the Swedish Radiation Safety Authority (SSM) in review of the recent license application submission by the Swedish Nuclear Fuel and Waste Management Co. (SKB). The work is contributing towards Working Group 6 of the International Atomic Energy Agency's (IAEA's) programme on Modelling and Data for Radiological Impact Assessments (MODARIA), which is developing guidance on addressing environmental change in long term safety assessments of radioactive waste disposal facilities. Complementing this is material from CIEMAT's development of detailed soil models capable of dealing with changes of soil hydrogeochemistry in response to changes in the depth of the water table.

I. BACKGROUND – MODEL REQUIREMENTS

What constitutes a "fit-for-purpose" model depends strongly on the assessment context, the site context, the regulatory context and, to a large extent, the stage in the iterative process that is the licensing process.[1]

In the late 1980s and 1990s SSM's forerunner (SSI) sponsored a series of intercomparisons to address different aspects of subject as applied to environmental radioactivity.[1,2,3] This was subsequently followed up by the IAEA's BIOMASS program which codified the *Reference Biospheres* approach.[4] At that time models for generic applications were relatively simple in structure and those intended for more clearly defined sites tended to be configured to the site-specific detail.[5] The two strands generic and specific are still discernable in today's ongoing model development.

Those organizations having recently submitted license applications for the construction of deep geologic disposal facilities for high-level radioactive waste (SKB, the Swedish Nuclear Fuel and Waste Management Company[6] and POSIVA, the corresponding organization in Finland[7]) have assembled detailed site descriptive modeling, since the site is known and well characterized. The dose assessment models supporting their applications are correspondingly complex and detailed.[8,9]

The regulatory framework in Sweden[10] and Finland[11] does not specify the way in which the calculations should be performed. Instead the protection objectives are set out so that the method to be used to assess future impacts is left open to the licensee. With a more prescriptive framework (e.g., in the USA[12]) the regulator has a more direct role in determining the nature of the calculation.

Detailed dose assessment models are not only used in HLW-assessments. Also in Sweden, SKB have recently submitted an application to the Swedish government to extend the existing I/LLW repository at Forsmark (the location of the proposed repository for spent fuel). In Spain, CIEMAT (Research Centre for Energy, Environment and Technology) have been engaged in development of models for the assessment of I/ILW repositories, specifically the facility at El Cabril.[13] The role of soil hydrology and the soil-plant interaction and how they evolve can be important in such assessments.[14,15,16] The interpretation and usage of standard models for the soil-plant interaction have also been studied in other dose assessments.[17,18]

Currently the International Atomic Energy Agency (IAEA) is finalizing its' MODARIA project.[19] The aim is to enhance confidence in dose assessment models with focus on long term climate change, in part by developing a consensus on modelling philosophies and approaches. This implies system evolution is an integral feature of assessments. Both CIEMAT and SSM are active in this forum with contributions involving the models described below.

This paper considers results from SSM's "alternate" models used to support the review of SKB's spent-fuel license application, specifically in respect to the treatment of long-term site evolution. We also consider the use of more detailed FEP-based models with higher spatiotemporal resolution. Results indicate how alternate models can be used to support the licensing process and indicate where future developments in dose assessment modelling are required.

II. MODELS AND APPLICATIONS

II.A. Types of model

Table I summarizes the models considered here. They can be categorised as “simple” (non-evolving, single ecosystem), “complex” (evolving, multi-ecosystem) and “advanced” (FEP-based, high spatiotemporal resolution) models. The applications for which they are intended are outlined below.

II.B. Models for Forsmark

The Forsmark site is located on the Baltic coast with a terrestrial landscape including lakes, mires, forest and arable land. The land at the site is projected to continue to rise due to post-glacial uplift (legacy climate change from the previous deglaciation) leading to significant ecosystem transitions over the next ten to twenty thousand years. SKB’s Radionuclide Model[8] is built on a landscape evolution model, whereby radionuclide releases to distinct hydrological basins/sub-catchments (termed ‘objects’) are represented as they evolve through land rise. The large number of data sets obtained by landscape development and site descriptive modeling[21,22] feed into the Radionuclide Model to describe the continuous development over time by varying the size and properties of aquatic and terrestrial areas according to the development of each specific biosphere object. “Landscape Dose Factors” (LDFs, (Sv $year^{-1}$)(Bq $year^{-1}$)$^{-1}$) for a range of relevant radionuclides in the disposed inventory are calculated to scale geosphere discharges so providing a measure of the potential radiological impact.

