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Title: TEP R&D

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Intended for: IO-US Bilateral Meeting on TEP

Los Alamos NATIONAL LABORATORY EST.1943

TEP R&D

Scott Willms, Bryan Carlson, Dave Dogruel, and the TEP team

US-IO Bilateral Meeting

LANL

Nov 20, 2008

LA-UR- 08-06499

Outline

- R&D Motivation
- Catalysts
- Impurity Processing
- Future Work

R&D Motivation

Project R&D

- Project R&D is performed to reduce project risk to acceptable levels. For example
  - Use published values/correlations or measure 1:1 values
  - Build prototype or just scale from equations

- For TEP the primary motivations for R&D are:
  - Impurity processing base technology performance evaluation and model benchmarking
  - Process scale-up
  - Control system development

Issues that drive TEP R&D

Issue	Activity
Need to size impurity processing to meet challenging product requirements. Limited catalyst performance data in TEP processing regime.	Determined WGS and MSR kinetics for candidate catalysts. Test prototype impurity processing systems
Considerable scale-up	Test IP at two sizes
Feed to IP will vary considerably over relatively short periods of time.	Perform dynamic performance
Successful operation requires addition of reactants	Perform control systems test
Need to be able to recover from unexpected operations	All of the above

Use computer modeling to generalize and scale results

Catalyst Testing

Reactions

Water gas shift

$$\mathrm{CO} + \mathrm{H_2O} \underset{k_{1,r}}{\overset{k_{1,f}}{\rightleftarrows}} \mathrm{H_2} + \mathrm{CO_2}$$

$$3\mathrm{H_2} + \mathrm{CO} \underset{k_{2,r}}{\overset{k_{2,f}}{\rightleftarrows}} \mathrm{CH_4} + \mathrm{H_2O}$$

$$\mathrm{CH_4} + \mathrm{H_2O} \underset{k_{1,r}}{\overset{k_{1,f}}{\rightleftarrows}} 3\mathrm{H_2} + \mathrm{CO}$$

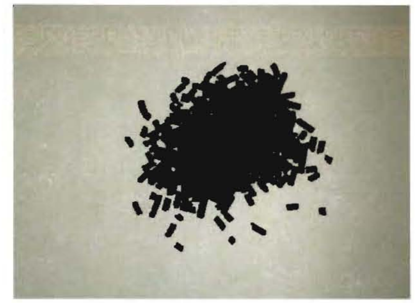
$$\mathrm{CO} + \mathrm{H_2O} \underset{k_{2,r}}{\overset{k_{2,f}}{\rightleftarrows}} \mathrm{H_2} + \mathrm{CO_2}$$

Methane steam reforming

Hydrogen Processing Laboratory

Catalysts

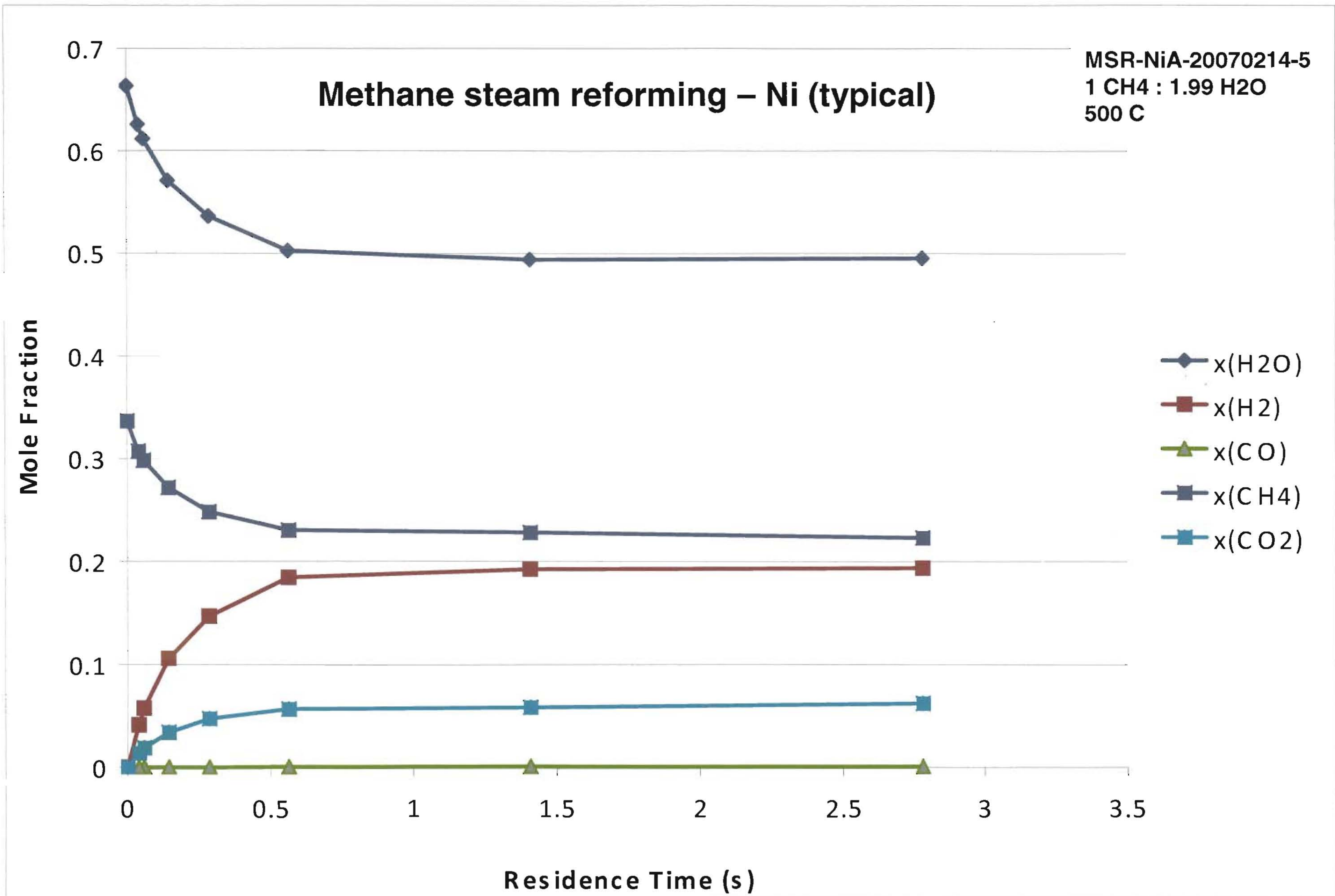
- **Catalyst 1: United Catalyst, 60-70% Ni/Al_2O_3, 1/16" extrusion**

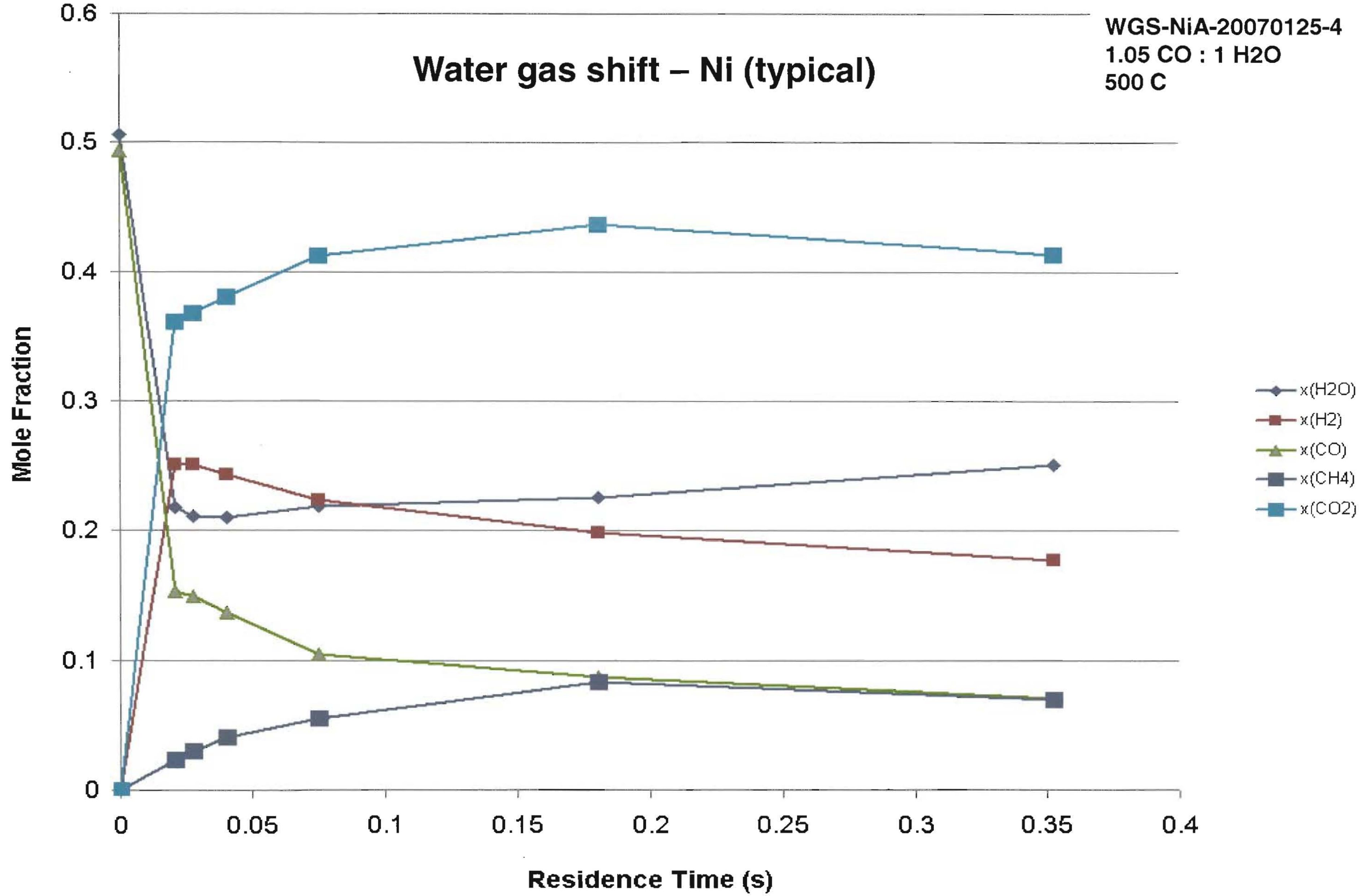


- **Catalyst 2: Degussa, 0.15% Pt/ 0.15% Pd on Al_2O_3, 2 mm spheres**

- **Catalyst 3: NIKKI, 50% Ni on diatomaceous earth, 2 mm pellets**

- **Catalyst 4: Engelhard, ~2% Pt on Al_2O_3**


Methane steam reforming – Ni (typical)
MSR-NiA-20070214-5
1 CH4 : 1.99 H2O
500 C
Mole Fraction
Residence Time (s)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
0.5
1
1.5
2
2.5
3
3.5
x(H2O)
x(H2)
x(CO)
x(CH4)
x(CO2)



