MBWR을 이용한 LNG 혼합물 Flash 공정모사

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LNG Mixture Flash Process Modeling for MBWR

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1.서론

본 연구에서는 BRMR(Bishinoi & Robinson Mixing Rules)를 적용한 MBWR 상태방정식(Modified Benedict-Webb-Rubin Equation of State)을 사용해서 기·액 상평형 물성 예측에 필요한 Flash 과정에 관하여 발표하고자 한다.

2. 이론

1) MBWR 상태방정식

Benedict-Webb-Rubin 상태방정식은 8개의 상수로 이루어져 있다.

$$P = \rho RT + (B_oRT - A_o - \frac{C_o}{T^2})\rho^2 + (bRT - a)\rho^3$$

$$a\alpha\rho^6 + \frac{c\rho^3}{T^2}(1 + \gamma\rho^2)\exp(-\gamma\rho^2) \qquad (2.4-1)$$

그 후 Starling et al. 은 BWR 상태방정식의 온도의존성에 대한 수정을 위해 상수 C_o와, 임계영역에서 물성예측의 개선을 위해 상수 a를 아래의 식과 같이 전개하였다.

$$C_o^* = C_{o1} - \frac{C_{o2}}{T} + \frac{C_{o3}}{T^2} \qquad (2.4-2)$$

$$a^* = a_1 + \frac{a_2}{T} \qquad (2.4-3)$$

그리고 등온의 enthalpy 분석으로 부터 얻어진 C_o^*와 a^*를 BWR식에 대입하여 다음의 MBWR 상태 방정식을 구했다.

$$P = \rho RT + (B_o RT - A_o - \frac{C_o}{T^2} + \frac{D_o}{T^3} - \frac{E_o}{T^4})\rho^2$$

$$+ (bRT - a - \frac{d}{T})\rho^3 + \alpha(a + \frac{d}{T})\rho^6$$

$$+ \frac{c\rho^3}{T^2}(1 + \gamma\rho^2)\exp(-\gamma\rho^2) \qquad (2.4-4)$$

11개의 순수물질 parameter는 다음 식으로 계산된다. (Han&Starling Correlation)

$$\rho_{ci} B_{oi} = A_1 + B_1 \omega_i$$

$$(\rho_{ci} A_{oi})/(R T_{ci}) = A_2 + B_2 \omega_i$$

$$(\rho_{ci}^2 C_{oi})/(R T_{ci}^3) = A_3 + B_3 \omega_i$$

$$\rho_{ci}^2 \gamma_i = A_4 + B_4 \omega_i$$

$$\rho_{ci}^2 b_i = A_5 + B_5 \omega_i$$

$$(\rho_{ci}^2 a_i)/(R T_{ci}^3) = A_6 + B_6 \omega_i$$

$$\rho_{ci}^3 \alpha_i = A_7 + B_7 \omega_i$$

$$(\rho_{ci}^2 c_i)/(R T_{ci}^3) = A_8 + B_8 \omega_i$$

$$(\rho_{ci} D_{oi})/(R T_{ci}^4) = A_9 + B_9 \omega_i$$

$$(\rho_{ci}^2 d_i)/(R T_{ci}^2) = A_{10} + B_{10} \omega_i$$

$$(\rho_{ci} E_{oi})/(R T_{ci}^5) = A_{11} + B_{11} \omega_i \exp(-3.8 \omega_i)$$

The Bishinoi-Robinson Mixing Rules

$$B_{oij} = \sum_{i=1}^{n} x_i B_{oi}$$

$$A_o = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j A_{oi}^{\frac{1}{2}} A_{oj}^{\frac{1}{2}} (1-k_{ij})$$

$$C_o = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j C_{oi}^{\frac{1}{2}} C_{oj}^{\frac{1}{2}} (1-k_{ij})^3$$

$$\gamma = \left[\sum_{i=1}^{n} x_i \gamma_i^{\frac{1}{2}} \right]^2$$

$$b = \left[\sum_{i=1}^{n} x_i b_i^{\frac{1}{3}} \right]^3$$

$$a = \left[\sum_{i=1}^{n} x_i a_i^{\frac{1}{3}} \right]^3$$

$$\alpha = \left[\sum_{i=1}^{n} x_i \alpha_i^{\frac{1}{3}} \right]^3$$

$$c = \left[\sum_{i=1}^{n} x_i c_i^{\frac{1}{3}} \right]^3$$

$$D_o = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j D_{oi}^{\frac{1}{2}} D_{oj}^{\frac{1}{2}} (1-k_{ij})^4$$

$$d = \left[\sum_{i=1}^{n} x_i d_i^{\frac{1}{3}} \right]^3$$

$$E_o = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j E_{oi}^{\frac{1}{2}} E_{oj}^{\frac{1}{2}} (1-k_{ij})^4$$