The LDF values are used in Section III to compare alternative interpretations of the future landscape. While the SKB model is a highly complex, spatially extended and evolving “landscape model”, SSM’s review models differ: GEMA-Site is an evolving model of a representative hydrologic basin typical of the future Forsmark landscape[20]. It takes the SKB database and, in particular, looks at the spatial discretisation of the basin and how this can influence the evolving flow system in the regolith of the basin. This too can be classed as a “complex” model.

The third model - the “simple” model has been developed by Walke using the BIOMASS Reference Biospheres Methodology for different ecosystem types.[23] Parameters describing the system are constant in time. As with GEMA-Site it is configured to use the common SR-Site dataset (as a first approximation).

There are commonalities in the structures of the SR-Site, GEMA-Site and models derived using the BIOMASS Reference Biospheres Methodology (RBM models) for dif-

TABLE I. Classification of models and characteristics. Vertical discretisation shows number of layers in the soil column. Horizontal indicates the spatial extent of the model. Models use either annual or monthly parameter values. Soil-plant interaction is by concentration ratio (CR) or as a dynamic uptake process.

Model and type		Ref.	Discretisation: Vert.	Discretisation: Horiz.	Discretisation: Time	Soil-plant model	Evolving
“Complex” – evolving, linked multi-ecosystem	SKB SR-Site	8	3	2[c]	Year	CR	Yes
	GEMA-Site [a]	20	3	3	Year	CR	Yes
“Simple” – constant, independent single ecosystem	RBM [b]	23	Variable	1	Year	CR	No
“Advanced” – FEP-based, high spatiotemporal resolution	CIEMAT	14, 15	10	1	Month	Dyn.	No
	GEMA-10 [a]	16	10	1	Month & year	CR or Dyn.	No

Notes:

a GEMA – Generic Ecosystems Modelling Approach. Several models in the GEMA series have been developed for SSM.

b RBM - “Reference Biosphere Models”. Multiple instances of different models are used to represent different ecosystem types. Based on the BIOMASS methodology, the discretisation is selected by the developer.

c Two lateral areas are defined for each basin in the landscape. Many basins are modelled separately and linked in the landscape model.

ferent ecosystems. GEMA-Site and the SR-Site model combine multiple ecosystems in the same model structure and different ecosystem types are active as the evolution progresses.

Where SR-Site's dose assessment model links different (largely independent) basins in the landscape, assessing the radiological consequence of release to each of the potential recipient basins, the single basin in GEMA-Site can be run in a probabilistic mode with varying characteristics. In this way both models "sample" the future landscape.

The essential difference between "complex" and "simple" models therefore lies in the way in which the models deal with system evolution. In the simpler approach multiple time-invariant models are used independently. In the more complex approach there are a considerable number of in-built switches that activate or deactivate specific processes according to the current state of the evolving system. During any particular system state the complexity of FEP representations is similar in "complex" and "simple" models.

II.C. "Advanced" models

Both CIEMAT and SSM have developed an interest in modeling redox effects in the soil column and the influence of a moving water table on interannual timescales, leading to models with more advanced FEP representations.

The main focus of the results presented in Section III.B is the CIEMAT model developed to assess radiological impacts of the I/LLW facility at El Cabril. The site is located in a semi-arid valley in the hills of the Sierra Albarrana, in the province of Córdoba. Ongoing anthropogenic climate change means that uncertainties in soil hydrology are important. This has prompted CIEMAT to develop tools to investigate time-varying soil conditions.

