Pruning in RMG-Py

Kehang Han

7/10/2014

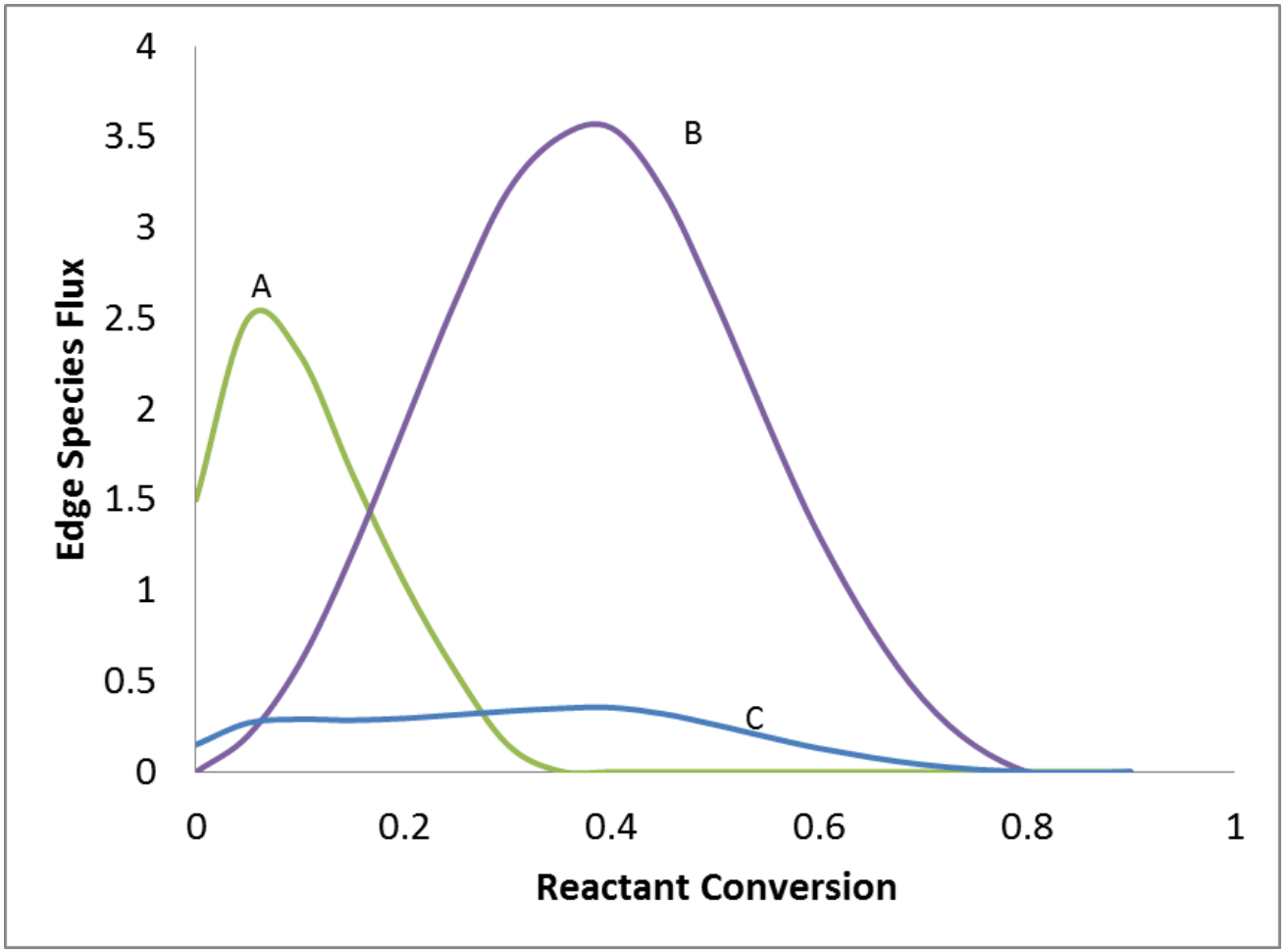
Why to Do Pruning

- For complex systems, memory limitation
- Most memory occupied by edge species
- Most edge species won't be included in final model
- Pruning is trying to get rid of edge species which have least possibility of entering core

