Combustion Chemistry

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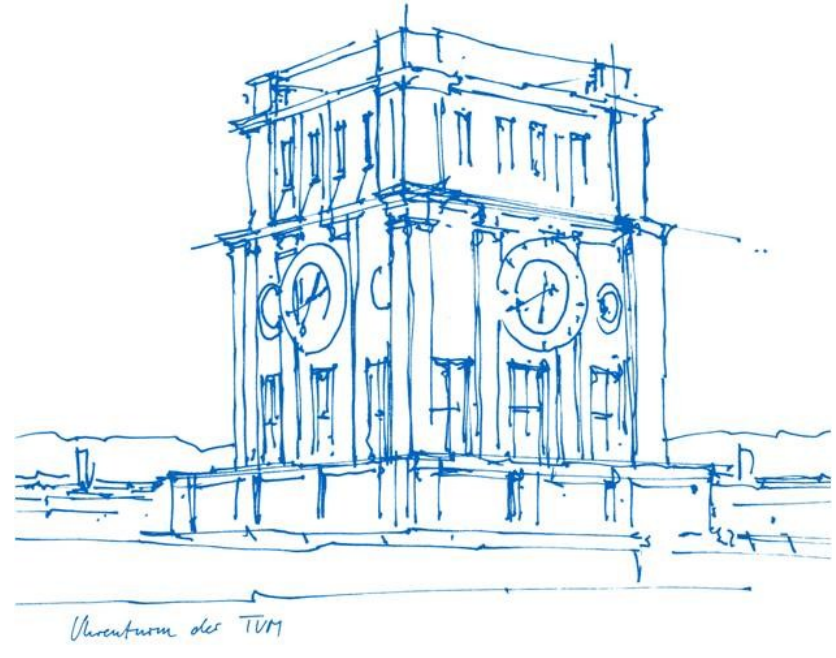
Exercise 9:
Development of a mechanism for a methane-air mixture using Reaction Mechanism Generator (RMG)



Problem statement

- Generate a detailed kinetic mechanism for methane-air combustion using RMG
- Determine freely propagating laminar flame speed of RMG generated mechanism for unburnt mixture temperature 298 K, initial pressure 1 bar and equivalence ratio ranging from 0.5-1.5
- Calculate the ignition delay time for temperatures ranging from 700-1400 K at equivalence ratio 1.1 and pressure 1 bar.
- Generate a reaction flux diagram at pressure 1 bar, temperature 1200 K and equivalence ratio 1.1
- Perform flame speed sensitivity analysis for the created mechanism at initial pressure 1 bar, unburnt gas temperature 298 K and equivalence ratio 1.1
- Compare the above results with the GRI-Mech3.0 mechanism and explain if there are inconsistencies

Levels of practical system development

Level 1:
Determination of thermodynamic and kinetic parameters

Level 2:
Development of a detailed kinetic model
(Species: 50-1000, Reactions: 500-20000, 0-D)

➡ Important for understanding combustion characteristics

Level 3:
Reduction of the detailed model
(species <50, reactions <200)

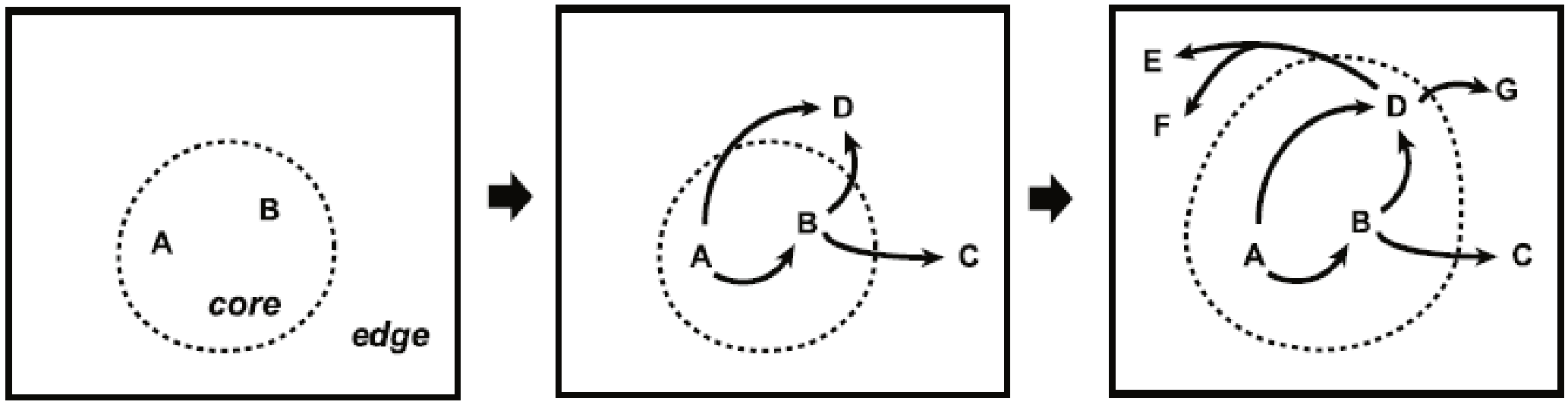
➡ Necessary to simulate practical systems

Level 4:
Computation fluid dynamics studies
(1-D,2-D,3-D using Cantera, CHEMKIN, FlameMaster)

