OLI Tips #46

Mixed Solvent Electrolyte (MSE) model Regression Parameters

The regression parameters for each variable are **Bold-faced**

K-VALUE COEFFICIENTS **A, B, C, D**
K-VALUE COEFFICIENTS **E, F, G**
BROMLEY **B1, B2, B3**
BROMLEY **C1, C2, C3**
BROMLEY **D1, D2, D3**
PITZER BETA0(1), BETA0(2), BETA0(3) (**B01,B02,B03**)
PITZER BETA1(1), BETA1(2), BETA1(3) (**B11,B12,B13**)
REACTION KINETICS **AF, BF, AR, BR**
REACTION KINETICS **ER1, ER2, ..., ER10**
REACTION KINETICS **EP1, EP2, ..., EP10**
ION EXCHANGE, **BEX1**
ION EXCHANGE, **AIJ, AJI, DIJ**
SRK **KIJ, GIJ**
SRK **KIJ0, KIJ1, KIJ2** (KIJ0 IS EQUIVALENT TO KIJ (NO. 56))
PITZER DENSITY BETA0(1), BETA0(2), BETA0(3) (**BD01,BD02,BD03**)
PITZER DENSITY BETA1(1), BETA1(2), BETA1(3) (**BD11,BD12,BD13**)
HELG **HW,HA1,HA2,HA3,HA4,HC1,HC2,GREF,SREF,HREF**

Mix Solvent UNIQAC

Q0IJ,Q0JI
Q1IJ,Q1JI
Q2IJ,Q2JI
Q3IJ,Q3JI
Q4IJ,Q4JI

Mix Solvent MID-RANGE

BMD0
BMD1
BMD2
CMD0
CMD1
CMD2
CMD3
CMD4
BMD3
BMD4

Full Pitzer Framework (Hanford)

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Binaries
beta(0) = PB01, PB02, ..., PB08
beta(1) = PB11, PB12, ..., PB18
beta(0) = PB21, PB22, ..., PB28
C(0)    = PC01, PC02, ..., PC08

Ternaries/Binaries
lambda  = PLAM1, PLAM2, ..., PLAM6
theta   = PTHE1, PTHE2, ..., PTHE6
psi     = PPSI1, PPSI2, ..., PPSI6
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Mix Solvent UNIQAC Density

D0IJ,D0JI
D1IJ,D1JI
D2IJ,D2JI

Mix Solvent Mid Range Density

DMD1
DMD2
DMD3
DMD4
DMD5
DMD6
DMD7
DMD8
DMD9
DMD0

Solid CP, G, H, S AND V

CP

CPS1
CPS2
CPS3
CPS4
CPS5

G, H, S, and V

GRFS
HRFS
SRFS
VRFS

Dielectric Constant

DIE0
DIE1
DIE2
DIE3

UNIQ R & Q

R_UQ
Q_UQ

Vapor CP, G and H

CPI1 JOULE/K/MOL
CPI2
CPI3
CPI4
CPI5
GRFV CAL/MOL
HRFV CAL/MOL
SRFV CAL/MOL/K