Water gas shift – Ni (typical)
WGS-NiA-20070125-4
1.05 CO : 1 H2O
500 C
Mole Fraction
Residence Time (s)
x(H2O)
x(H2)
x(CO)
x(CH4)
x(CO2)
0.6
0.5
0.4
0.3
0.2
0.1
0
0.05
0.15
0.25
0.35

Methane-steam reforming and water-gas shift - Key equations

$$CH_4 + H_2O \underset{k_{1,r}}{\overset{k_{1,f}}{\rightleftarrows}} 3H_2 + CO$$

$$CO + H_2O \underset{k_{2,r}}{\overset{k_{2,f}}{\rightleftarrows}} H_2 + CO_2$$

$$\frac{d(Fx_{CH_4})}{dz} = -AV_f\{k_{1,f}[CH_4][H_2O] - k_{1,r}[H_2]^3[CO]\}$$

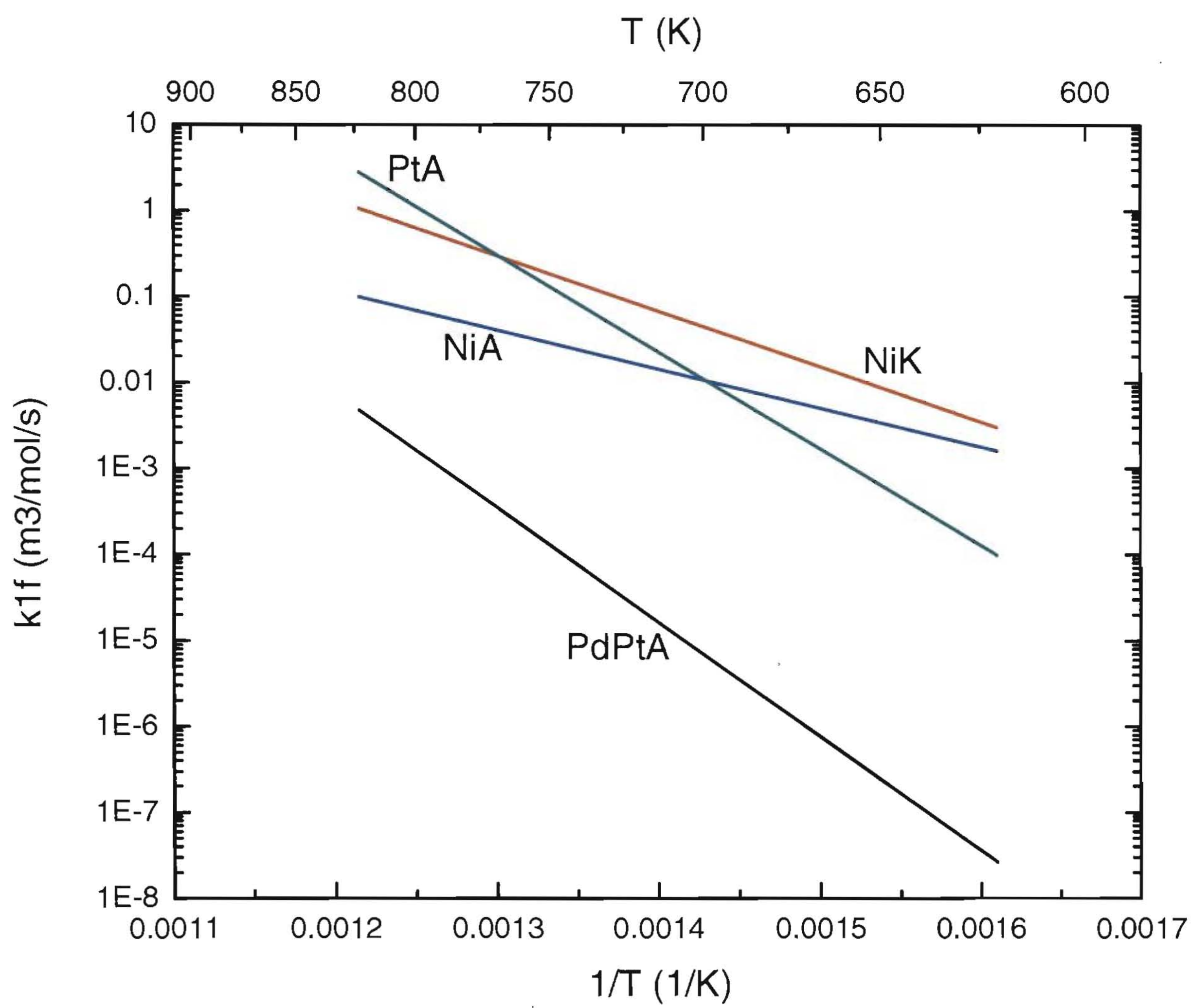
$$\frac{d(Fx_{H_2O})}{dz} = -AV_f\{k_{1,f}[CH_4][H_2O] - k_{1,r}[H_2]^3[CO] + k_{2,f}[CO][H_2O]\} - k_{2,r}[H_2][CO_2]$$

$$\frac{d(Fx_{H_2})}{dz} = -AV_f\{3k_{1,r}[H_2]^3[CO] - 3k_{1,f}[CH_4][H_2O] + k_{2,r}[H_2][CO_2] - k_{2,f}[CO][H_2O]\}$$

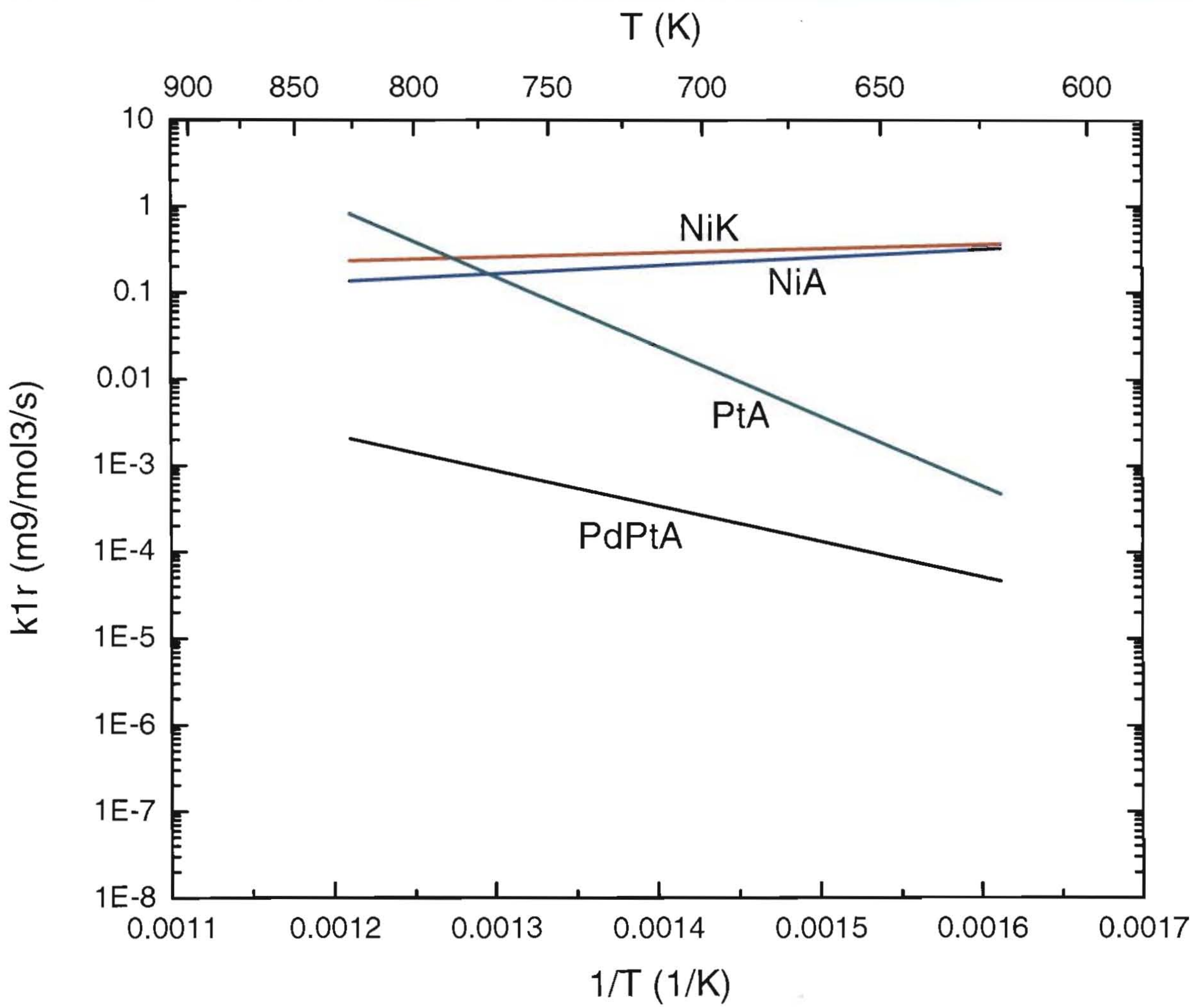
$$\frac{d(Fx_{CO})}{dz} = -AV_f\{k_{1,r}[H_2]^3[CO] - k_{1,f}[CH_4][H_2O] + k_{2,f}[CO][H_2O] - k_{2,r}[H_2][CO_2]\}$$