Table 1. Interaction parameter, k_{ij}

이 성 분 계	k_{ij}	이 성 분 계	k_{ij}
Methane - Ethane	0.01	Methane - n-Heptane	0.06
Methane - Propane	0.023	Methane - n-Octane	0.07
Methane - n-Butane	0.031	Methane - n-Nonane	0.081
Methane - n-Pentane	0.041	Methane - n-Decane	0.092
Methane - n-Hexane	0.05	-	-

Table 2. Generalized Constant A_j and B_j for MBWR EOS

매개변수의 첨자	매 개 변 수 값	
	A_j	B_j
1	0.443690	0.115449
2	1.284380	-0.920731
3	0.356306	1.708710
4	0.544979	-0.270896
5	0.528629	0.349261
6	0.484011	0.754130
7	0.0705233	-0.044448
8	0.504087	1.322450
9	0.0307452	0.179433
10	0.0732828	0.463192
11	0.006450	-0.022143

Sample(input data): Methane-Propane Binary System

```
    1
     .1E-6      .2E-6      .3E-6      .1E-5   1.000001    2.
    2    2   30
METHANE             1   16.042     -116.43    0.013      0.6274      673.40
-5.58114 0.564874 0.101132E-03 0.417399E-06 -1.525576E-101.958857E-14 -0.623373
PROPANE             2   44.0940    206.13     0.157      0.3121      616.30
-1.22301 0.179733 0.664580E-04 0.250998E-06 -1.247461E-101.893509E-14  0.178189
0.023
    1
0.948       0.052
    5
    1
-100.       500.
    2
-100.       500.
    3
-100.       300.
    4
-100.       500.
    5
-100.       500.
```

