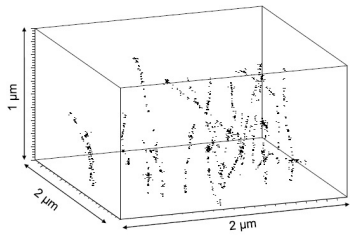
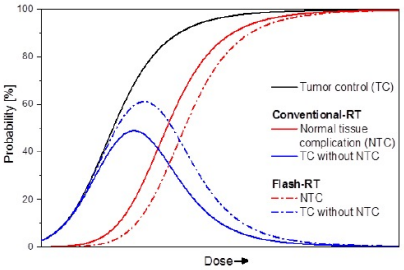
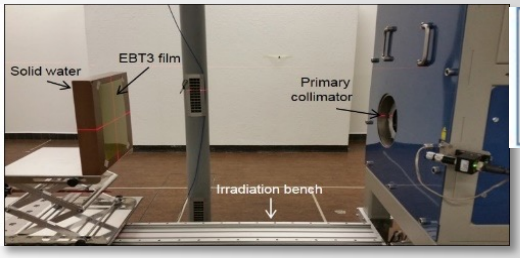
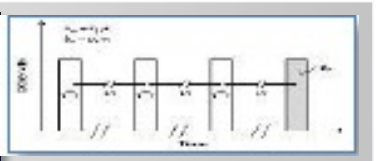
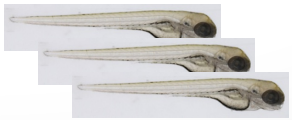










Geant4 Annual Collaboration Meeting

Ngoc Hoang Tran, CENBG

G4DNA chemistry example for Water radiolysis with Scavengers

in collaboration with Laurent Desorgher, Flore Chappuis and Sébastien Incerti

Water radiolysis with Scavengers

Many applications of water radiolysis using scavengers

- **Calculate initial G-values (G°) of radio-induced species**
- **Study biological materials**

Simulation of Scavengers

The implementation of scavenger effect in the Monte Carlo model introduces some problems:

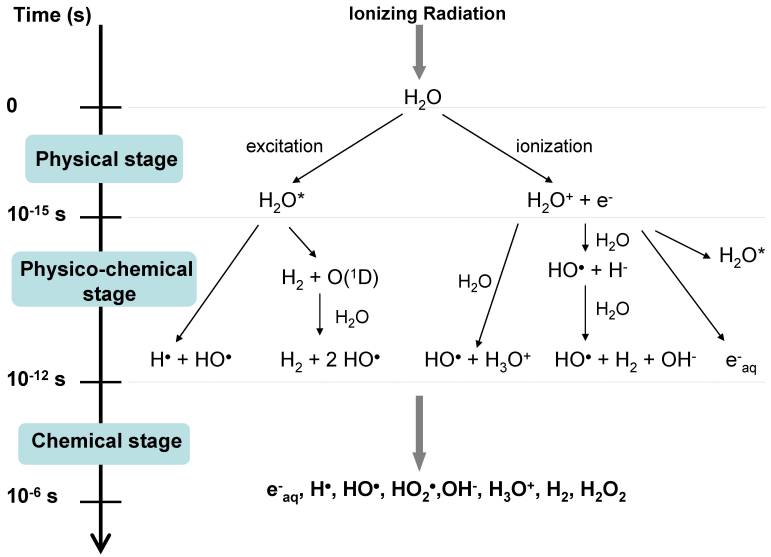
- Due to large number of scavenger particles in the system, the particle-based representation cannot be used

- In an approximation, the scavenging molecules are modeled as a continuum which is presented in standard deterministic treatments:

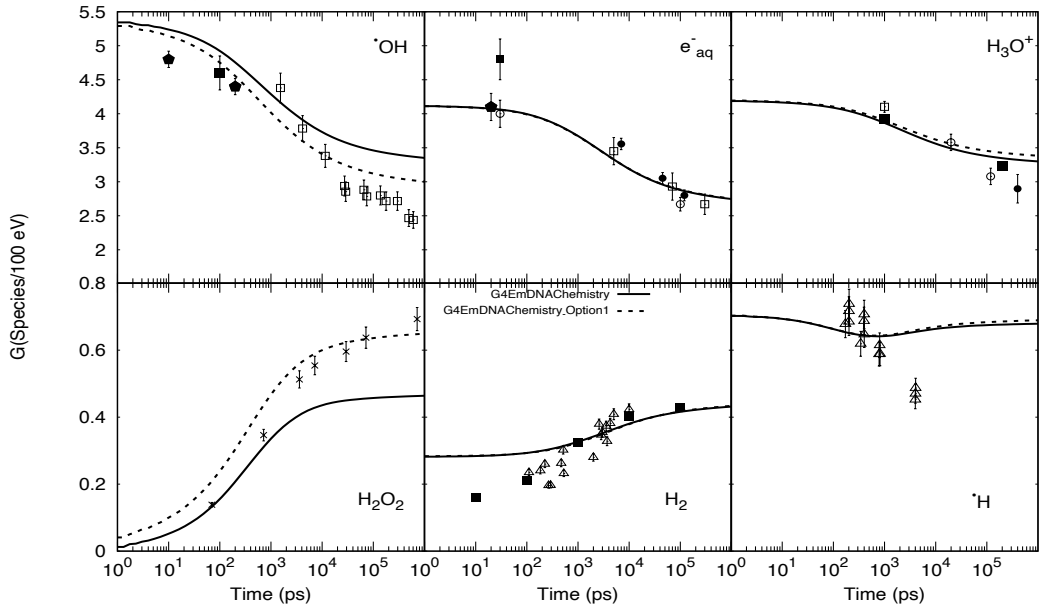
$$\frac{dX}{dt} = -kC_sX$$

C_s : is oxygen concentration,
X : is the survival probability of the species
k : is the reaction rate

GEANT4-DNA chemistry



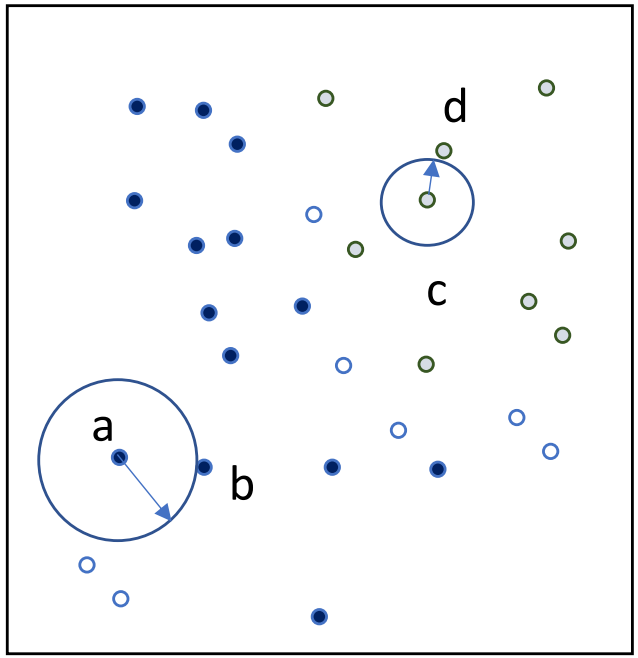
Electronic state	Decay channel	Fraction
All ionization states	$H_2O^+ + H_2O \rightarrow H_3O^+ + {}^\bullet OH$ (through proton transfer)	100 %
Excitation state A1B1: (1b1) → (4a1/3s)	$H_2O^* \rightarrow {}^\bullet OH + H^\bullet$ $H_2O^* \rightarrow H_2O + \Delta E$	65 % 35 %
Excitation state B1A1: (3a1) → (4a1/3s)	$H_2O^* \rightarrow HO^+ + {}^\bullet OH + e^-_{aq}$ $H_2O^* \rightarrow {}^\bullet OH + {}^\bullet OH + H_2$ $H_2O^* \rightarrow H_2O + \Delta E$	55 % 15 % 30 %
Excitation state : Rydberg, diffusion bands	$H_2O^* \rightarrow HO^+ + {}^\bullet OH + e^-_{aq}$ $H_2O^* \rightarrow H_2O + \Delta E$	50 % 50 %



