Two-Phase Flash Logic

Assume P and z_i are given.

We require $R_{ic} \to 0$ where

$$R_{ic} = \ln \varphi_{ic}^{l} - \ln \varphi_{ic}^{v} - \ln K_{ic} \qquad (1)$$

and φ_{ic}^{α} is the fugacity coefficient for phase α.
The fugacity coefficient can be expressed as

$$\ln \varphi_{ic}^{\alpha} = f(z^{\alpha}, n_{ic}^{\alpha}, p) \qquad (2)$$

the functional form of f is identical for both phases.

The mole numbers for each phase satisfy

$$n_{ic}^{l} = (1-v)\frac{n_{ic}}{1+(K_{ic}-1)v} \qquad (3a)$$

$$n_{ic}^{v} = v K_{ic} \frac{n_{ic}}{1+(K_{ic}-1)v} \qquad (3b)$$

The vapor fraction satisfies

$$R_v \equiv \sum_{ic} \frac{(K_{ic}-1)\, n_{ic}}{1+(K_{ic}-1)v} = 0 \qquad (4)$$

The Z^α factors satisfy

$$1 = \frac{1}{Z^\alpha - B^\alpha + C^\alpha} - \frac{A^\alpha}{(Z^\alpha + e_1 B^\alpha + C^\alpha)(Z^\alpha + e_2 B^\alpha + C^\alpha)} \tag{5}$$

where A^α, B^α, and C^α functions of n_{ic}^α and p.

Solution logic is:

Assume K_{ic} is given:

(1) Solve (4) for v and use (4) to express δv in terms of $\delta \ln K_{ic}$

(2) Determine n_{ic}^α from (3)

(3) Solve (5) for Z^α

(4) Calculate $\ln \varphi_{ic}^\alpha$ from (2)

(5) Check (1) for convergence

(6) Expand (1) in terms of $\delta \ln K_{ic}$ to calculate an update for $\ln K_{ic}$

The expansion of (2) produces

$$\delta \ln \varphi_{ic}^{\alpha} = \frac{\partial \ln \varphi_{ic}^{\alpha}}{\partial Z^{\alpha}} \delta Z^{\alpha} + \sum_{jc} \frac{\partial \ln \varphi_{ic}^{\alpha}}{\partial x_{jc}^{\alpha}} \delta x_{jc}^{\alpha} \qquad (6)$$

where the pressure term is not included since pressure does not vary during the flash iterations.

From (5) we have

$$R_e^{\alpha} + \frac{\partial R_e^{\alpha}}{\partial Z} \delta Z^{\alpha} + \sum_{jc} \frac{\partial R_e^{\alpha}}{\partial n_{jc}^{\alpha}} \delta n_{jc}^{\alpha} = 0 \qquad (7)$$

From (4)

$$R_v + \frac{\partial R_v}{\partial v} \delta v + \sum_{j} \frac{\partial R_v}{\partial \ln K_{jc}} \delta \ln K_{jc} = 0 \qquad (8)$$

From (3)

$$\delta n_{ic}^{\alpha} = \frac{\partial n_{ic}^{\alpha}}{\partial v} \delta v + \sum_{jc} \frac{\partial n_{ic}^{\alpha}}{\partial K_{jc}} K_{jc} \delta \ln K_{jc} \qquad (9)$$

To form the Jacobian for (1):

(1) Use (8) in (9) to express δn_{ic}^{α} in terms of $\delta \ln K_{jc}$

(2) Use this δn_{ic}^{α} in (7) to express δZ^{α} in terms of $\delta \ln K_{jc}$

(3) Substitute for δn_{ic}^{α} and δZ^{α} in (6) and use in expansion of (1)

(4) Solve $R_{ic} + \sum_{jc} \frac{\partial R_{ic}}{\partial \ln k_{jc}} \delta \ln k_{jc} - 1$

for new $\delta \ln k_{jc}$

(5) We do not update δv, δz^{α} or δn^{α}_{ic} since we iterate separately on v and z and calculate δn^{α}_{ic} directly from k_{ic} and v.