$$\frac{d(Fx_{CO_2})}{dz} = -AV_f\{k_{2,r}[H_2][CO_2] - k_{2,f}[CO][H_2O]\}$$

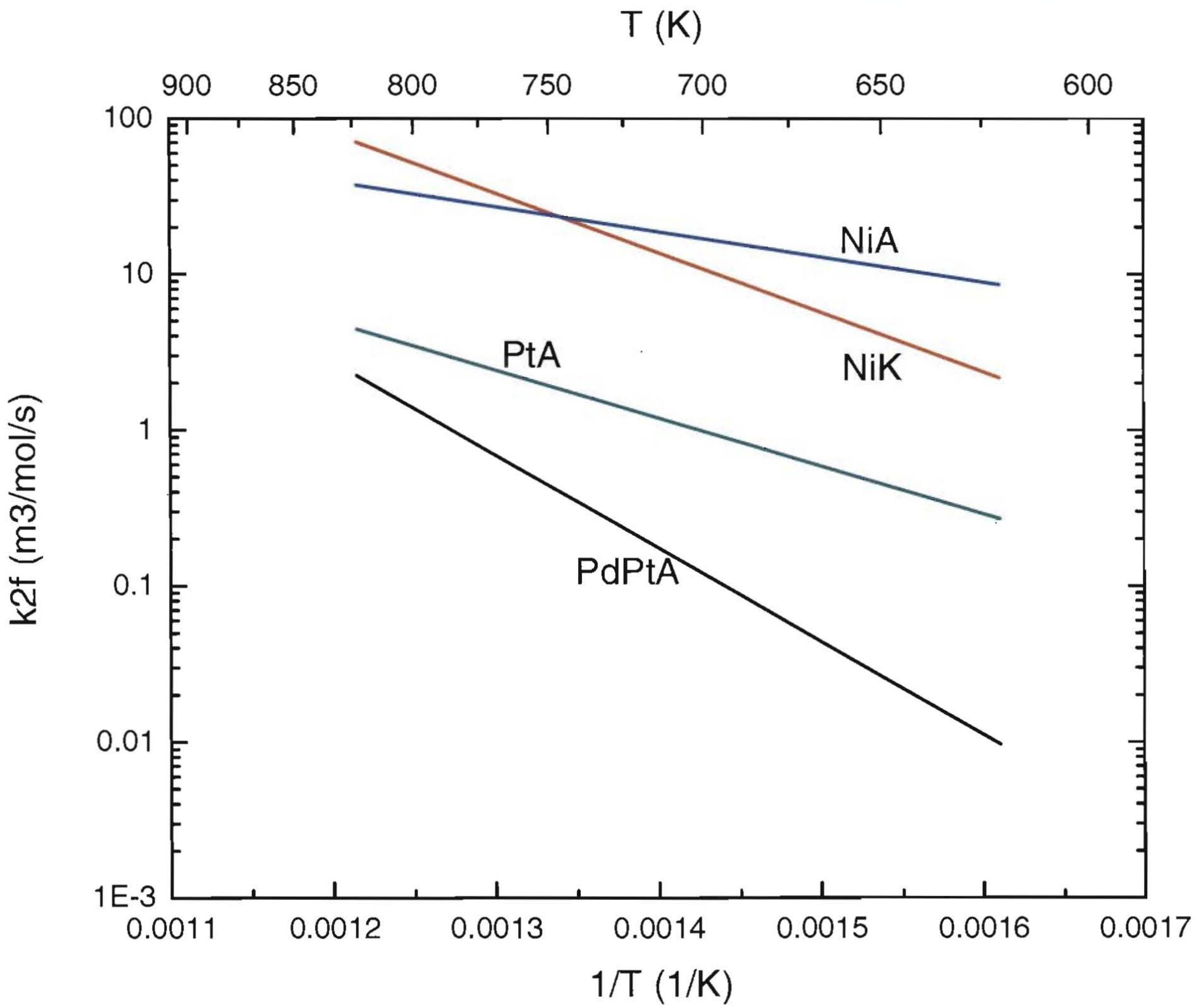
Arrhenius plot for forward MSR reaction (k1f)



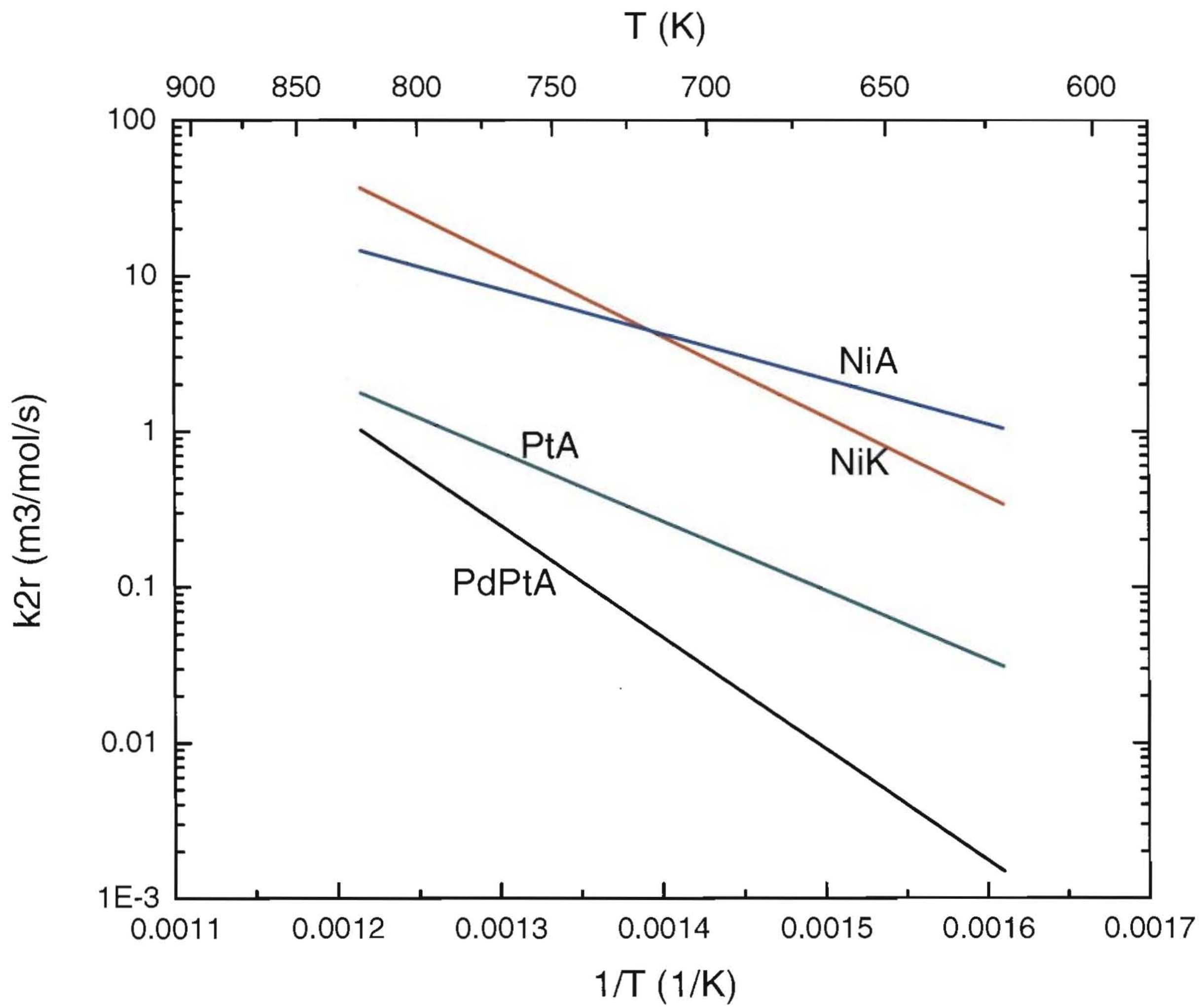
Arrhenius plot for forward MSR reaction (k1r)



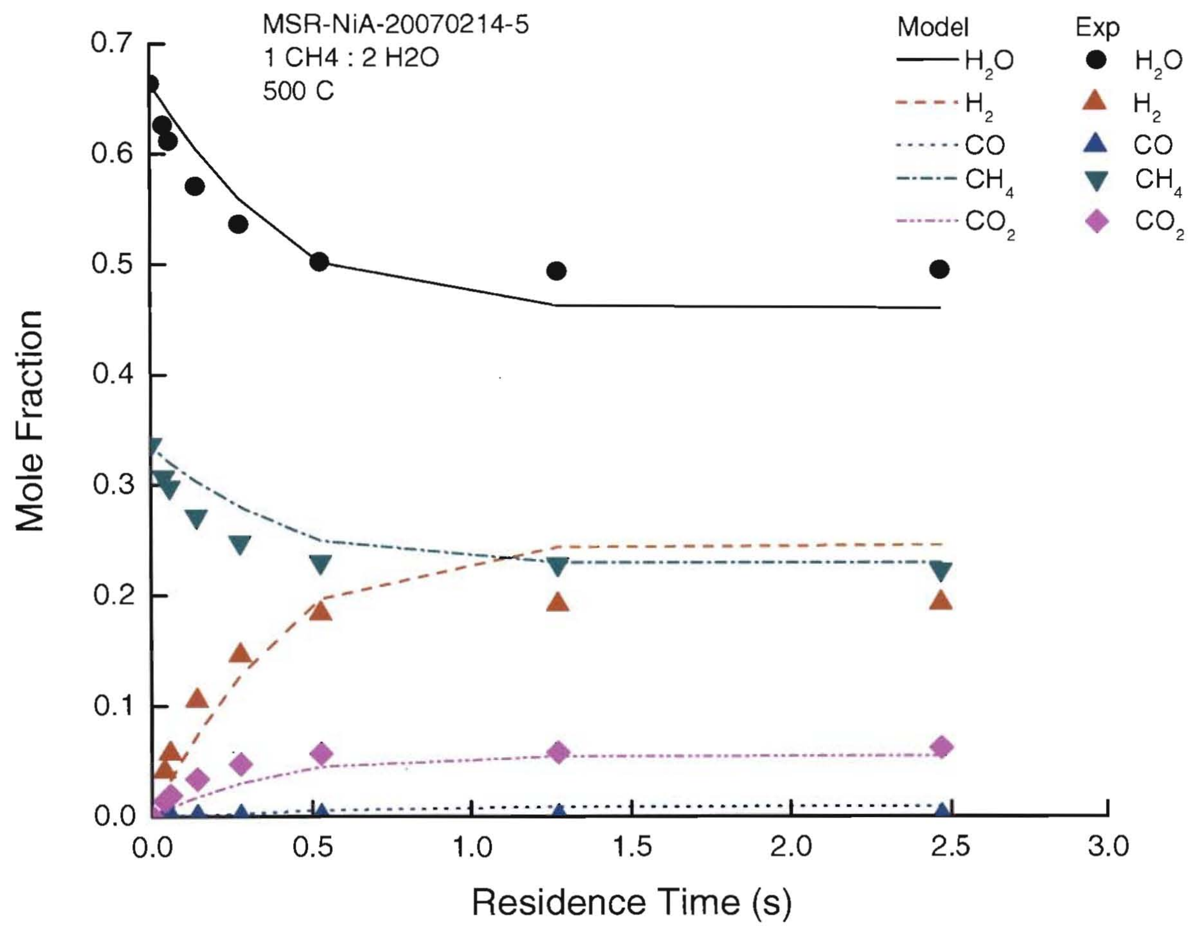
Arrhenius plot for forward WGS reaction (k2f)



Arrhenius plot for forward WGS reaction (k2r)