Geant4-DNA: Step by Step (SBS) and Independent Reaction Time (IRT) methods

- Using the dynamic time step model
- Describing the diffusion process corresponding to the Brownian motion (SBS)
- Simplifying the multiple particle problem to the two-particle problem in an approximation (IRT)

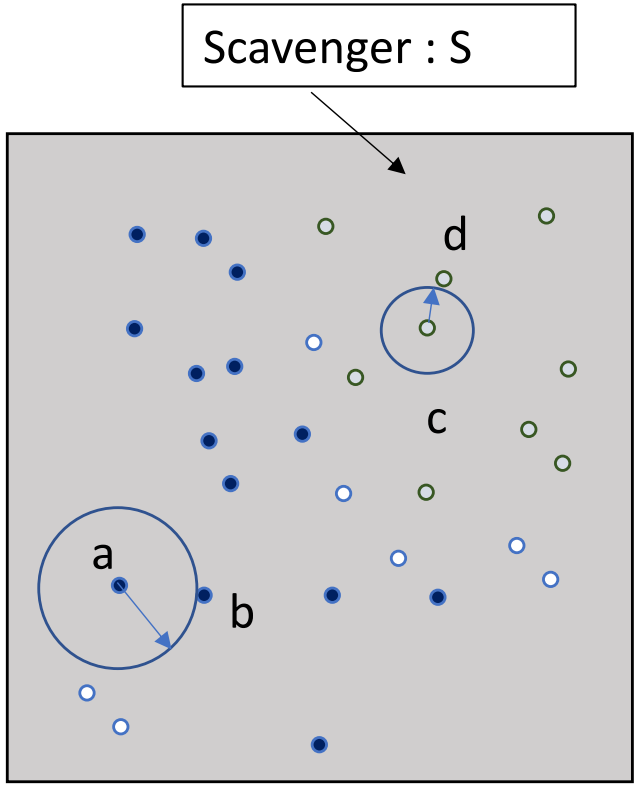
Independent Reaction Time Model



#	reactions	time
1	c + d	t_1
2	a + b	t_2

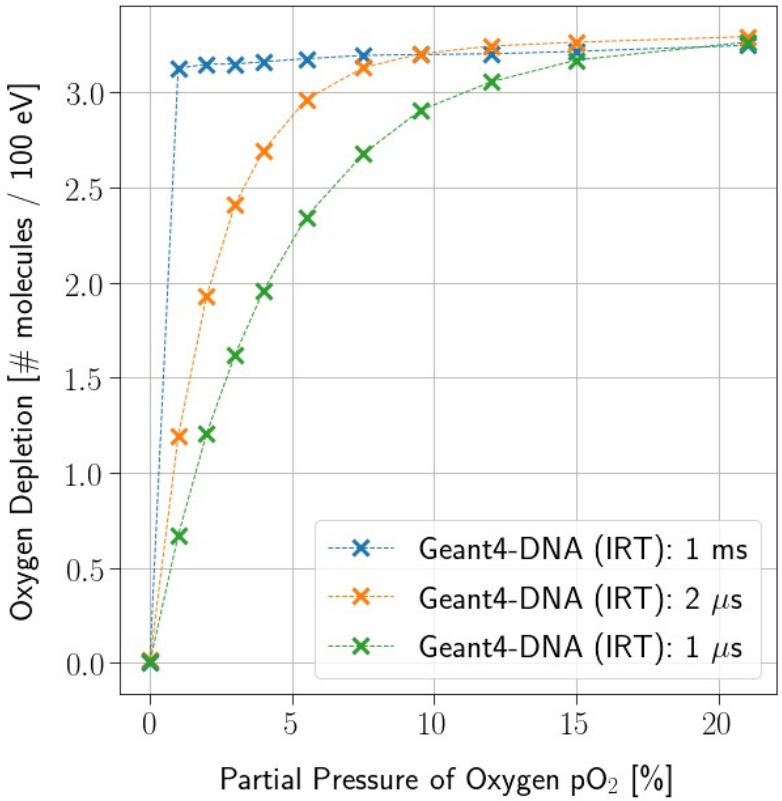
Thanks Wook-Geun and collaborators for this work !