The initial CIEMAT model[15] addressed selenium transport and accumulation in soils, accounting for variation in sorption as a function of water saturation linked to local redox-sensitive behavior in each of the ten soil layers. A development[16] was reconfigured and run for ^{238}U and ^{226}Ra. The model adopts a 1D vertical compartment model, employing a mass balance approach so that net precipitation inputs are balanced against losses by evaporation, transpiration and drainage, allowing for changes in storage in the soil layers. Monthly rather than annual averages are used as input parameters.

The GEMA-10 model developed on behalf of SSM was motivated from similar considerations and is similar in structure. The water table in Sweden is close to the surface – within 1 m in many agricultural situations (see Ref. 23). Bioturbation was included between the non-saturated layers and the model, otherwise simplified with respect to the CIEMAT interpretation, was configured from the outset to be a flexible assessment-level model, incorporating a range of radionuclides: ^{79}Se, the ^{226}Ra chain, ^{129}I, those relevant to the Swedish HLW program.

Compared to the models for Forsmark described in Section II.A, the CIEMAT[14,15] and GEMA-10 (Ref. 16) models feature higher vertical resolution in the soil column as well as monthly averaged parameters to describe water fluxes and soil chemistry. They also allow for the modelling of the soil-plant interaction to be addressed as a dynamic process (see also Refs. 10, 17). Both models originated with the aim of modeling the effects of variability in water table height. Notwithstanding the difference in climate state at the Forsmark (temperate/boreal) and El Cabril (Mediterranean) sites, there is a high degree of commonality in the models, albeit with different input data.

In comparison to the structures of the SR-Site models, these models are more detailed in that they include more processes (bioturbation, dynamic root uptake) with higher (fixed) vertical resolution and with monthly rather than yearly temporal resolution of input parameters. In this way they are beyond the standard modeling approach employed by the models in Section II.A. They can therefore be described as more "advanced" than the standard assessment models.

III. RESULTS AND DISCUSSION

III.A. "Complex" Landscape and "simple" models

Fig. 1 compares the SR-Site best-estimate LDF results[6] with the corresponding values from Walke's "simple" models[23] and a set of alternate results from GEMA-Site.[20] SKB's LDFs are based on the assumption of 1 Bq year^{-1} input to the base of the regolith and this same source term is used for each of the "simple" and GEMA-Site models. Results are presented for ^{79}Se, ^{94}Nb, ^{129}I and ^{226}Ra. These are important radionuclides in the disposed spent-fuel inventory with different sorption properties – selenium and iodine are relatively weakly sorbing and niobium and radium (with contributions from ingrowing daughters ^{210}Pb and ^{210}Po) are all relatively strongly sorbing. Doses are calculated for foodstuffs available in the evolving ecosystems. Wells in the bedrock provide drinking water resources for both the SKB and "simple" models. GEMA-Site assumes water from lakes (when present) or the surface drainage streams (agricultural period). Results for the reference model with a well in the lower regolith are also shown.

SKB's LDFs are derived as the highest dose from all landscape objects over the time period of the assessment. The set of landscape objects is the sample space from which the LDF is obtained. It constitutes objects of different sizes.