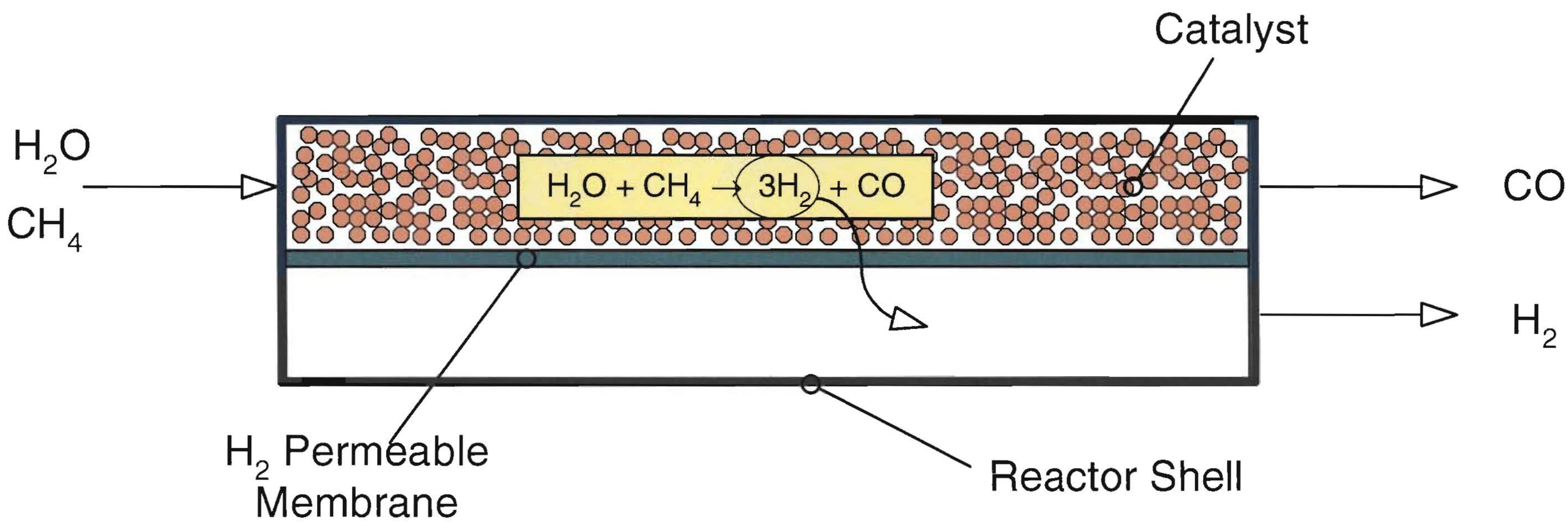


Example comparison of model to experiment-MSR over NiA

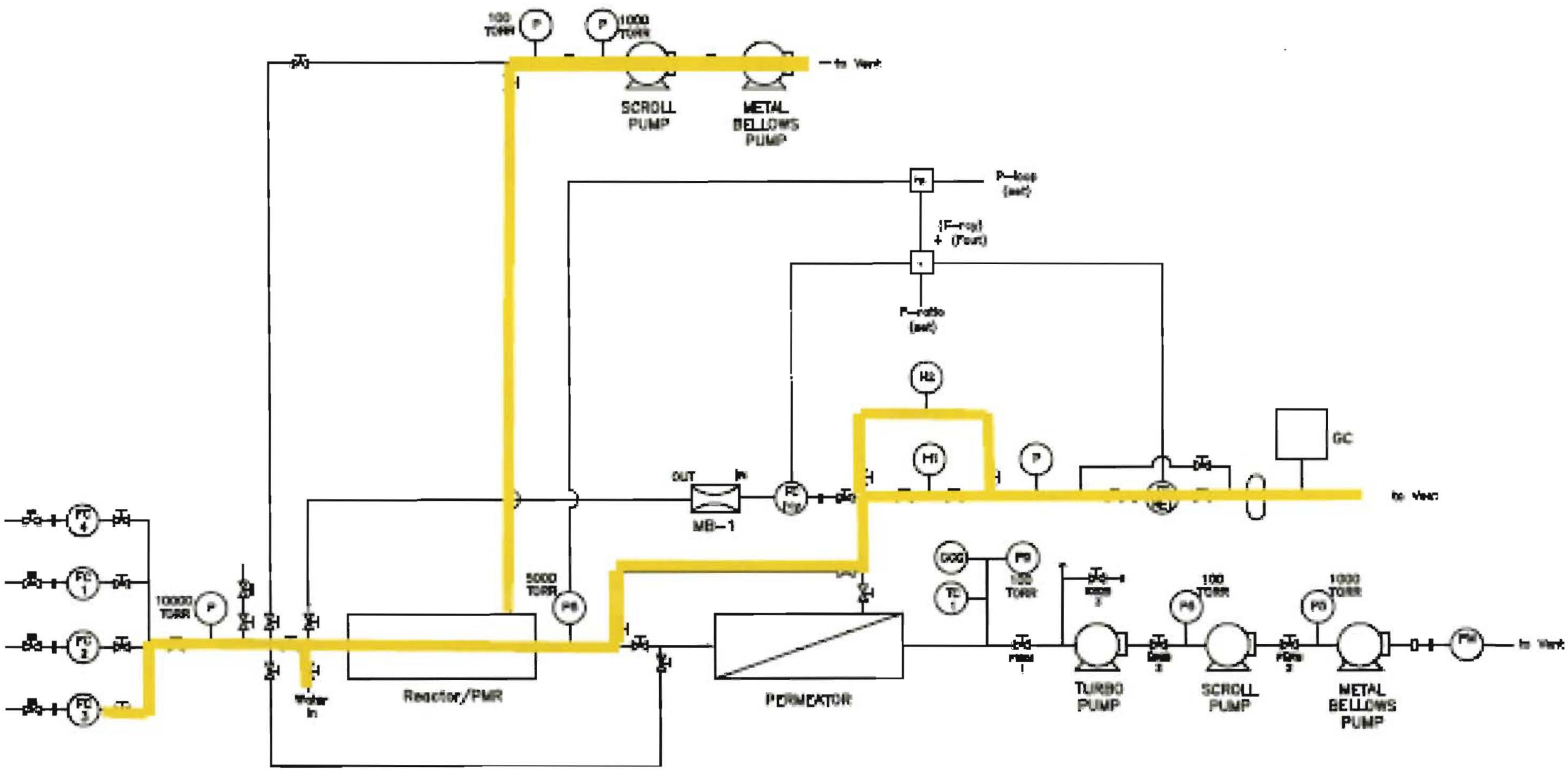


PMR --Preliminary Data--

By removing hydrogen as it is produced, thermodynamic barriers are circumvented and process can be greatly simplified



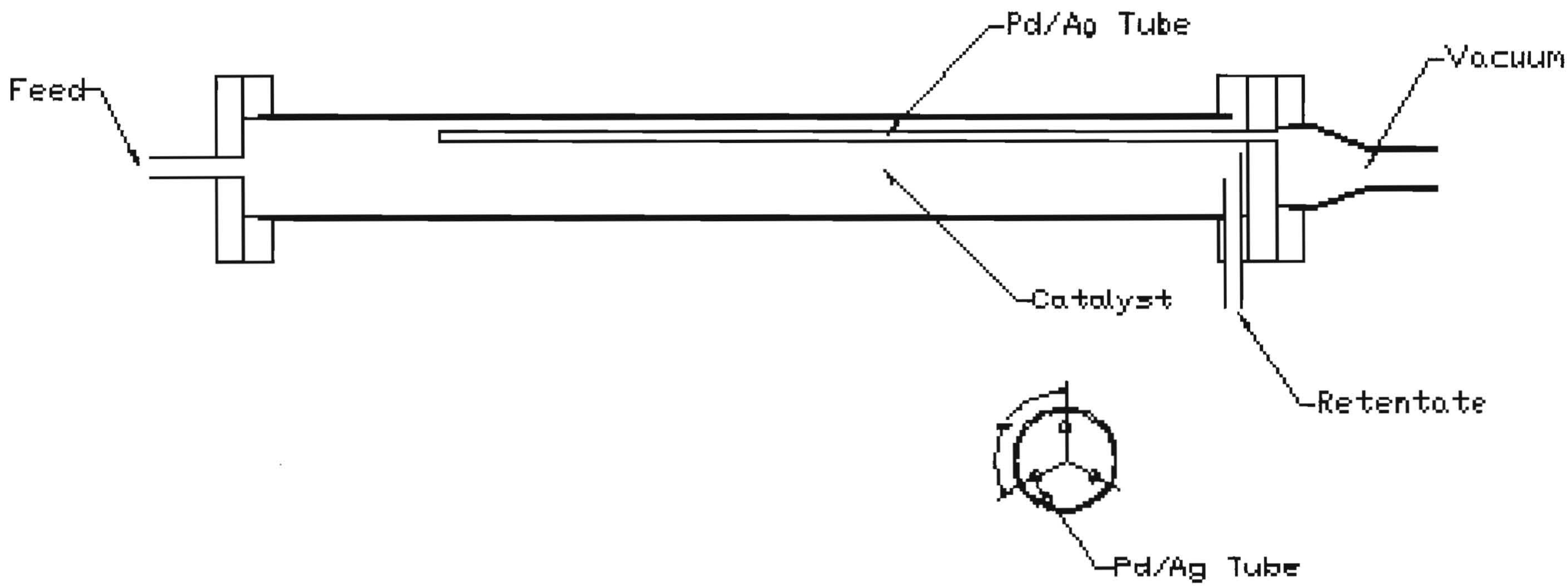
TEP R&D Test Stand – Highlighted for PMR test



