\*.cti … Cantera Format

\*.inp here the mechanisms in chemkin format

There is a tool to convert those (ck2cti.py – see cantera homepage)

Literature to the mechanisms is in the folder

Some useful information below:

One-Step Mechanism

|  |  |  |
| --- | --- | --- |
|  | Value | Unit |
| A | 9.48683e+11 |  |
|  | 0 | - |
|  | 1.9e2 |  |

ODE-System consists of 4 equations:

Two-Step Mechanism

|  |  |  |
| --- | --- | --- |
|  | Value | Unit |
|  | 2.8e9 |  |
|  | 0 | - |
|  | 48.4 |  |
|  | 3.98e14 |  |
|  | 0 | - |
|  | 40 |  |
|  | 5e8 |  |
|  | 0 | - |
|  | 40 |  |
|  |  |  |

General data

Name definitions:

…concentration of species i in kmol/m³ for One-Step and in mol/cm³ for Two-Step

…mass fraction of species i in kg/kg

for one-step and for two-step

….density in kg/m³

…molar mass of component i in kg/kmol

…enthalpy of a species I in J/kg

…number of species

…reaction rate of a species =

…specific heat capacity in

(approximation for methane combustion – 1 reaction)

approximately taken as cp of air at high temperatures

|  |  |
| --- | --- |
| Component | Molar Mass |
|  | 16.04 g/mol |
|  | 15.99 g/mol |
|  | 18.015 g/mol |
|  | 44.01 g/mol |
|  | 28.01 g/mol |

R…gas constant 8.314e-3

**Cp calculation & data**

Above high cp coeffs used, below low cp coeffs used. Model only valid between and . The fifth and sixth coefficients are not relevant here.

O2

{

thermodynamics

{

Tlow 200;

Thigh 3500;

Tcommon 1000;

highCpCoeffs ( 3.28253784 0.00148308754 -7.57966669e-07 2.09470555e-10 -2.16717794e-14 -1088.45772 5.45323129 );

lowCpCoeffs ( 3.78245636 -0.00299673416 9.84730201e-06 -9.68129509e-09 3.24372837e-12 -1063.94356 3.65767573 );

}

}

H2O

{

thermodynamics

{

Tlow 200;

Thigh 3500;

Tcommon 1000;

highCpCoeffs ( 3.03399249 0.00217691804 -1.64072518e-07 -9.7041987e-11 1.68200992e-14 -30004.2971 4.9667701 );

lowCpCoeffs ( 4.19864056 -0.0020364341 6.52040211e-06 -5.48797062e-09 1.77197817e-12 -30293.7267 -0.849032208 );

}

transport

}

CH4

{

thermodynamics

{

Tlow 200;

Thigh 3500;

Tcommon 1000;

highCpCoeffs ( 0.074851495 0.0133909467 -5.73285809e-06 1.22292535e-09 -1.0181523e-13 -9468.34459 18.437318 );

lowCpCoeffs ( 5.14987613 -0.0136709788 4.91800599e-05 -4.84743026e-08 1.66693956e-11 -10246.6476 -4.64130376 );

}

}

CO2

{

thermodynamics

{

Tlow 200;

Thigh 3500;

Tcommon 1000;

highCpCoeffs ( 3.85746029 0.00441437026 -2.21481404e-06 5.23490188e-10 -4.72084164e-14 -48759.166 2.27163806 );

lowCpCoeffs ( 2.35677352 0.00898459677 -7.12356269e-06 2.45919022e-09 -1.43699548e-13 -48371.9697 9.90105222 );

}

}

N2

{

thermodynamics

{

Tlow 250;

Thigh 5000;

Tcommon 1000;

highCpCoeffs ( 2.92664 0.0014879768 -5.68476e-07 1.0097038e-10 -6.753351e-15 -922.7977 5.980528 );

lowCpCoeffs ( 3.298677 0.0014082404 -3.963222e-06 5.641515e-09 -2.444854e-12 -1020.8999 3.950372 );

}

}

CO

{

thermodynamics

{

Tlow 200;

Thigh 3500;

Tcommon 1000;

highCpCoeffs ( 2.71518561 0.00206252743 -9.98825771e-07 2.30053008e-10 -2.03647716e-14 -14151.8724 7.81868772 );

lowCpCoeffs ( 3.57953347 -0.00061035368 1.01681433e-06 9.07005884e-10 -9.04424499e-13 -14344.086 3.50840928 );

}

}

Initial Conditions

Different Test cases with initial composition and temperature would be nice:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 0.5 | 0.2 | 0.3 | 0.6 |
|  | 0.5 | 0.8 | 0.3 | 0.4 |
|  | 0 | 0 | 0.4 |  |

Start Temperature=1600K/1800K/2000K/2200K

Number of sub time intervals: 10/100/1000/10000 (to simulate “CFD”-conditions)

Reversible Reaction Rate

… reverse reaction rate

…forward reaction rate

…standard pressure

RR… universal gas constant in J/(kmol K)

T… temperature

p….pressure

… absolute enthalpy in J/kg

…Entropy in J/(kg K)

…Gibbs free energy in J/kg

…Equilibrium constant in terms of partial pressures

…Equilibrium constant in terms of molar concentration