HIGH PRESSURE COAL COMBUSTION KINETICS (HPCCK) PROJECT

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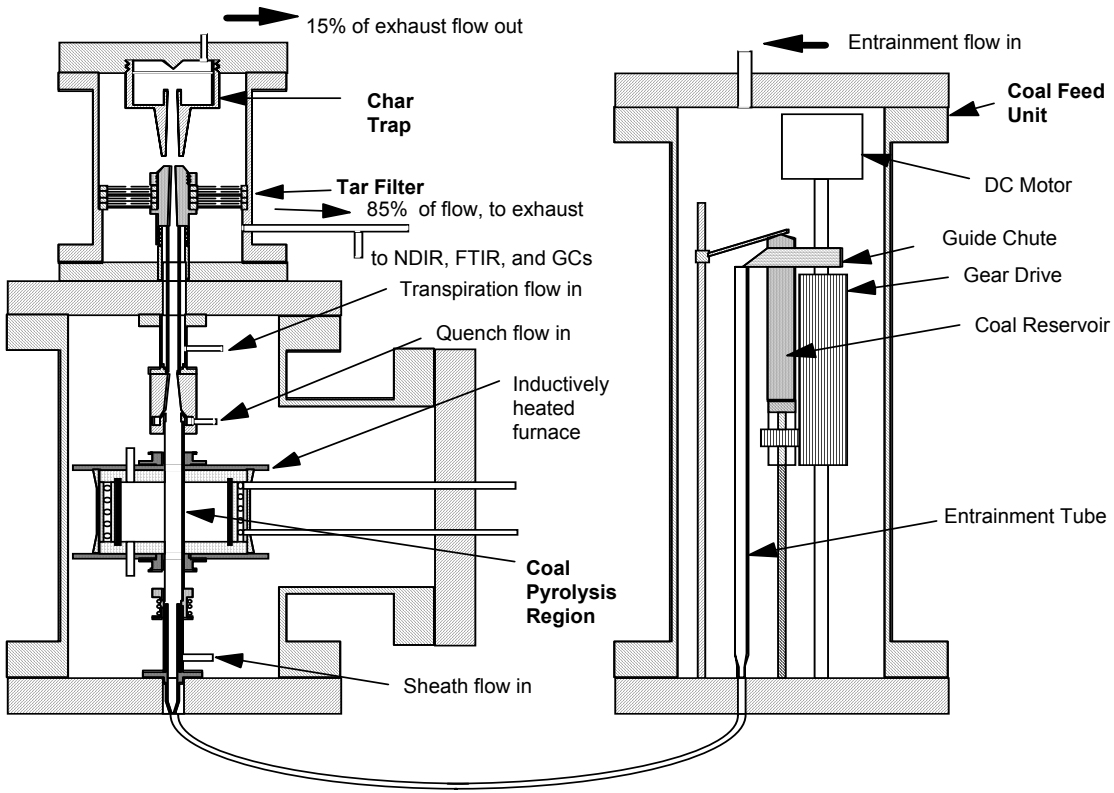
Roles and Team Organization Under the HPCCK Project

- **Pressurized coal combustion datasets – *SRI International*.**
- **Interpretations with CFD and full chemistry - *NEA*.**
- **Submodels for devolatilization and volatiles conversion – *NEA*.**
- **Char oxidation submodel – *Brown*.**
- **Ash behavior submodel- *UCONN*.**
- **Demonstration simulations – *Fluent*.**
- **Program management – *Fluent*.**
- **Vision 21 Design Exercise with Aspen Plus– *Foster Wheeler***
- **Supplement for high CO_2 levels – *Air Liquide***

SRI's Pressurized-Radiant Coal Flow Reactor (p-RCFR)

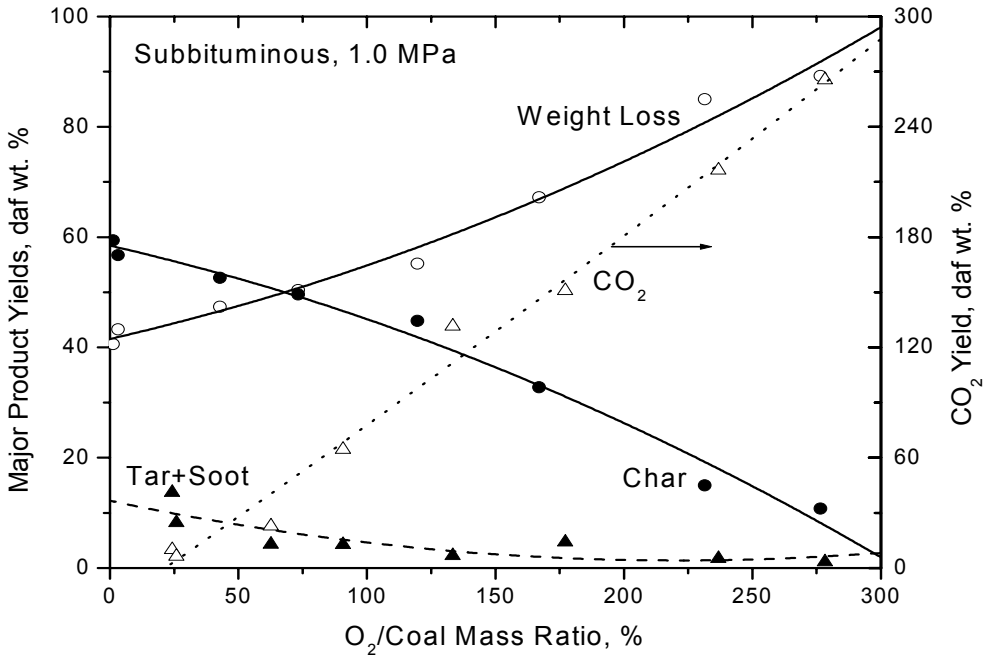


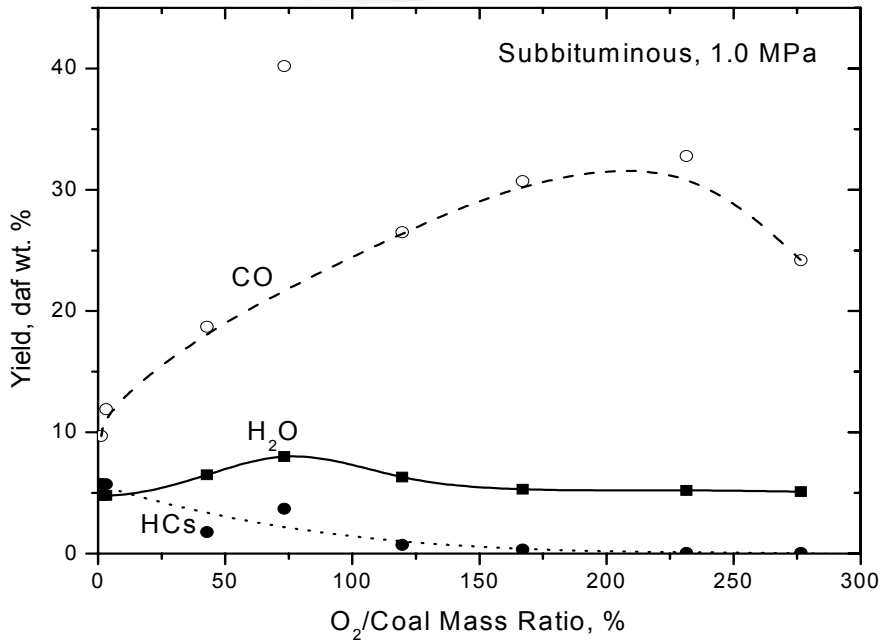
- *Realistic radiant heat fluxes of **60 W/cm^2** impose realistic temperature histories.*
- *Heat release determines the maximum temperature.*
- *Realistic suspension loadings impose the **same chemical environment** in the gas phase.*
- *All major products monitored, and all char and soot are recovered.*
- *C/H/N **balances are closed** in individual runs.*