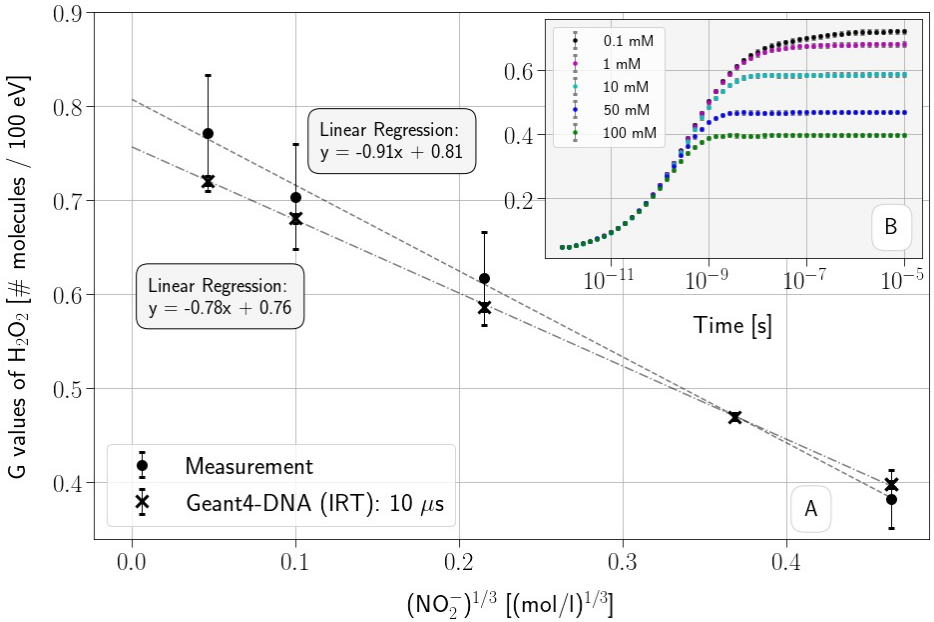
Independent Reaction Time Model



#	reactions	time
1	c + d	t_1
2	a + b	t_2
3	a + S	t_3
4	b + S	t_4
…	…	…

For 1 MeV electrons





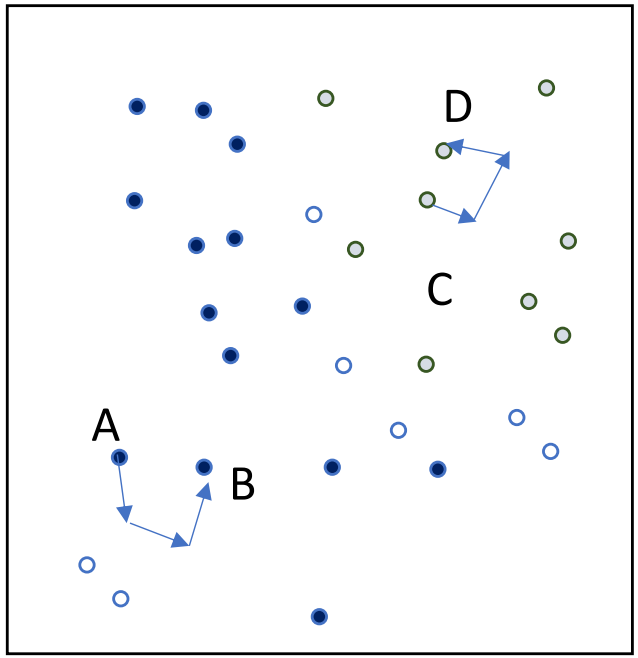
H_2O_2 G value: Scavengers NO_2^-/NO_3^-

Reaction	(1e^{10} M-1s-1)
$e^-_{aq} + O_2 \rightarrow O_2^-$	1.74
$H^\bullet + O_2 \rightarrow HO_2$	2.10

Thanks Flore for this work !

