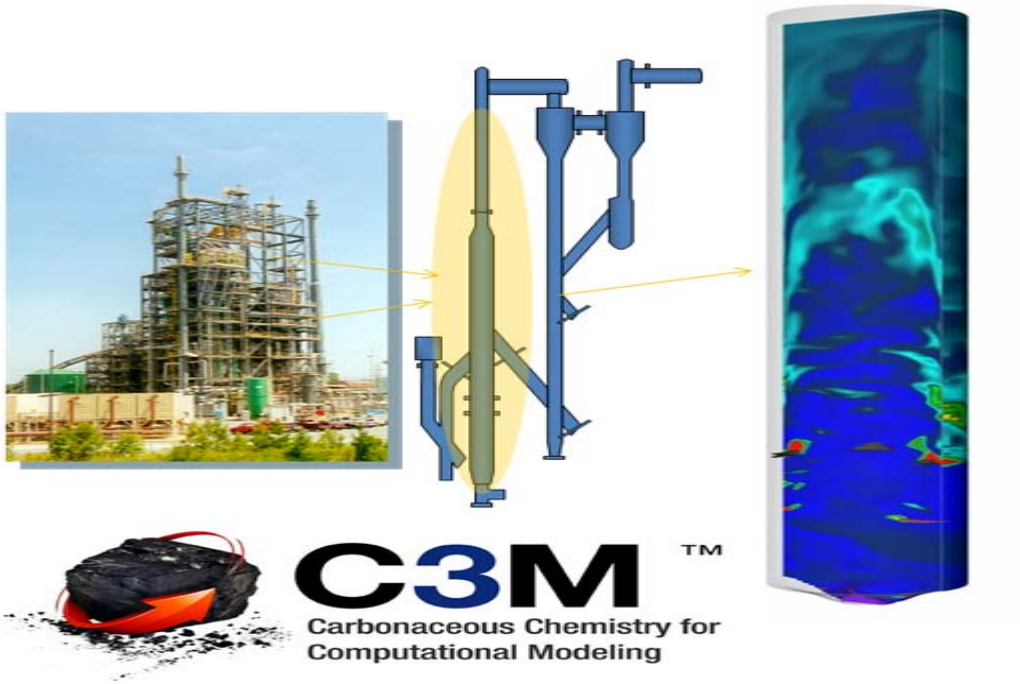
Reacting Flow Modeling with C3M



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NETL 2012 Conference on Multiphase Flow Science
NRCCE, Morganotwn WV.
May 24th 2012

Outline

- Introduction
  - Background
  - MGAS
- Kinetic Packages
  - PC Coal Lab (PCCL)
  - Chemical Percolation Model for Coal Devolatilization (CPD)
  - The Functional-Group, Depolymerization, Vaporization, Cross linking (FGDVC)
  - Experimental data
- Objective
- Carbonaceous Chemistry for Computational Modeling (C3M)
- C3M Highlights
- Summary
- Future Work
- Acknowledgement

Introduction
Background

- New gasifiers coming on-line in the 21st century will require greater fuel flexibility, reliability, availability, maintainability, and higher throughput and conversion.

- There has been growing interest in mathematical modeling of coal processing.

- CFD models such as MFIX, ANSYS-FLUENT and BARRACUDA are doing a great job in modeling coal gasification and other process.

- The accuracy and validity of CFD models depends on the kinetic models used to describe the homogeneous and the heterogeneous reactions that take place in the gasifier.

Introduction
Background

- Sometimes the kinetic models used have the limitations in operating condition range and fuel types.
- Hence there is a need for sophisticated models for coal devolatilization, combustion and gasification at various operating conditions and wide variety of coal.
- Experimental data is used to verify the simulations results. Experiments on other hand could be expensive and time consuming.
- Kinetic packages such as PC Coal Lab, CPD and FGDVC do a good job in predicting kinetics and product yields at various operating conditions using wide variety of coals.

Introduction
Background

- Currently there is no software platform available through which a user has access to the information from the kinetic packages and that easily converts the predictions of the models into usable, correctly formatted, reaction expressions that can be subsequently used directly to run the CFD codes.

- The aim of this research is to develop a graphical user interface (GUI) that allows detailed kinetic expressions for the gasification of a wide variety of coals and biomass to be seamlessly implemented in existing CFD codes.

METC Gasifier Advanced Simulation (MGAS)

- METC Gasifier Advanced Simulation (MGAS) by Syamlal and Bissett (1992)[a] can describe the transient operations of co flow , counter flow or fixed bed gasifiers .

- Reaction scheme and kinetics used was based on literature available at that time for four types of coal.

- MGAS now which includes gasification kinetics for five type of coal has received the National Award for Excellence in Technology Transfer from the Federal Laboratory Consortium (FLC) in 2008.

a: Syamlal M., and Bissett, L.A., "METC Gasifier Advanced Simulation (MGAS) Model," Technical Note, NTIS report No. DOE/METC-92/4108 (DE92001111), 1992.

METC Gasifier Advanced Simulation (MGAS)

- MGAS has been implemented in MFIX, ANSYS FLUENT and BARRACUDA.

- MGAS doesn't account for:
  - Effect of coal heating rate or reactor pressure on devolatilization yield
  - Soot formation or polyaromatic hydrocarbon (PAH) formation
  - Biomass/Petcoke gasification process

- MGAS has successfully been used in modeling transport gasifiers (Guenther et al., 2002 and Guenther et al., 2003)[b,c] , although some reaction rates adjustment had to be made.

b: Guenther C., Syamlal M., Longanbach J., and Smith P., "CFD modeling of a transport gasifier Part II", Proceedings of the 20th Annual Pittsburgh Coal Conference, Pittsburgh, PA, September 15-19, 2003.

c:: Guenther C., Shahnam M., Syamlal M, Longanbach J, Cicero D., and Smith P., "CFD modeling of a transport gasifier", Proceedings of the 19th Annual Pittsburgh Coal Conference, Pittsburgh, PA, September 23-27, 2002.

PC Coal Lab

- It is a mathematical model developed by Dr.Niksa and his group.
- It predicts kinetics and composition of products from devolatilization; tar cracking along with secondary pyrolysis and gasification reactions for over 2000 coals along with biomass and pet coke.
- It can predict effect of pressure, temperature and heating rate on devolatilization.
- It can simulate two types of tests
  - Drop tube method
  - Electrically heated wire grid method
- It requires license agreement.

Chemical Percolation Model for Coal Devolatilization (CPD)

- It is developed by Sandia National Laboratories, and University of Utah (Fletcher et al, 1992)[d].
- It describes the devolatilization behavior of rapidly heated coal based on the chemical structure of the parent coal.
- It enables user to specify the chemical structure of the coal as measured directly by ^{13}C NMR analyses.
- The current version can only predict devolatilization of coal.
- It is available for free.

d:Fletcher, T. H. and Hardesty D. H., "Compilation of Sandia Coal Devolatilization Data: Milestone Report," Sandia Report No. SAND92-8209, available NTIS, 1992.

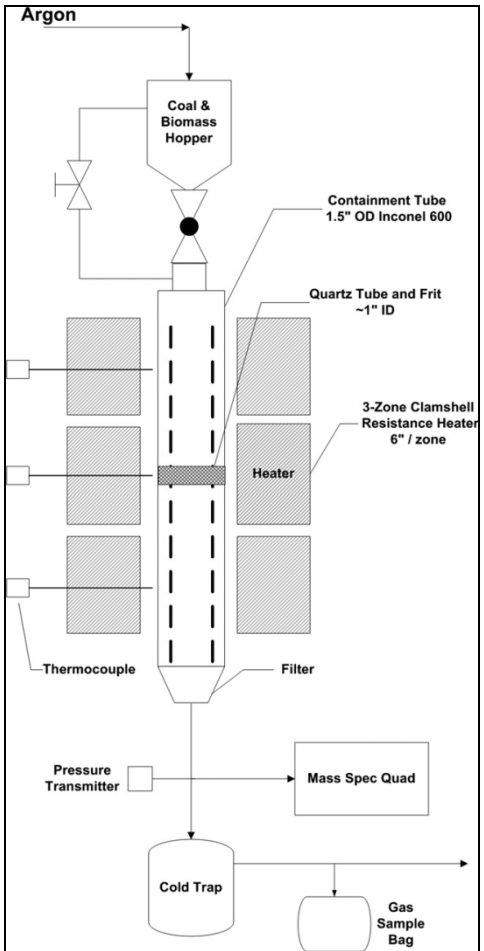
The Functional-Group, Depolymerization, Vaporization, Cross-linking (FG-DVC)

- FG-DVC model is a comprehensive code for predicting yields and compositions of coal pyrolysis products (gas, tar, and char).
- FG-DVC can handle fuels such as coal, biomass and waste organic material such as car tires, etc.
- FGDVC requires the ultimate analysis for the coal as input but better results are obtained if the TG-FTIR for the coal is used.
- The FG-DVC model combines two previously developed models by Solomon and workers [e,f ,g]
  I. Functional Group (FG) model : gas evolution and functional group composition
  II. Depolymerization, Vaporization, Cross-linking (DVC) model: amount and molecular weight of macromolecular fragments

e:Solomon, P.R. "The Evolution of Pollutants During the Rapid Devolatilization of Coal" Rep. R76-952588-2, United Technologies Research Center, East Hartford. 1977.
f:Solomon, P.R, Hamblen, D.G., Carangelo, R.M., Serio, M.A., and Deshpande, G.V. "A Genaral Model of Coal Devolatilization". In: Energy & Fuels (1988), pp. 405–422.
g::Solomon, P.R., Serio, M.A., and Suuberg, E.M. "Coal pyrolysis: experiments, kinetic rates and mechanisms". In: Progress in Energy and Combustion Science 18 (1992), pp. 133–220.