Level 5:
Practical system design with improved efficiency and less emissions

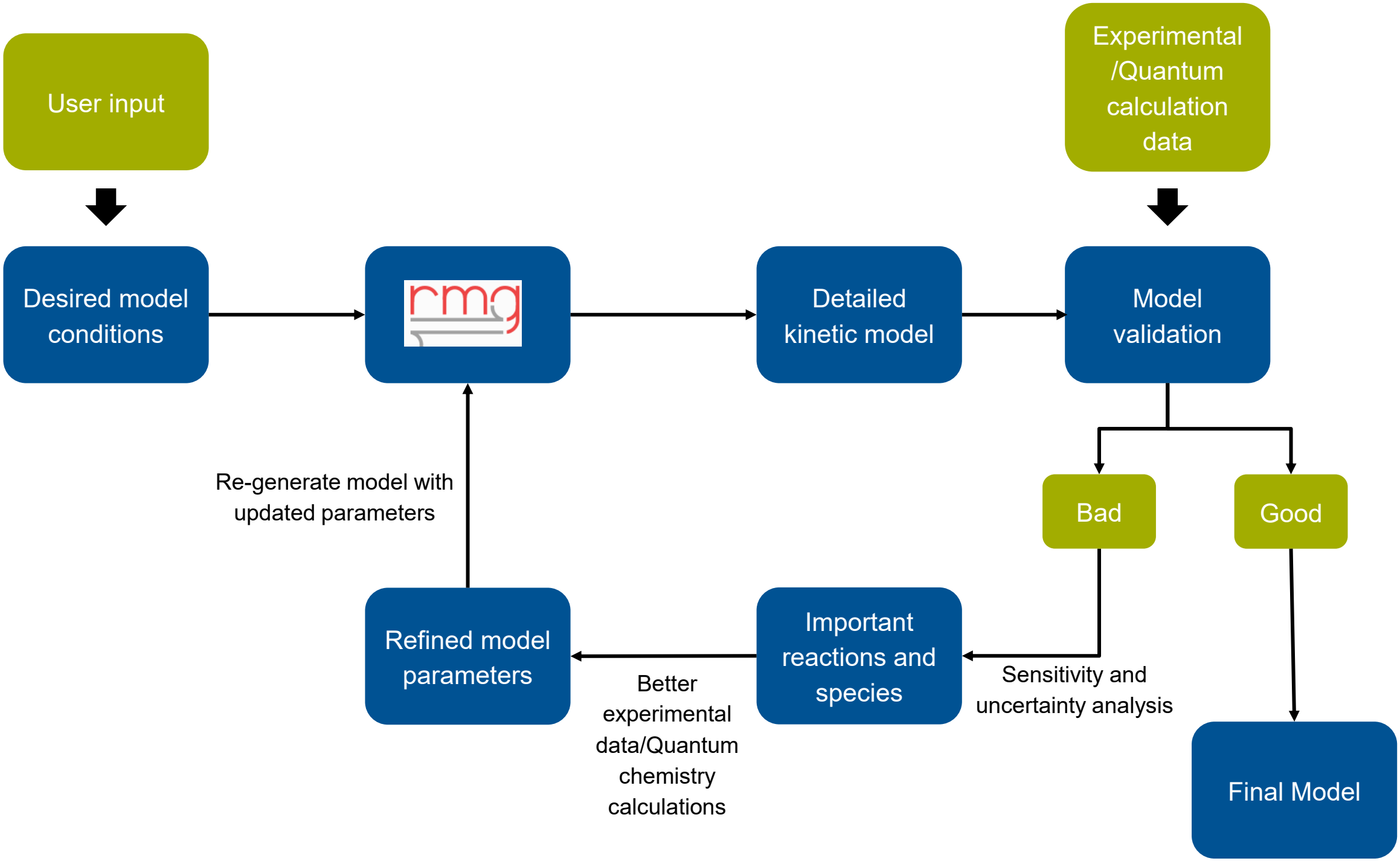
Model generation and expansion in RMG

- RMG is an automatic chemical reaction mechanism generator that constructs kinetic models composed of elementary chemical reaction steps using a general understanding of how molecules react
- Initially, reactants are placed at the model core
- All the possible reactions are generated for the species in the model core
- New species and reactions are added to the core based on the conditions defined in the input file
- Reactions and species not meeting the specified conditions in the input file are kept in the model edge



Gao et al. Compu. Phy. Commu., 203, 2016, https://doi.org/10.1016/j.cpc.2016.02.013