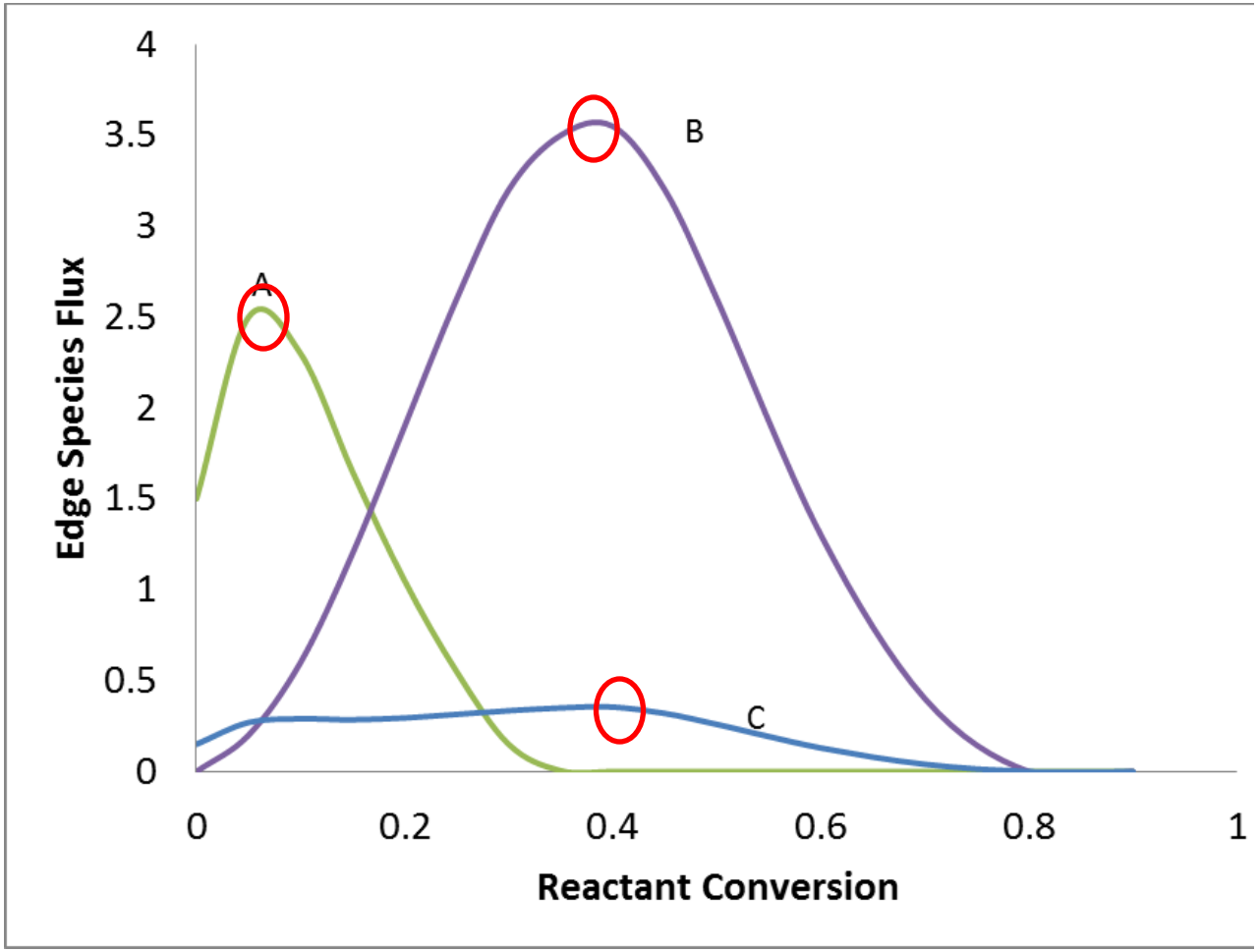
Key Params in Pruning

- toleranceInterruptSimulation
- toleranceMoveToCore
- toleranceKeepInEdge
- maximumEdgeSpecies