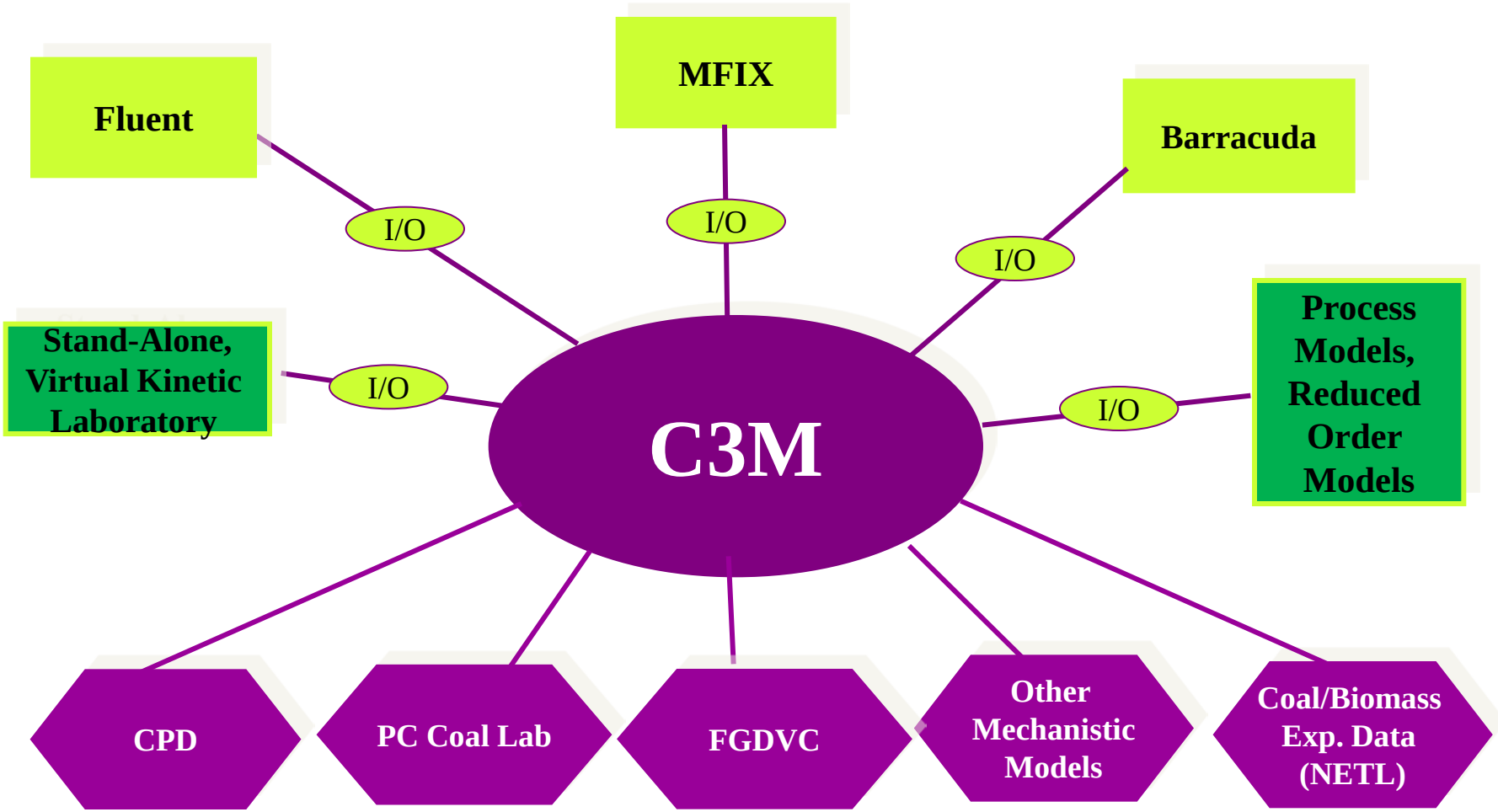
Experimental Data

- Experiments performed at NETL site with coal and biomass gasification.



- An experimental study to investigate the effects of co-feeding on pyrolysis product distributions under conditions relevant to transport gasifiers for coal and biomass. (done by Nathan Weiland and group).

Objective


Fluent
MFIX
Barracuda
I/O
I/O
I/O
Stand-Alone, Virtual Kinetic Laboratory
I/O
C3M
I/O
Process Models, Reduced Order Models
CPD
PC Coal Lab
FGDVC
Other Mechanistic Models
Coal/Biomass Exp. Data (NETL)

Carbonaceous Chemistry for Computational Modeling (C3M)

- C3M provides connection to access a variety of kinetic processes and reaction mechanisms typically found in coal gasification, gas clean-up, and carbon capture processes.

- The C3M GUI allows users easily enter fuel properties and operating conditions, select one or more kinetic packages from the C3M GUI menu, and compare graphically their output to show the sensitivity of fuel properties and/or operating conditions on predicted rates and yields.

- C3M allows modelers to extract kinetic rates and yields for devolatization and tar cracking steps from leading kinetic databases and models.

- The desired kinetic output is automatically updated into a specified computational model.

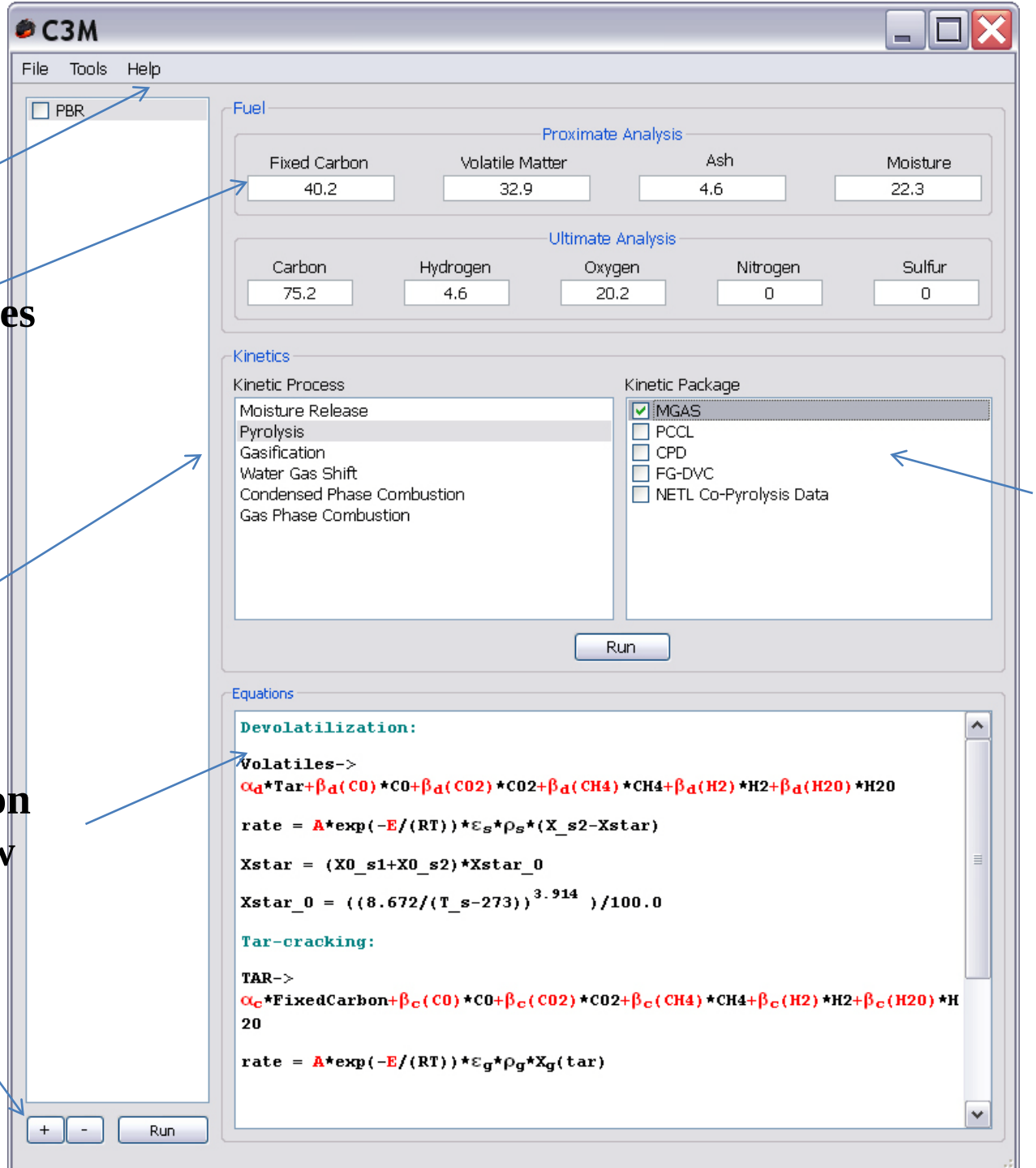
Uncertainty Quantification (UQ)

- It is a unique feature that can be coupled with C3M.
- Utilizing a UQ engine and toolbox (e.g., PSUADE, DAKOTA), the user can observe and predict the uncertainties/variations in product yields and reaction rates with the prescribed variability in the operating conditions and fuel properties.
- This is achieved by conducting systematically designed runs on the kinetic packages available in C3M and analyzing the output with the UQ toolbox.
- This is a very cheap and cost effective method in terms of time and computer capability