Mechanism Development



RMG Input Database

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

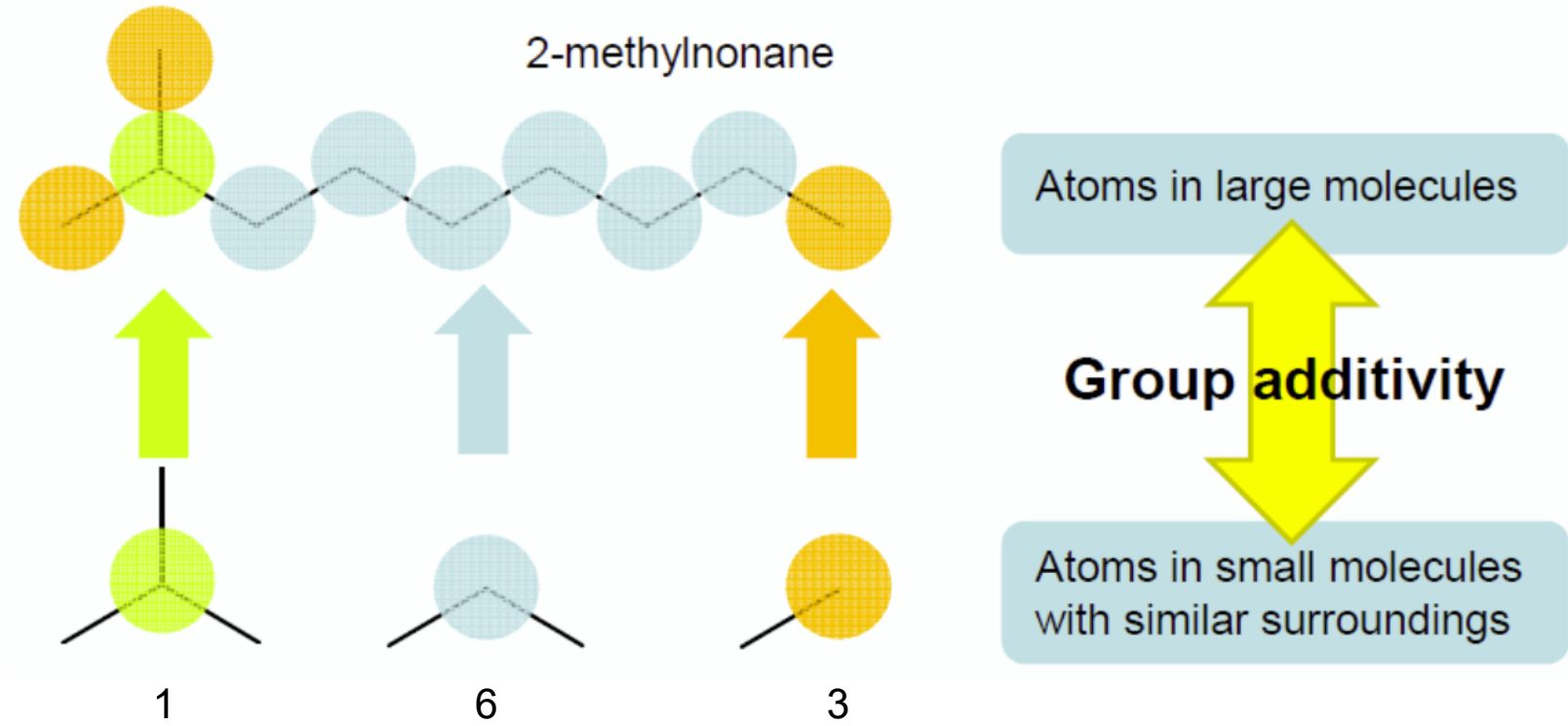

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)
```

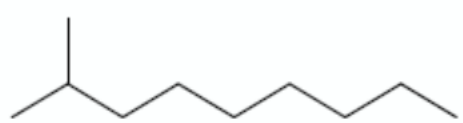

- **kineticsFamilies**: Defines reaction classes to be included (H abstraction, Unimolecular fuel decomposition etc.)
- **thermoLibraries**: Species thermodynamics data (G, H, S, C_p) (Otherwise: Group additivity, Hydrogen Bond Increment)
- **reactionLibraries**: Kinetic data for reactions ($A, n\ and\ E_a$)
- **seedMechanism**: Reactions and species are included in the mechanism
- **kineticsDepositories**: Store reactions for rate estimation
- **kineticsEstimator**: Specifies the type of rule to estimate unknown rates

Important: Order of preference

Seed mechanisms > Reaction libraries > Kinetic depositories> Rate rules

RMG input Database –Group Additivity



Additivity:  = 1 + 6 + 3

The value for each group is obtained from thermo group database

$$\Delta_f H^o_{298}(X) = \sum_i GAV(C_i)$$

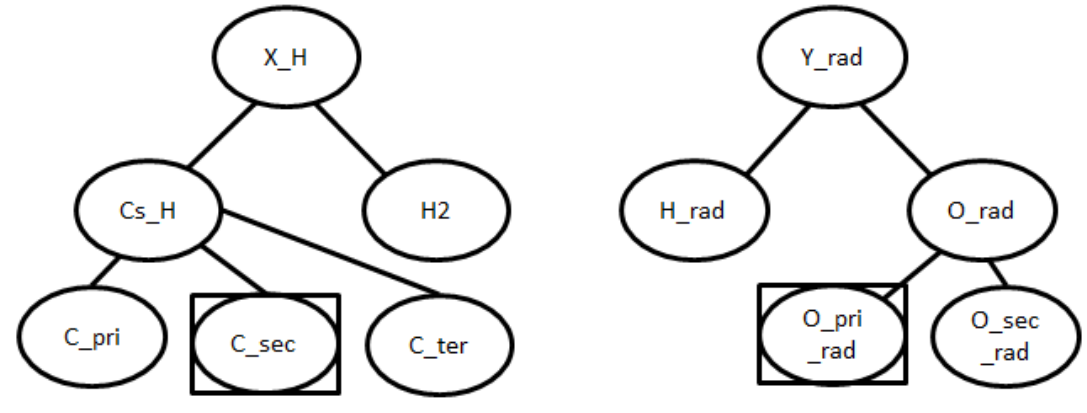
RMG input Database – Rate Rules

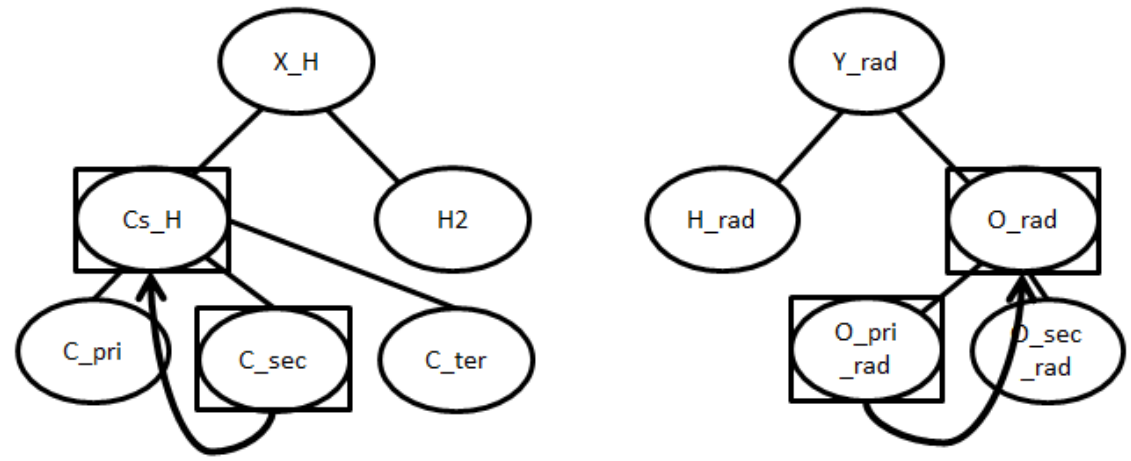
Estimation by rate rules: H-abstraction

Reaction template: 

- RMG's rate rule-based estimator uses a tree structure to determine unknown rates
- When the reaction is proposed, it descends the tree to find the best corresponding rate rule
- If there is no estimation available for the required nodes, the rule will attempt to "fall up" to a more general node and an estimate will be written for that.

Portion of rate rule tree:





RMG Input - Define Initial Species

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

```
# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)
```

- Reactant species (reactive or non-reactive) are provided in this section
- Can be defined in 3 ways: SMILES, Adjacency list and InChI

For methane

SMILES
C

Adjacency list
1 C u0 p0 c0 {2,S} {3,S} {4,S} {5,S}
2 H u0 p0 c0 {1,S}
3 H u0 p0 c0 {1,S}
4 H u0 p0 c0 {1,S}
5 H u0 p0 c0 {1,S}

InChI
InChI=1S/CH4/h1H4

RMG Input – Reactor System

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