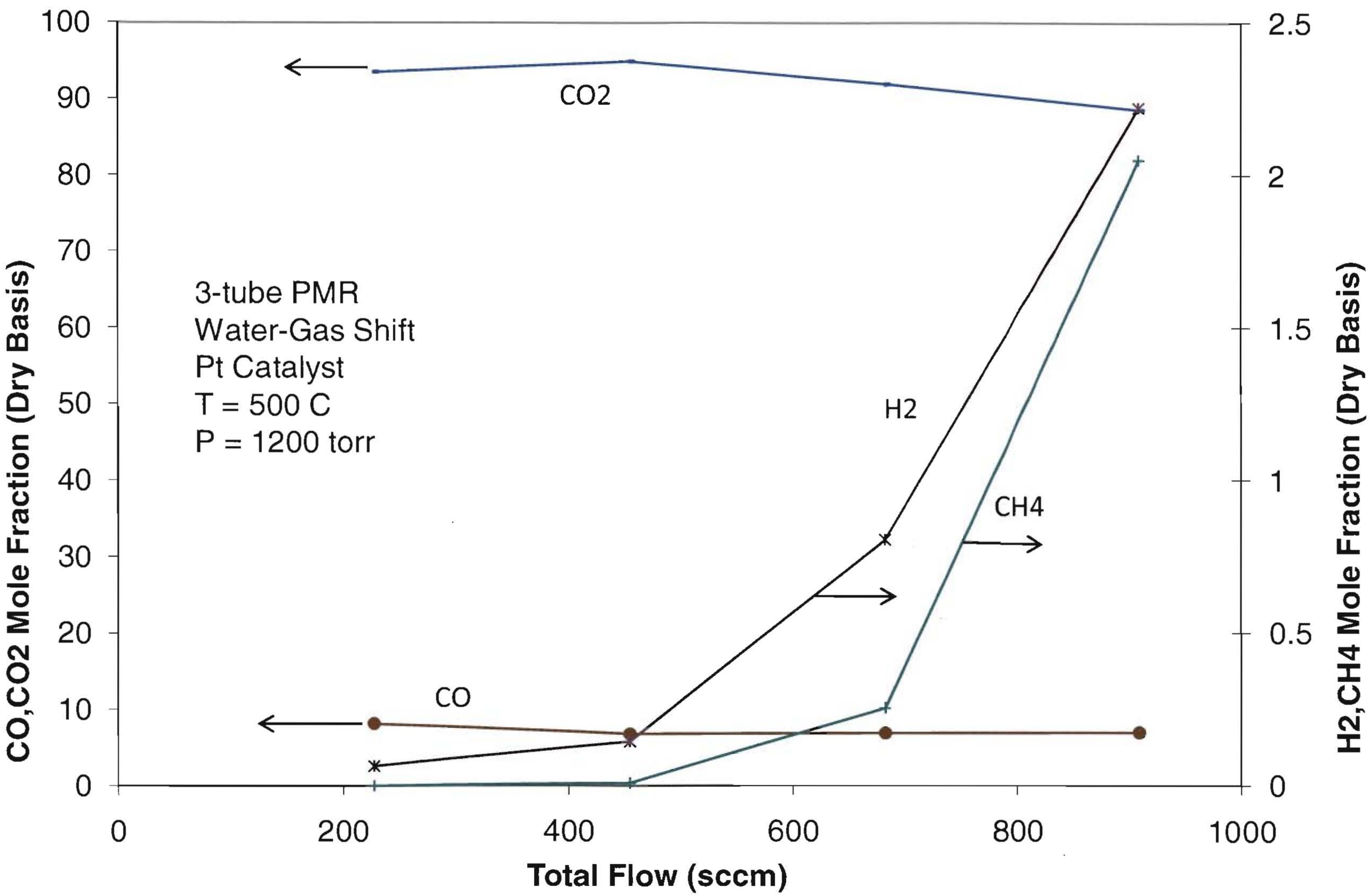
PMR – recent accomplishment summary

- Completed design and fabrication of 3-tube and prototype (1/6th scale) PMR
- Developed conditioning procedure
- Developed method for preventing tube crushing
- Tested 3-tube PMR with Pt catalyst
  - Performed baseline and parametric testing
- Testing 3-tube PMR with Nikki catalyst