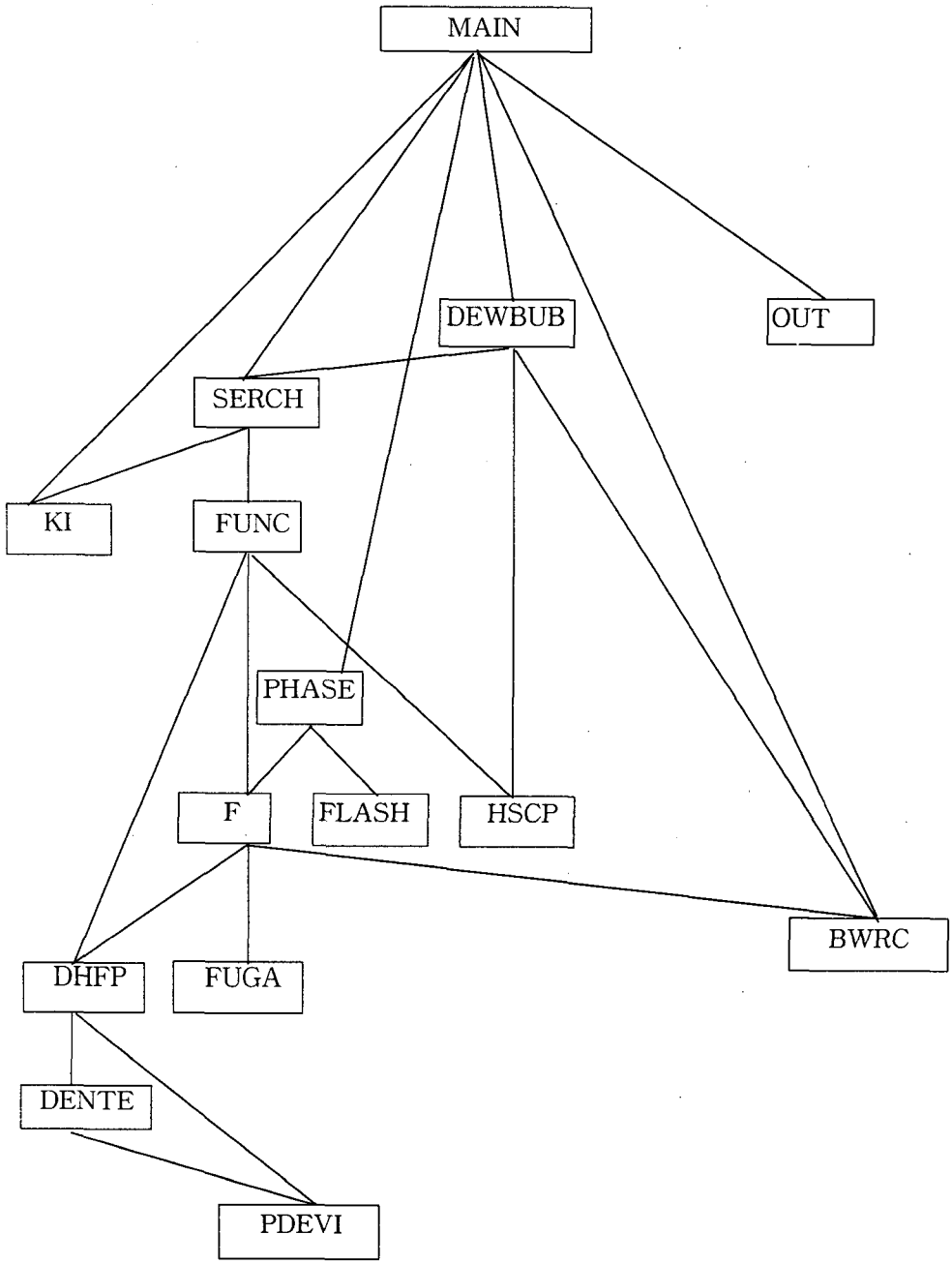

Fig1. Algorithm of MBWR EOS Program

3. 결과 : MBWR EOS를 이용한 flash 계산결과(METHANE-PROPANE)

```
1       NRUN
          1
         EPSD          EPSV          FUGERR          EPSS       STEP       DMAX
        .10E-06       .20E-06       .30E-06       .10E-05  1.0000010        2.0
         NC       NPHASE    ITNM      IPRNT
         2          2         90          0
COMP              IDCOM    CMW       TC         ACF        CD         PC
 METHANE            1   16.0420 -116.4300      .0130      .6274   673.4000
CI   -5.58114        .564874        .101132E-03    .417399E-06    -.152558E-09    .195886E-13    -.623373
 PROPANE            2   44.0940  206.1300      .1570      .3121   616.3000
CI   -1.22301        .179733        .664580E-04    .250998E-06    -.124746E-09    .189351E-13    .178189
CKIG      .0230
1***** FLUID  THERMODYNAMIC   BEHAVIOR  PREDICTOR  USINGHAN-STARLING  GENERALIZED
CORRELATION *****

    INLET CONDITIONS

    FLASH CALCULATION( P AND T SPECIFIED, V,L,X AND Y VARIABLE,NTYPE = 1)

    TEMPERATURE= -100.000     F      PRESSURE=  500.000     PSIA

    COMPONENT                  MOLE FRACTION                K VALUE              FUGAICITY
    ------------------------------------------------------------------------------------------

                          FEED      VAPOR     LIQUID                    VAPOR         LIQUID
    METHANE              .948000   .989250   .553183       1.78829     388.512       388.512
    PROPANE              .052000   .010750   .446817       .240582E-01 1.59112       1.59112

        PROPERTY              FEED          VAPOR          LIQUID
    ---------------------------------------------------------------
    MW                      17.5007        16.3435        28.5761
    VOLUME FRACTION          1.00000        .982893        .171068E-01

        LBMOLE BASIS
    PHASE MOLE FRACTION      1.00000        .905404        .945964E-01
    VOLUME, CU-FT/LBMOLE     5.10832        5.54552        .923791
    DENSITY, LBMOLE/CLFT     .195759        .180326        1.08250
    ENTHALPY, BTU/LBMOLE     2572.66        3022.06        -1728.67
    ENTROPY, BTU/LBMOL-R     37.3846        37.6508        34.8364
    HEAT CAP.,BTU/LBM-R      22.2184        20.0957        42.5348

        LBMASS BASIS
    PHASE MASS FRACTION      1.00000        .845538        .154462
    VOLUME, CU-FT/LB         .291892        .339310        .323274E-01
    DENSITY, LB/CU-FT        3.42592        2.94716        30.9335
    ENTHALPY, BTU/LB         147.003        184.908        -60.4935
    ENTROPY, BTU/LB-R        2.13617        2.30371        1.21908
    HEAT CAP.,BTU/LB-R       1.26957        1.22958        1.48847
```