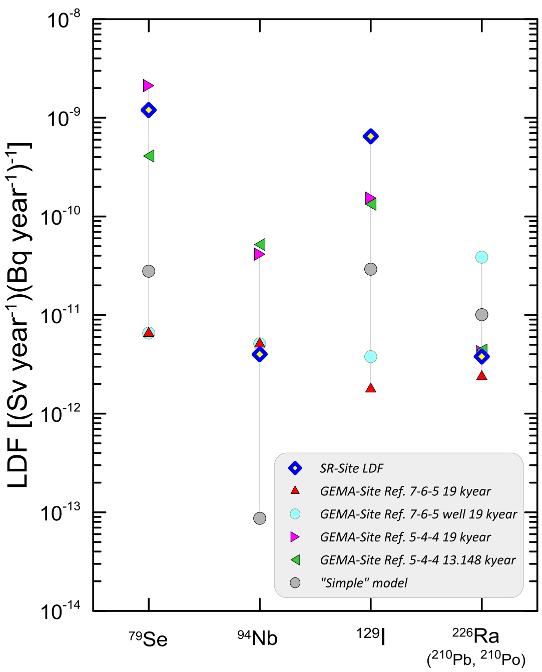
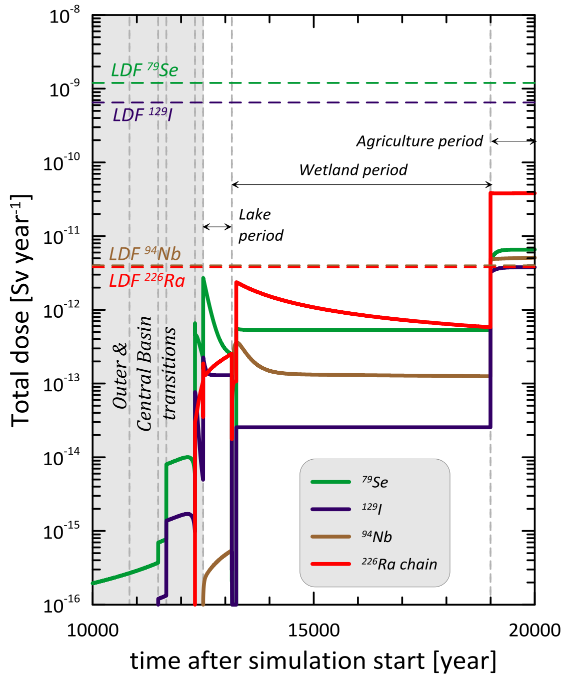


Fig. 1. Comparison of calculated doses for unit release of ^{79}Se, ^{129}I and ^{226}Ra to the base of the regolith. SR-Site results are the peak dose over all landscape objects and are used for comparison. The "simple" model assumes a small object and results from the GEMA-Site model are shown for four alternative implementations.

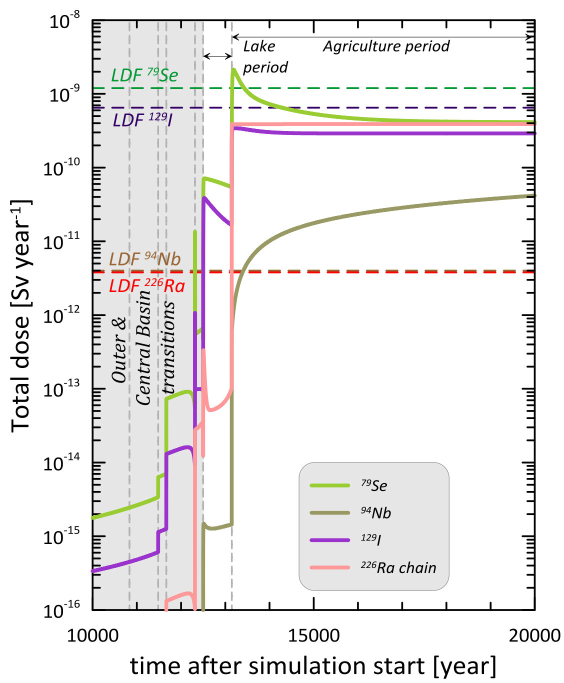
The "simple" model assumes a small object if 10^4 m², comparable to small agricultural areas in the SR-Site landscape description. GEMA-Site employs two sets of area data - the reference object (see Ref. 20) with Outer, Inner and Central basin areas in the ratio 10^7:10^6:10^5 m² respectively - the 7-6-5-model. A small basin 10^5:10^4:10^4 m² is also modelled - the 5-4-4-model. The effect of the time of conversion to agriculture in the Central basin is shown, with t_{agri} = 19 kyear compared to conversion as soon as possible, at the end of the lake stage at 13.148 kyear (determined by the model at run time in response to the initial configuration of the system and the land uplift parameter).