C3M Highlights

C3M™

Carbonaceous Chemistry for Computational Modeling



Menu

Fuel Properties

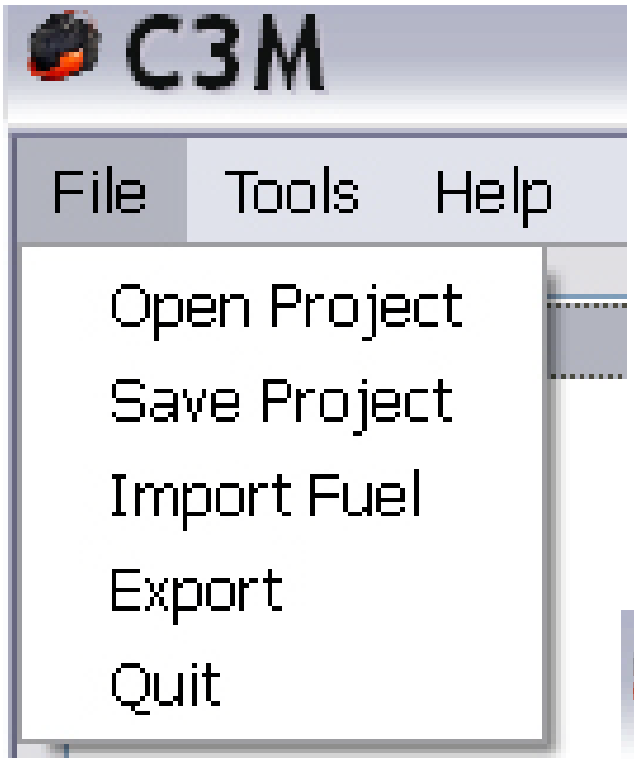
Kinetic Process

Equation Window

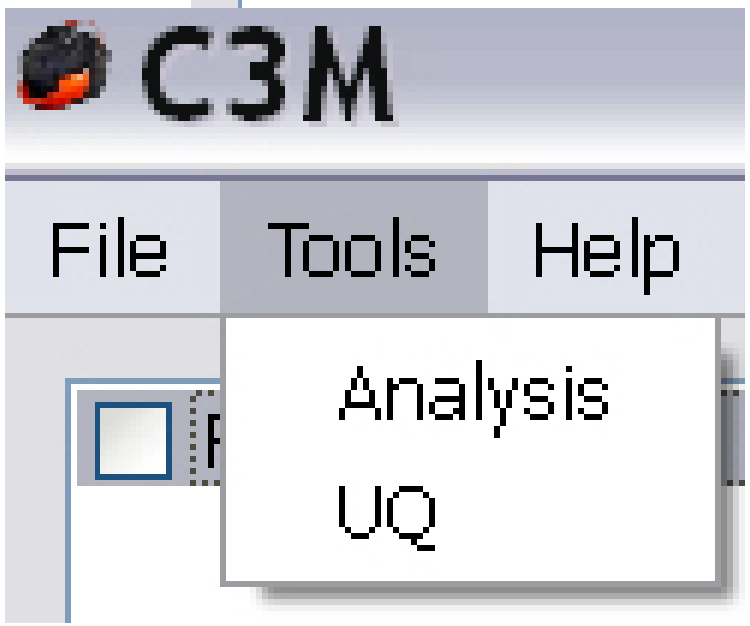
Adding Fuel

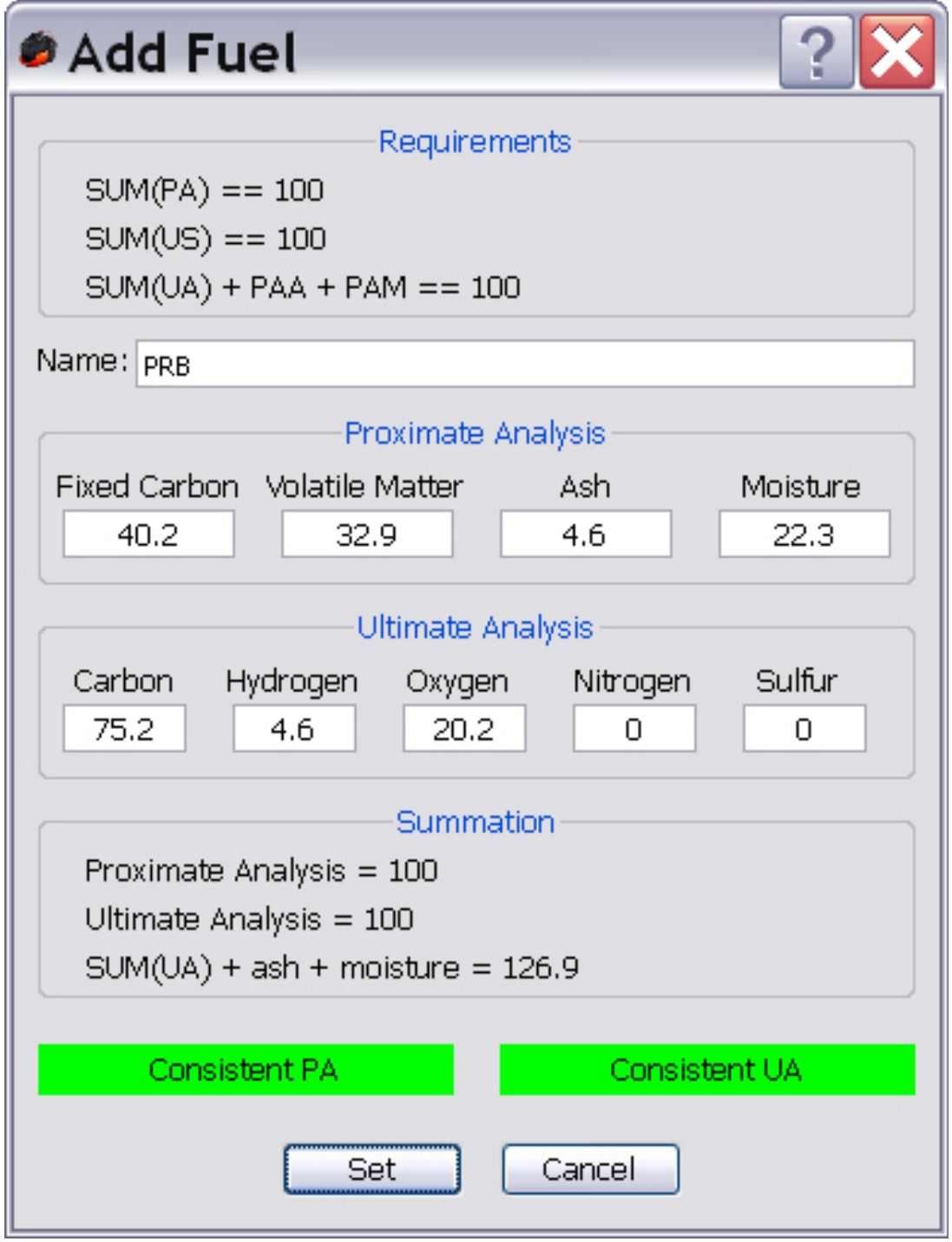
Kinetic Packages

Menu


C3M
File
Tools
Help
Open Project
Save Project
Import Fuel
Export
Quit


C3M
File
Tools
Help
PBR
About
Context Help


C3M
File
Tools
Help
Analysis
UQ


Add Fuel
Requirements
SUM(PA) == 100
SUM(US) == 100
SUM(UA) + PAA + PAM == 100
Name: PRB
Proximate Analysis
Fixed Carbon
Volatile Matter
Ash
Moisture
40.2
32.9
4.6
22.3
Ultimate Analysis
Carbon
Hydrogen
Oxygen
Nitrogen
Sulfur
75.2
4.6
20.2
0
0
Summation
Proximate Analysis = 100
Ultimate Analysis = 100
SUM(UA) + ash + moisture = 126.9
Consistent PA
Consistent UA
Set
Cancel

FUEL

FUEL

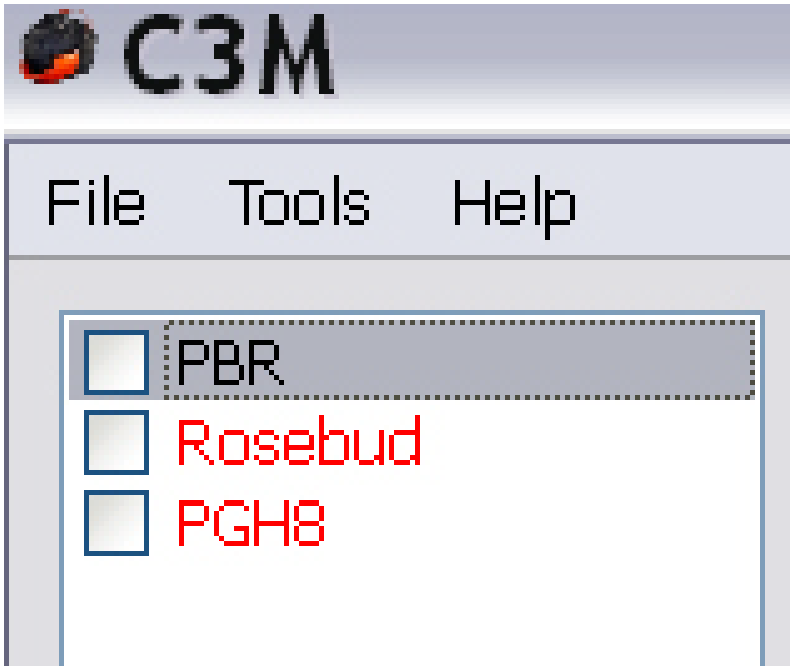
Fuel

Proximate Analysis

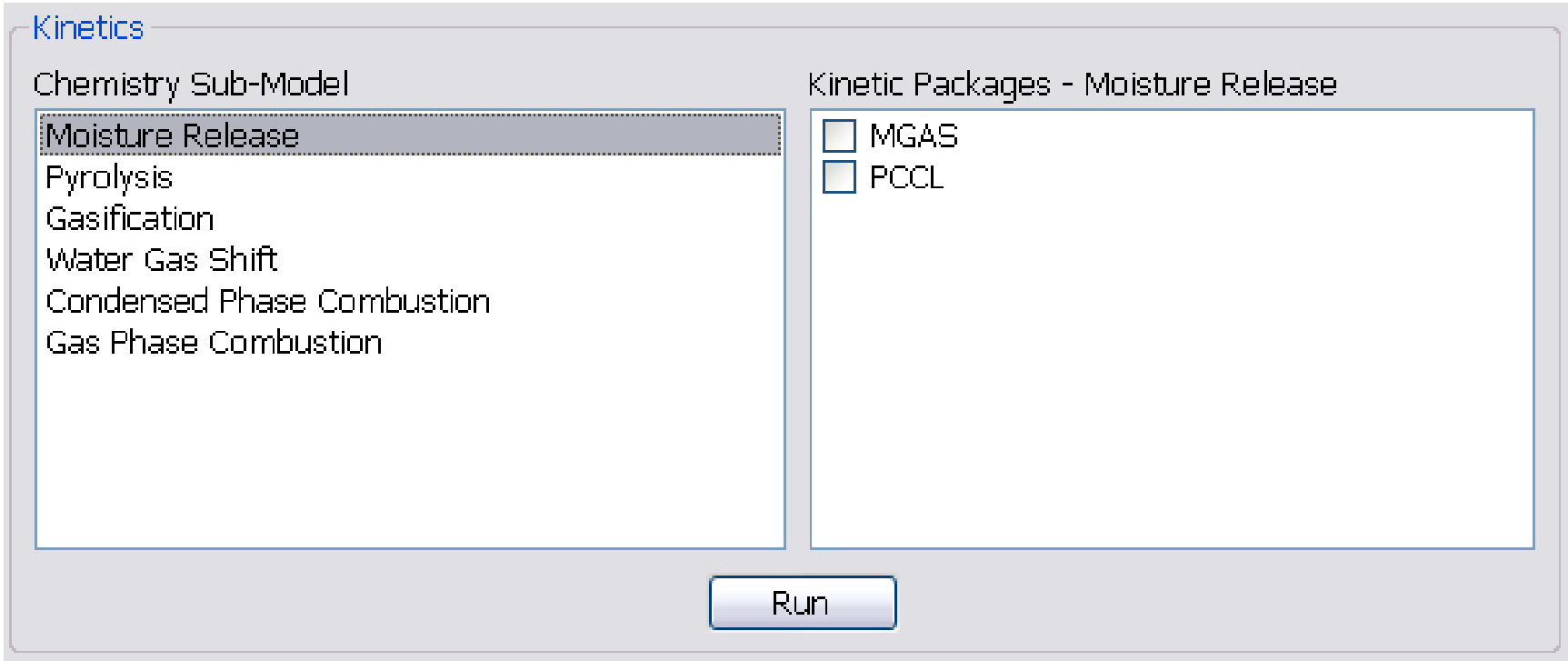
Fixed Carbon	Volatile Matter	Ash	Moisture
40.2	32.9	4.6	22.3

