Simulation of CO2 Reduction via Ion Impact in-Reactor

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INTRODUCTION

Carbon neutrality is a new paradigm for the modern world in the light of climate crisis. However, the actual methods available for CO2 dissociation present a challenge due to their high energy cost and inefficiencies. A special integrated system of CO2 reduction to CO for nuclear reactors via ionizing radiation may present a new solution.

Such a system, too, represents a high cost of manufacturing and testing; thus, simulation of CO2 dissociation may be used to assess the viability of nuclear reactor CO2 reduction systems.

There are already empirical results for electromagnetic radiation-induced CO2 dissociation available, so this simulation endeavor will focus on ion impacts from fuel fragments.

SOFTWARE

- There are numerous quantum chemistry packages available.
  - MOPAC, NWChem, ORCA, Q-Chem
- There are many molecular dynamics applicaitons.
  - LAMMPS, Q, VENUS
- Unmet need for independent quantum mechanical trajectory dynamics.
- Solution: An interface between a quantum chemistry package and classical dynamics program.
- VENUS/NWChem chosen based on existing research.[1-3]

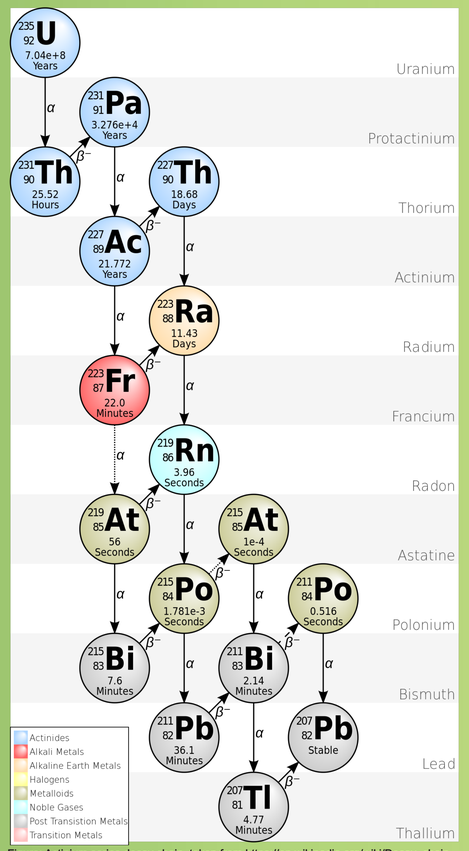

Figure: Actinium series decay chain, taken from https://en.wikipedia.org/wiki/Decay_chain

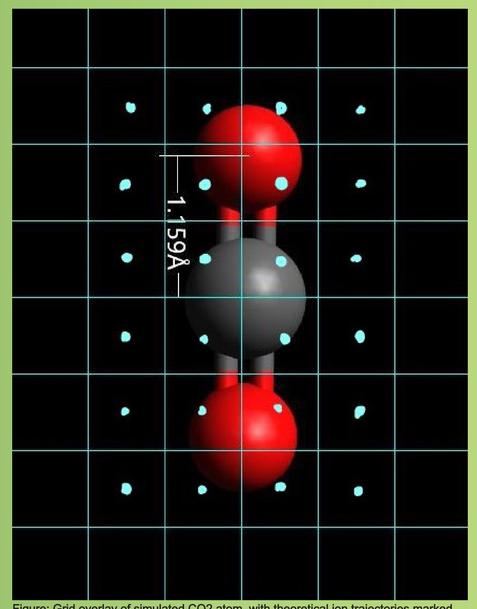

Figure: Grid overlay of simulated CO2 atom, with theoretical ion trajectories marked.

SIMULATION METHOD

- Density Functional Theory (DFT) manages atom bonds using electron density.
  - Geared toward ground-state, static systems.
- Time-Dependent DFT (TDDFT) functions similarly to DFT, but is intended for time-dependent processes.
  - Can manage excited states.
  - Provides approximate, but more accurate, results than DFT.
  - Significantly more expensive computationally.[4]
- TDDFT is the ideal quantum mechanical algorithm for

SIMULATION DESIGN

There are several key elements to consider:

- Pressurization of simulated CO2 vessel:
  - Managed using simulation cell size control.
- Ions involved in impact:
  - All ions involved in the nuclear decay chain (U-235 shown on the left) will be considered candidates for CO2 impact.
- Trajectories:
  - Different orientations of CO2 covered by setting up a “trajectory grid” (see left, below).
    - + Each square represents a trajectory simulation.
  - Trajectory grid performed for each ion.

REFERENCES

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