For the weakly sorbing radionuclides (^{79}Se, ^{129}I) the LDFs calculated by SKB are at the upper end of the range, with the results from the "simple" models more than an order of magnitude lower. With agricultural transition at 19 kyear, the 7-6-5 (reference basin) model gives the lowest doses and it is only the small basin (5-4-4-model) that approaches the SKB LDFs. Notably the early conversion to agriculture with such a small basin gives a higher dose for ^{79}Se. Usage of lower regolith wells does not significantly increase the dose for these nuclides in the GEMA-Site modeling.

For the more strongly sorbing ^{94}Nb and the members of



(a) Reference basin (7-6-5), $t_{agri} = 19000$ year .



(b) Small basin (5-4-4), $t_{agri} = 13148$ year (conversion as soon as possible)

Fig. 2. Evolving doses in the model described in the GEMA-Site model (including well usage for domestic and livestock water consumption). Reference and "small basin" models. See Ref. 20 for a brief description of the model.

the ^{226}Ra chain the role of k_d is clearly important. Niobium is more mobile in the lower regolith than in the superficial media. The GEMA-Site 5-4-4 model therefore gives an order of magnitude higher dose than the SKB LDF. Members of the ^{226}Ra chain are more strongly retained at depth in the system and there is relatively little variation in the dose from the release of ^{226}Ra system. Only in the case of the well in the lower regolith (GEMA-Site, 7-6-5 model) is the dose higher than the values calculated in the "simple" model and the SR-Site implementation.

GEMA-Site (and the SR-Site model) evaluate the evolution of the system from the end of the previous glaciation out to 20 kyear in the future. In this way the aim is to model all of the major changes to the biosphere. Fig. 2 clearly demonstrates that agricultural systems give rise to the highest doses. Before year 10000 all of the basin is beneath the Baltic and doses from marine foodstuffs are lower than those at later times from terrestrial ecosystems.

The dynamics of dose evolution in the GEMA-Site model demonstrate the effect of changes to the hydrological regime in the basin. With the reference model in Fig. 2(a), there is some accumulation in the upper regolith upto the end of the lake stage in the Central basin. On conversion to wetland this is progressively leached out, as net precipitation drains through the wetland. In Fig. 2(b) agriculture starts as soon as the lake is shallow enough to allow the emplacement of drainage pipes in the mid-regolith. The residual activity concentration in the upper regolith is therefore available for uptake in agricultural crops before leaching through the rooting zone becomes effective. Agricultural doses from ^{79}Se peak at this time.

The two variables – area and time of transition to agriculture have an important role. Overall the SR-Site model predicts relatively high doses from the low k_d radionuclides (^{79}Se and ^{129}I) but there is an indication in Fig. 1 that the doses from higher k_d radionuclides could be higher with alternative interpretations of hydrology.

For the ^{226}Ra chain, it is well water that dominates dose. The well water sub-models differ between the three models considered here. SR-Site and the "simple" model assume a deep well in the bedrock as the source. In the GEMA-Site model well abstraction is from the lower regolith where there can be significant accumulations of sorbing radionuclides.

Overall, the "alternate" models applied to the SR-Site dataset build confidence in the license model – doses are conservative. They also suggest that additional model development might be needed in respect of the more highly sorbing radionuclides.

III.B. Advanced soil-plant modeling

In contrast to the site-specific model discussed above, the *raison d'être* of the "advanced" models is to investigate alternative representations of FEPs. The context remains the development of assessment-level models; reviewing what FEPs might be required in assessment models and seeing how they can be practically added. We focus here on results affecting uptake in plants.

Kłos & Wörman noted that there are alternatives in the representation of the soil-plant uptake and that there can be considerable uncertainties in plant concentration (and thereby dose) as a result.[17] These results used the standard annual temporal resolution approach with a ten layer 1 m soil column. Results were presented for soil-plant interaction by concentration ratio as well as dynamic uptake. Similarly structured soil models with higher temporal resolution[14,15,16] show similar variation.

The issue is with the appropriate value of the concentration ratio. Fig. 3 shows the derived interannual variation for the soil-plant concentration ratio (CR) calculated by the CIEMAT model.[16] This is simply the ratio of the dynamic plant concentration to the concentration in the soil column. The appropriate value that should be used in the dose assessment model would therefore be that at harvest (month 9). The implication of a simply interpreted constant CR value for use in assessment models is therefore of questionable utility. Further investigation is suggested.

