1 Input File - New Style

```
<InitialConditions>
Temperature
EndTime - followed by end time and time step
</InitialConditions>

<Species>
Species Name - followed by concentration
Optional:
Species Name - followed by concentration - followed by ConstantConcentration
</Species>

<SolverParameters>
Jacobian
Force Stability
Use General Solver
hm
initialh
Tolerance a b
Threshold
RTOL
IRREV
Print Rates
Stoichiometry Matrix For Opt
</SolverParameters>

<Analysis>
RatesMaxAnalysis
StreamRatesAnalysis
RatesSpeciesAllAnalysis
RatesAnalysisAtTime - followed by times (sorted)
RatesOfSpecies - follwoed by species names
</Analysis>

<PressureVessel>
Sample Size=
Vessel Size=
Initial Pressure=
Maximum Pressure=
Gas Solubility=
Gas Species=
PetroOxy Temperature Rise=

Experimental: Henry Law Diffusion Limit
</PressureVessel>

<MechanismReduction>
Use New Lumping
Use Slow Lumping
ReduceReactions
</MechanismReduction>

Experimental:
GasPhasePressure
```

```
GasPhaseVolume
```

2 Input File - Old Style

2.1 Required

```
Temperature 423   ! initial temperature/K
EndTime  5e4 1.0e0! second entry is time step
O2(2)      0.02 ! concentrations of initial species, assumes mol/L
C12H26(1)   4.7
```

2.2 Either of

```
Threshold  1.0e-13
RTOL 1.0e-7
```

or

```
Tolerance 1.0e-7    1.0e-13 ! relative tolerance and threshold
```

2.3 Optional

```
IRREV ! flag to make scheme irreversible, set automatically where necessary
PrintReac ! prints reaction rates
RatesMaxAnalysis ! find the maximum rates for every reaction
RatesAnalysisAtTime x y z ! print rates at timex xyz
%TimeStepChange 1.0e5 1.0e-3  ! time to change the timestep to the new step
ReduceReactions 7 ! orders of magnitude difference to the fastest rate
hm 1.e-12 ! minimum timestep if other is desired
initialh 1.e-3 ! initial timestep for solver if other is desired

GasPhasePressure 101.325 ! input is in kPa
GasPhaseVolume 1         ! input is in L

PetroOxySolvent Sample=5
PetroOxyInitialPressure=700
PetroOxyMaximumPressure=1015
PetroOxyGasSpecies=O2(2)
PetroOxyGasSolubility=0.002

Use General Solver ! uses dodesol_rkm9mkn for non-stiff to stiff problems,
! else uses dodesol_mk52lfn which is specific to stiff problems
```

2.3.1 PetroOxy

Additional Commands in the Input File, example given below. The module will not be activated if any parameters are missing.

2.4 Files

2.4.1 Species Lumping

File with name "species_mapping.txt". Unmapped or ungrouped species are internally assigned class 0, hence the labelling from 1.

```
MAPPING
C12H26(1)
O2(2)
HO2J(4)
C12H25J(5)
SPC(54)  ! C12H25O2J(54)
H2O2(38)
SPC(92)  ! C12H25O2J(92)
SPC(113) ! C12H25O4J(113)
SPC(114) ! C12H26O4(114)
SPC(13) 1 ! C12H25J(13)
SPC(213) 2 ! C12H25O2J(213)
SPC(214) 3 ! C12H26O2(214)
C12H25J(9) 1
END
```

2.4.2 Species Removal

File with name "kill.txt" and a species list, "!" for comments

```
SPC(190) !4 ! C12H25O2J(190)
SPC(203) !4 ! C12H25O2J(203)
SPC(250)
```

2.4.3 Species Picking

File wih name "SpeciesPicking.txt", the first line with "ONLY" results in only reactions with chosen species to be picked otherwise all reactions that include a desired species are selected

```
ONLY
C12H26(1)
O2(2)
HO2J(4)
C12H25J(5)
SPC(54)  ! C12H25O2J(54)
H2O2(38)
SPC(92)  ! C12H25O2J(92)
SPC(113) ! C12H25O4J(113)
SPC(114) ! C12H26O4(114)
SPC(13) 1 ! C12H25J(13)
SPC(213) 2 ! C12H25O2J(213)
SPC(214) 3 !
```