Run chemical reaction flow

To run chemical reacting flow, user must download the **thermdat** and the **trandat** files from Sandia National Laboratories. And put those two file under the **esdc** folder.

Currently the chemical reaction flow, can only be run by command mode.

Under esdc directory, type “command_line” to setup environment variables.

Then go to the folders under D:\ESDC\GAS.VRF\CHEMICAL\g1-Sod's-shock-tube

Then type “flusol” with g1.da as input to solve the problem.

Chemical reacting flow model format

To solve the chemical reacting flow problems, following input are needed:

**begin
solver = compressible flow

chemical = off, For single component gas flow (Solving Navier Stokes equations ,Euler equations or conical flow equations)
= on**,** For multi-component gas flow (for chemical reacting or mixing flow problems)
endu = off, The energy diffusive term in the energy equation is set equal to zero. Usually this option is used for equilibrium problem.
= on, The energy diffusive term will be calculated.
diffusion = **off**, The species diffusive term is set equal to zero. Usually, this option is used for equilibrium problems.
= on, The species diffusive will be calculated.
*head

Sod's shock tube problem

```
*chemical
ELEMENTS
H O N
END
SPECIES
O2 H2 H2O H O OH N2
END
REACTIONS
H2+O2=2OH       1.70E13    0.00  47780.0
H+O2=OH+O       1.42E14    0.00  16507.0
H2+OH=H2O+H     3.16E07    1.30   3626.0
O+H2=OH+H       2.07E14    0.00  13751.0
2OH=O+H2O       5.50E13    0.00   7000.0
H+OH+M=H2O+M    2.21E22   -2.00      0.0
 H2O/20/
H+H+M=H2+M      6.53E17   -1.00      0.0
 H2O/0.0/
 H2/0.0/
END
```

***initial conditions for mixture**

** n1, n2, increment, density, ux,vy,wz,pressure

1, 101,1, 0.125,0.0,0.0,0.0,1.0E+4

1, 51,1, 1.0 ,0.0,0.0,0.0,1.0E+5

***ckinitial conditions (Initial conditions for real gas flow problems)**

**Under this group control card, the moral ratio (or volume ratio) of each spice is

**inputed by the following format :

****begin, last, inc,label, moral number,label,moral number, -----**

**example : 1, 101,1 ,O2,20.9476 ,N2,78.084 , AR,0.934 , CO2, 0.0314

The above example shows the moral number composition of each gas species for air. n1, ** n2, increment, ** Specie (such

**O2),

1, 101,1,O2,20.9476,N2,78.084, AR,0.934, CO2, 0.0314

***ckbcds (boundary conditions for species' mass fraction at specified node**

locations)

begin, last, inc, label, value of mass fraction

3137, O2, 0.0, 3137, 1

3137, N2, 0.0, 3137, 1

3137, HE, 2.7514, 3137, 1

*output

1,101,1,pres

1,101,1,density

1,101,1,mach

1,101,1,ux

1,101,1,temperature

1,101,1,O2

*last card