What impact does this uncertainty in the appropriate soil-plant model have on plant concentrations? Fig. 4 illustrates the results of using the GEMA-10 model[16] with the distribution of ^{79}Se, ^{129}I and ^{226}Ra resulting from GEMA-Site reference model (Fig. 2a).

There are clear differences between the plant concentrations for three variants of the soil-plant interaction. The highest plant concentrations come from the case with monthly parameters used in the calculation (precipitation and evapotranspiration influencing a range of soil parameters) with dynamic soil-plant transfer. The same model using annual-average soil hydrology with a dynamic model gives lower crop values. Slightly higher are results for the annually averaged hydrology using CR to model plant concentrations.

The influence of this model feature on plant concentration is nuclide dependent. For ^{129}I and ^{226}Ra it is around 1 to 1½ orders of magnitude. For ^{79}Se – with its CR values – the overall uncertainty is fairly constant in time; less than one order of magnitude. There is scope for further research and this is being undertaken by CIEMAT and SSM.

III.C. Synthesis – impact on uncertainties

Two assessment contexts have been presented here: a detailed site-specific assessment related to an application for a license to construct a deep-geologic repository for spent fuel and the development of assessment-level models that "push the envelope" beyond what is traditionally considered in dose assessment modelling.

By the nature of the advanced stage of disposal program in Sweden, the license application and associated review models also deal in advanced concepts. System change and the consequences of climate change are prominent. Over the timescale of the dose assessment (up to 20 kyear) the legacy of climate change at the end of the latest glacial episode is still working itself out in Fennoscandia.

Results in Section II.A indicate that alternative approaches to the modelling of system change lead to similar conclusions in respect of the radiological impact of release to the future landscape at Forsmark. There are two features of interest; retention in the upper regolith and the interpretation of the hydrology in the regolith that has a major influence on the distribution in the components of future hydrologic units – the basins in the future landscape.

Changes of ecosystem state are important. Currently models are relatively crude in the way in which these transitions are modeled with step changes apparent in Fig. 2. As indicated changes in the flow system concomitant with ecosystem change can lead to differences in dose depending on when they occur in the evolutionary sequence.

As part of the overall verification and confidence building the "simple" models have an important role. They can be used to bound the results from more "complex" evolving models.

It is the way in which the more complex models capture changes to the system that is important. In the examples shown there are differences between the SR-Site (licensee) and GEMA-Site (review) models that can be traced to the way in which the hydrologic flow system in the regolith of the basins is interpreted. In the SR-Site model the relative water fluxes in the model remain constant in time whereas in the GEMA-Site model the flow vectors are time-dependent, contingent on the nature of the ecosystems. This feature accounts for the differences in the landscape dose conversion factors for weakly and strongly sorbing radionuclides.

The "advanced" models discussed here have another role. They ask questions about the way in which FEPs are included in assessment level models. A common theme arising from this type of high spatiotemporal resolution model is that there is a need to review the model implemen-

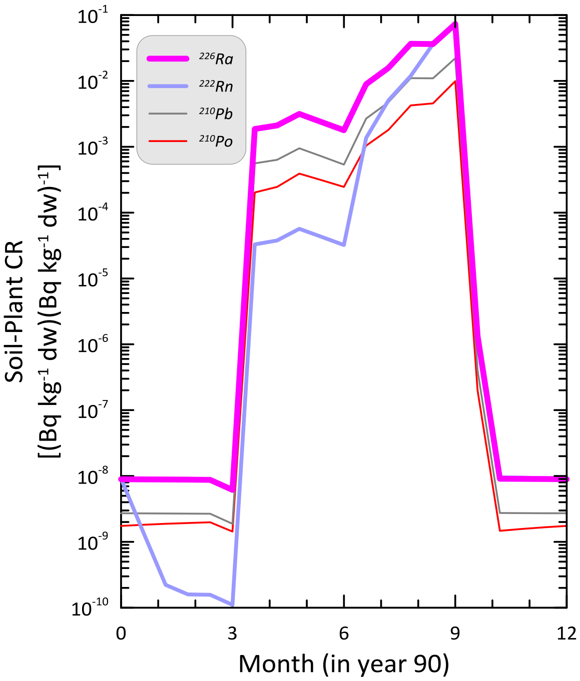


Fig.3.Interannual soil-plant concentration ratio derived for ^{226}Ra and long-lived progeny in the CIEMAT model[14]. Results for the 90th year in a 500 year simulation. Constant 1 Bq year^{-1} input at the base of the soil column. (Plot modified from Ref. 16).