Near-Burner Flame Zone (NBFZ) Test Strategy

- *At each pressure, run a series of tests with progressively more O_2.*
- *Gaseous fuels, soot, and char compete for the available O_2.*
- *O_2 depletion is an effective quench.*
- *Monitor all major products, including N-species.*
- *The data characterize fuel-N conversion over the broad range of S. R. values in near-burner flame zones.*
- *Run test series at 1.0, 2.0, and 3.0 MPa.*

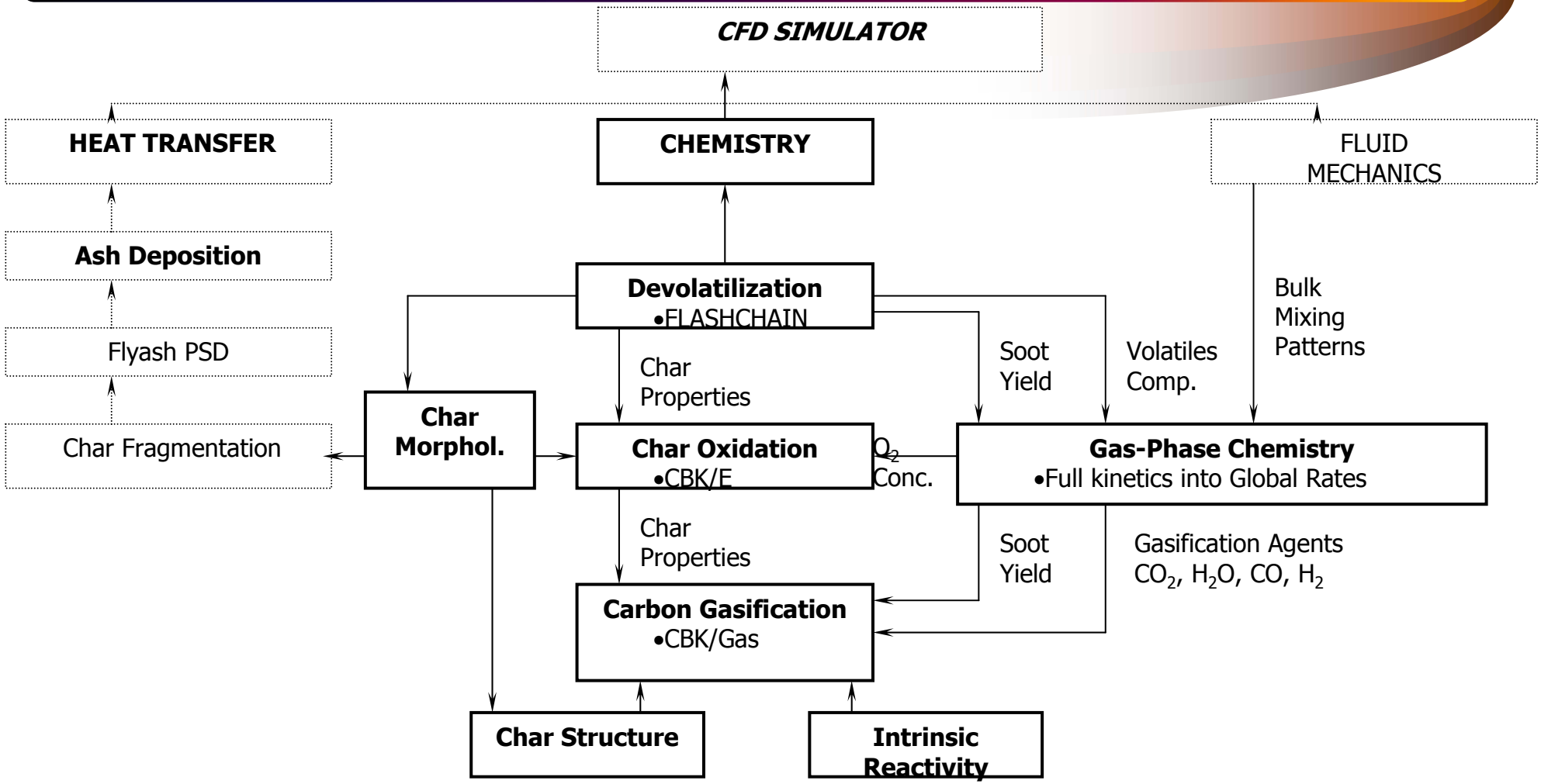
All Fuel Compounds Are Monitored for Any S.R., Including Gasification





- Similar datasets already recorded at 2.0 and 3.0 MPa

Chemistry Submodels Determine Conversions, Compositions, and Flyash Deposition Rates



FLASHCHAIN® for Devolatilization, CBK/E for Char Burnout, and CBK/G for Char Gasification are Distributed in PC Coal Lab®

•FLASHCHAIN® was validated against a database of 332 independent tests involving **99 coals** and broad ranges of heating rates, temperatures, and pressures to 16.7 MPa.

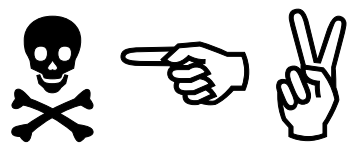
• Expanded the theory behind CBK for char oxidation at elevated pressures.

• CBK/E was validated against a database of 235 independent tests that characterized **11 coals, 2 coal chars**, and a graphite, heating rates approaching 10^6 °C/s, furnace temperatures to 1527 °C, pressures to 2.0 MPa, and O_2 levels to 100 %.

• Formulated CBK/G for gasification by CO_2, H_2O, and H_2.

•CBK/G validated against 452 gasification tests that characterized **26 coals**, temperatures to 1400 °C, and steam and CO_2 mole fractions from 0 to unity.