```
#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)
```

- **simpleReactor**: Gas phase (isothermal & isobaric) reactor
- **Temperature** and **pressure** for the reactor system
- **nSims**: number of time variable condition reactor run each reactor cycle
- **initialMoleFractions**: Initial mole fraction of the reactant species
- **Termination Criteria**: Specific conversion of reactant species, specific time
- **balanceSpecies**: Mole fraction of the given species will be adjusted to keep overall mole fraction 1

RMG Input – Simulator Tolerances

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

```
simulator(
    atol=1e-16,
    rtol=1e-8,
)
```

- **atol**: Absolute tolerance of ODE solver
- **rtol**: Relative tolerance of ODE solver

RMG Input – Model Tolerances

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

```
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)
```

- **toleranceMoveToCore**: Indicates how high the edge flux for a species must get to enter the core model
- **toleranceInterruptSimulation**: Indicates how high the edge flux ratio must get to interrupt simulation
- **maximumEdgeSpecies**: Number of species in edge to interrupt simulation

RMG adds species to the core when species edge flux $R_i = \frac{dC_i}{dt}$ exceeds εR_{char} (characteristics flux of the system).

C_i: Concentration of species i

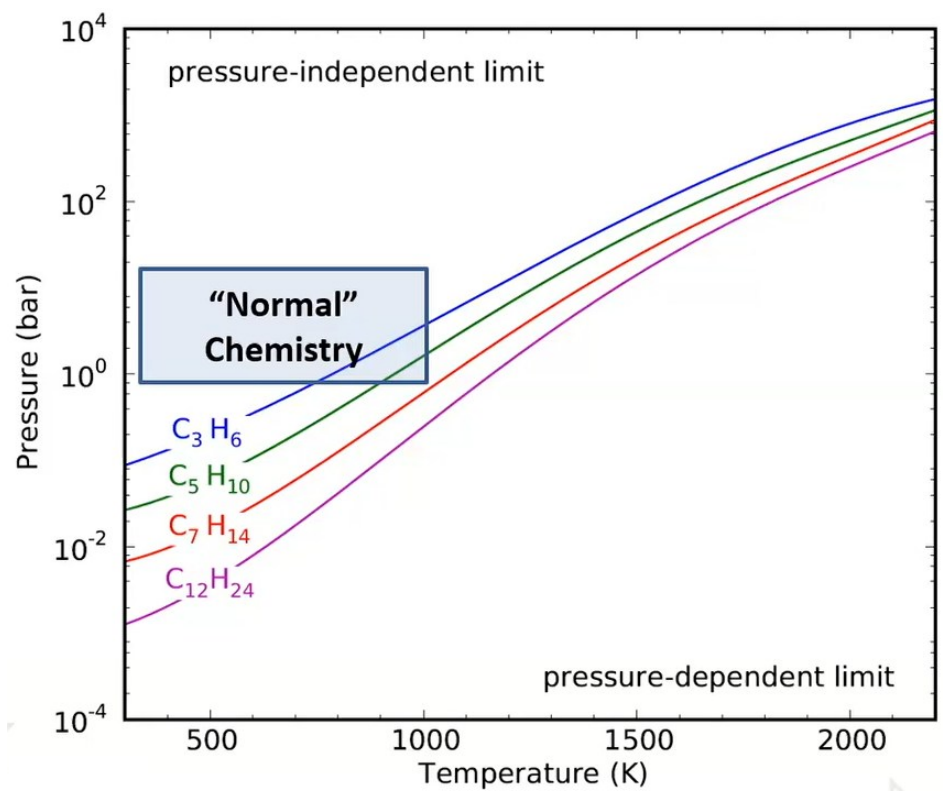
ε: Tolerance move to core

$R_{char} = \sqrt{\sum_j R_j^2}$ where species j belongs to core

RMG Input – Pressure Dependence

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

```
pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('PDepArrhenius', 6, 4),
)
```



Pressure dependence is important at low pressures and higher temperatures.

RMG Input – Pressure Dependence

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

```
pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('PDepArrhenius', 6, 4),
)
```

- Pressure-dependent reactions are similar to regular Arrhenius, but P-dependent
- Rate coefficient is a function of the overall energy of the molecule
- k(T,P) is obtained from k(E) using Modified Strong Collision or Reservoir State Method
- Interpolation scheme and limits for pressure and temperature have to be specified for the determination of k(T, P)

RMG Input – Constraints on Species

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

```
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)
```

- **maximumCarbonAtoms**: Limits chemistry only up to C_3 species
- **allowed**: Allow species from the input file, seed mechanisms and reaction libraries to bypass other constraints specified in this section

RMG Input – Output Control

```
# Data sources
database(
    thermoLibraries = ['GRI-Mech3.0','primaryThermoLibrary'],
    reactionLibraries = ['GRI-Mech3.0','Klippenstein_Glarborg2016'],
    seedMechanisms = ['GRI-Mech3.0'],
    kineticsDepositories = ['training'],
    kineticsFamilies = 'default',
    kineticsEstimator = 'rate rules',
)

# List of species
species(
        label='CH4',
        reactive=True,
        structure=SMILES("C"),
)

species(
    label='O2',
    reactive=True,
    structure=SMILES("[O][O]"),
)

species(
    label='N2',
    reactive=False,
    structure=SMILES("N#N"),
)

#Equivalence ratio ranging from 0.6 to 1.4
simpleReactor(
    temperature=[(700,'K'),(1400,'K')],
    pressure=(1,'bar'),
    nSims=10,
    initialMoleFractions={
        "CH4": [0.0593,0.1282],
        "O2": 0.19,
        "N2": 0.71
    },
    terminationConversion={
        'CH4': 0.99,
    },
    terminationTime=(1e6,'s'),
    balanceSpecies = "N2",
)

simulator(
    atol=1e-16,
    rtol=1e-8,
)
model(
    toleranceMoveToCore=0.1,
    toleranceInterruptSimulation=0.1,
    maximumEdgeSpecies=5000,
)

pressureDependence(
    method='modified strong collision',
    maximumGrainSize=(0.5,'kcal/mol'),
    minimumNumberOfGrains=250,
    temperatures=(300,3000,'K',8),
    pressures=(0.001,100,'bar',5),
    interpolation=('Chebyshev', 6, 4),
)
# Constraints on generated species
generatedSpeciesConstraints(
    maximumCarbonAtoms = 3,
    allowed=['input species','seed mechanisms','reaction libraries'],
)

# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

```
# Miscellaneous options
options(
    units='si',
    generateOutputHTML=True,
    generatePlots=False,
    saveSimulationProfiles=True,
    verboseComments=False,
    saveEdgeSpecies=True,
)
```

- **units**: RMG currently has only SI units
- **generateOutputHTML**: Saves 2-D images of all species and data related to reactions in the generated core model
- **generatePlots**: Generates plots describing the statistics of the RMG job, if set to True
- **saveSimulationsProfile**: Saves .csv files of the simulation. This file will provide the time, reactor in m^3, as well as the mole fractions of the individual species.
- **verboseComments**: Generates chemkin files with complete verbose commentary for the kinetic and thermodynamic parameters, if set to True
- **saveEdgeSpecies**: Generate Chemkin files of the edge reactions, if set to True

Results – Final Model

```
MODEL GENERATION COMPLETED

The final model core has 43 species and 685 reactions
The final model edge has 1730 species and 6330 reactions

RMG execution terminated at Wed Jul  3 11:53:57 2024
```

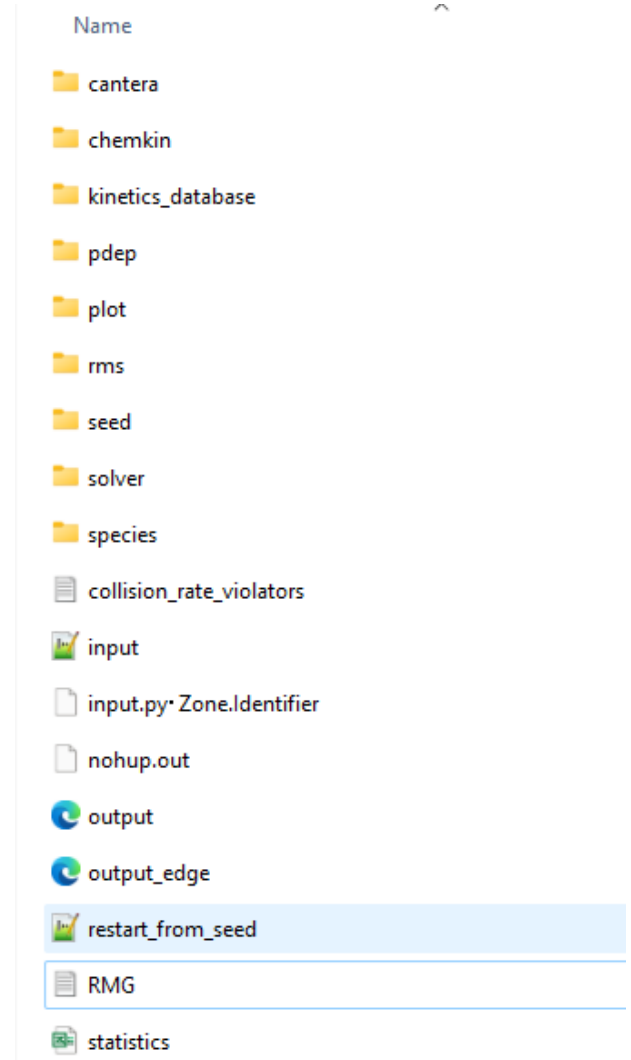
- Convert **chem.cti** file to .yaml format using inbuilt cti2yaml function in CANTERA.
- Command: **python -m cantera.cti2yaml "<filename>.cti"**

Common error while converting .cti to .yaml:

To resolve this, keep the more generalized reaction and comment out the other one

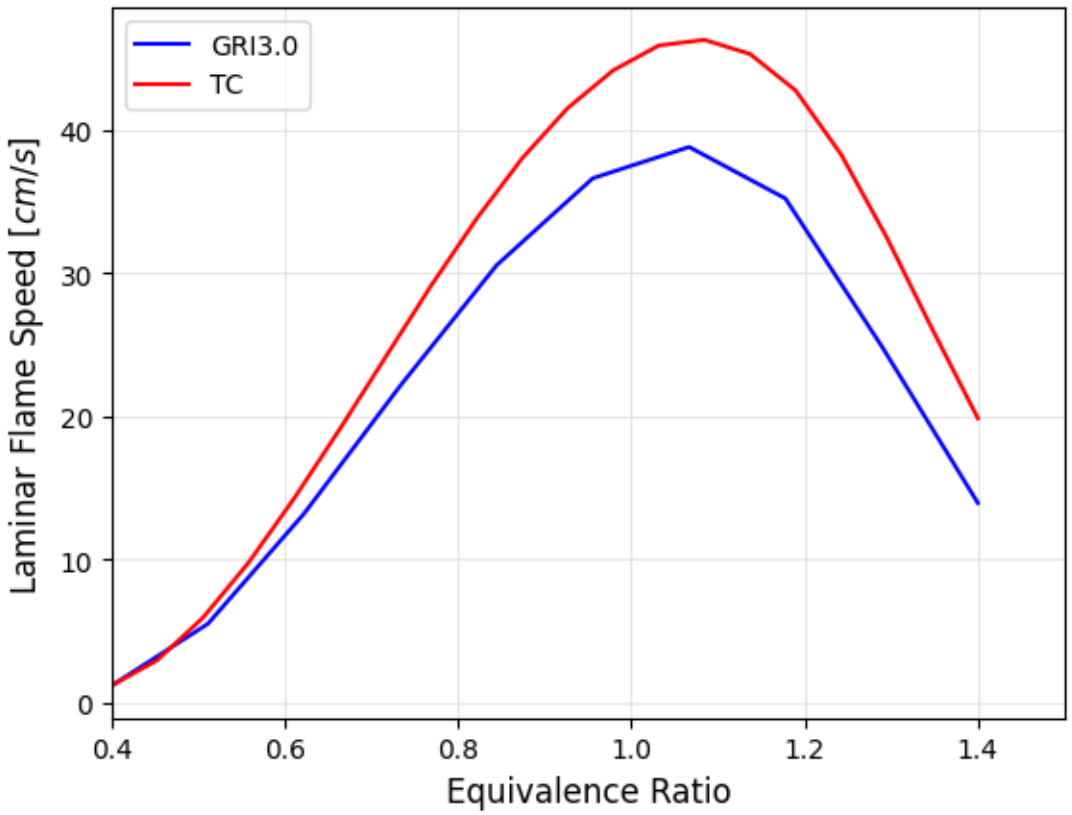
```
(ct-env) pnema@Pooja:~/miniconda3/envs/ct-env/lib/python3.11/site-packages/cantera/
hon -m cantera.cti2yaml TC-36.cti
Wrote YAML mechanism file to 'TC-36.yaml'.
Mechanism contains 49 species and 1 reactions.
Validating mechanism...
FAILED

*******************************************************************************
InputFileError thrown by Kinetics::checkDuplicates:
Error on lines 1184 and 1342 of ./TC-36.yaml:
Undeclared duplicate reactions detected:
Reaction 205: H(5) + OH(6) + M <=> H2O(28) + M
Reaction 177: H2O(28) + H2O(28) <=> H(5) + OH(6) + H2O(28)
```

```
# Reaction 177
three_body_reaction('H(5) + OH(6) + M <=> H2O(28) + M', [2.200000e+22, -2.0, 0.0],
                    efficiencies='C2H6(27):3.0 CH4(1):2.0 H2(4):0.73 H2O(28):3.65',options='duplicate')
```