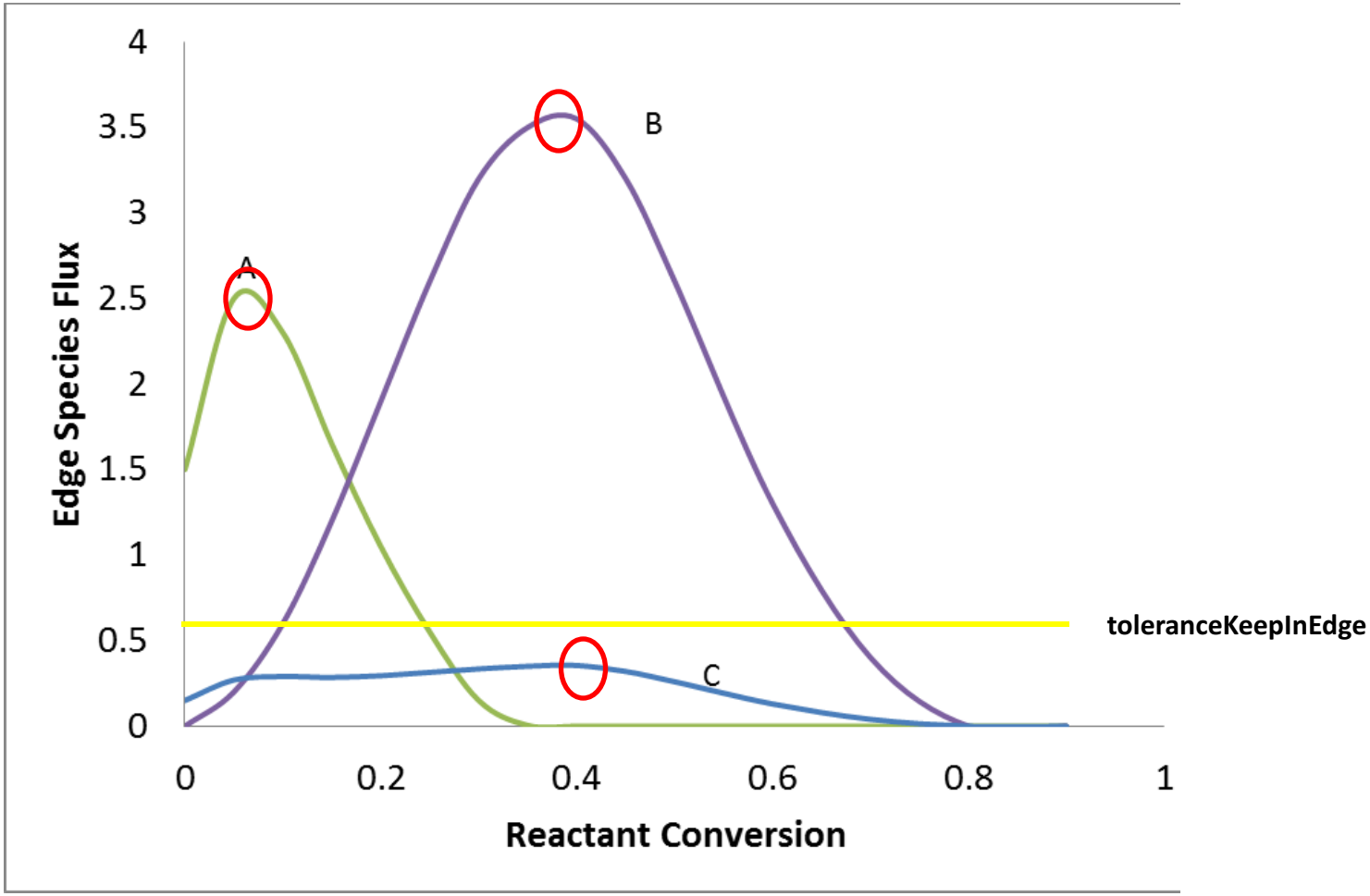
How Pruning Works



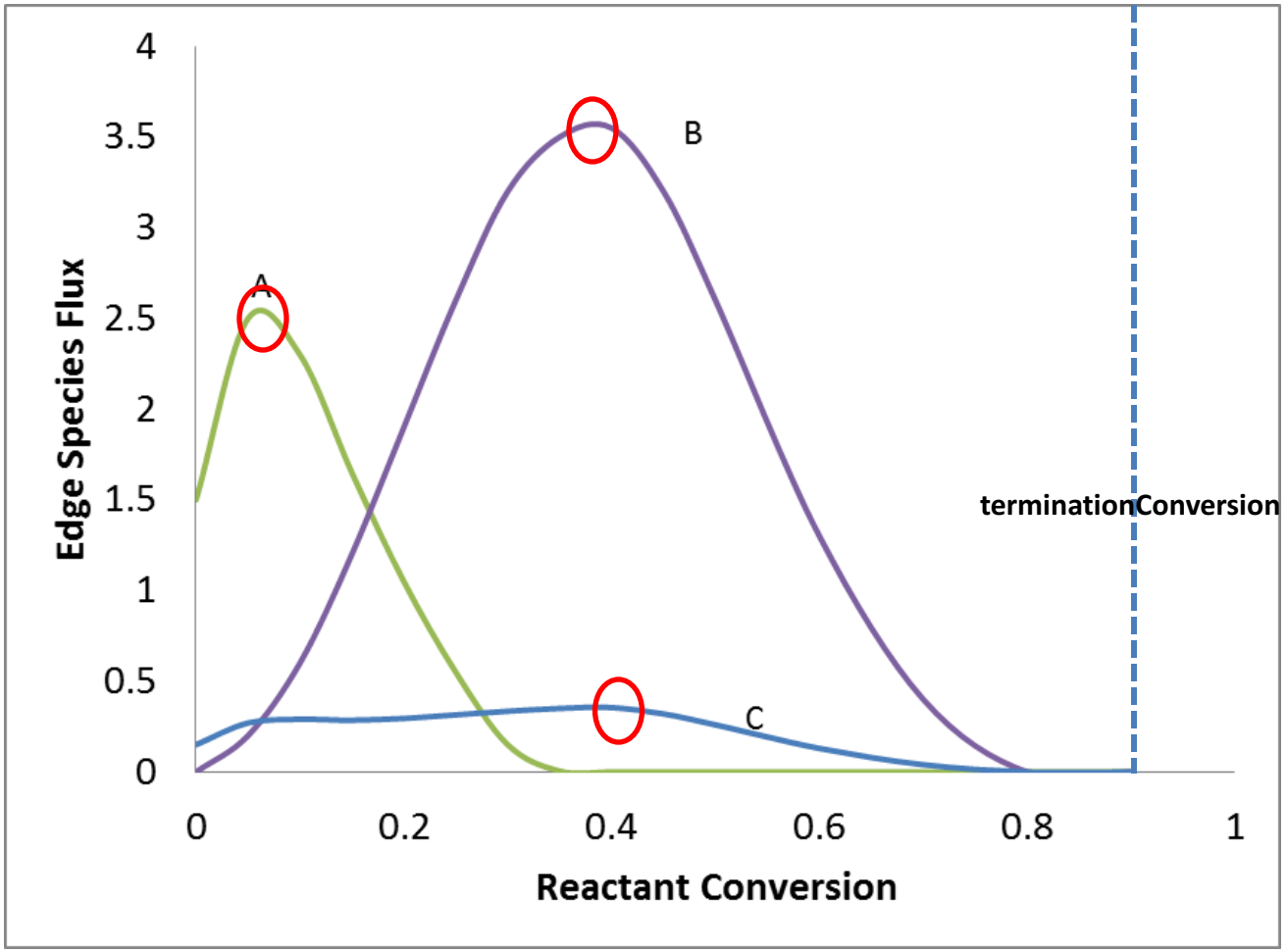
Which Species to Prune



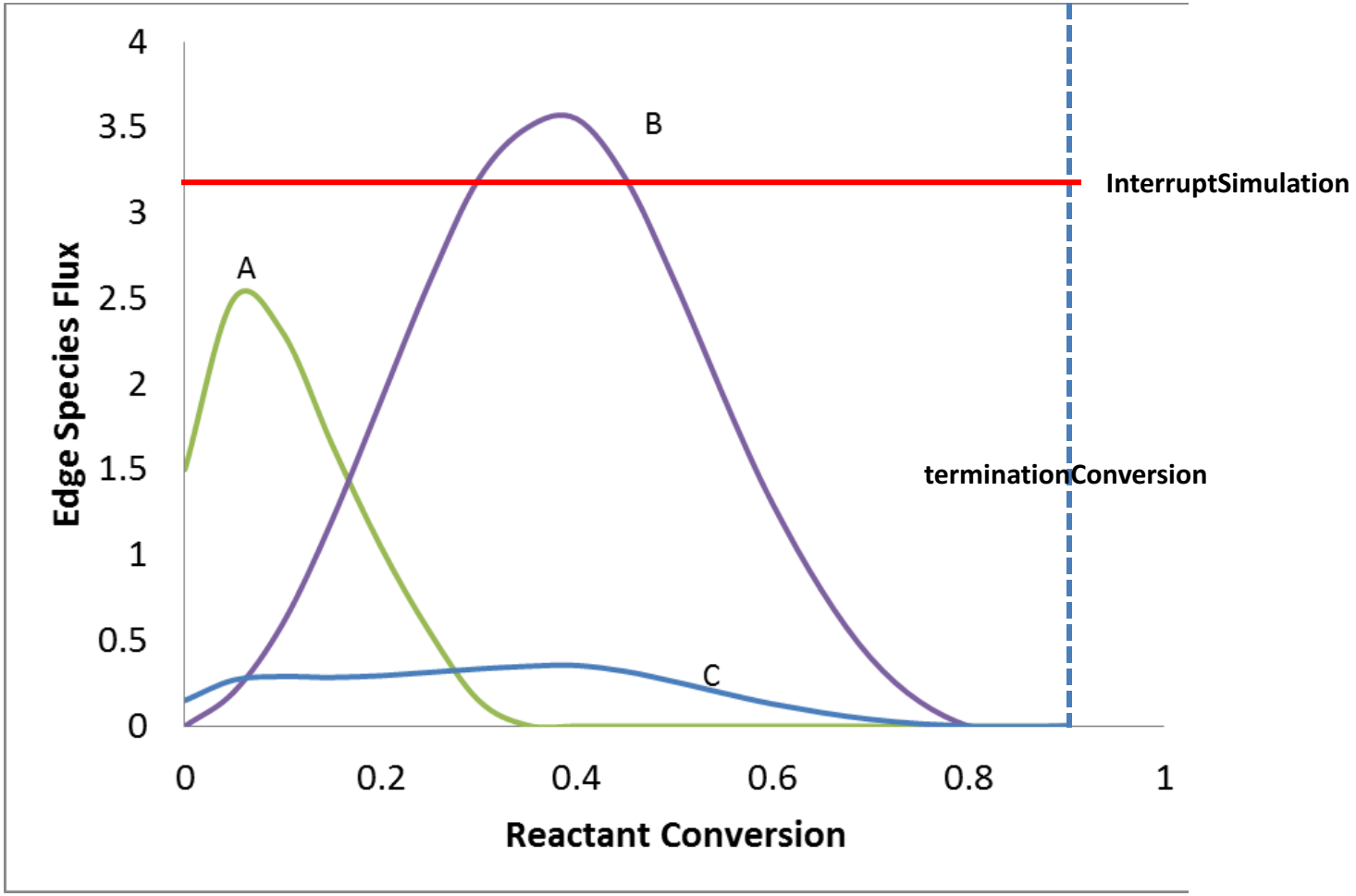
Which Species to Prune