See PECS, 29(5):425-77 (2003)



NEA's ChemNet™ Post-Processing (CNPP) Starts With Conventional CFD

Conventional Post-Processing

CFD → Flowfield T-Field Major Species → NO_X Post-Processor → NO_X Predictions

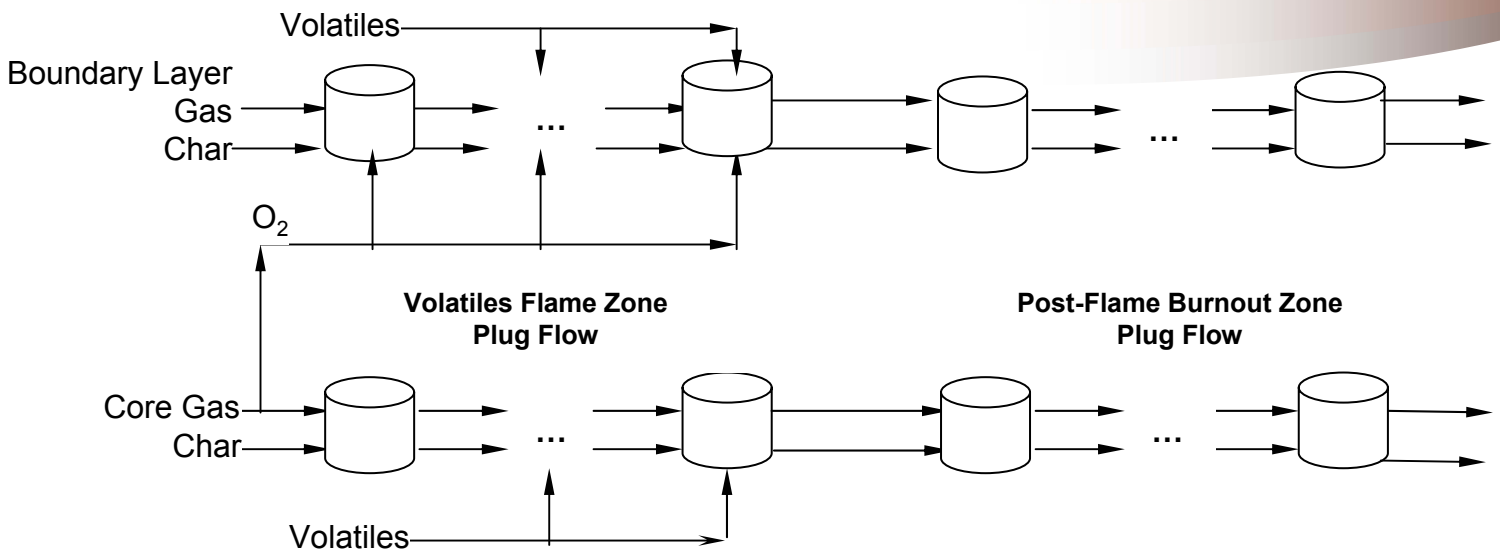
ChemNet™ Post-Processing

CFD → Flowfield T-Field D_{TURB} Conserved Scalars → ChemNet™ Post-Processor → Equivalent Reactor Network → Detailed Chemistry Calculations → NO_X, LOI Predictions

CHEMKIN

FLASHCHAIN® and CBK

p-RCFR Network Has Parallel Channels in Plug Flow with O_2 Entrainment

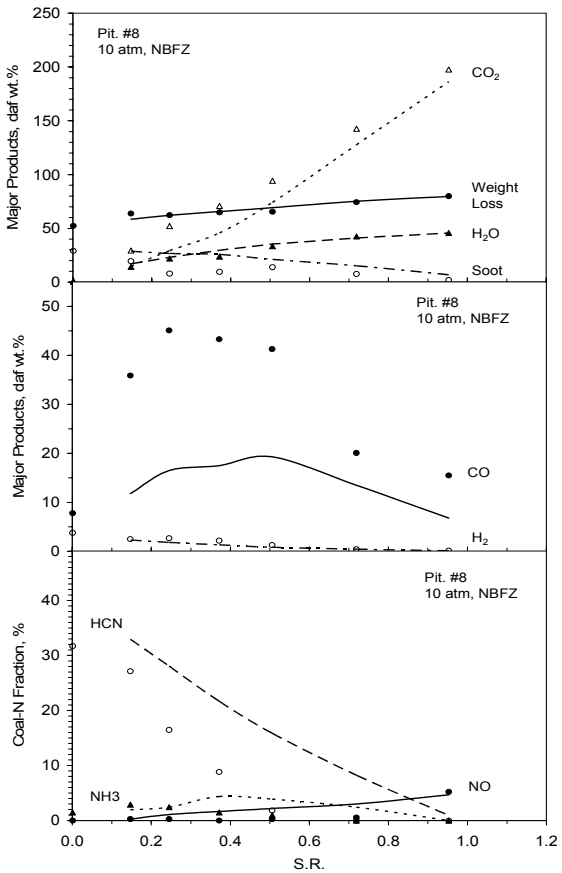


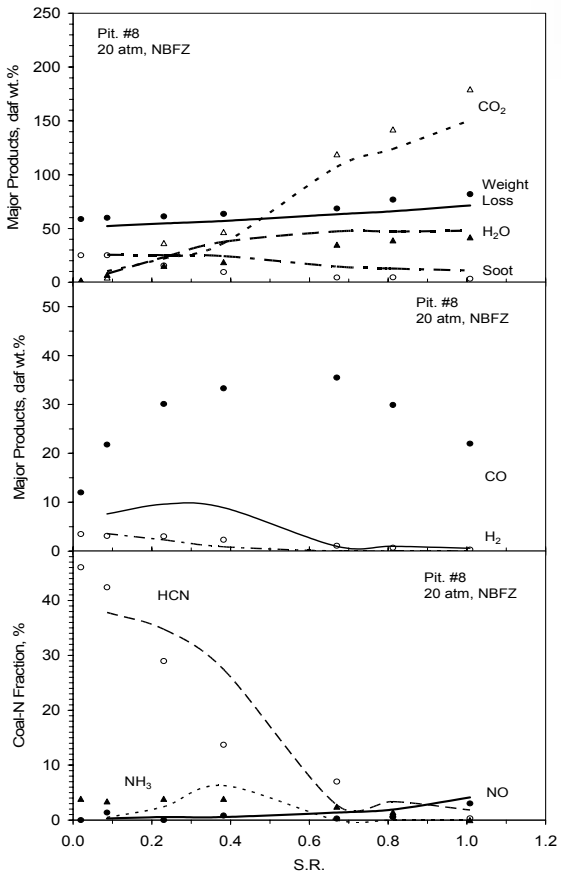
- *Calibrate O_2 entrainment to match case with S. R. =1.*
- *All other conditions from CFD simulations.*
- *Specify char reactivity, char –NO fraction from case with S. R. =1.*

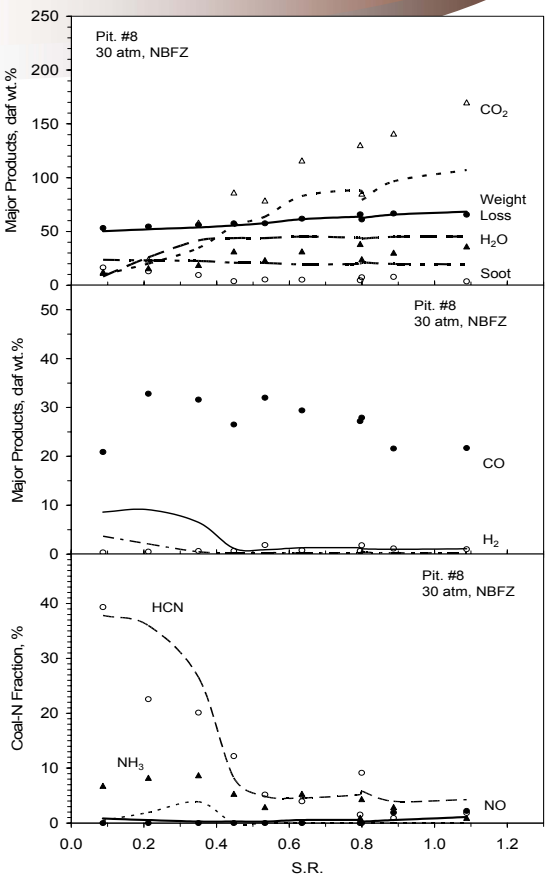
Complete Reaction Mechanisms for All Stages of Combustion