Reaction	(1e^{10} M-1s-1)
$OH + NO_2^- \rightarrow NO_2 + OH$	0.8
$e^-_{aq} + NO_2^- \rightarrow NO_2^{--}$	0.35
$e^-_{aq} + NO_3^- \rightarrow NO_3^{--}$	0.97

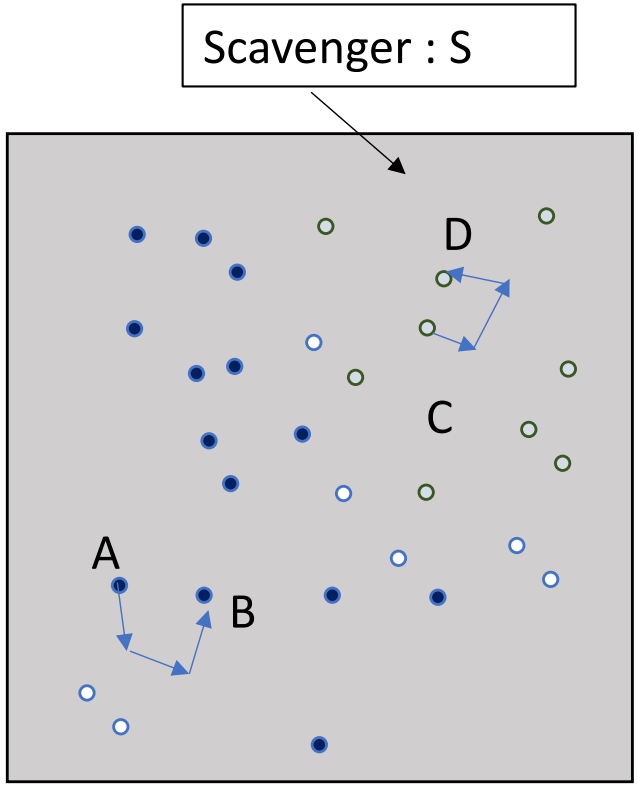
Step-By-Step Model



Synchronize in time the steps of all tracks

1. Define a minimum step time : ts_{min}
2. For all tracks, compute the minimum interaction time : ti_{min}

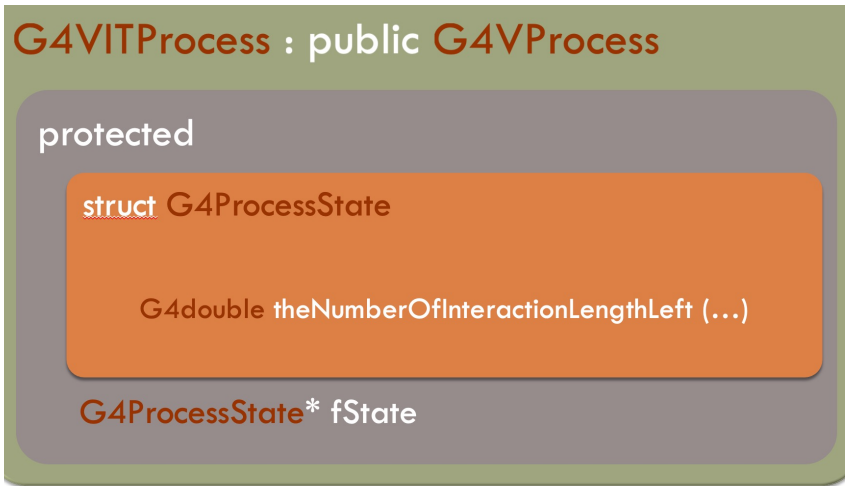
Step-By-Step Model