Ultimate Analysis

Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur
75.2	4.6	20.2	0	0

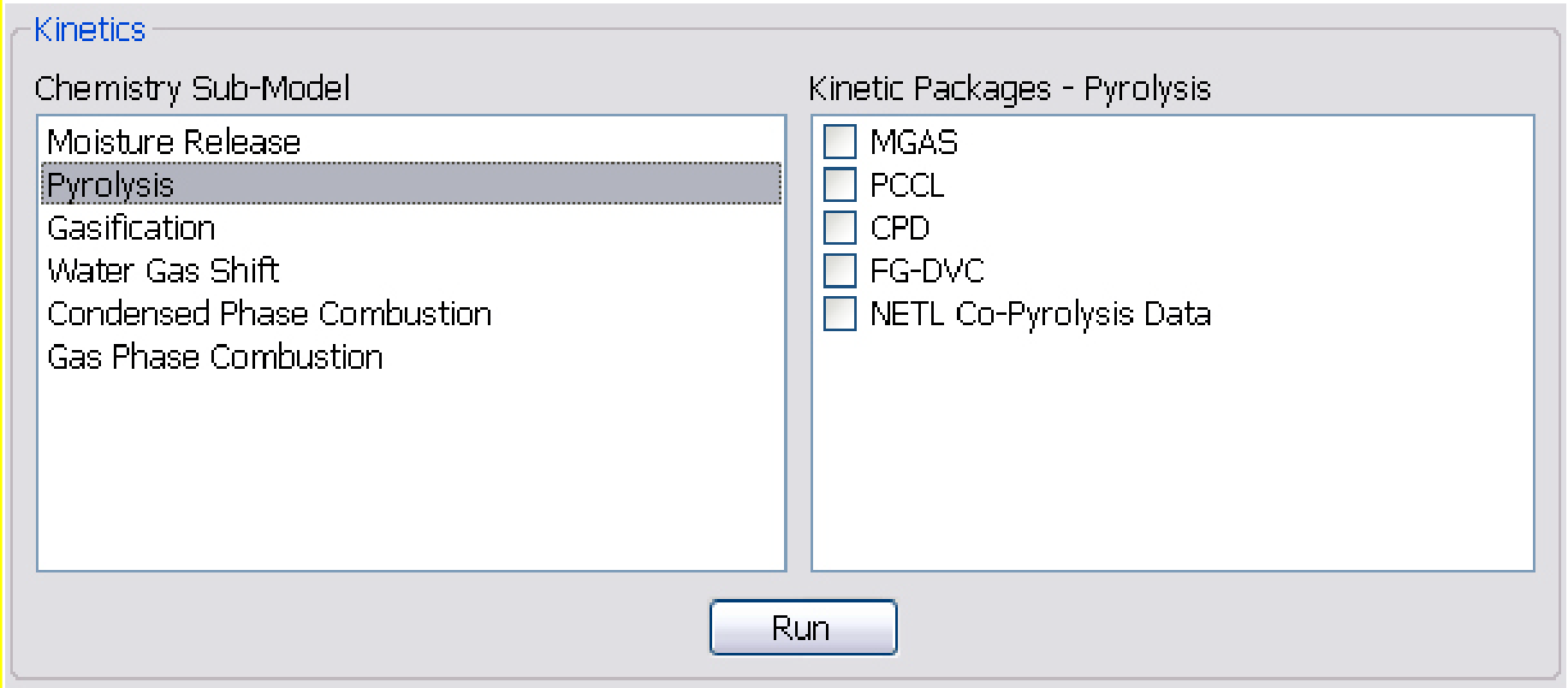


Kinetic Process Selection



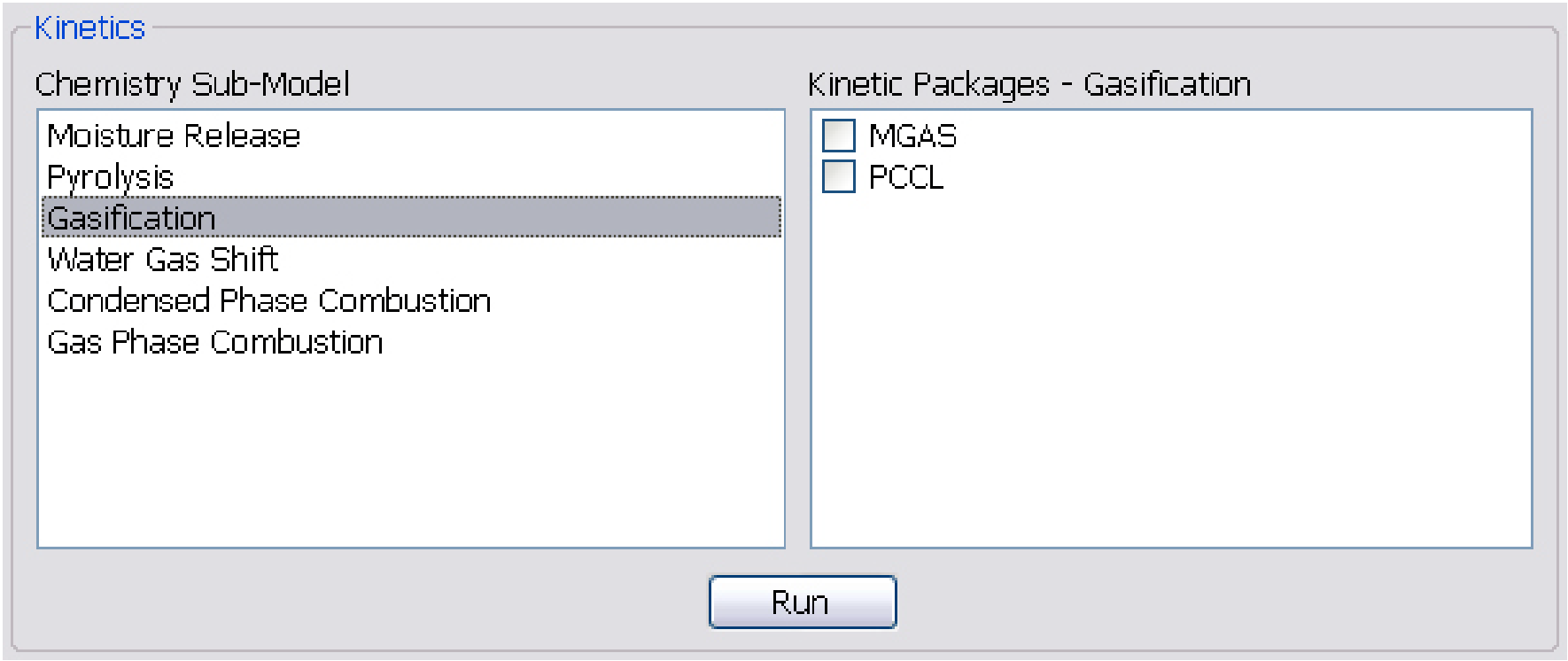
Kinetic Process Selection

Devolatilization



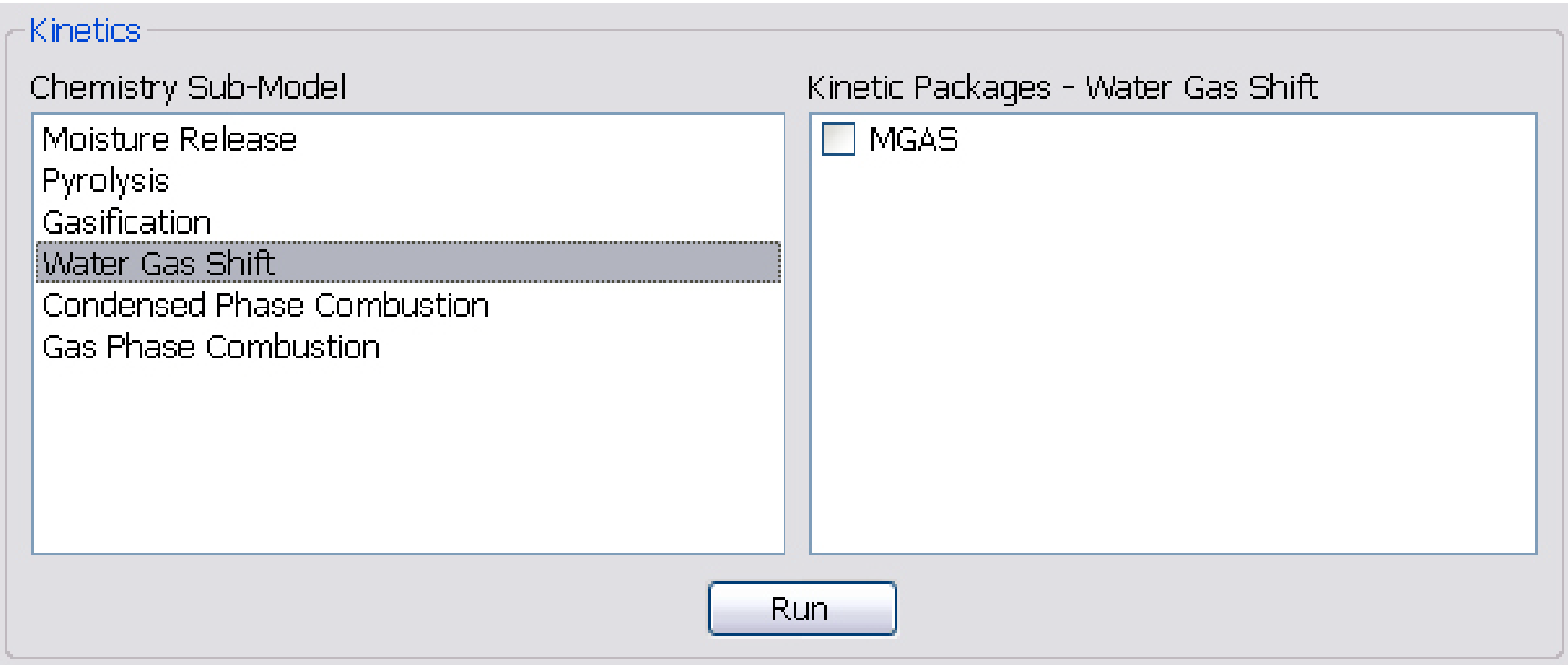