- *FLASHCHAIN® predicts fluxes of all fuels (CO, H_2, CH_4, C_2H_2, HCN, soot) for the gas phase reaction mechanism.*
- *FLASHCHAIN® predicts all char properties for the CBK simulations.*
- *Soot chemistry represents oxidation by O_2, O, OH plus H, OH recombinations & NO reduction.*
- *Prof. Glarborg's 444-step reburning mechanism for N-species conversion and volatiles combustion (66 species).*
- *Prof. Hurt's CBK/E model for char burnout.*

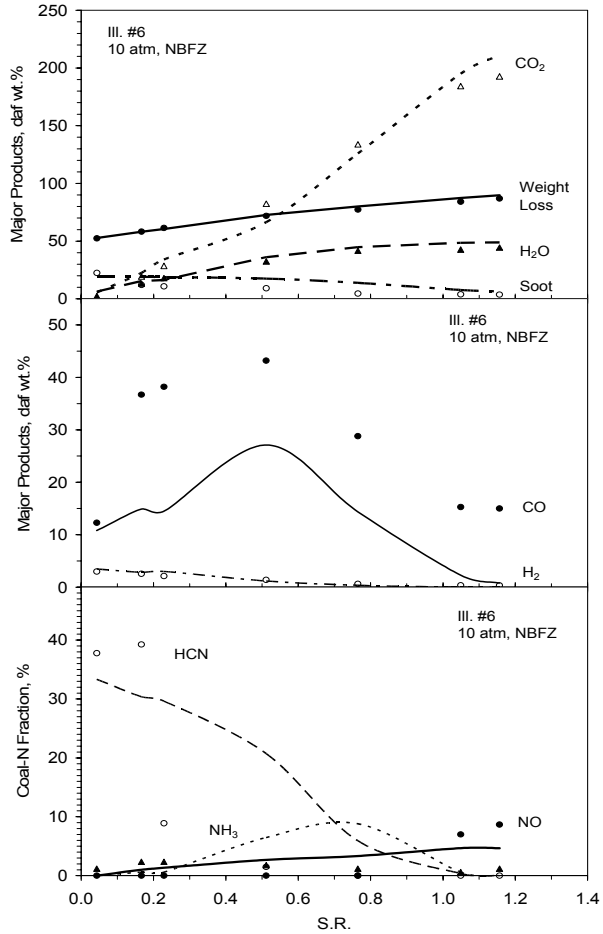
Pit. #8 at 1.0, 2.0, and 3.0 MPa

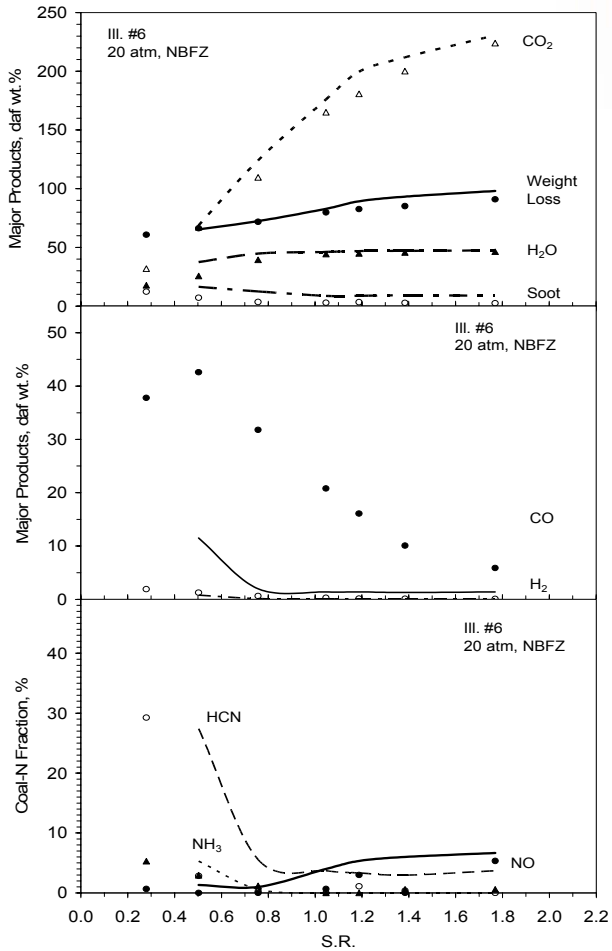


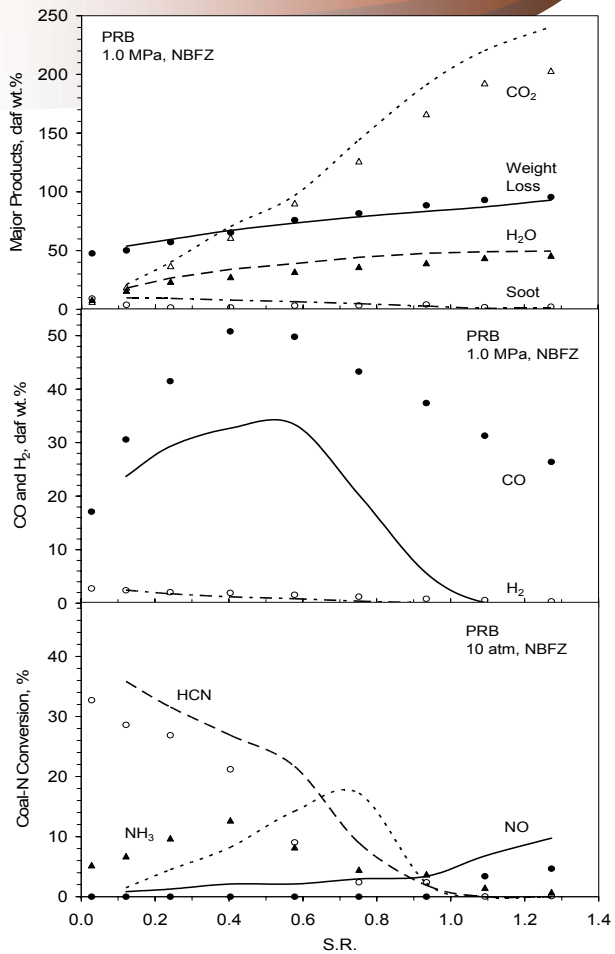




Ill. #6 at 1.0 and 2.0 MPa, PRB at 1.0 MPa







Predicted Impact of Pressure on NO is Accurate for Pit. #8

Pressure, MPa	NO @ S. R. =1, daf wt. %	
	Predicted	**Measured**
1	0.17	0.19
2	0.15	0.11
3	0.04	0.08