Synchronize in time the steps of all tracks

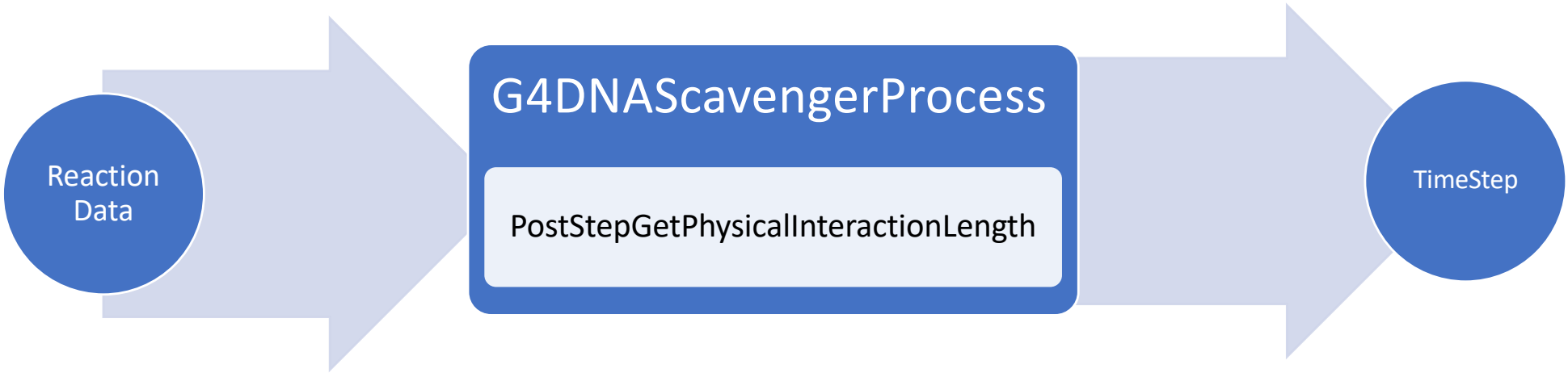
1. Define a minimum step time : ts_{min}
2. For all tracks, compute the minimum interaction time : ti_{min}

New G4DNAScavengerProcess is implemented:



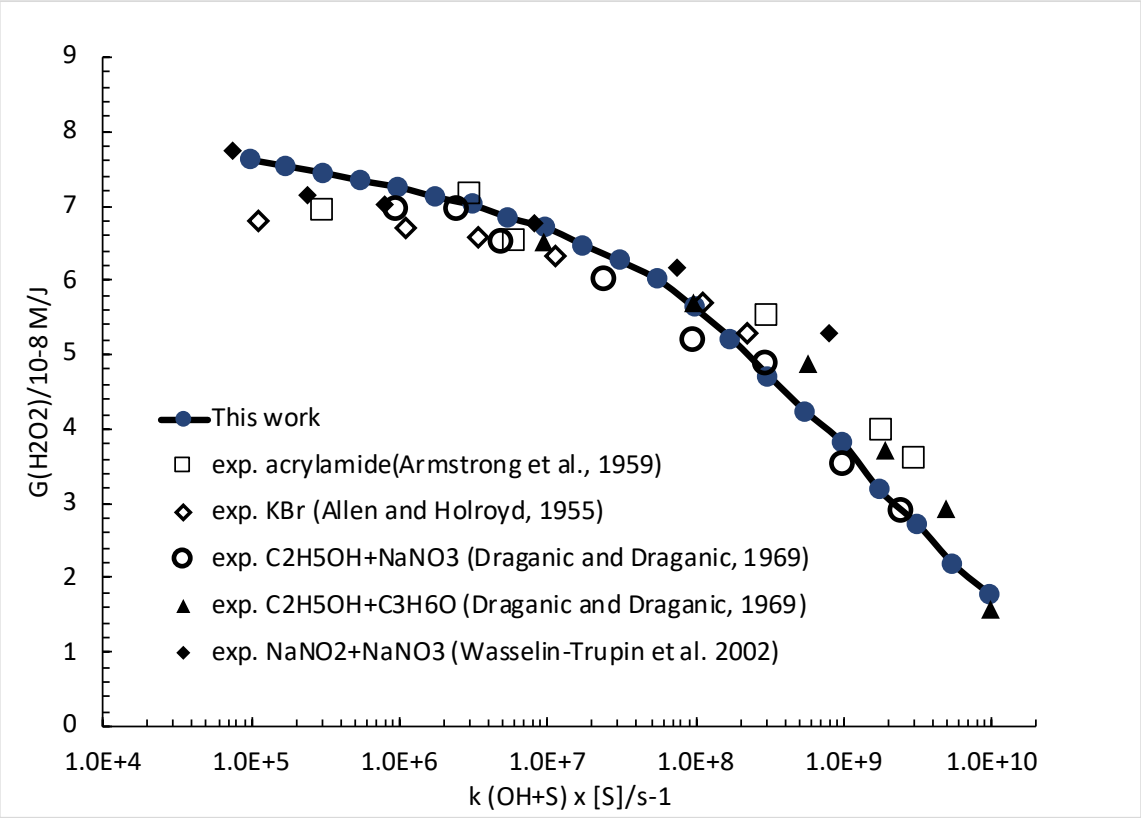
- G4DNAScavengerProcessState : public G4ProcessState
- Added to G4EmDNAChemistry constructors by G4PhysicsListHelper
- SetProcessSubType(65)