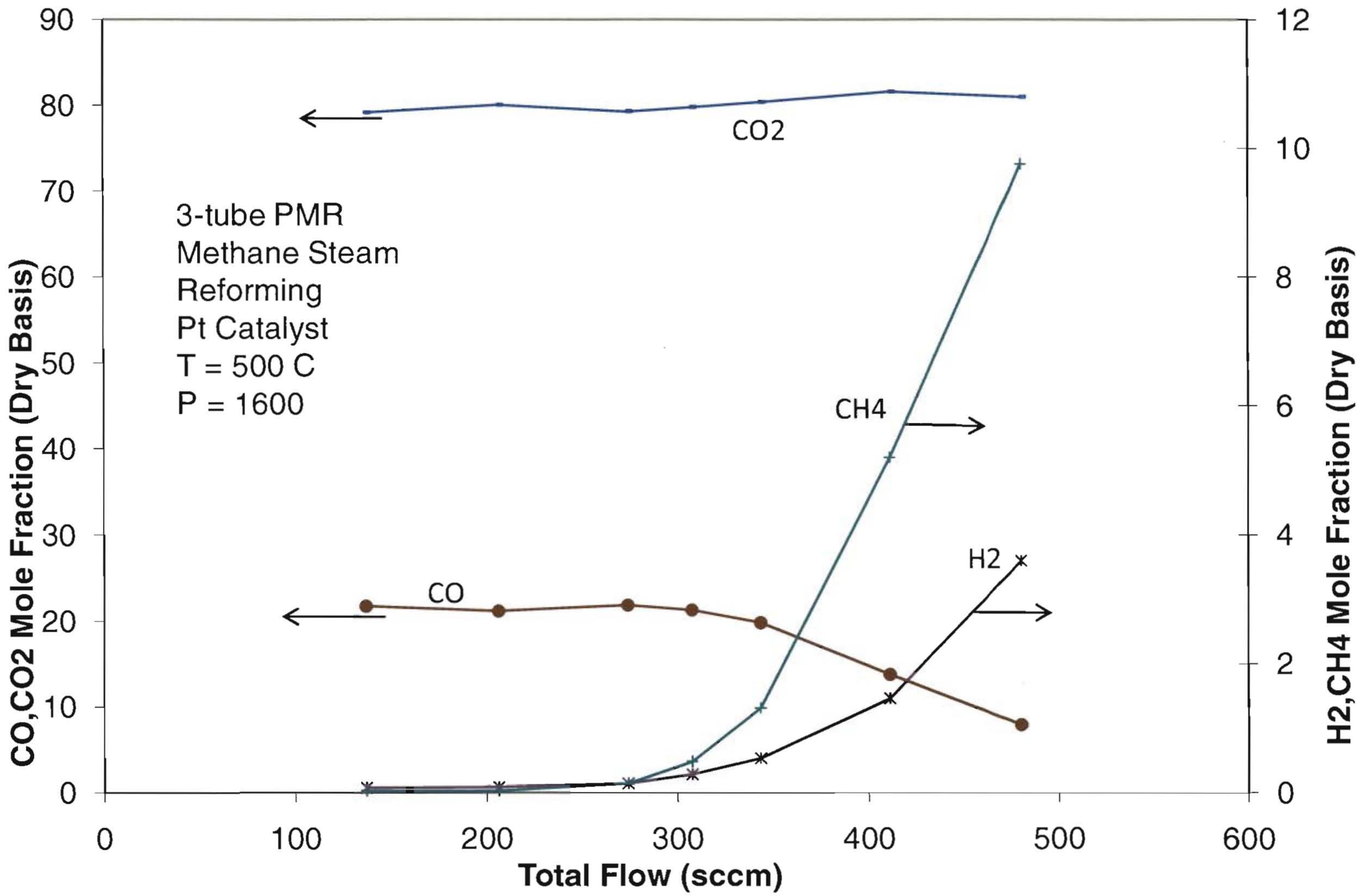
3-tube PMR Sketch



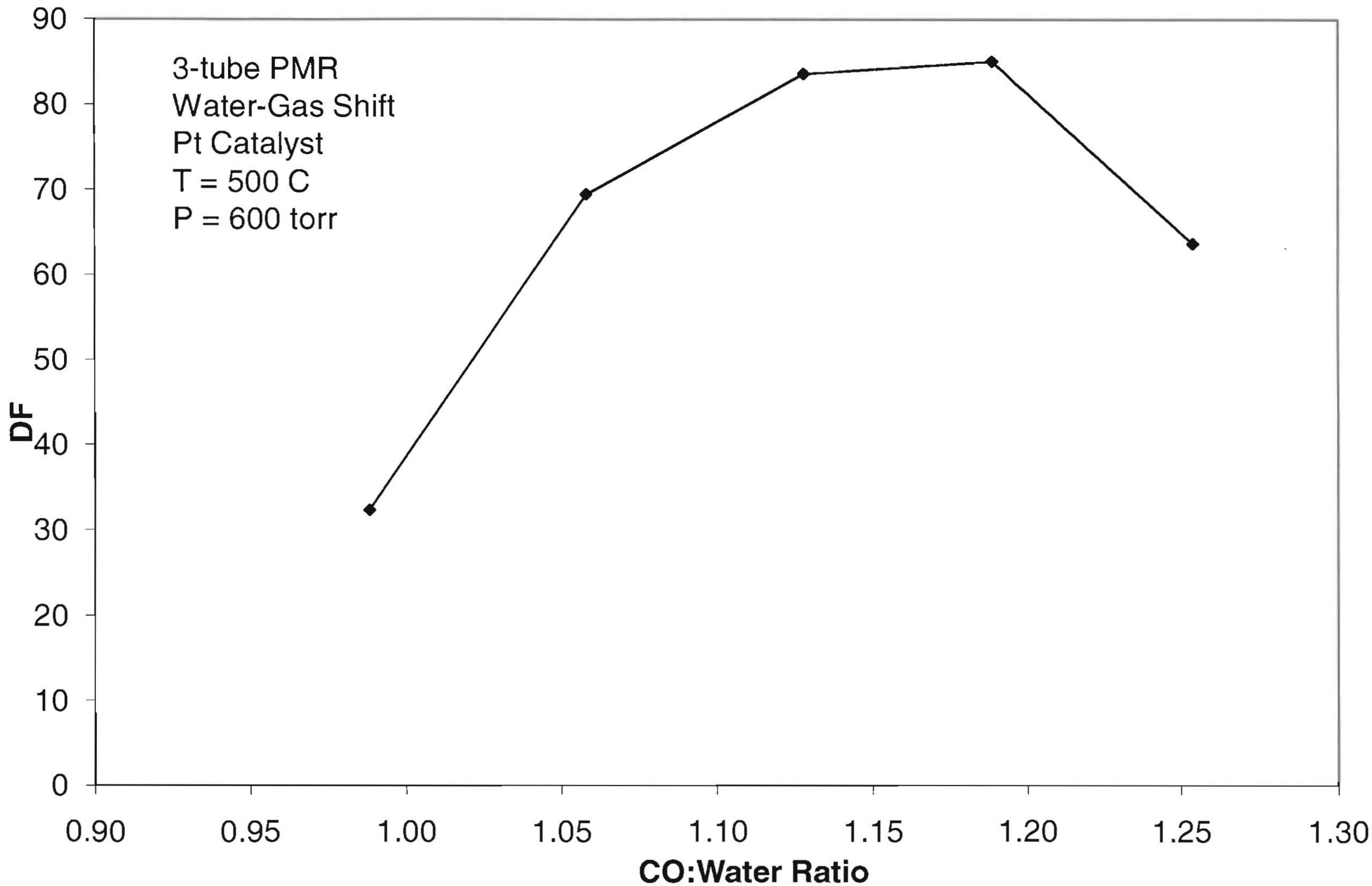
PMR – baseline data – water-gas shift



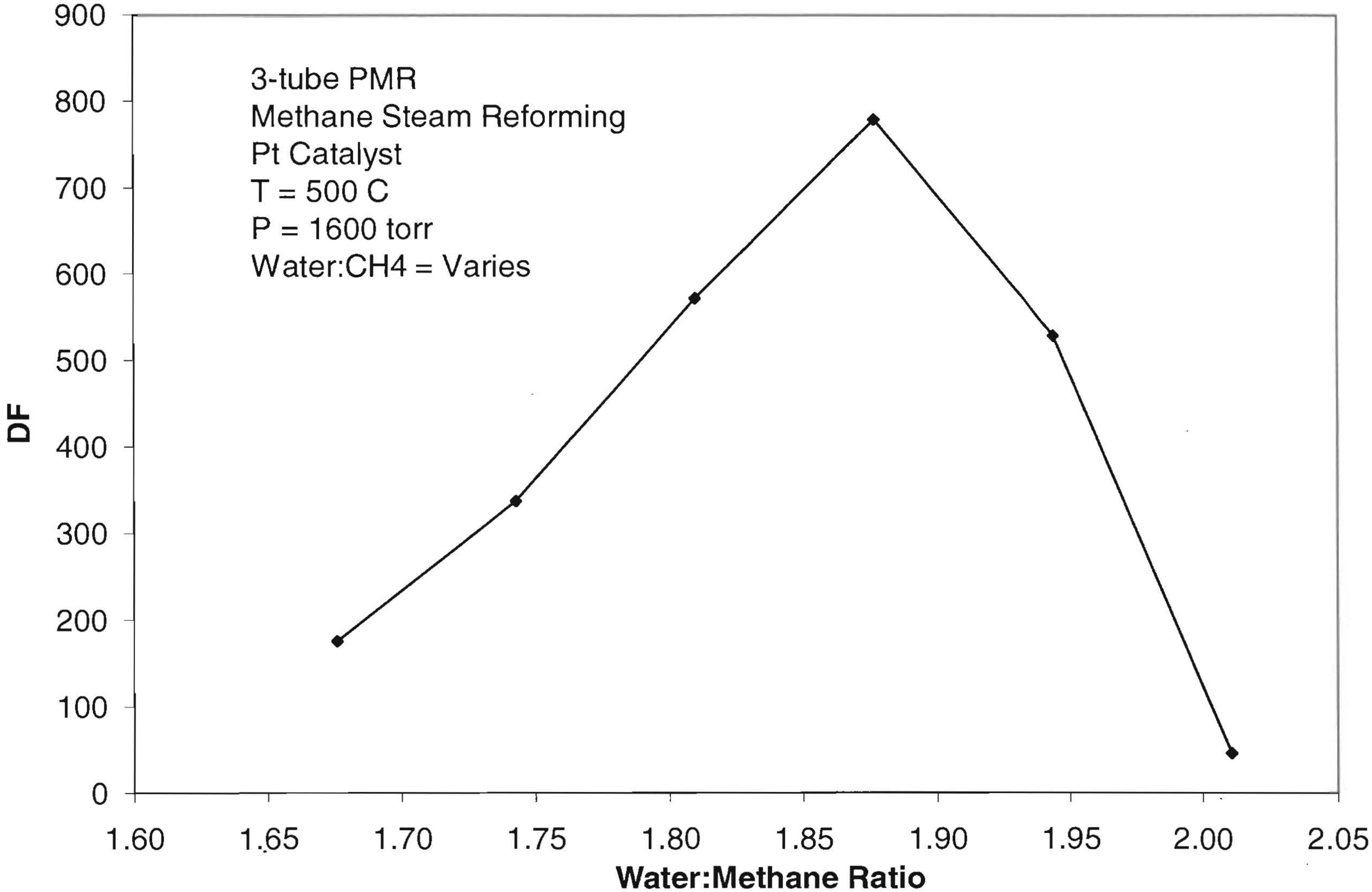
PMR – baseline data – methane-steam reforming