- *CNPP also correctly predicts substantial HCN at 3.0 MPa, in accord with the measurements.*

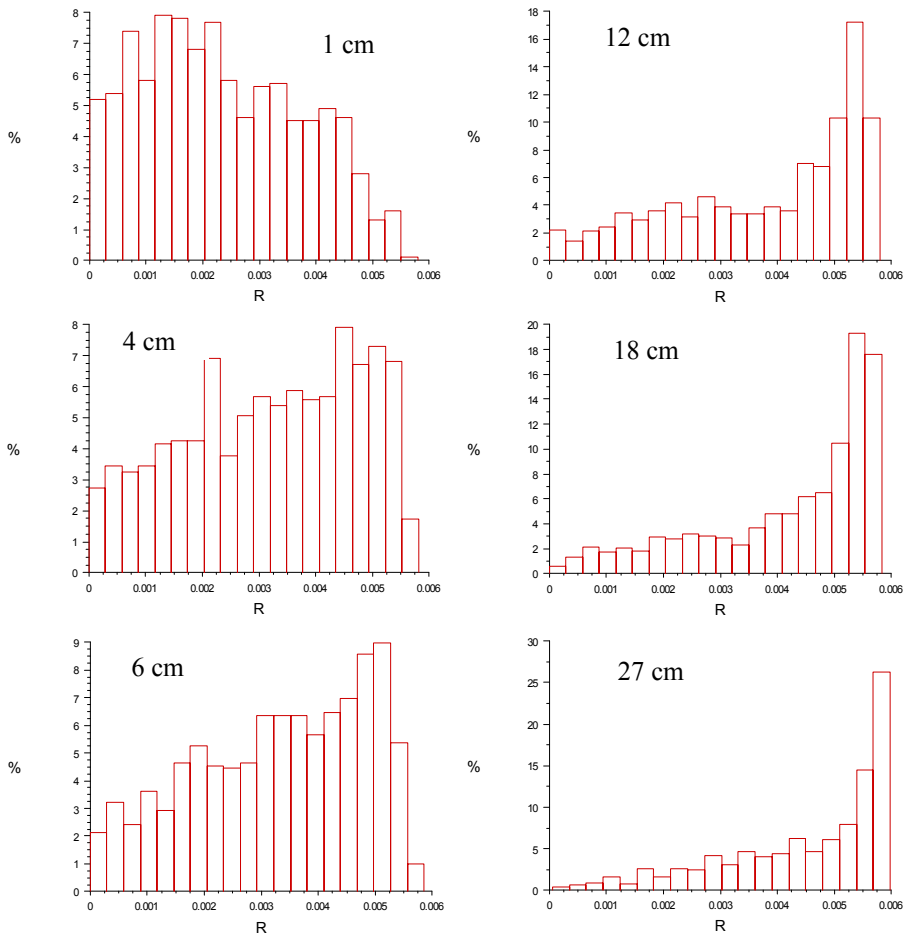
Practical Implications

- *Expect substantial particle agglomeration in pressurized burners.*
- *Current reaction mechanisms sufficient for wide range of coal quality at elevated pressures.*
- *ChemNet™ post-processing delivers accurate simulations for all NBFZ tests, including accurate predictions for fuel-N release and for the very low N-conversion to NO at elevated pressures.*
- *All input for N-conversion submodel in hand.*

CFD Simulations

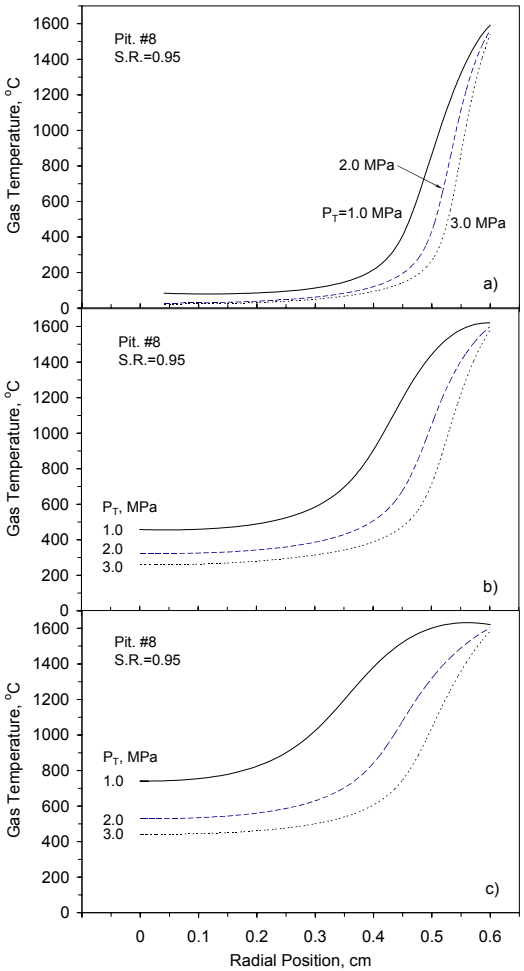
- *Fluent.*
- *Separate kinetics for HCs, CO/H_2, soot, and char.*
- *Adjust parameters to match measured extents of fuel conversion in each test.*
- *The heat release must therefore be accurate.*
- *Characterize operating conditions in depth.*

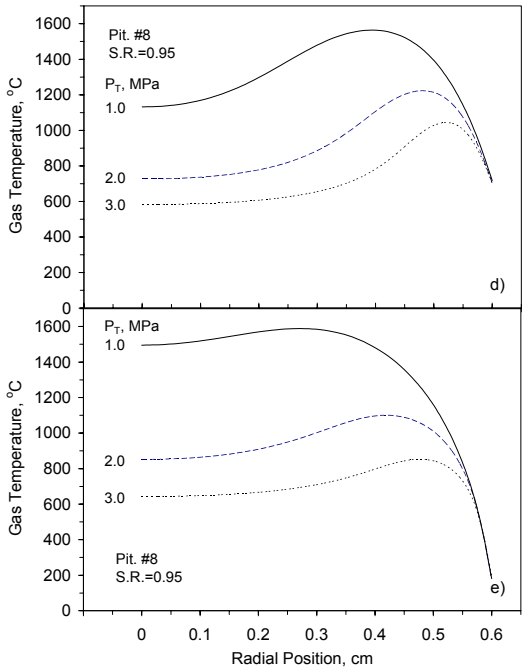
Particle Accumulation Near Walls Has Important Consequences