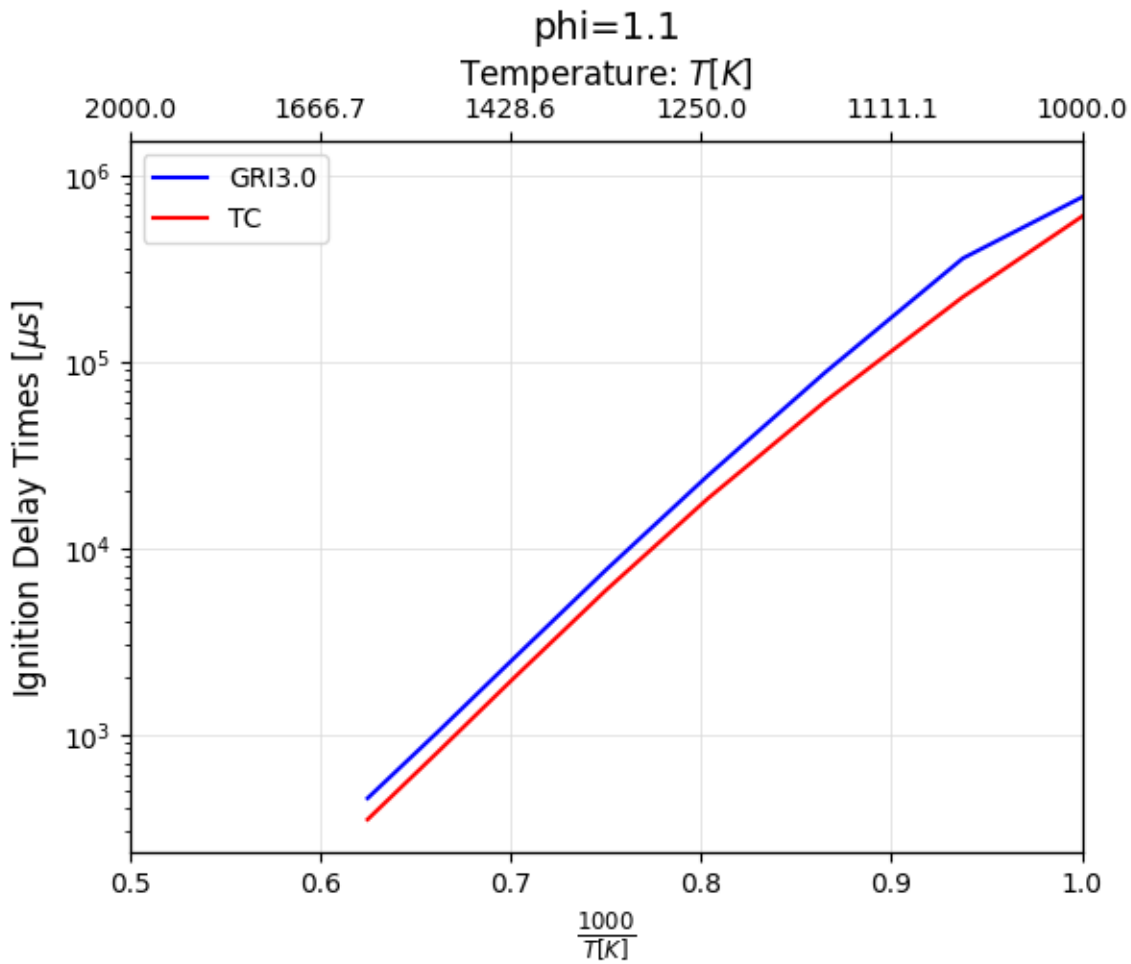


Results – Laminar Flame Speed and Ignition Delay

Laminar flame speed



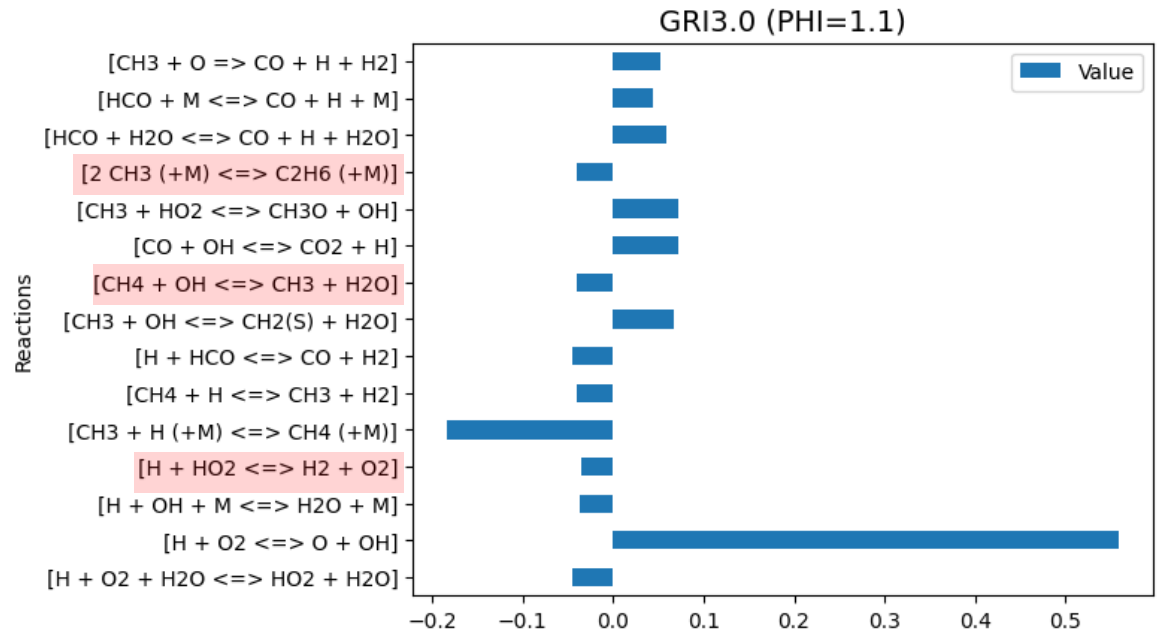
Ignition delay

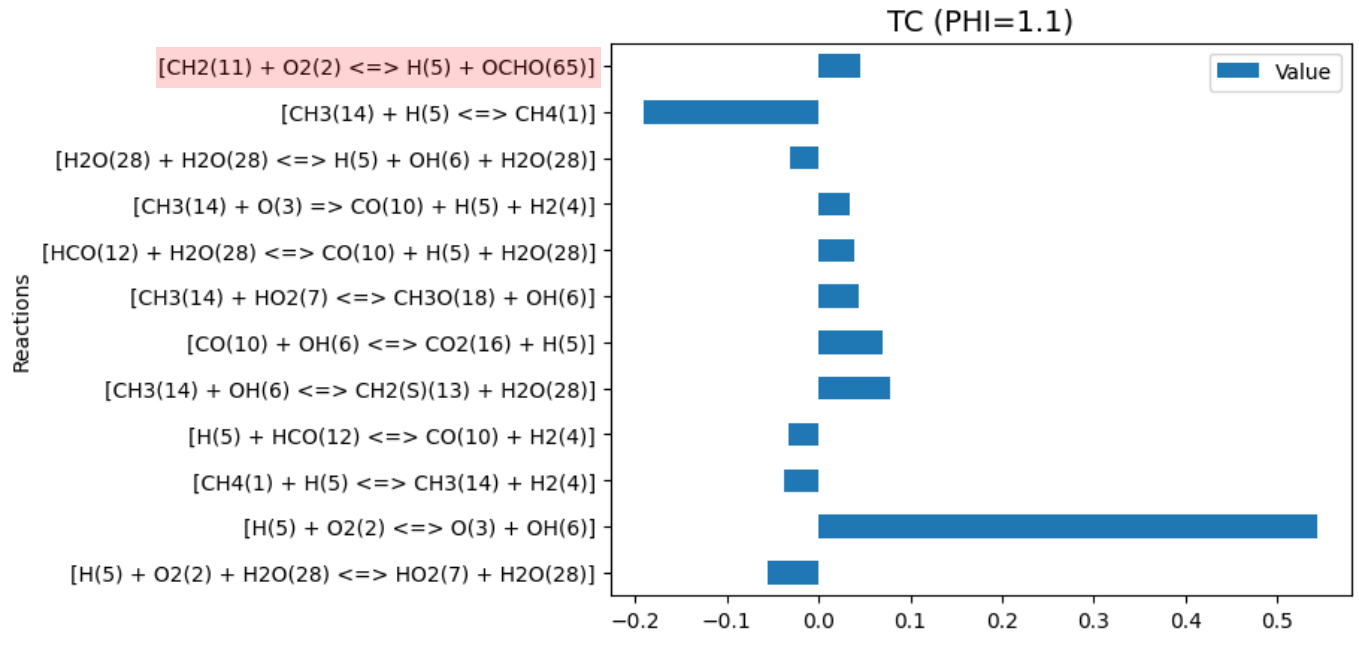