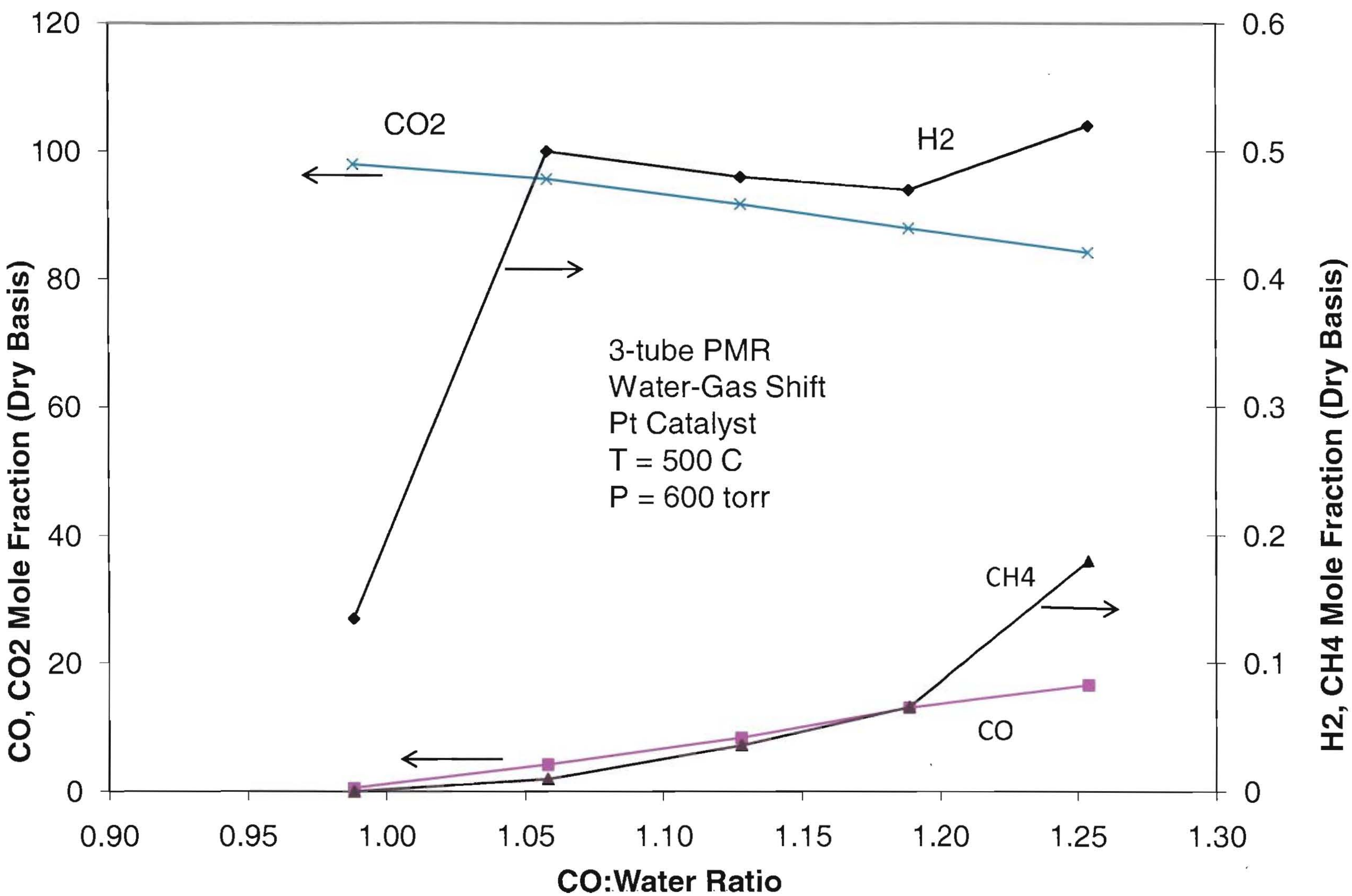
PMR – WGS - effect of feed composition



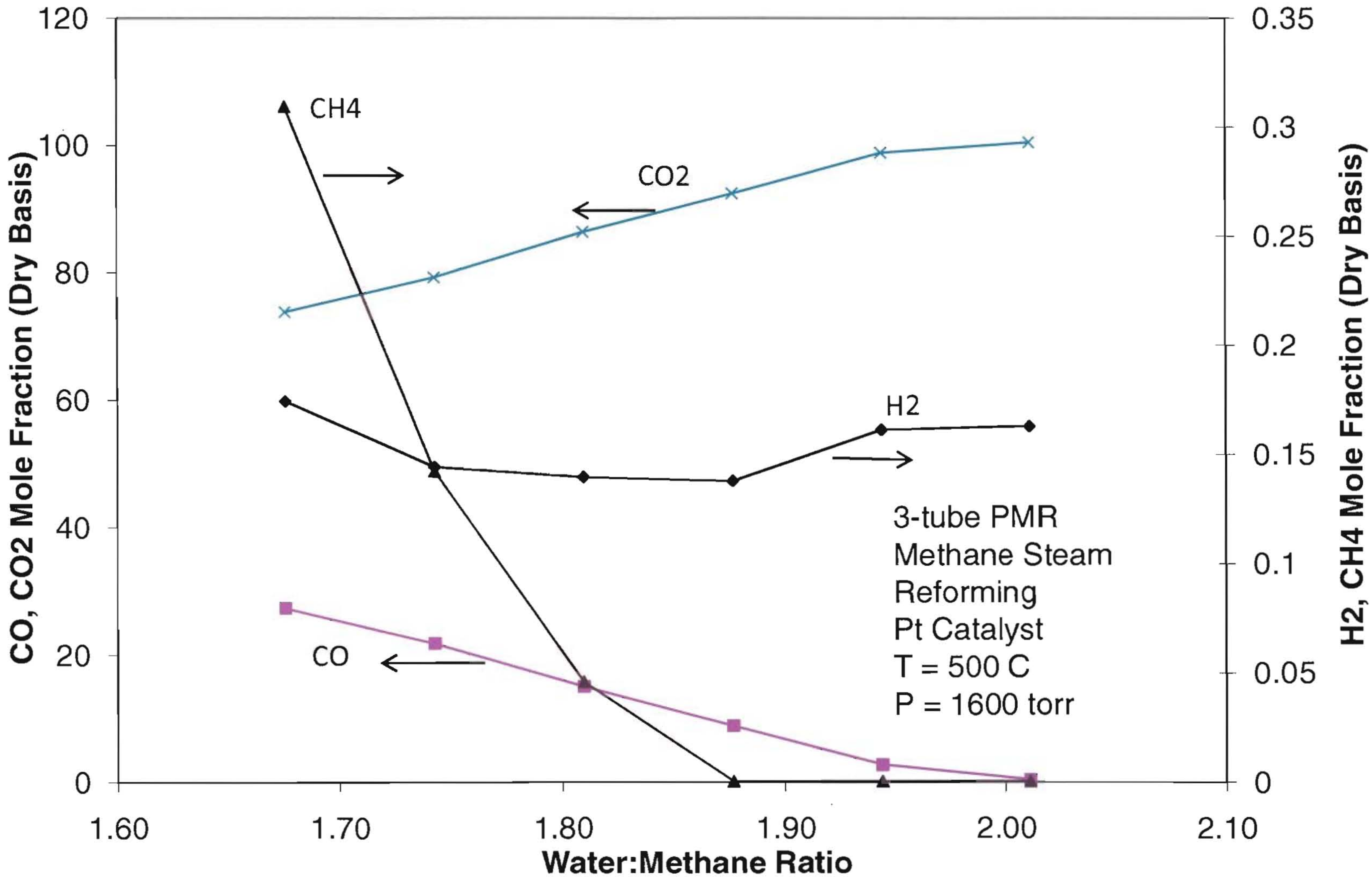
PMR – MSR - effect of feed composition



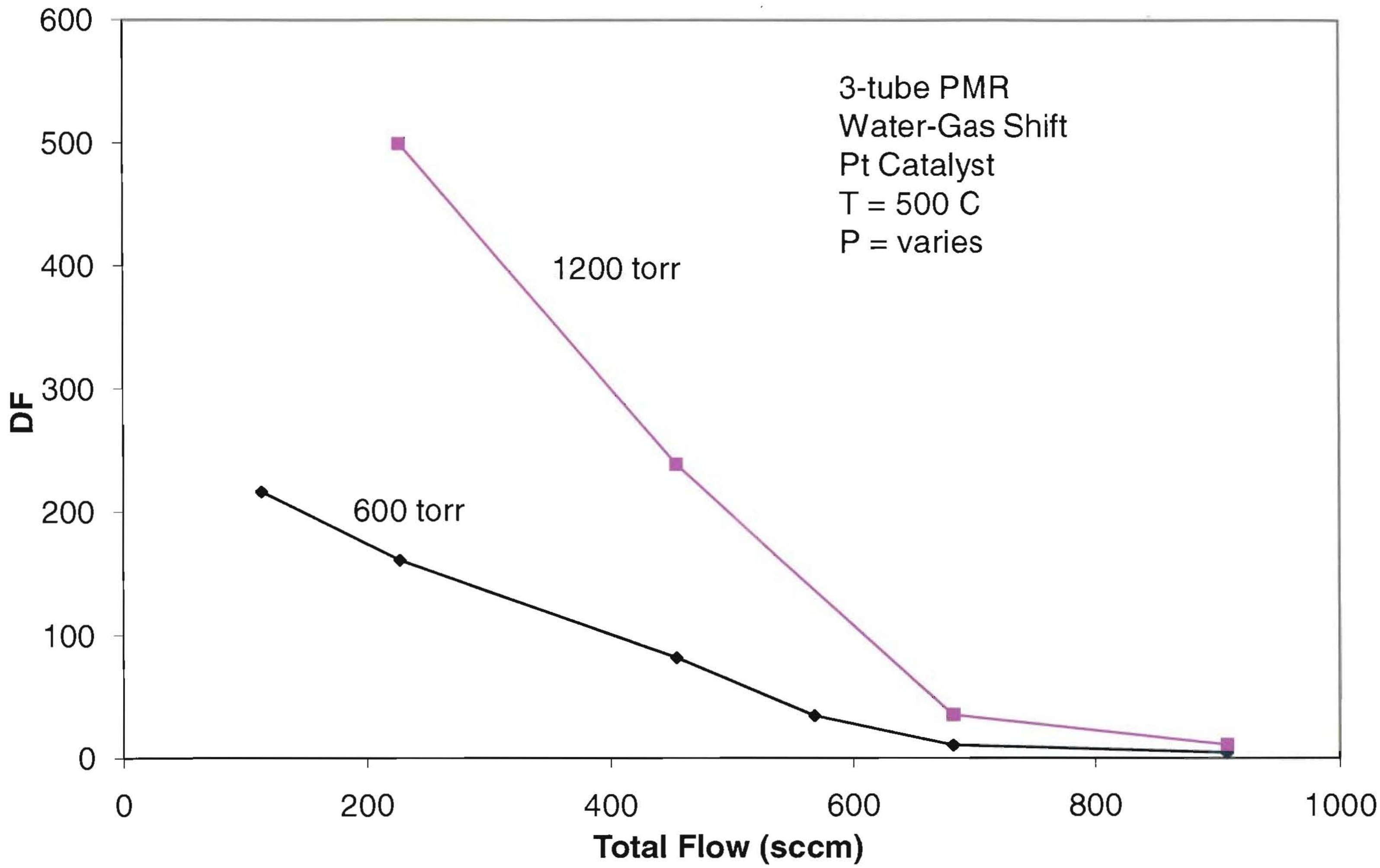
PMR – WGS – effect of feed composition



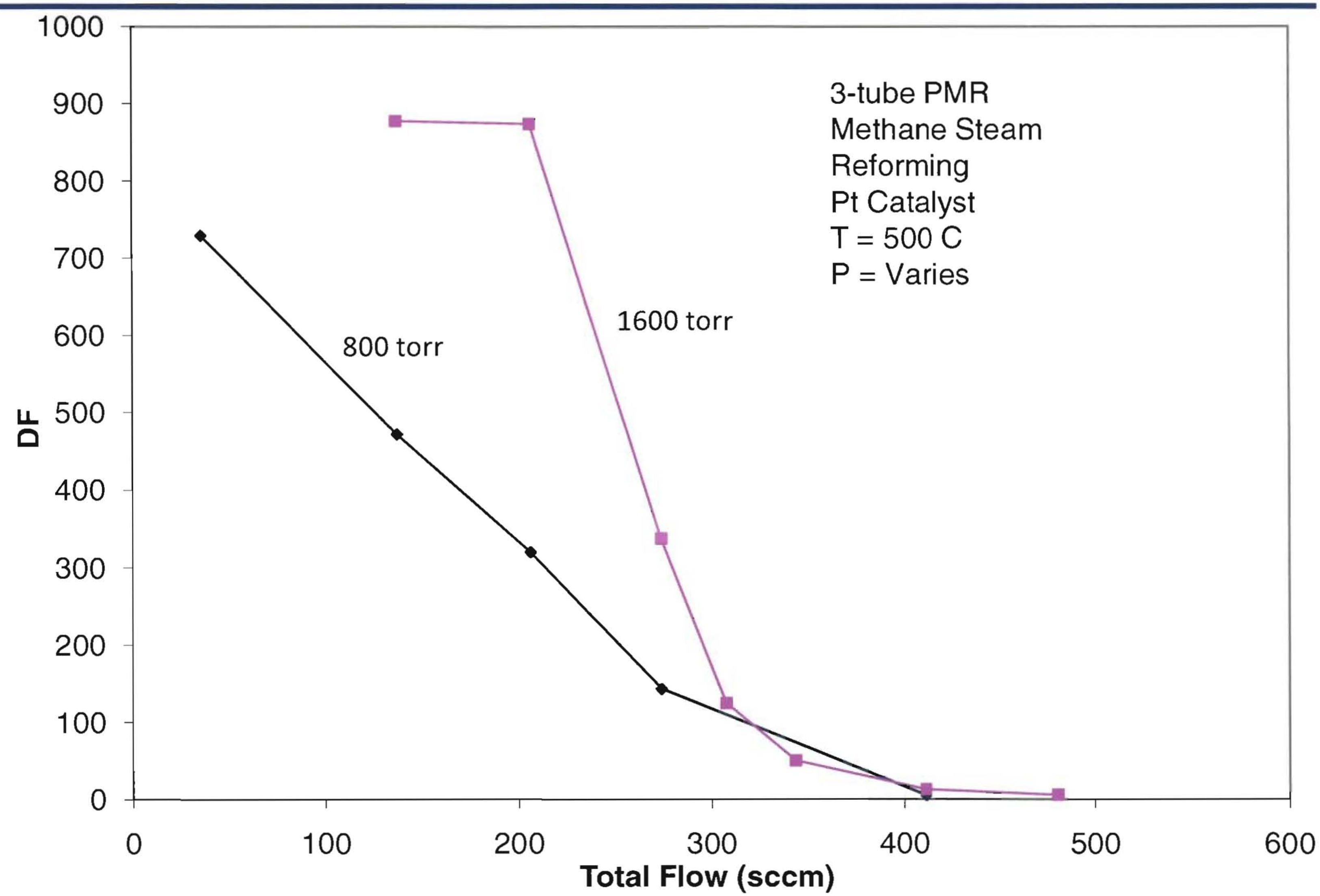
PMR – MSR – effect of feed composition



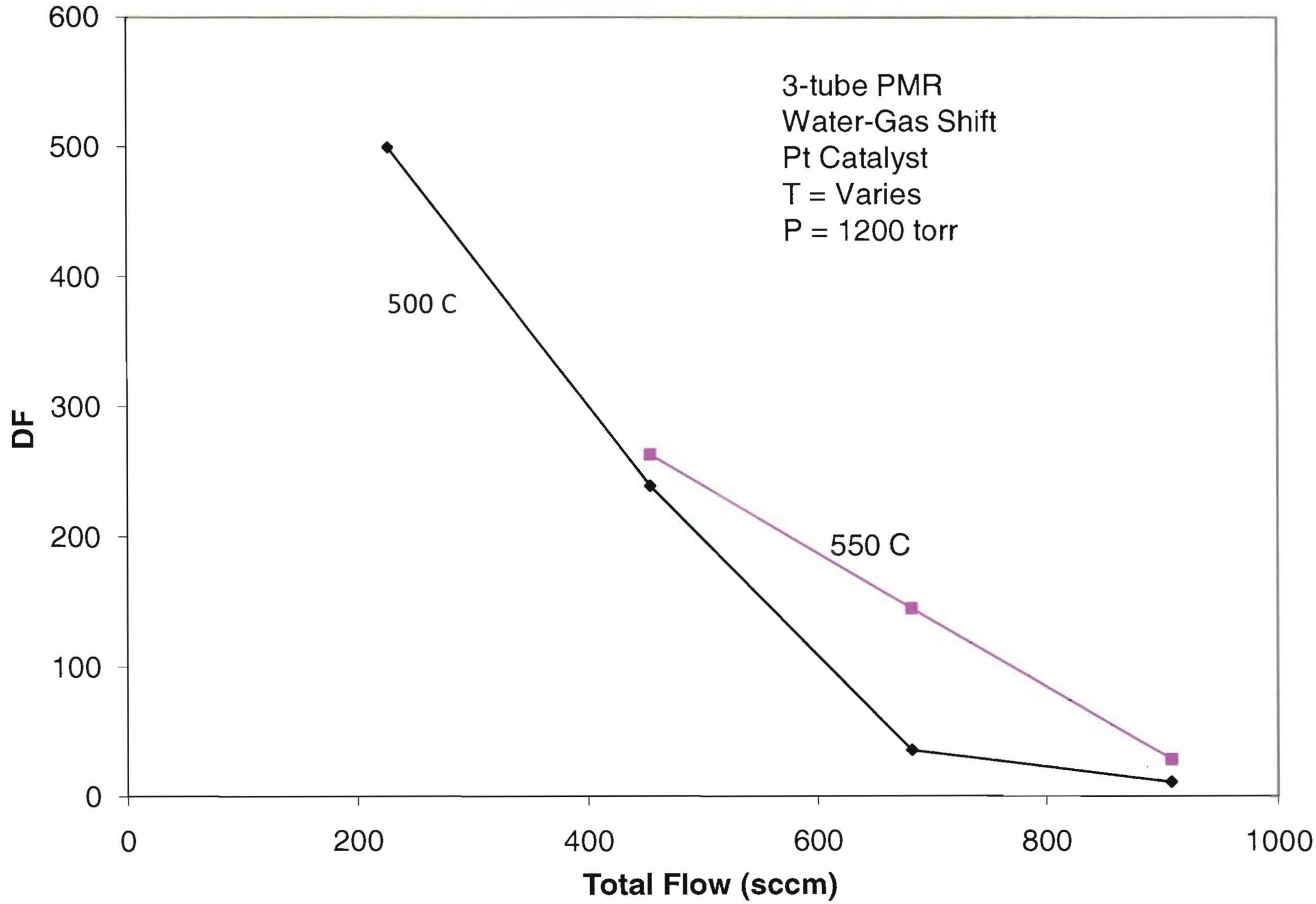
PMR – WGS – effect of retentate pressure