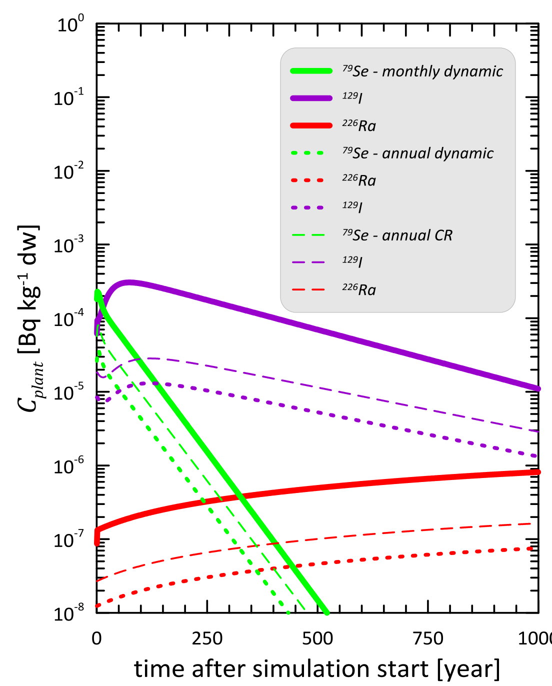


Fig. 4. Evolution of the GEMA-10 plant inventories (winter wheat) assuming the initial distribution in the agricultural soil profile taken from the GEMA-Site reference model (Fig. 2a). Results for alternative assumptions for the soil-plant model are illustrated.

tation of the soil-plant relationship. Such alternative interpretations could account for around an order of magnitude increase in dose factors† compared to the standard modeling approach.

Both SSM and CIEMAT are active in these respects. Further results will be reported to the IAEA's MODARIA project, the final meeting of which will take place in the Fall of 2015.

IV. CONCLUSIONS

As is generally the case in biosphere dose assessments, the treatment of hydrology is fundamental to the results obtained. The main differences between the "simple" approach and the SKB SR-Site models on the one hand and the GEMA-Site model on the other is the way in which the flow system changes in the latter. There remains scope for a better implemented understanding of the evolution of the flow in the regolith layers. The "complex" models here illustrate how a quasi-3D approach might be used in the future. Similarly the "advanced" models describing, in particular, the soil-plant interaction are also a useful method for improving model capabilities.

Understanding of current and future "complex" and "advanced" models can best be aided by the application of simpler modeling to the same site and assessment context. The inherent uncertainties in the long-term development of biosphere systems coupled to the detail in some of the models that have recently been used in performance assessments mean that simple and transparent models can illuminate the workings of more sophisticated models. Complex models use more of the available site-specific information and contribute to an understanding of process interactions and effects of system heterogeneity. However, the degree of conservatism associated with complex modelling approaches can be difficult to interpret. A balance between the two approaches is fruitful and there are clear benefits to applying both to the same assessment.

There can be no "one-size-fits-all" dose assessment model. Complex and simple models should be used in mutual support. To do so brings benefits in terms of clarity from the descriptive power of the models as well as providing enhanced confidence in the overall assessment.

The development of more advanced models is therefore necessary to "push the envelope" and to raise additional questions – e.g. the soil-plant hysteresis implied by high spatiotemporal resolution models. Such models can give confidence that nothing of importance has been overlooked by the use of overly-simplistic approaches.

† Remembering that dose factors scale radionuclides discharges across the geosphere-biosphere interface.

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