Results – Sensitivity Analysis

Unique reactions

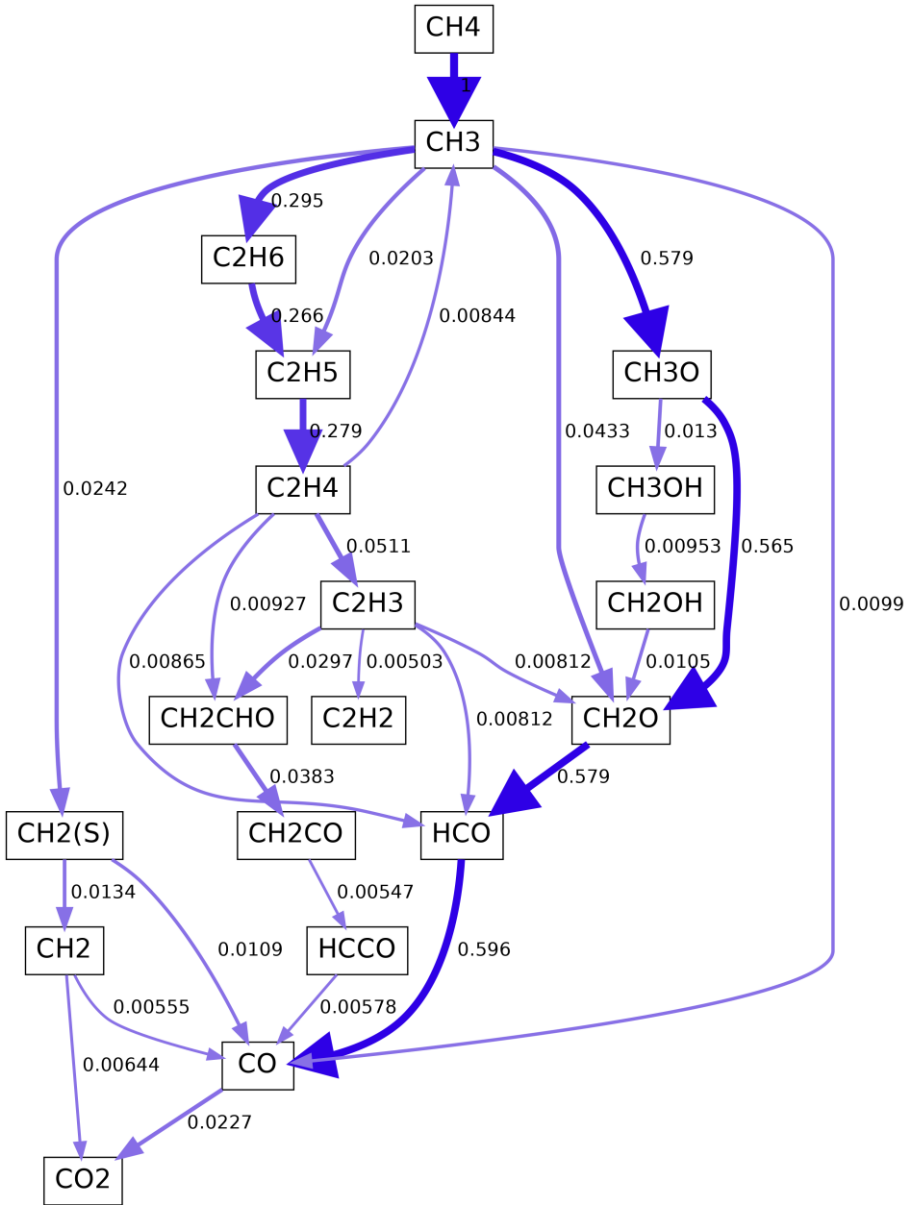
Flame speed sensitivity



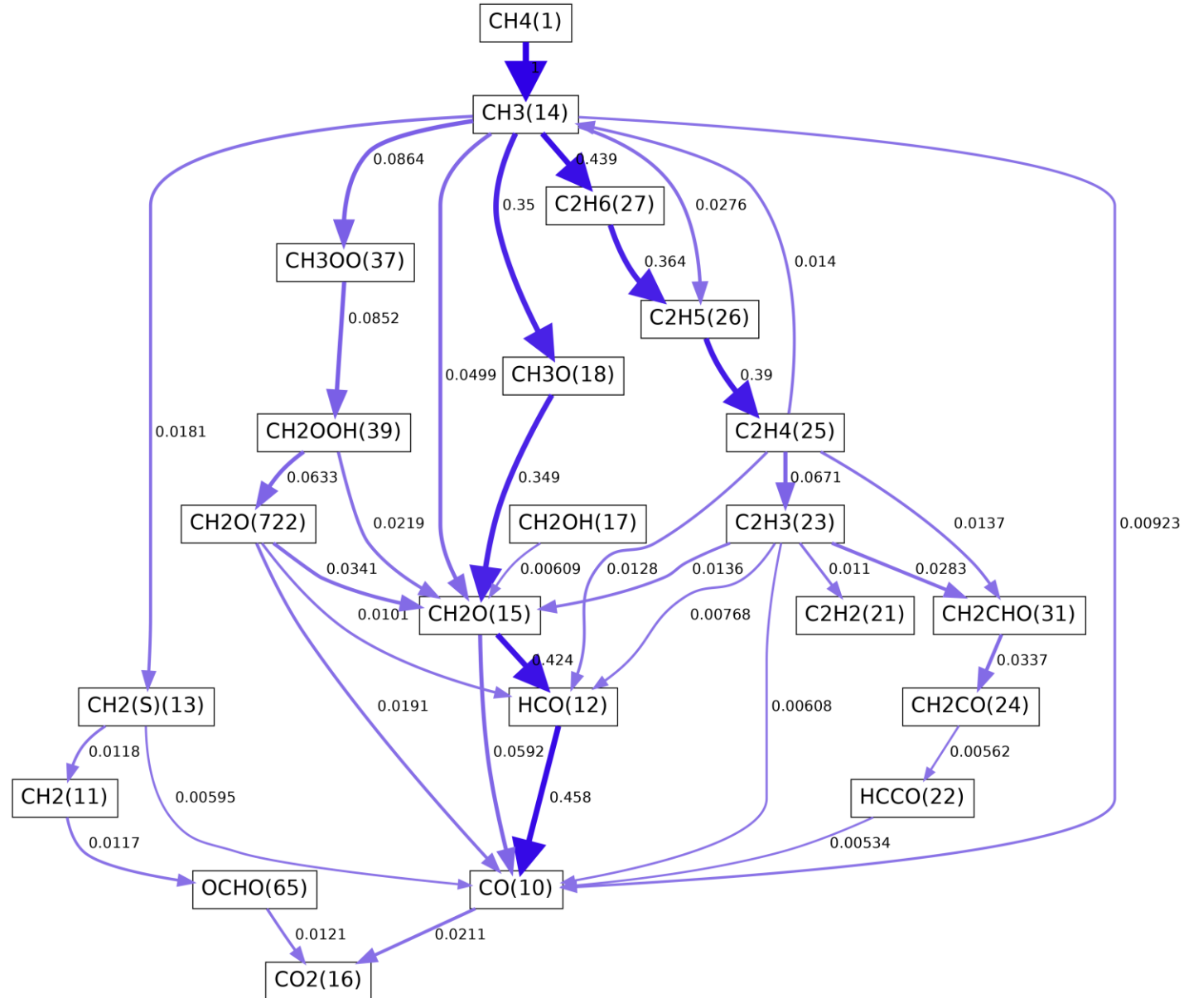


Results – Path Flux Analysis

Path flux diagrams



GRI3.0, PHI=1.1, T=1200 K



TC, PHI=1.1, T=1200 K

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Thank you!

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