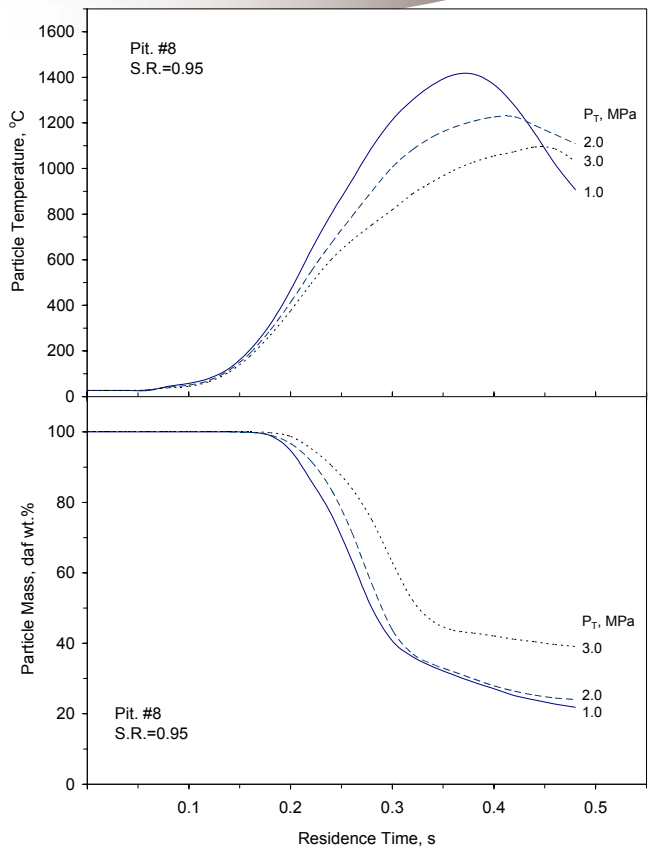


- *High local solids loading causes agglomeration.*
- *Depleted O_2 concentration near the wall.*
- *Unconverted CO, H_2 near the wall.*
- *Cooler core temperatures.*

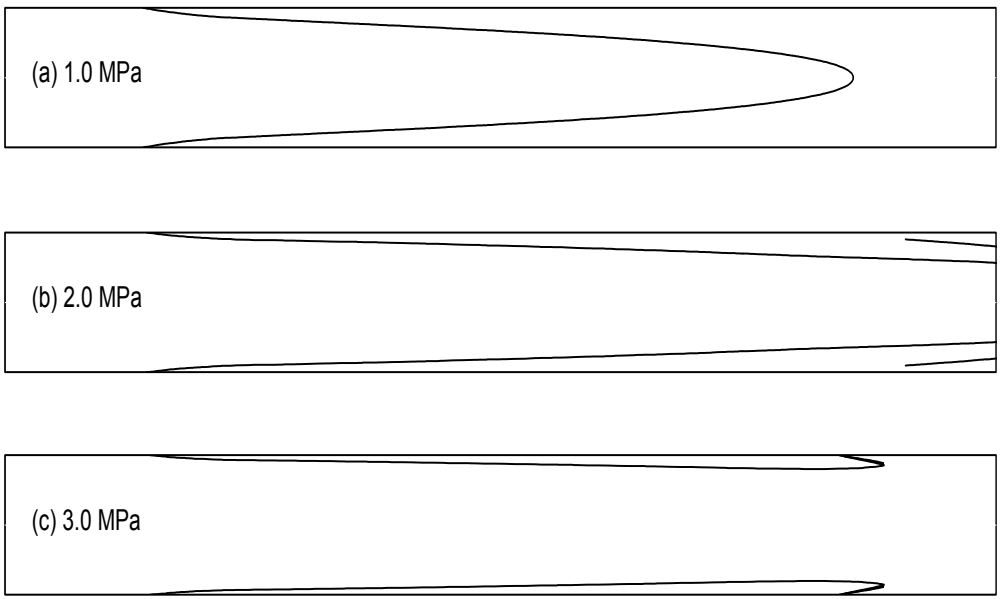
Much Cooler Flow at Progressively Higher Pressures





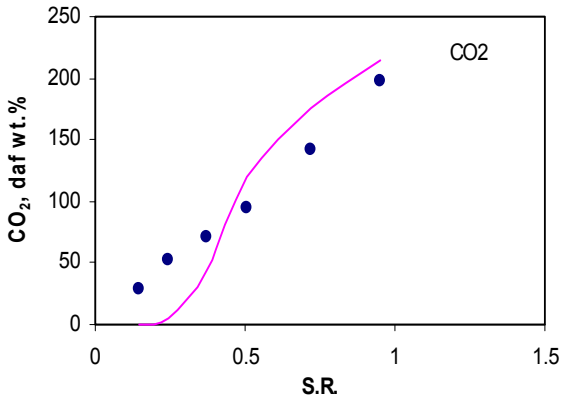


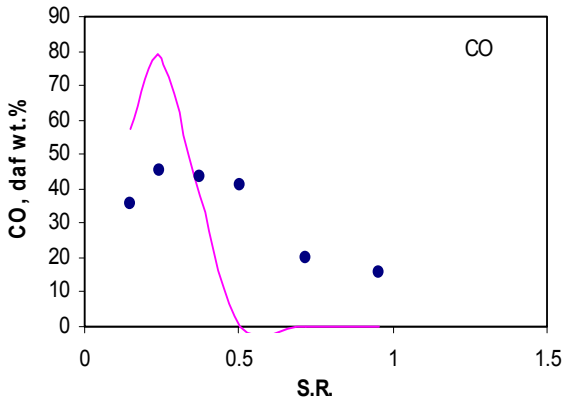
At Fixed S. R., Flames Open at Higher Pressures

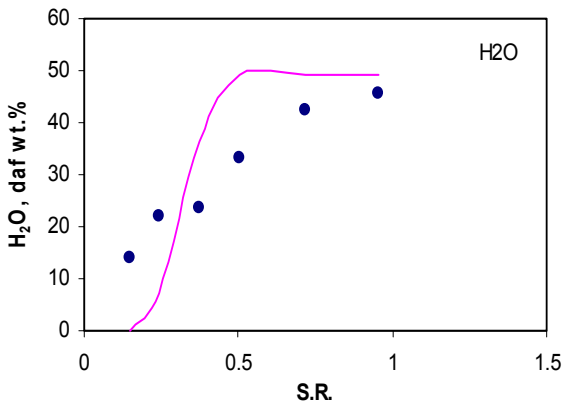


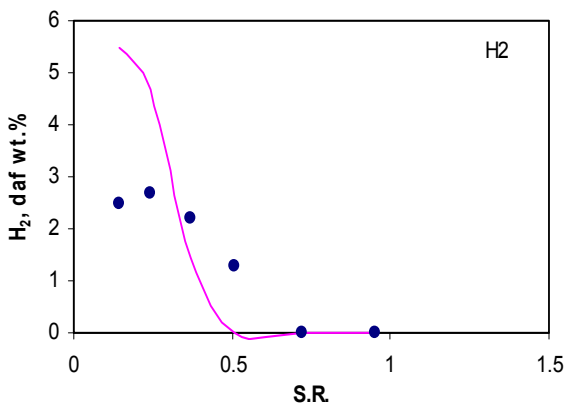
- *Cores become too cool to ignite.*
- *Flue gases contain burned and unburned species.*
- *Same tendency with progressively lower S. R.*
- *Ill.#6 most likely to form open flames.*