Kinetic Process Selection

Char and soot Gasification



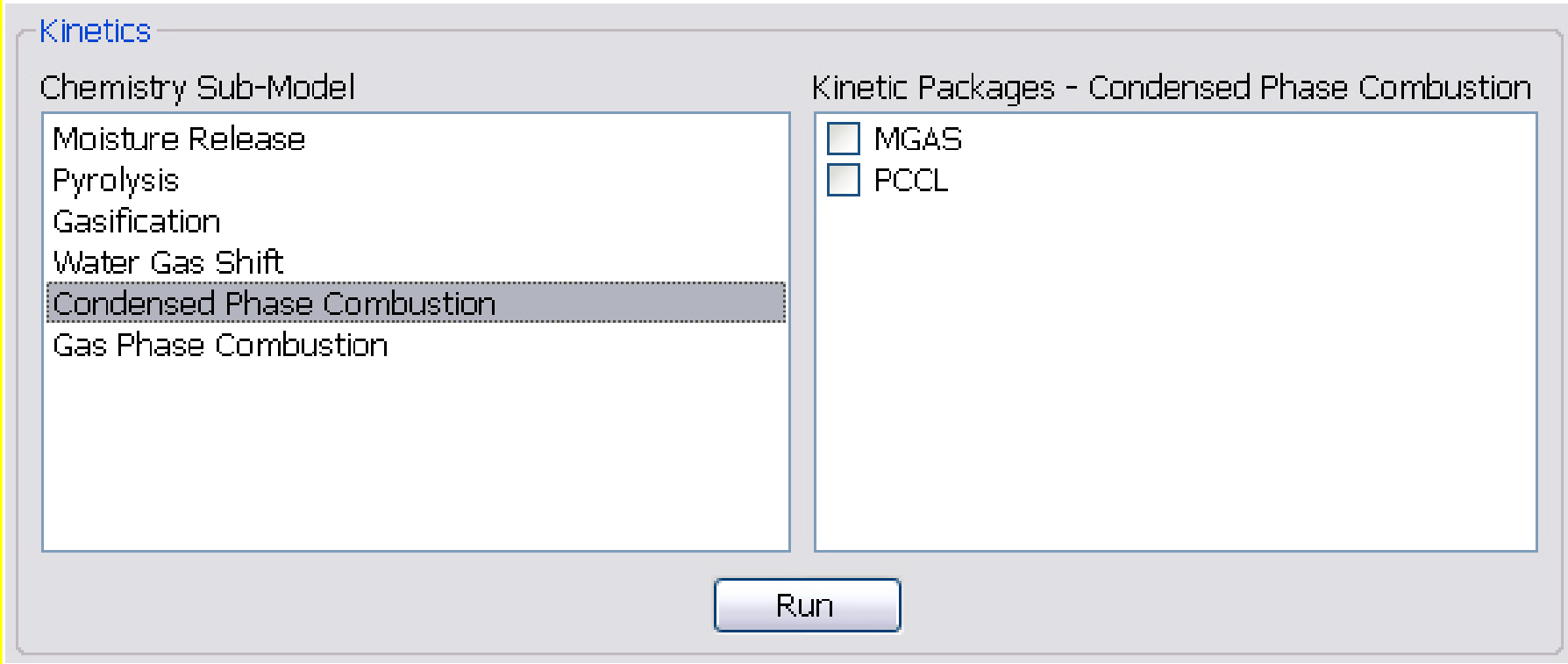
Kinetic Process Selection

Water Gas Shift



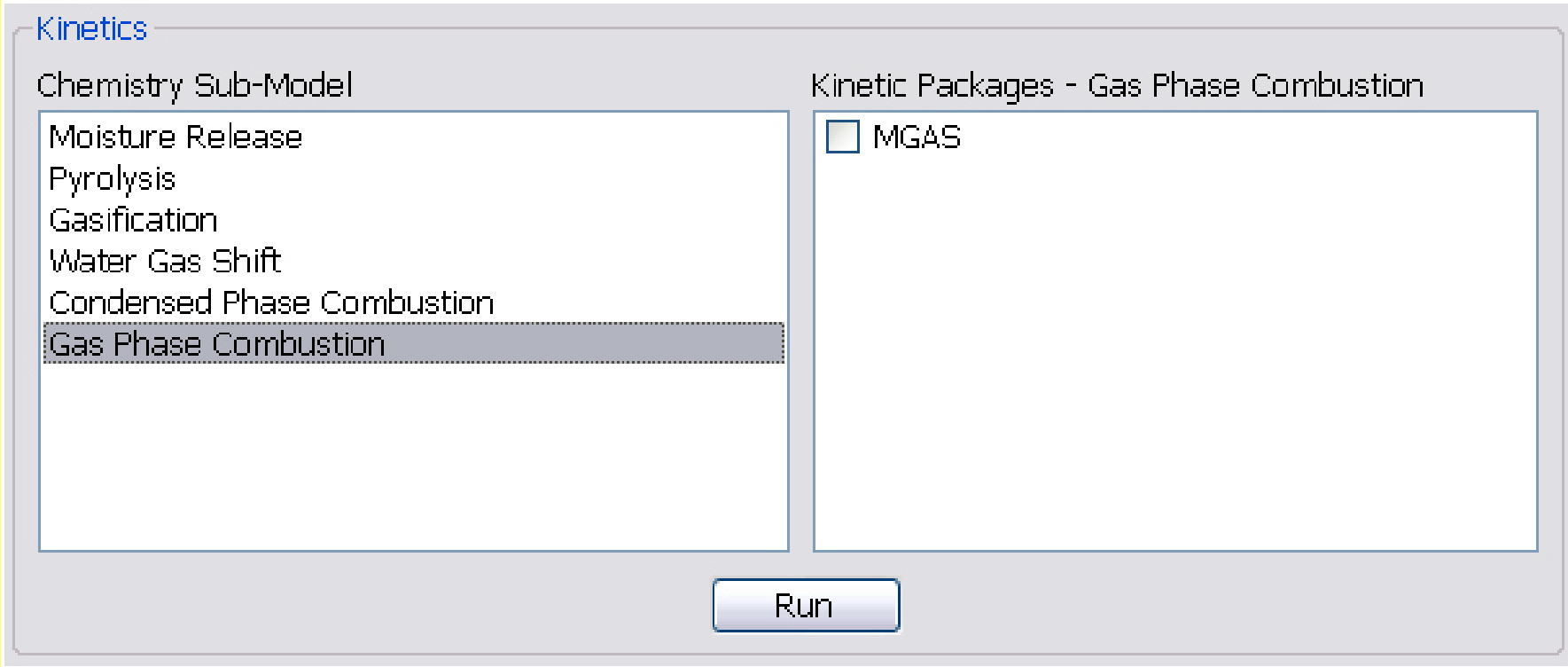
Kinetic Process Selection

Condensed Phase Combustion

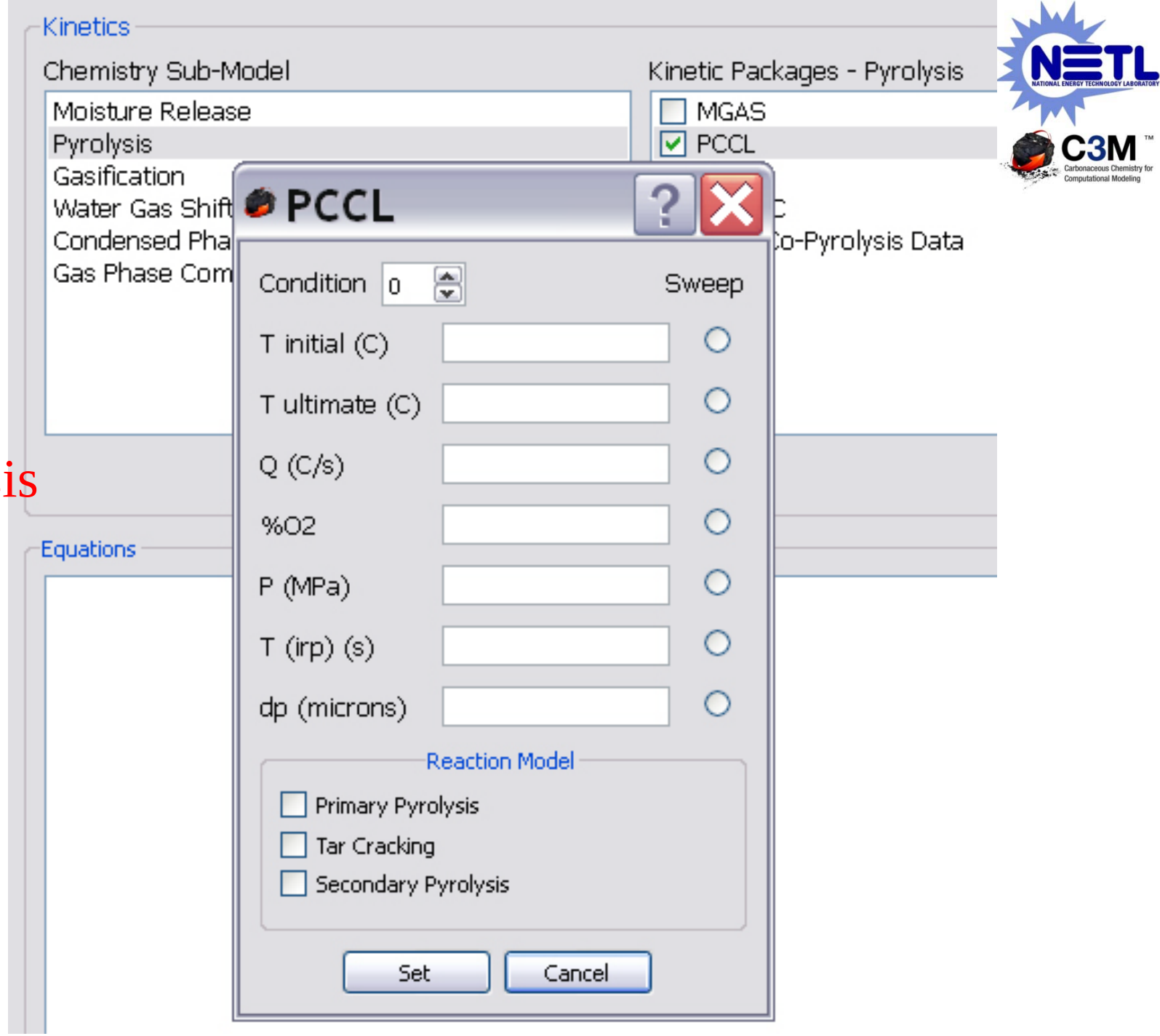