G4DNAScavengerProcess:: PostStepGetPhysicalInteractionLength



- Multi-Scavengers are randomly chosen by propensity functions
- A scavenger table is used to count the change of scavenger concentration in time
- Compatible with the new **mesoscopic model** for simulations beyond 1 us (please, see : Parallel EM: EM – 2)

Initial G-value as function of scavengering capacity



- $[NO_2^-]$ from [0.125 uM- > 1.25 M]
- $[NO_3^-]$ = 5x10-4 M

User interface : No need to change reactions from G4EmDNAChemistry_OptionX

Read from a file

```
#
####################################
# Definition of Reservoir Molecules
####################################
reservoir_molecule: NO2-    10.00e-3
reservoir_molecule: NO3-    1.00e-3
#
####################################
# Reactions Implemented in Geant4-DNA
####################################
reaction_III: e_aq + e_aq + [H2O] + [H2O] -> H2 + OH- + OH- ,  6.36e9
reaction_II:  e_aq + OH -> OH- ,                               2.95e10
reaction_I:   e_aq + H + [H2O] -> H2 + OH- ,                   2.50e10
reaction_IV:  e_aq + H3O+ -> H + [H2O] ,                       2.11e10
reaction_II:  e_aq + H2O2 -> OH- + OH ,                        1.10e10
reaction_II:  OH + OH -> H2O2 ,                                5.50e9
reaction_II:  OH + H -> [H2O] ,                                1.55e10
reaction_I:   H + H -> H2 ,                                    5.03e9
reaction_III: H3O+ + OH- -> [H2O] + [H2O] ,                    1.13e11
#
####################################
# Reactions with Medium NO2-/NO3-
####################################
reaction_VI: OH + [NO2-] -> NO2 + OH- ,  8.e9
reaction_VI: e_aq + [NO2-] -> NO2-- ,    3.5e9
reaction_VI: e_aq + [NO3-] -> NO3-- ,    9.7e9
#
```

concentration in [mol/l]

second order reaction rate in [l/(s mol)]

reaction with reservoir rate in [l/(s mol)]

Full macro file

```
#second order reaction
#/chem/reaction/add e_aq + OH -> OHm
#/chem/reaction/add H + H -> H2
#/chem/reaction/add e_aq + H -> H2 + OHm
#/chem/reaction/add e_aq + e_aq -> H2 + OHm + OHm
#/chem/reaction/add H3Op + OHm ->
#/chem/reaction/add OH + H ->
#/chem/reaction/add OH + OH -> H2O2
#/chem/reaction/add e_aq + H2O2 -> OHm + OH
#/chem/reaction/add e_aq + H3Op -> H + H2O

# pH and Scavenger in environment (env)
/chem/env/pH 1
/chem/env/Scavenger O2 19 %
#/chem/env/Scavenger NO2m 1 mM

/chem/reaction/print

/run/verbose 1
#/primaryKiller/setSize 3 3 3 um
/tracking/verbose 0
/scheduler/verbose 1
/scheduler/endTime 1000 s
#/scheduler/maxNullTimeSteps 50
/scheduler/ResetScavengerForEachBeamOn true
```

Conclusion

- New chemistry example of Geant4-DNA for scavengers
- The example may be released from version Geant4 11 and feedback is welcome

Thank you very much