The Persistence of CO and H_2 Is Most Unusual



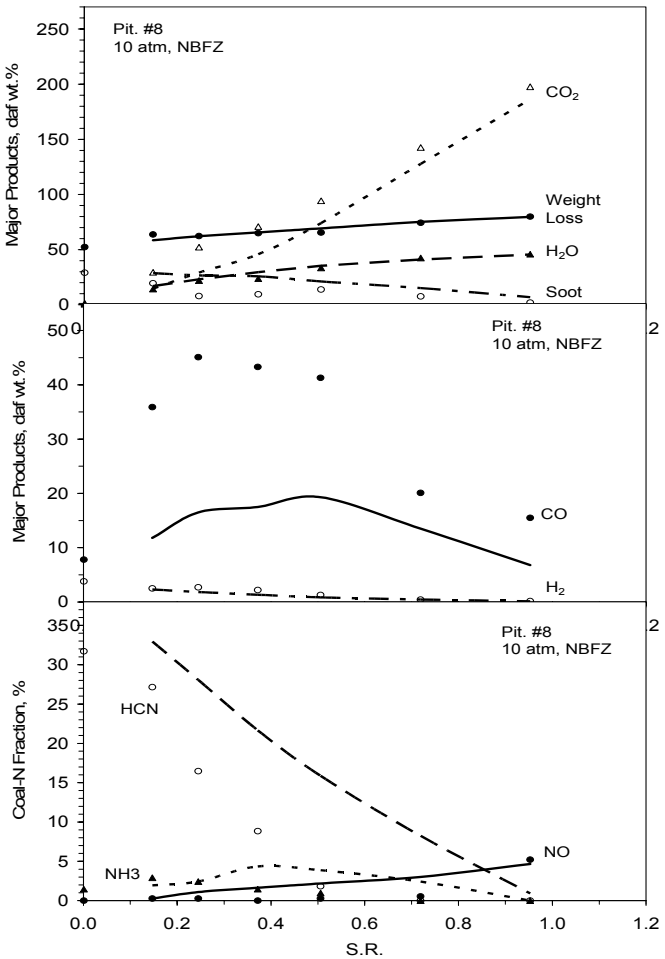






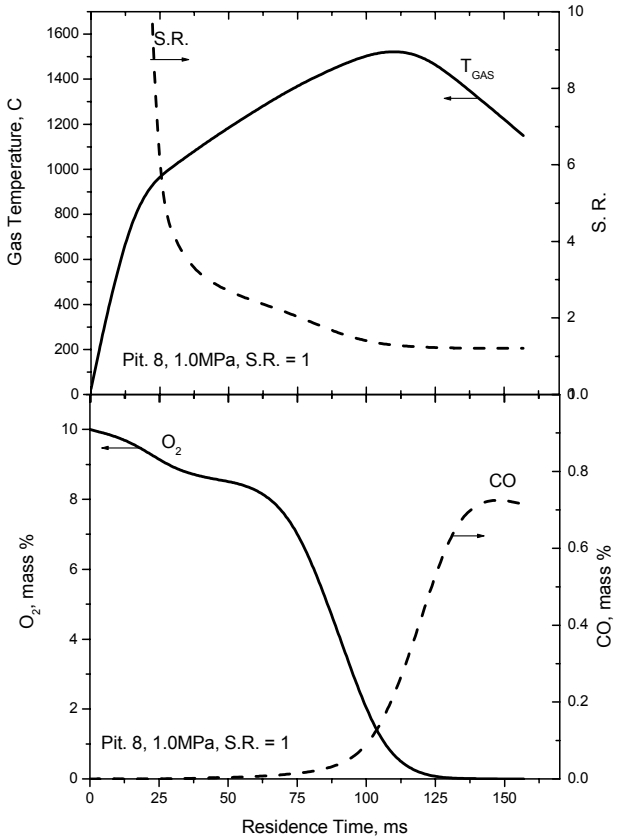
- *Flames not equilibrated, even when closed at the hottest temperatures.*
- *Particle-rich boundary layers burn much richer than the nominal S. R.*
- *Products always reflect a mixture of the boundary layer and core flows.*

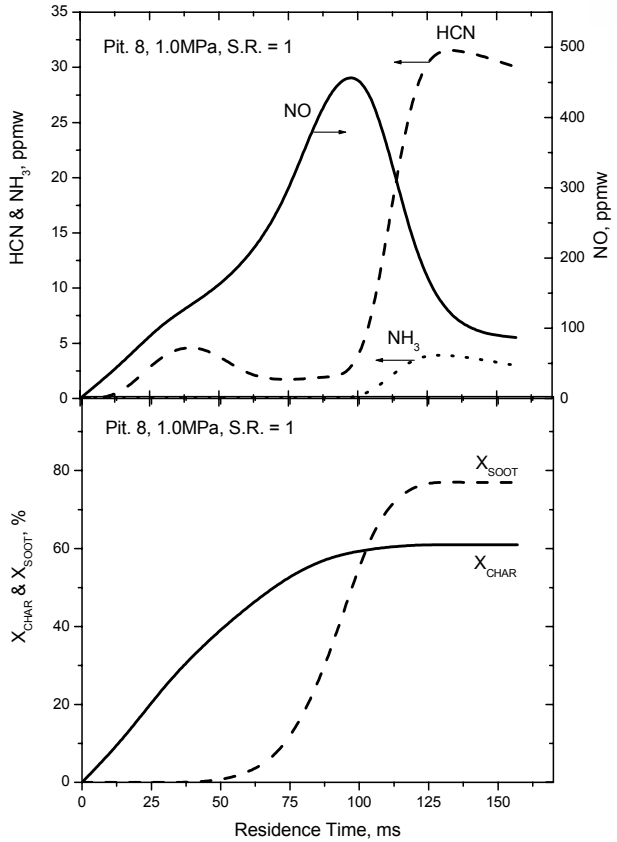
Accurate Predictions for Pit. #8 at 1.0 MPa



- *Accurate major species levels.*
- *Coexistence of CO and O_2 in flue gas.*
- *Qualitatively correct CO, like 0.1 MPa.*
- *Accurate total N-release and NO level.*
- *Only 5 % N-conversion to NO.*
- *Qualitatively correct HCN, NH_3 profiles.*