Kinetic Process Selection

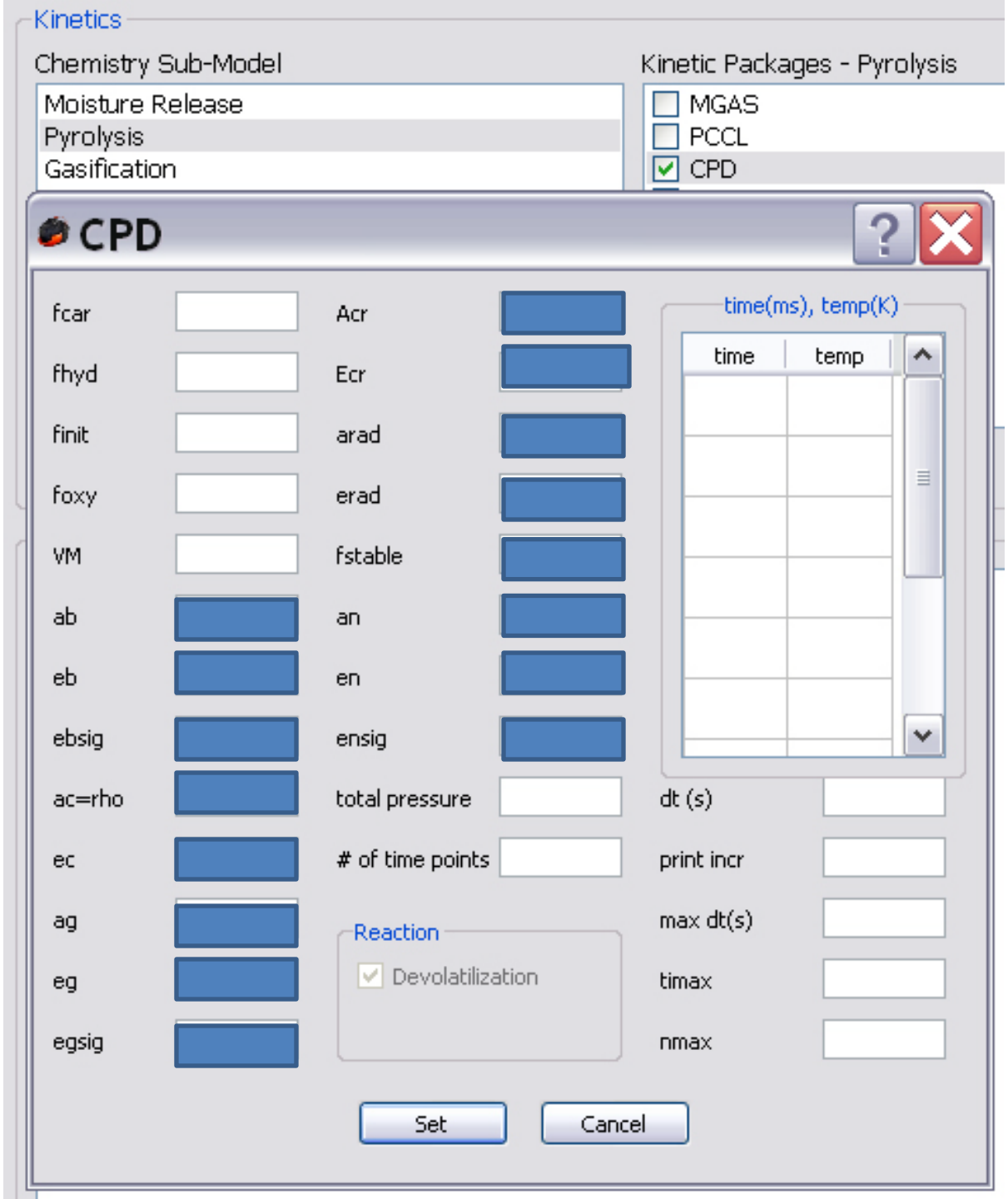
Gas Phase Combustion



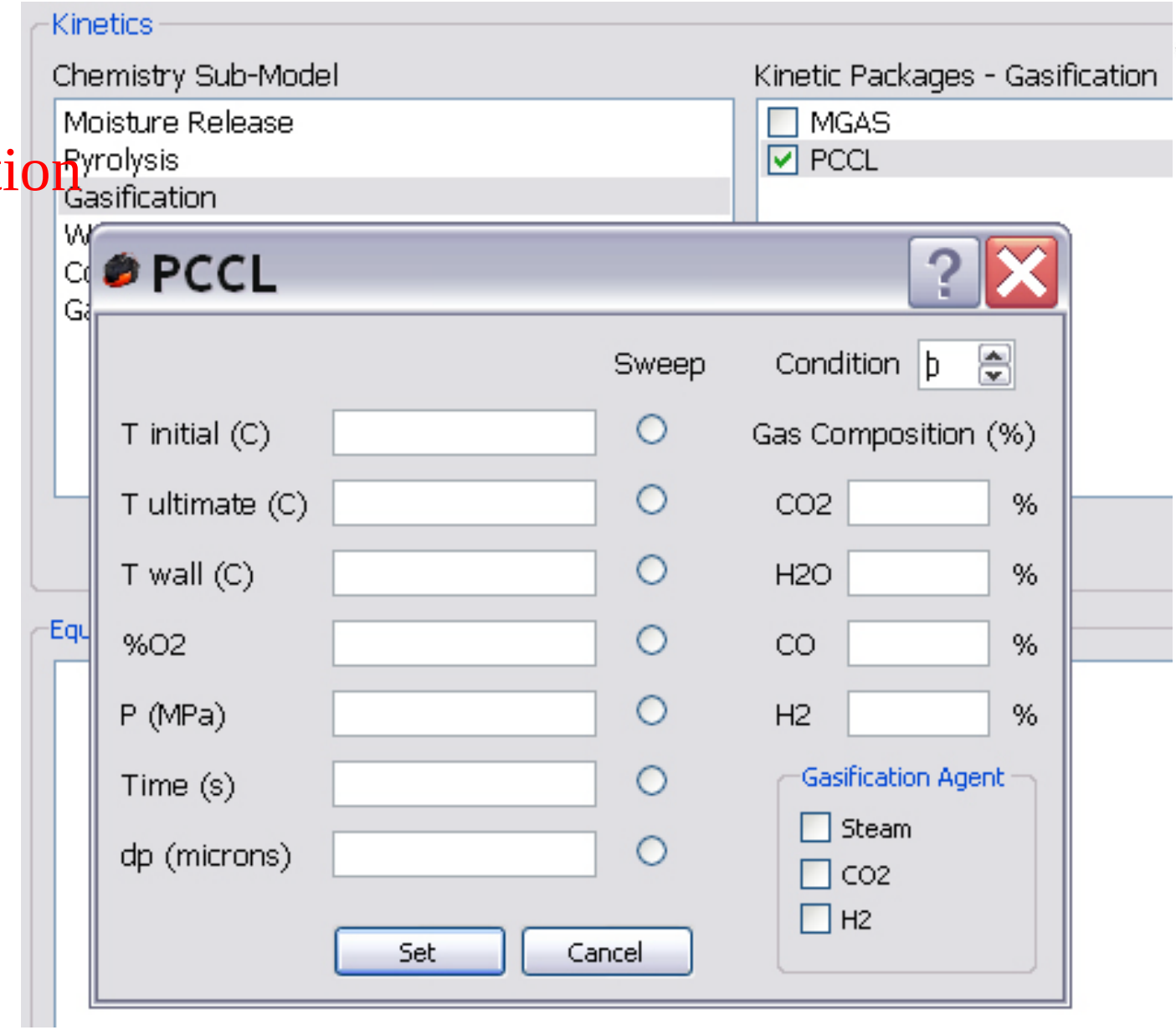
PCCL Pyrolysis



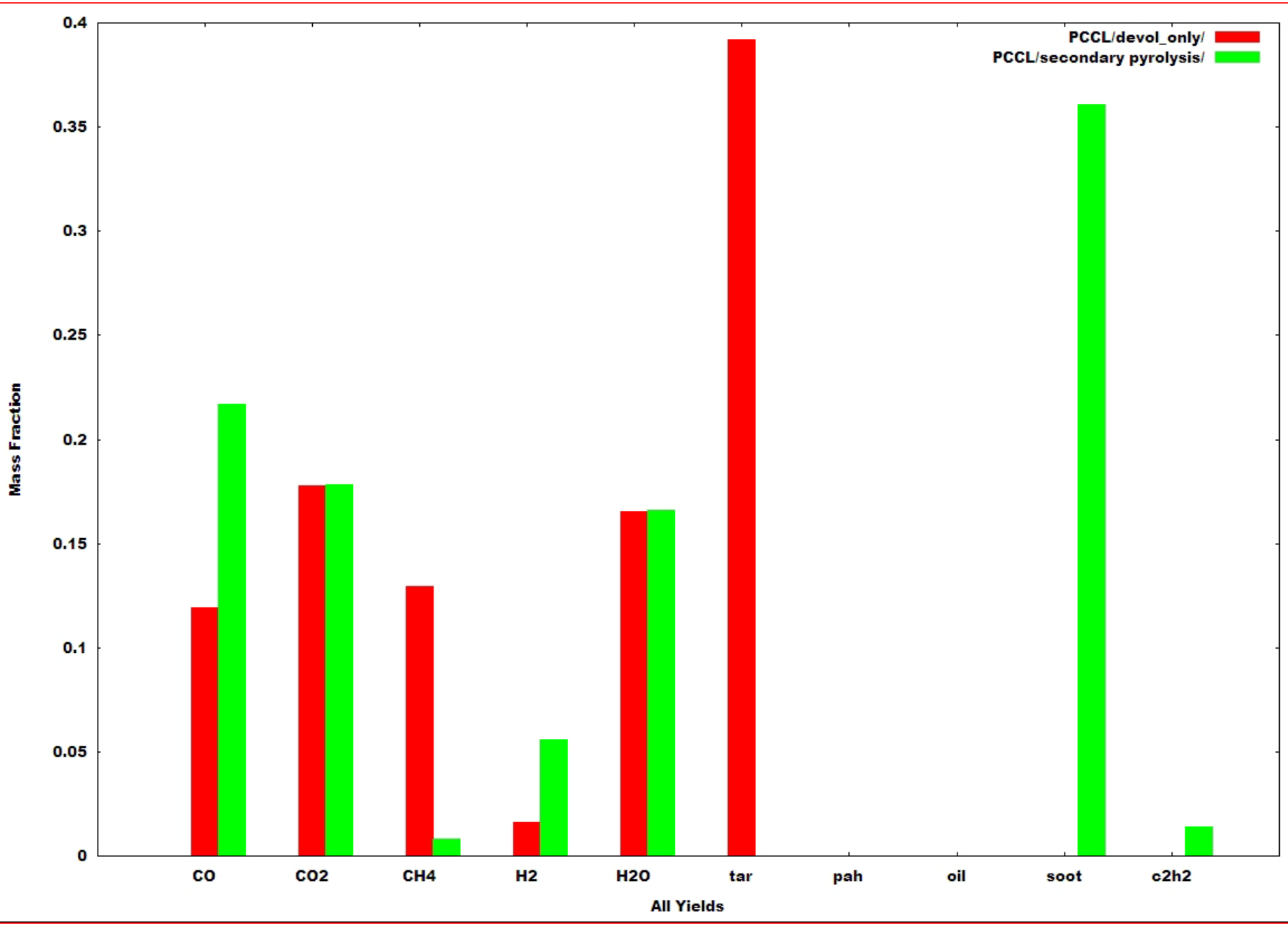
CPD Pyrolysis

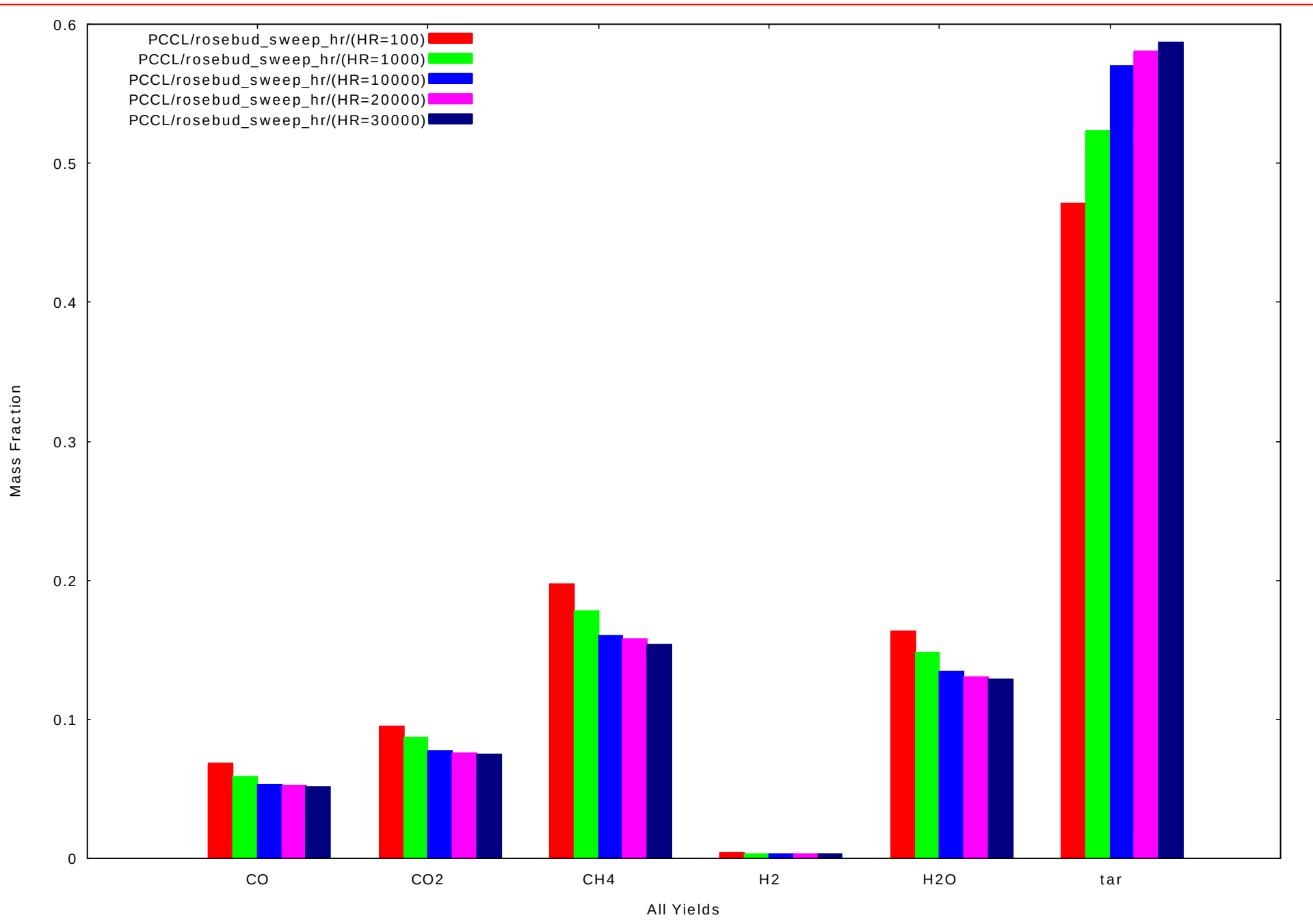


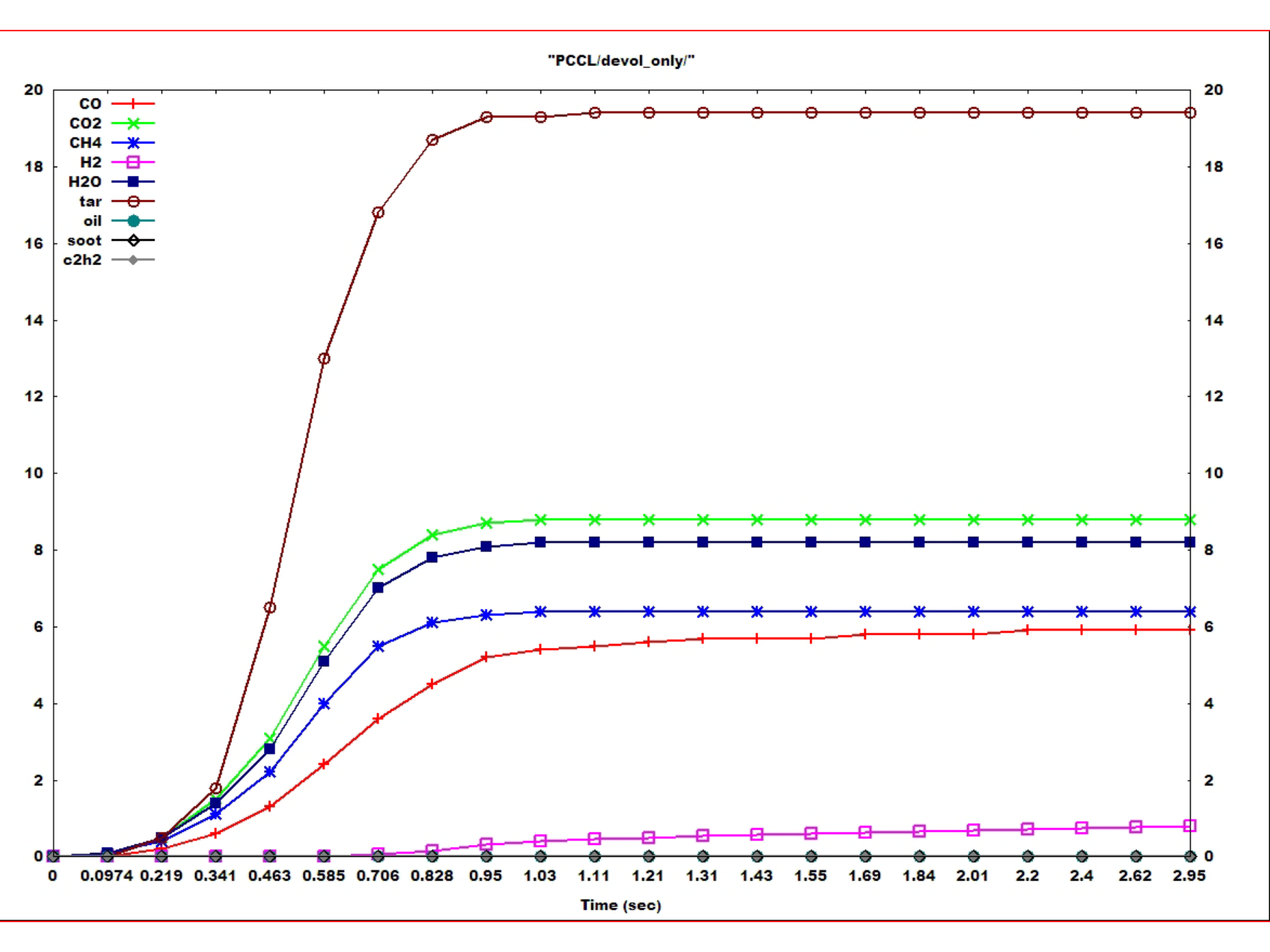
PCCL Gasification