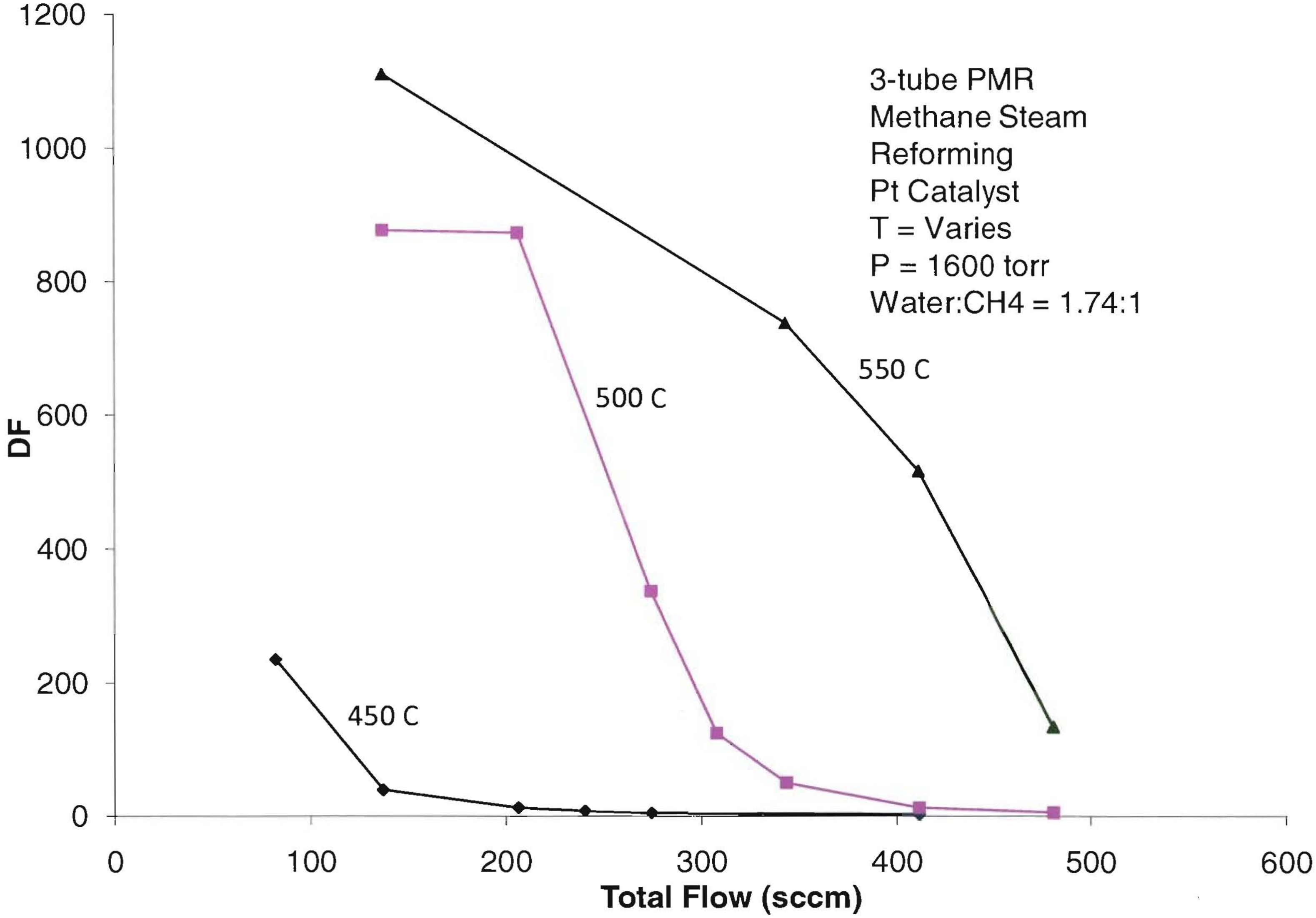
PMR – MSR – effect of retentate pressure



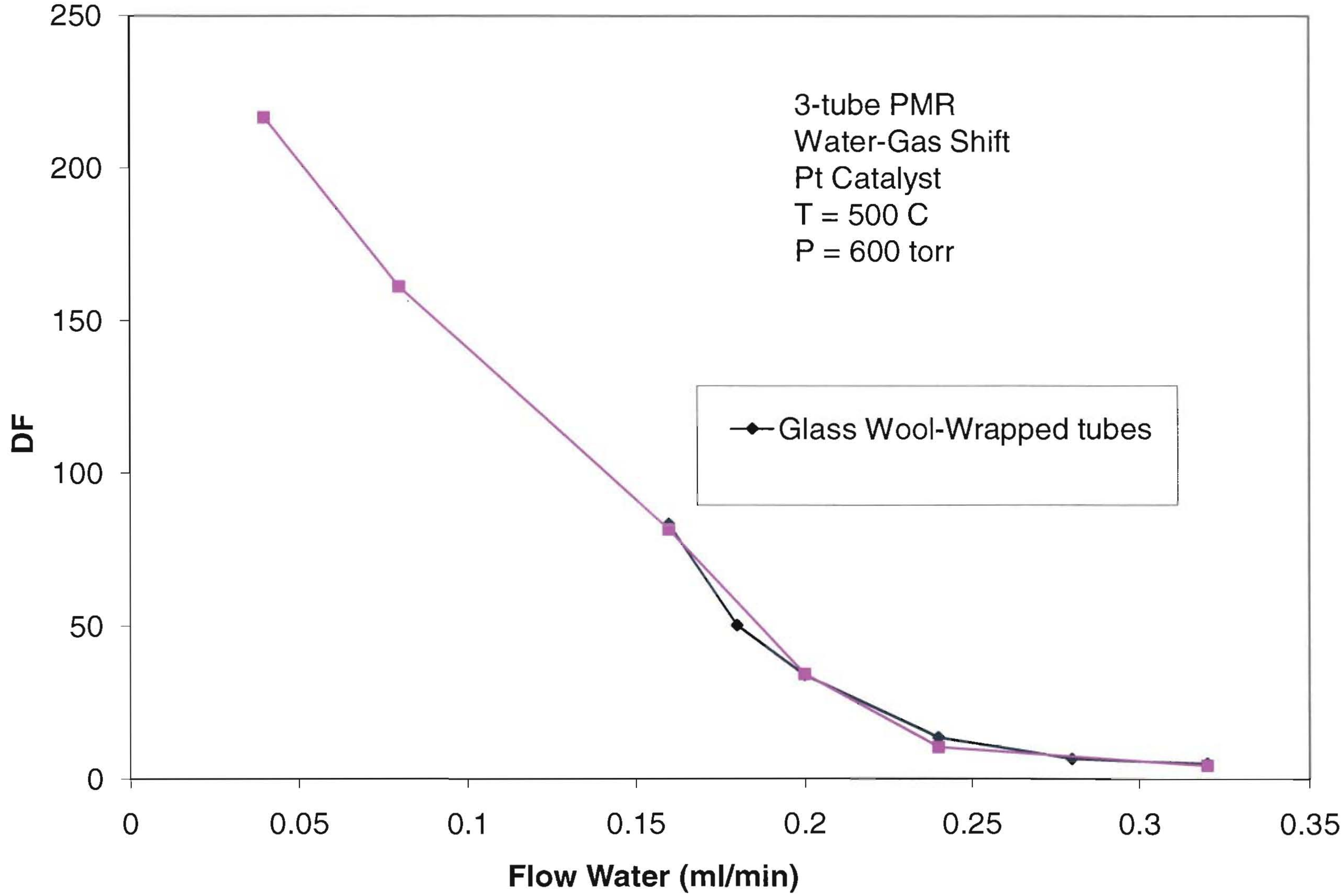
PMR – WGS – effect of temperature



PMR – MSR – effect of temperature



PMR – WGS – effect of perforated metal shields on Pd/Ag tubes

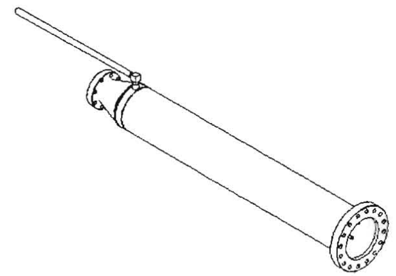


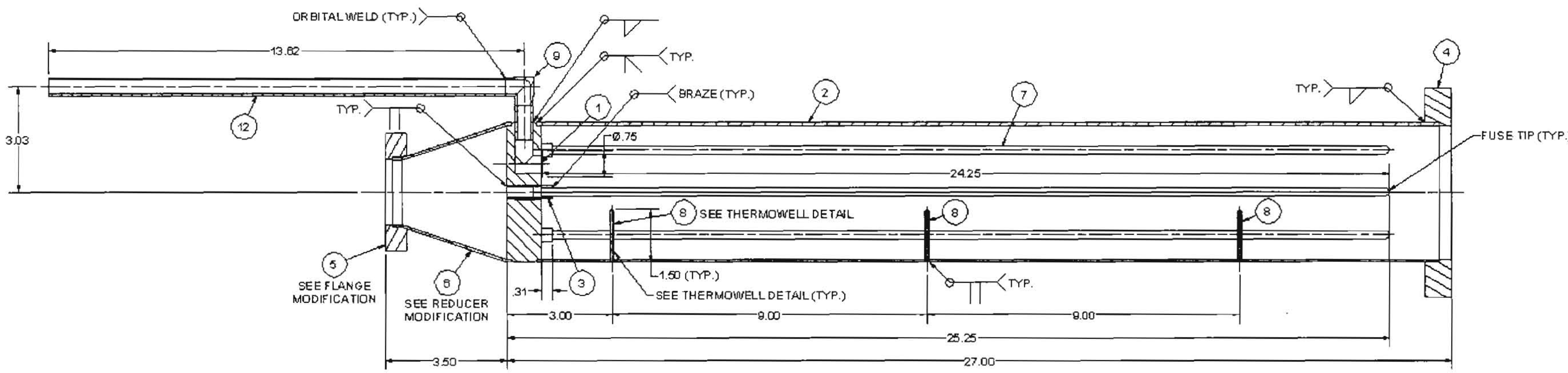
PMR Nikki results

ALP/WLP testing next steps

- ALP/WLP performance/sizing tests
  - Test 3-tube with Nikki (non-tritium)
  - Prototype Test (7-tube, non-tritium)
- ALP processing control
  - Dynamic performance tests
  - Control system tests

TEP prototype PMR





Tubes: 0.25" x 23.8" long Pd/Ag tubes, qty 7
Total Area: 0.084 m2
Prototype to ITER scale factor: 5.9

Conclusions