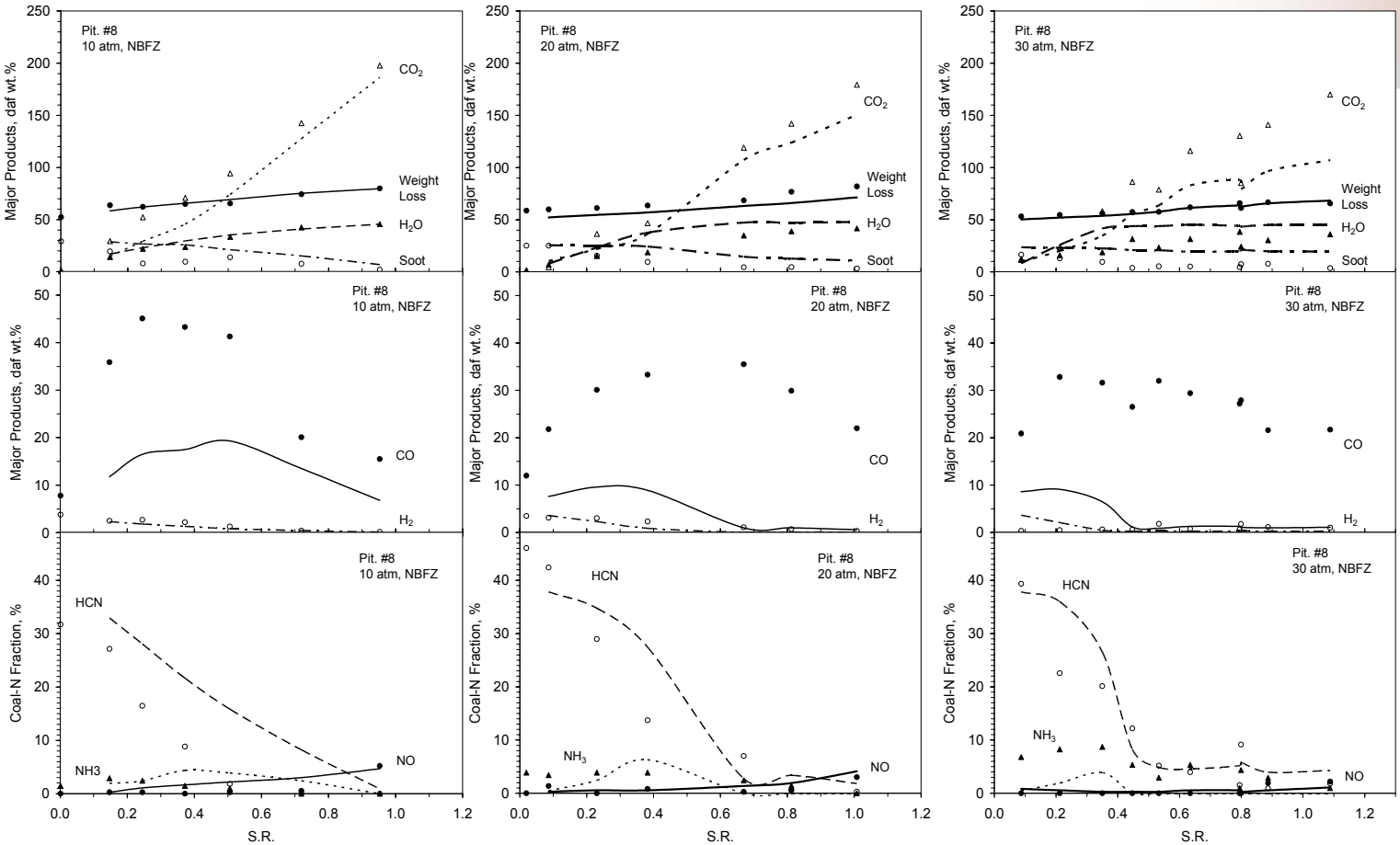
Chemical Structure of the Boundary Layer Flow Resembles Burners





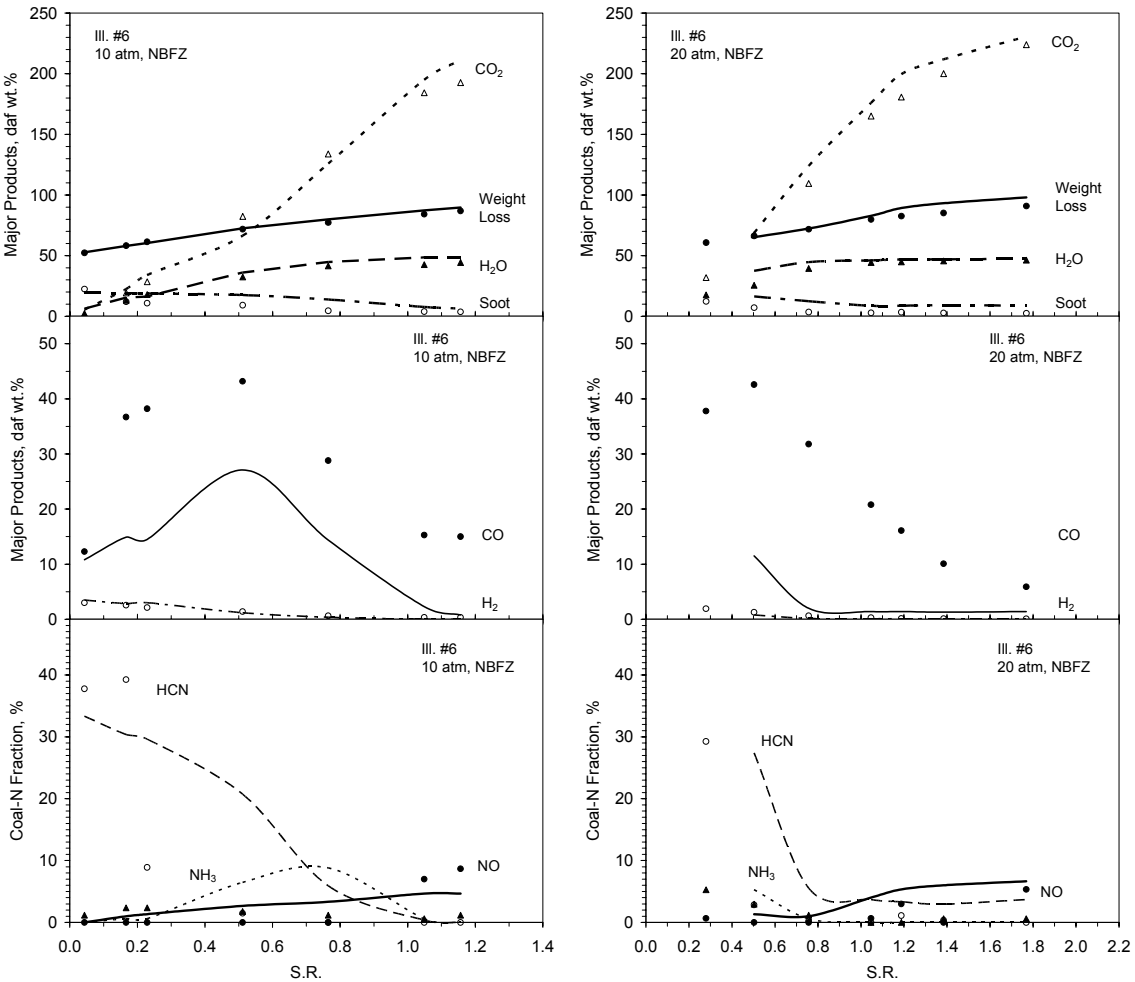
- *S. R. falls as volatiles and oxidation products are added.*
- *Realistic T- and O_2-histories.*
- *NO forms early, then reduced away (by CO, H_2).*
- *CO, HCN, NH_3 produced late.*
- *Char effectively competes for O_2 during the early stages.*
- *Soot is difficult to ignite but burns out faster than char.*

Predicted Impact of Pressure is Reasonable



- ***Accurate char BO.***
- *Soot burns too slowly at higher pressures.*
- *Correct shift to lower CO levels.*
- *Correct N-species transformations.*
- ***Accurate NO levels** at all pressures.*

Similar Performance with Ill. #6



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Immediate Extensions

- *Use ChemNet™ simulations to develop and evaluate the fuel-N conversion submodel for elevated pressures.*
- *Qualify HPBO test data.*
- *Interpret HPBO test data with CBK/E.*