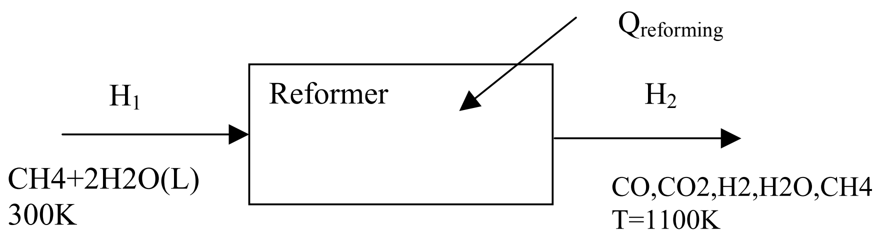
HW 3 SOLUTION

1.



Using Equil one can calculate the mole fractions of the final stage and enthalpies of the initial and final stages. In the "Gas Chemistry input" (chem.inp) file in Equil, you need to specify CO, CO2, H2, H2O and CH4. Also, you need to supply "Surface chemistry input" for H2O in liquid form.[1] An example of input files is as follow:

"Gas Chemistry Input"
```
ELEMENTS C H O END
SPECIES CO H2 CO2 CH4 H2O END
```

"Surface Chemistry Input"
```
BULK
H2O(L)
END
```

"Application Input"
```
REAC CH4 1
REAC H2O(L) 1
TP
PRES 1
TEMP 300
CNTN
END
REAC CH4 1
REAC H2O(L) 1
TP
PRES 1
TEMP 1100
END
```

Using the above input files, you will get the following answer:

[1] You should not put H2O(L) in the "Gas Chemistry input". The gas chemistry input is for gases only.

```
**********************************************************
*          CHEMKIN Collection Release 3.7                *
*              EQUIL Application                         *
*          CHEMKIN INTERFACE FOR STANJAN                 *
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```

```
            WORKING SPACE REQUIREMENTS
             PROVIDED      REQUIRED
 INTEGER         494         494
 REAL           1281        1281
 CHARACTER        37          37
```

Initializing CHEMKIN Gas-phase Library, a component of CHEMKIN Release 3.7.
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Initializing SURFACE CHEMKIN Library, a component of CHEMKIN Release 3.7.

```
          KEYWORD INPUT

 REAC CH4 1
 REAC H2O(L) 2
 TP
 PRES 1
 TEMP 300
 CNTN
 END

  Constant temperature and pressure problem.
  Calling SUBROUTINE EQUIL

        WORKING SPACE REQUIREMENTS
          PROVIDED      REQUIRED
 INTEGER       282          282
 REAL         963          963
 CHAR           6            6

  MIXTURE:        INITIAL STATE:     EQUILIBRIUM STATE:
```

P (atm)	1.0000E+00	1.0000E+00
T (K)	3.0000E+02	3.0000E+02
V (cm3/gm)	4.7205E+02	4.8916E+02
H (erg/gm)	-1.2410E+11	-1.2380E+11
U (erg/gm)	-1.2458E+11	-1.2429E+11
S (erg/gm-K)	6.2814E+07	6.3889E+07
W (gm/mol)	1.7358E+01	1.7358E+01
Mol Fractions		
H2	0.0000E+00	1.3448E-05
CO2	0.0000E+00	3.3621E-06
CH4	3.3333E-01	3.3333E-01
H2O	0.0000E+00	1.2061E-02
H2O(L)	6.6667E-01	6.5459E-01

GAS PHASE

Mols	1.0000E+00	1.0362E+00
W (gm/mol)	1.6043E+01	1.6112E+01
V (cm3/gm)	1.5345E+03	1.5279E+03
Mol Fractions		
CO	0.0000E+00	1.1463E-13
H2	0.0000E+00	3.8935E-05
CO2	0.0000E+00	9.7337E-06
CH4	1.0000E+00	9.6503E-01
H2O	0.0000E+00	3.4919E-02

BULK PHASE: BULK1

Mols	2.0000E+00	1.9638E+00
Mol Fractions		
H2O(L)	1.0000E+00	1.0000E+00

**** CONTINUING TO NEW PROBLEM*******

KEYWORD INPUT

REAC CH4 1
REAC H2O(L) 2
TP
PRES 1
TEMP 1100
Reached end of input ...

Constant temperature and pressure problem.

MIXTURE: INITIAL STATE: EQUILIBRIUM STATE:

P (atm)	1.0000E+00	1.0000E+00
T (K)	1.1000E+03	1.1000E+03
V (cm3/gm)	1.7327E+03	8.6517E+03
H (erg/gm)	-5.6216E+09	-4.4884E+10
U (erg/gm)	-7.3773E+09	-5.3651E+10
S (erg/gm-K)	4.8881E+07	1.9509E+08
W (gm/mol)	1.7358E+01	1.0432E+01
Mol Fractions		
CO	0.0000E+00	1.5953E-01
H2	0.0000E+00	6.3843E-01
CO2	0.0000E+00	3.9961E-02
CH4	3.3333E-01	8.4767E-04
H2O	0.0000E+00	1.6123E-01
H2O(L)	6.6667E-01	0.0000E+00

GAS PHASE

Mols	1.0000E+00	4.9915E+00
W (gm/mol)	1.6043E+01	1.0432E+01
V (cm3/gm)	5.6263E+03	8.6522E+03
Mol Fractions		
CO	0.0000E+00	1.5953E-01
H2	0.0000E+00	6.3843E-01
CO2	0.0000E+00	3.9961E-02
CH4	1.0000E+00	8.4767E-04
H2O	0.0000E+00	1.6123E-01

BULK PHASE: BULK1

Mols	2.0000E+00	0.0000E+00
Mol Fractions		
H2O(L)	1.0000E+00	0.0000E+00

Total CPUtime: 1 (seconds)

Mole fractions after reformer

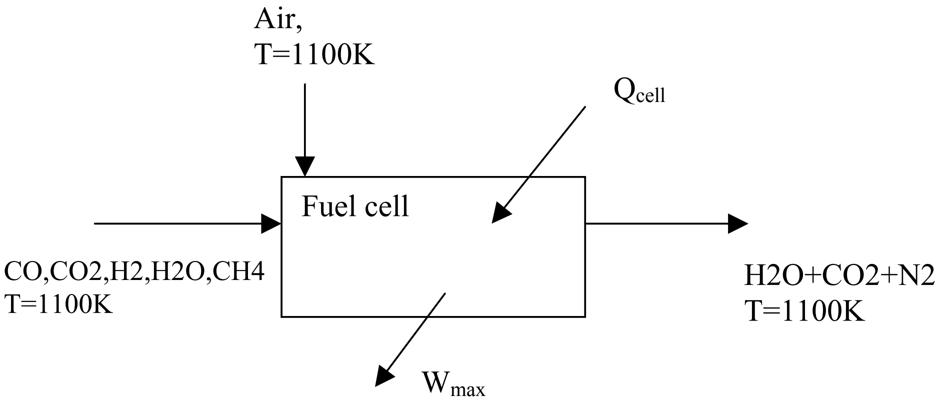
	CH4	CO	CO2	H2	H2O
Mole fractions	8.48e-4	0.16	0.04	0.638	0.161
Number of moles/ (per kg mixture of CH4 and 2H2O)	0.08	15.4	3.8	61.3	15.5

2.

$Q_{reforming}=H_2-H_1$

$Q_{reforming}$=7.910MJ/(kg mixture of CH4 and 2H2O)

3.



Required O2 in the cell per one mole of mixture after reformer can be calculated as

		O2 Required
CH4	8.48e-4	8.48e-4*2
CO	0.16	0.16/2
H2	0.638	0.638/2
Total		0.4

Hence, 0.4 mole of O2 and 0.4*3.76=1.504 mole of N2 is required in the cell per one mole of mixture. In terms of mass, 5.25kg of air is required per kg of (CH4+2H2O)

To calculate ΔG, we use Equil again and an example of input files is as follow:

```
"Gas Chemistry Input"
ELEMENTS C H O N END
SPECIES CO CO2 CH4 O2 H2 H2O N2 END

"Application Input"
REAC CH4 8.48E-4
REAC CO 0.16
REAC CO2 0.04
REAC H2 0.638
REAC H2O 0.161
REAC O2 0.4
REAC N2 1.504
PT
PRES 1
TEMP 1100
END
```

Solutions are as follow:

Constant temperature and pressure problem.
Calling SUBROUTINE EQUIL

WORKING SPACE REQUIREMENTS

	PROVIDED	REQUIRED
INTEGER	341	341
REAL	1196	1196
CHAR	7	7

MIXTURE:	INITIAL STATE:	EQUILIBRIUM STATE:
P (atm)	1.0000E+00	1.0000E+00
T (K)	1.1000E+03	1.1000E+03
V (cm3/gm)	4.0094E+03	3.4593E+03
H (erg/gm)	1.3874E+08	-3.1069E+10
U (erg/gm)	-3.9238E+09	-3.4574E+10
S (erg/gm-K)	1.0306E+08	9.3398E+07
W (gm/mol)	2.2513E+01	2.6092E+01
Mol Fractions		
CO	5.5099E-02	1.1214E-04
CO2	1.3775E-02	8.0049E-02
CH4	2.9203E-04	1.0086E-16
O2	1.3775E-01	8.7922E-13
H2	2.1971E-01	4.4343E-04
H2O	5.5444E-02	3.1913E-01
N2	5.1793E-01	6.0027E-01

Total CPUtime: 2 (seconds)

$$W_{\max} = -\Delta G = -(H_2 - TS_2) + (H_1 - TS_1)$$

=-(-3.1069E+10-1100*9.3398E+07)+(1.3874E+08-1100* 1.0306E+08)

= $2.06\text{x}10^{10}$erg/gm=2.06MJ/(kg mixture)

We can get W_{max} per unit mass of the reformer mixture by

W_{max} =2.06MJ/(kg mixture)*(1kg+5.25kg)/ (kg mixture of CH4 and 2H2O)
=12.9MJ/(kg mixture of CH4 and 2H2O),

Q_{cell} can be calculate from energy balance as

$Q_{cell} - W_{\max} = H_2 - H_1$=-6.66MJ/(kg mixture of CH4 and 2H2O)

4.

Mole fractions after reformer

	CH_4	CO	CO_2	H_2	H_2O
Mole fractions	8.48e-4	0.16	0.04	0.638	0.161
Number of moles/ (per kg mixture of CH_4 and $2H_2O$)	0.08	15.4	3.8	61.3	15.5

If we represent W_{max} per mole of H_2 and CO used,
12.9MJ/(kg mixture of CH_4 and $2H_2O$)* (kg mixture of CO and$2H_2$)/(61.3+15.5 moles of H_2 and CO)=168J/mol

Voltage= 168*1000J/mol /(2*96485C/mol)=0.87Volt