SUPPORTING INFORMATION TEXT

Thermo-physical properties of pseudo components

Thermo-physical properties of pseudo components with carbon number up to eight are determined by assuming equilibrium amongst the corresponding individual species. A free-energy minimization method is used to determine equilibrium chemical composition of gaseous mixture of corresponding species at constant temperature (500^0C) and constant pressure (30 bar). For the fractions C_{9+} fractions average thermo-physical properties are used. Thermo-physical properties of pure components are extracted from electronic form of DIPPR thermo-physical databank [1]. Calculated thermo-physical properties such as standard enthalpy of formation H_{form}, standard free energy of formation G_{form}, as well as the coefficients of polynomial heat capacity equation for all pseudo-components are listed in Table 1

Reaction rate equilibrium constants

Equilibrium constants of reverse reactions are calculated from change in Gibbs free energy using following thermodynamic relationship (eq. 1)

$$-RT\ln\left[K_{eq}(T)\right] = \Delta G_{Rx}(T) \qquad (1)$$

Where:

R denotes ideal gas constant (kJ/kmol/K)

T denotes temperature (K)

ΔG_{Rx} denotes free energy (J/kmol)

$K_{eq}(T)$ – equilibrium constant at temperature T (atm^i)

$K_{eq}(T)$ is a function of temperature only, and the temperature dependence of K_{eq} are given by integrated form of van't Hoff equation (2), and coefficients of equation for all reverse reactions are

listed in Table 2

$$K_{eq}(T) = K_{eq}(773.15)\exp\left[\frac{\Delta H_{Rx}}{R}\left(\frac{1}{773.15} - \frac{1}{T}\right)\right] \qquad (2)$$

Table 1 Thermo-physical properties of pseudo-components

Comp	H_{form} (J/kmol)	G_{form}(J/kmol)	Cp (J/kmol/K)				
			A	B	C	D	E
H2	0.00E+00	0.00E+00	27617.0	9560.0	2466.0	3760.0	567.6
P1	-7.45E+07	-5.05E+07	33298.0	79933.0	2086.9	41602.0	992.0
P2	-8.38E+07	-3.19E+07	40326.0	134220.0	1655.5	73223.0	752.9
P3	-1.05E+08	-2.44E+07	51920.0	192450.0	1626.5	116800.0	723.6
P4	-1.30E+08	-1.86E+07	68980.0	244900.0	1612.0	153100.0	720.4
P5	-1.52E+08	-1.23E+07	79440.0	318800.0	1574.0	189500.0	690.4
nP6	-1.67E+08	-6.63E+04	104400.0	352300.0	1694.6	236900.0	761.6
iP6	-1.75E+08	-4.96E+06	88070.0	386000.0	1583.0	242600.0	682.5
nP7	-1.88E+08	8.17E+06	120150.0	400100.0	1676.6	274000.0	756.4
iP7	-1.95E+08	4.53E+06	101100.0	437500.0	1567.0	283600.0	676.8
nP8	-2.09E+08	1.60E+07	135540.0	443100.0	1635.6	305400.0	746.4
iP8	-2.15E+08	1.33E+07	115000.0	485600.0	1550.0	320200.0	673.6
nP9	-2.29E+08	2.50E+07	151750.0	491500.0	1644.8	347000.0	749.6
iP9	-2.36E+08	2.04E+07	136300.0	523900.0	1565.0	349800.0	694.3
N6	-1.07E+08	3.60E+07	65840.0	350100.0	1562.0	230600.0	720.1
N7	-1.38E+08	3.80E+07	94070.0	401700.0	1724.0	292900.0	795.1
N8	-1.73E+08	3.87E+07	109000.0	457600.0	1639.0	322800.0	775.3
N9	-1.89E+08	5.05E+07	122600.0	517700.0	1646.0	360700.0	759.0
A6	8.29E+07	1.30E+08	44767.0	230850.0	1479.2	168360.0	677.7
A7	5.02E+07	1.22E+08	58140.0	286300.0	1440.6	189800.0	650.4
A8	1.91E+07	1.21E+08	78120.0	337000.0	1501.0	223300.0	678.5

A9	-9.00E+06	1.22E+08	97860.0	386100.0	1509.0	248000.0	684.2

Table 2 Reaction rate equilibrium constants

Reaction	K_{eq} (773.15 K)	UNIT	ΔHr (KJ/kmol)
N6↔A6+3H2	70437.3086	atm^3	206042.8285
N7↔A7+3H2	1706326.1	atm^3	201731.7124
N8↔A8+3H2	8476751.35	atm^3	203344.2951
N9↔A9+3H2	32511972.7	atm^3	191182.0506
nP6↔iP6	1.02320227	-	-7220.540362
nP7↔iP7	0.76284955	-	-6180.398136
nP8↔iP8	0.70367737	-	-7435.462647
nP9↔iP9	1.10748818	-	-6433.832538
nP6↔N6+H2	1.29261336	atm	59983.67257
nP7↔N7+H2	1.39141946	atm	51244.76956
nP8↔N8+H2	0.8704456	atm	39116.44748
nP9↔N9+H2	0.75853236	atm	42850.52429
iP8↔N8+H2	1.2369953	atm	46551.90986
iP9↔N9+H2	0.68491238	atm	49284.35707

REFERENCES

(1) http://dippr.byu.edu/