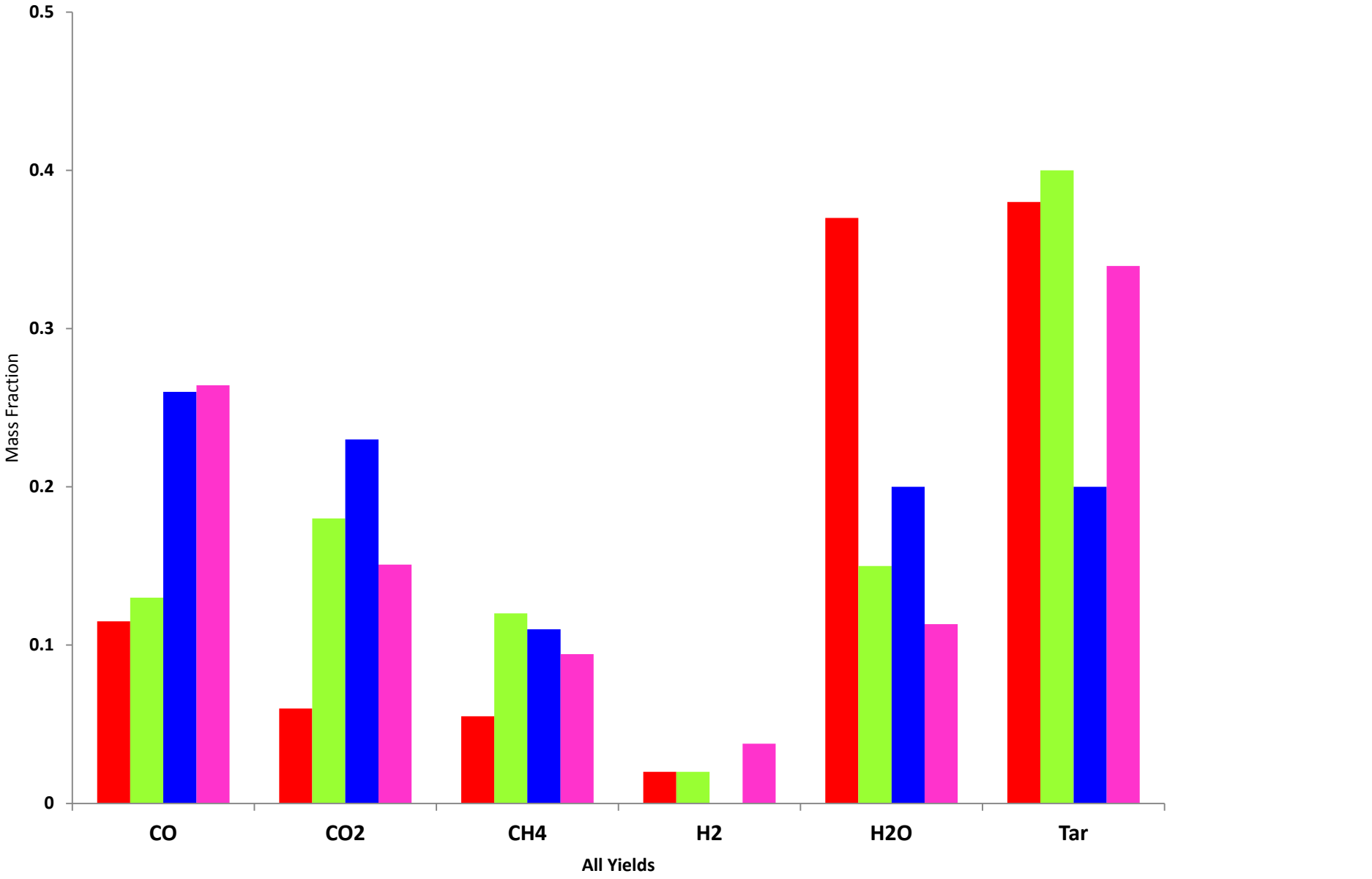


Analysis of Kinetic Package Outputs

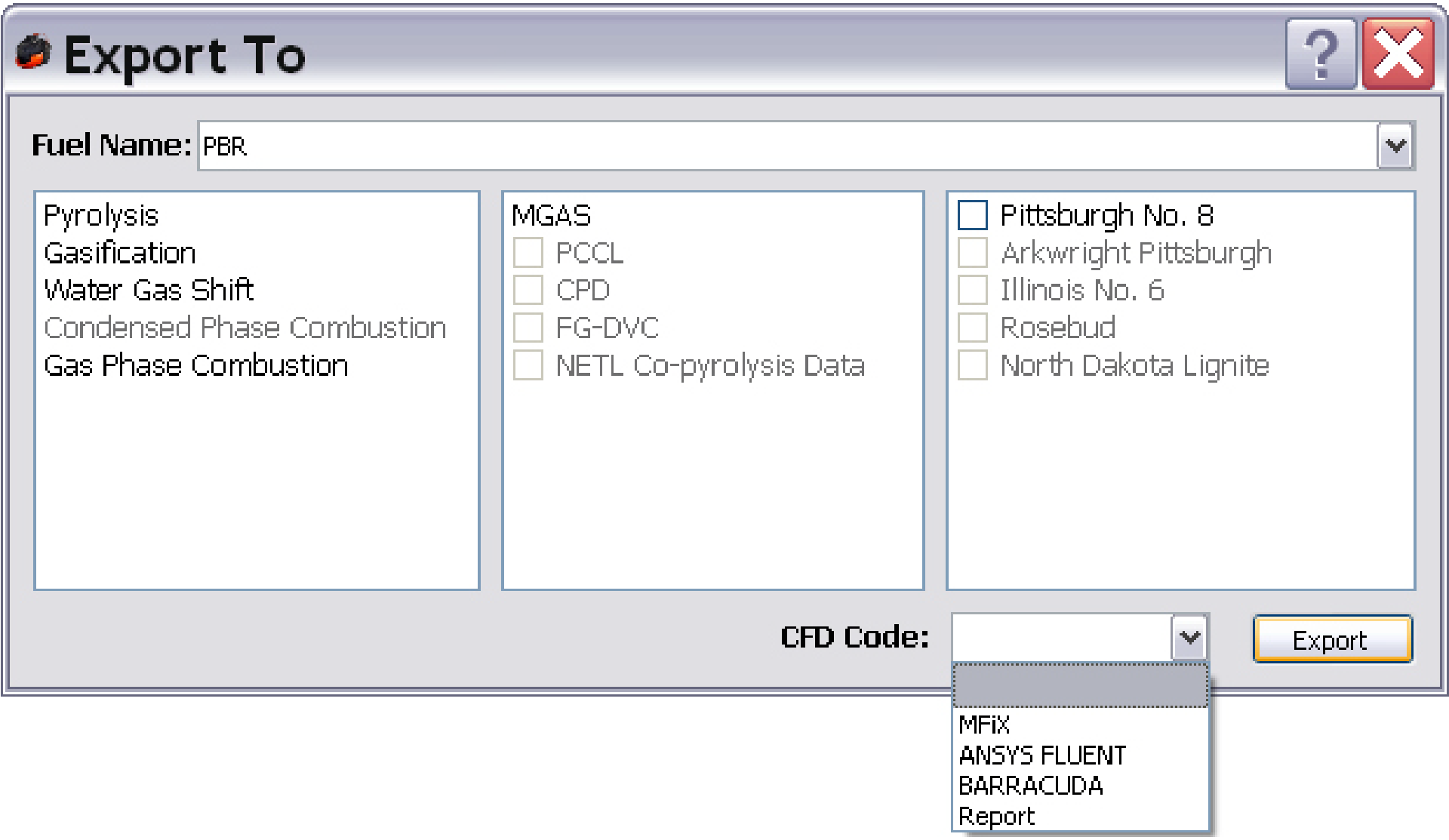

PCCL/devol_only/
PCCL/secondary pyrolysis/
Mass Fraction
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
CO
CO2
CH4
H2
H2O
tar
pah
oil
soot
c2h2
All Yields