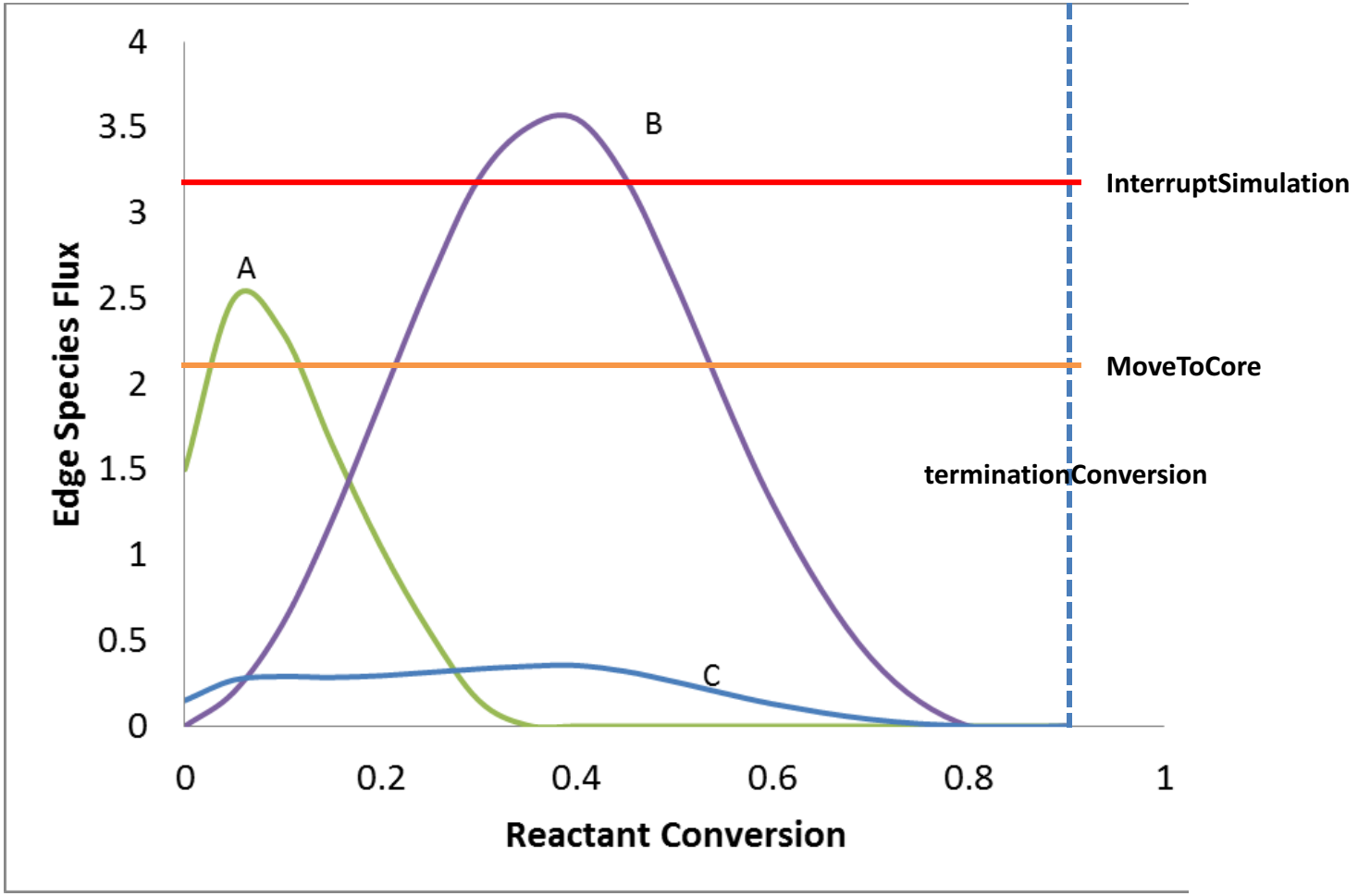
Simulation Runs to Termination



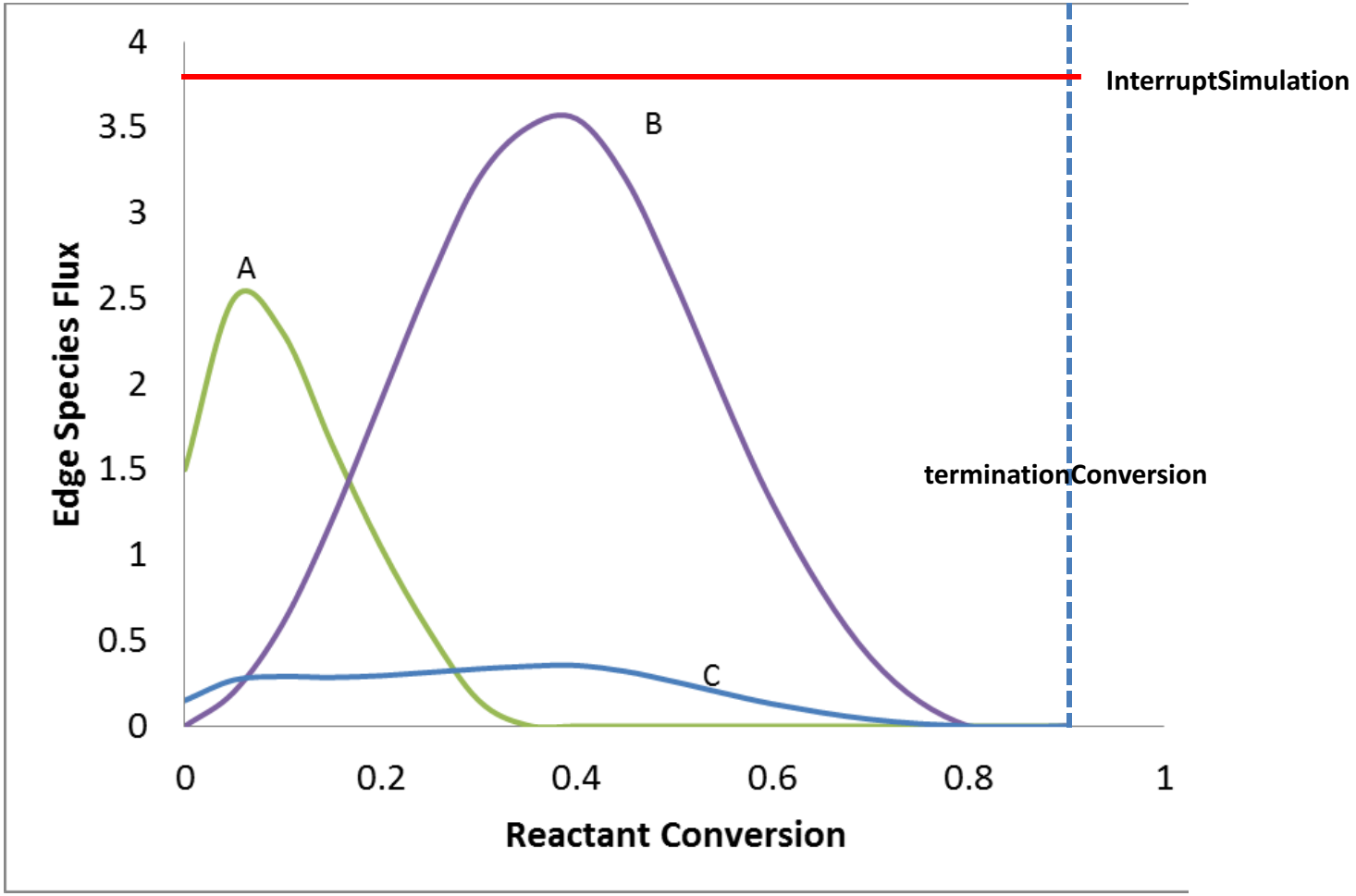
ToleranceInterruptSimulation



ToleranceMoveToCore



ToleranceInterruptSimulation



Normal Rules for Params

- toleranceInterruptSimulation≥toleranceMoveToCore
  - Otherwise, always interruption without enlarging core
  - Special cases: equal to each other; Interruption tol→infinity
- toleranceKeepInEdge has the unit for flux
  - Not convenient, maybe can do pruning just based on rank
- maximumEdgeSpecies
  - Start deleting species with lowest fluxes if total edge species number exceeds maximumEdgeSpecies

Further Questions to Ask

- How effective it can save memory when dealing with complex kinetics system?
- How it affects model generation/model content?
  - By compare models with and without pruning
- ….