Chemistry Café

- Unify updates of chemical reactions
- Track changes to Mechanisms (Tags)
- Mechanism reports for preprocessors
 - KPP
 - CESM chemistry preprocessor
- Comments and references for reactions, species, tags
- Species data as well (tracking unclear)

Mechanisms are collections of reactions



CH2O + HO2 -> HOCH2OO rate:(9.7e-15,625)

H2 + O -> OH + H rate:(1.6e-11, -4570)

Tropospheric Mechanism OH + H2 -> H2O + H rate:(2.8e-12, -1800)

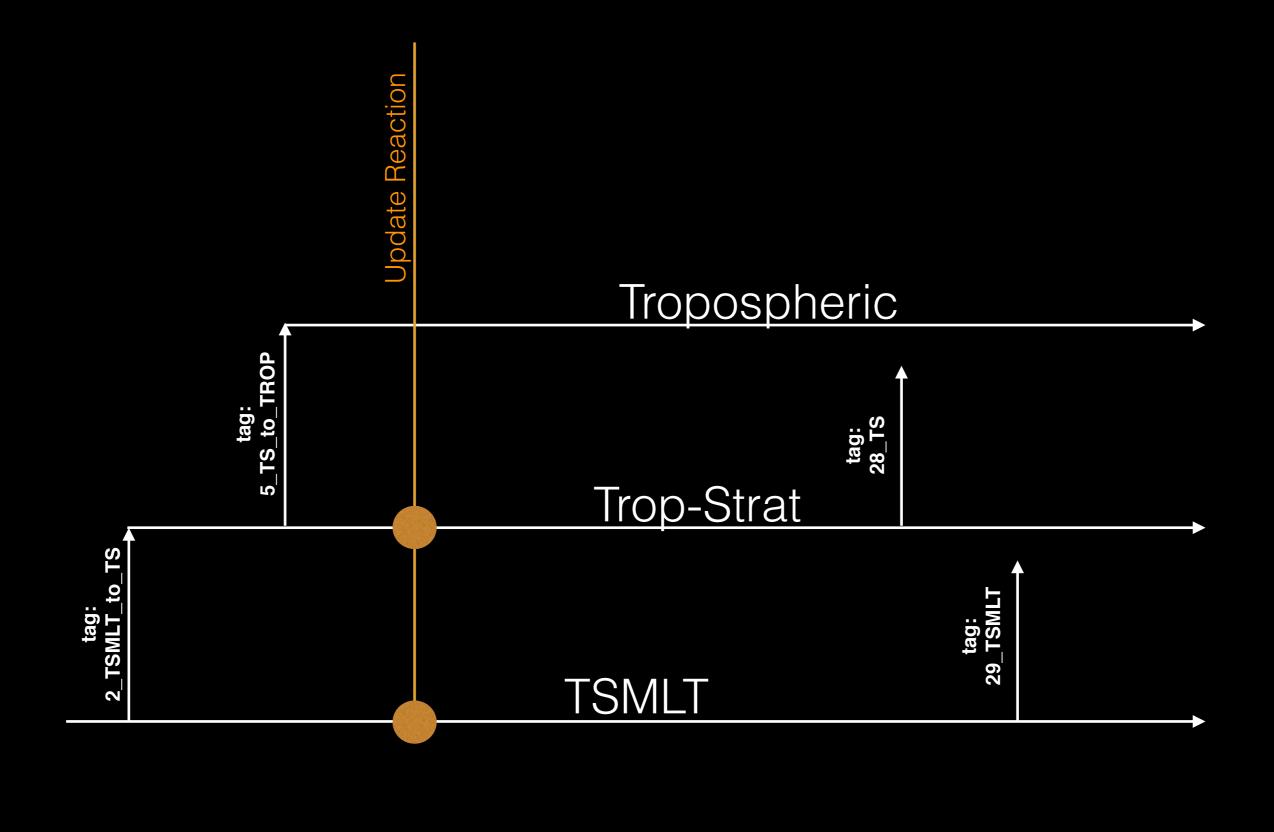
OH + H2 -> H2O + HO2 rate:(2.8e-12, -1800)

. . .

OH + H2 -> H2O + HO2 rate:(5.5e-12, -1800)

Versioning: Mechanisms and Tags

- Mechanisms change when a reaction is edited
- Tags do not change when a reaction is edited
- Tags are a snapshot of a mechanism at some point in time
- A new mechanism is created from a tag of another mechanism



Edit Reaction (what the Café does for the user)

- Copy old reaction -> new reaction
- User edits new reaction
- Move all Mechanism pointers to new reaction
- Leave all Tag pointers with old reaction
- old reaction and new reaction stay in the database