PCCL/rosebud_sweep_hr/(HR=100)
PCCL/rosebud_sweep_hr/(HR=1000)
PCCL/rosebud_sweep_hr/(HR=10000)
PCCL/rosebud_sweep_hr/(HR=20000)
PCCL/rosebud_sweep_hr/(HR=30000)
Mass Fraction
0.6
0.5
0.4
0.3
0.2
0.1
0
CO
CO2
CH4
H2
H2O
tar
All Yields


"PCCL/devol_only/"
CO
CO2
CH4
H2
H2O
tar
oil
soot
c2h2
0
2
4
6
8
10
12
14
16
18
20
0
0.0974
0.219
0.341
0.463
0.585
0.706
0.828
0.95
1.03
1.11
1.21
1.31
1.43
1.55
1.69
1.84
2.01
2.2
2.4
2.62
2.95
Time (sec)

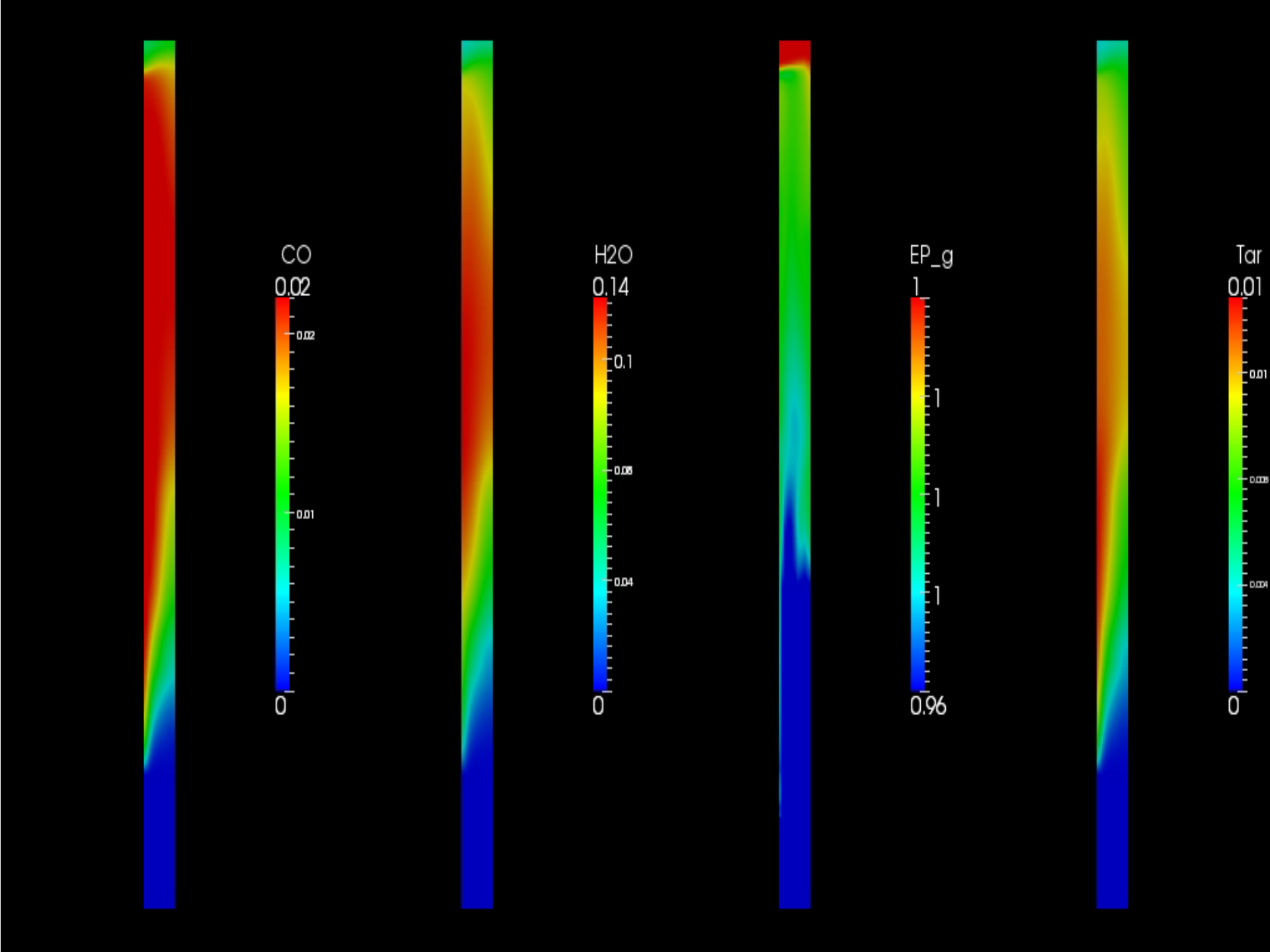

MGAS
PCCL Devol Only
CPD
HPTR Exp
0.5
0.4
0.3
0.2
0.1
0
Mass Fraction
CO
CO2
CH4
H2
H2O
Tar
All Yields

Exporting output to CFD model


Export To
Fuel Name:
PBR
Pyrolysis
Gasification
Water Gas Shift
Condensed Phase Combustion
Gas Phase Combustion
MGAS
PCCL
CPD
FG-DVC
NETL Co-pyrolysis Data
Pittsburgh No. 8
Arkwright Pittsburgh
Illinois No. 6
Rosebud
North Dakota Lignite
CFD Code:
Export
MFiX
ANSYS FLUENT
BARRACUDA
Report

```
##########################################################################
############################  Pyrolysis ##################################
##########################################################################

# Volatile Matter --> C3M_ALPHAD * Tar + C3M_BETAD(2) * CO
#                                      + C3M_BETAD(3) * CO2
#                                      + C3M_BETAD(4) * CH4
#                                      + C3M_BETAD(5) * H2
#                                      + C3M_BETAD(6) * H2O
#
        C3M_BETAD(2,1) =   0.0274134    # CO
        C3M_BETAD(3,1) =   0.0332876    # CO2
        C3M_BETAD(4,1) =     0.15469    # CH4
        C3M_BETAD(5,1) =  0.00724496    # H2
        C3M_BETAD(6,1) =   0.0939886    # H2O

        C3M_ALPHAD(1) =   0.683376  #

# rate = C3M_AKD * exp (-C3M_AED/(RT)) * e_s * p_s * (X_s2 - Xstar)

        C3M_AKD(1) =      10820
        C3M_AED(1) =      13350

#     Moisture Release

# rate = C3M_AKM * 6 * e_s / Dp * (X_s3)

        C3M_AKM(1) =    0.01555


##########################################################################
#########################  Water Gas Shift ###############################
##########################################################################

# rate = C3M_WG3 * 2.877 * F3 * p^(0.5-p/250)
#           * exp (-27760/(RT)) * (X_g2 * X_g6 - X_g3*X_g5)/K3

        C3M_WG3(1) =      0.014


##########################################################################
############################  Gasification ###############################
##########################################################################

        PCCL_mw_soot= 0
        PCCL_w1= 0
        PCCL_w2= 0
        PCCL_w3= 0
        PCCL_t1= 0
```

```
    6  2.9E-06  1.6E-05  6.6E-04  1.7E-03  7.5E-05  8.7E-04  V0
    7  1.5E-06  8.0E-06  3.4E-04  8.4E-04  3.7E-05  4.4E-04  V0
    8  8.2E-07  4.1E-06  1.7E-04  4.2E-04  1.8E-05  2.2E-04  V0

 Time =  0.43224E-03  Dt =  0.16935E-04    CPU time left =    12.408 days
  Nit      P0       P1       U0       V0       U1       V1    Max res
    1  1.0E-03  5.2E-02  1.7E-02  5.4E-02  2.7E-03  2.8E-02  X0 6
    2  1.4E-04  3.1E-04  8.5E-03  2.6E-02  1.4E-03  1.4E-02  V0
    3  2.0E-05  1.2E-04  4.8E-03  1.3E-02  6.2E-04  6.9E-03  V0
    4  1.1E-05  6.2E-05  2.4E-03  6.5E-03  3.0E-04  3.4E-03  V0
    5  5.5E-06  3.1E-05  1.2E-03  3.2E-03  1.5E-04  1.7E-03  V0
    6  2.9E-06  1.6E-05  6.4E-04  1.6E-03  7.4E-05  8.5E-04  V0
    7  1.5E-06  8.1E-06  3.3E-04  8.2E-04  3.6E-05  4.3E-04  V0
    8  8.1E-07  4.1E-06  1.7E-04  4.1E-04  1.8E-05  2.1E-04  V0

 Time =  0.44917E-03  Dt =  0.16935E-04    CPU time left =    12.408 days
  Nit      P0       P1       U0       V0       U1       V1    Max res
    1  1.0E-03  5.2E-02  1.5E-02  5.2E-02  2.7E-03  2.7E-02  X0 6
    2  1.4E-04  3.1E-04  7.7E-03  2.5E-02  1.4E-03  1.4E-02  V0
    3  1.9E-05  1.2E-04  4.3E-03  1.3E-02  6.0E-04  6.7E-03  V0
    4  1.0E-05  6.2E-05  2.2E-03  6.3E-03  2.9E-04  3.3E-03  V0
    5  5.4E-06  3.1E-05  1.1E-03  3.2E-03  1.5E-04  1.7E-03  V0
    6  2.8E-06  1.6E-05  5.8E-04  1.6E-03  7.2E-05  8.3E-04  V0
    7  1.5E-06  8.1E-06  3.0E-04  8.0E-04  3.6E-05  4.2E-04  V0
    8  8.0E-07  4.2E-06  1.5E-04  4.0E-04  1.8E-05  2.1E-04  V0

 Time =  0.46611E-03  Dt =  0.16935E-04    CPU time left =    12.408 days
  Nit      P0       P1       U0       V0       U1       V1    Max res
    1  1.0E-03  5.2E-02  1.3E-02  5.1E-02  2.6E-03  2.7E-02  X0 6
    2  1.4E-04  3.1E-04  6.7E-03  2.4E-02  1.3E-03  1.3E-02  V0
    3  1.9E-05  1.2E-04  3.8E-03  1.2E-02  5.8E-04  6.6E-03  V0
    4  1.0E-05  6.2E-05  1.9E-03  6.1E-03  2.9E-04  3.3E-03  V0
```


CO
0.02
0.02
0.01
0
H2O
0.14
0.1
0.06
0.04
0
EP_g
1
1
1
1
0.96
Tar
0.01
0.01
0.006
0.004
0

Summary

- C3M has developed a seamless integration between PC Coal Lab, CPD , FG-DVC, and Experimental data to leading multiphase CFD solvers MFIX, ANSYS-FLUENT and BARRACUDA.

- C3M allows a scientist to choose a kinetic process of interest (e.g., pyrolysis, gasification, sorbent based CO_2 capture etc.) and evaluate it as a function of fuel and/or operating conditions

- C3M provides the user the ability to conduct virtual kinetic experiments using leading kinetic packages and available experimental data to evaluate kinetic predictions as a function of fuel and sorbent type and/or operating conditions.

- C3M allows modelers to quickly incorporate detailed chemical reactions in multiphase CFD models for a variety of carbonaceous fuels and gasifier operating conditions.

Future Work

- Develop the UQ tool.
- Experimental Kinetic Data:
  - Soot formation reaction
  - Coal and biomass gasification
  - Entrained Flow reactor gasification
  - High pressure, high temperature water gas shift reaction
  - Chemical Looping
  - CO_2 adsorbent

Acknowledgement

- This technical effort was performed in support of the National Energy Technology Laboratory's ongoing research in development of C3M for coal gasification kinetics under the RES contract DE-FE0004000.

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