Implementation of PCGC-3 Coal Combustion Submodels into STAR-CD

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Introduction

- STAR-CD has limited coal combustion models.
- This research involves the implementation of some coal combustion submodels.
- This implementation has 3 steps:
  - Modification of PCGC-3 coal submodels for implementation into STAR-CD.
  - Verification of the individual submodels.
  - Validation of STAR-CD using the implemented coal submodels on a coal combustion system.

Background

- Many phenomena affect the performance of coal combustion and gasification equipment.
  - Flow
  - Heat transfer (Radiation, convection, conduction)
  - Reactions (Coal reactions, gas-phase reactions, pollutant formation reactions)
- All these are important to accurately predict in order to model a combustion system.
- Modeling is used to make improvements to the overall performance (increased efficiency, reduced pollutant emissions).

Background

- Most fundamental research on coal combustion is focused in three areas:
  - Model development
  - Laboratory experiments
  - Process development
- Coal combustion models developed include:
  - Coal structure and properties
  - Coal reactions
  - Gas-phase reactions
  - Pollutant formation (NOx)
  - Deposition

Background

- Coal reactions models available in STAR-CD
  - Devolatilization (1-step, constant rate)
  - Char Oxidation (1st-order, constant rate)
- Coal reactions models available in PCGC-3
  - Moisture Vaporization
  - Devolatilization
    - 1-Step
    - 2-Step
    - Distributed Activation Energy
    - Chemical Percolation Devolatilization (CPD)
  - Char Oxidation
    - Global nth-order
    - Char Burnout Kinetic (CBK)

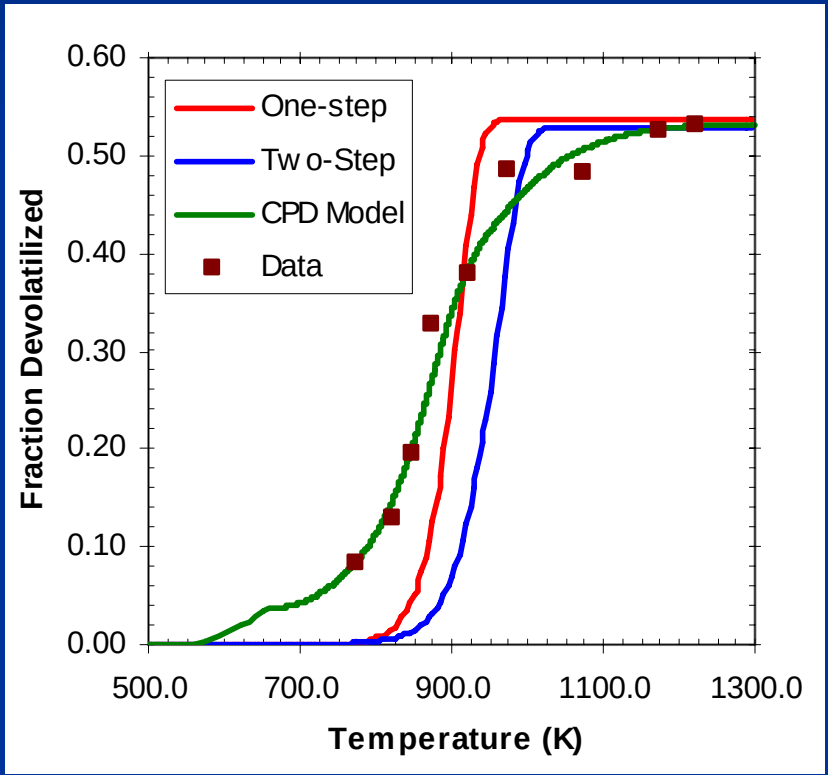
Modification and Implementation

- Some coal submodels (CPD and CBK) existed as stand-alone programs meant to predict a specific coal reaction rate.
- Other submodels existed as PCGC-3 submodels.
- General modifications made to the submodels included:
  - Adapting models to enable interfacing with STAR-CD.
  - Restructuring models to remove redundancies.

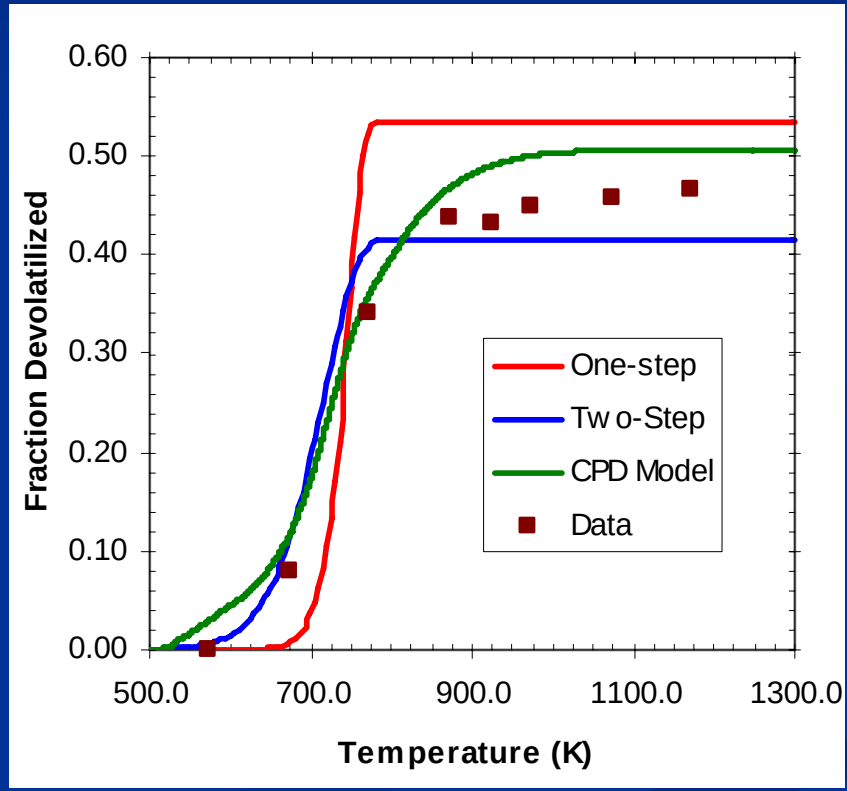
Verification

- Verification involved comparison between predictions and experimental data for each individual submodels.
- Verification was performed on the devolatilization and char oxidation models.

Verification of Devolatilization Models

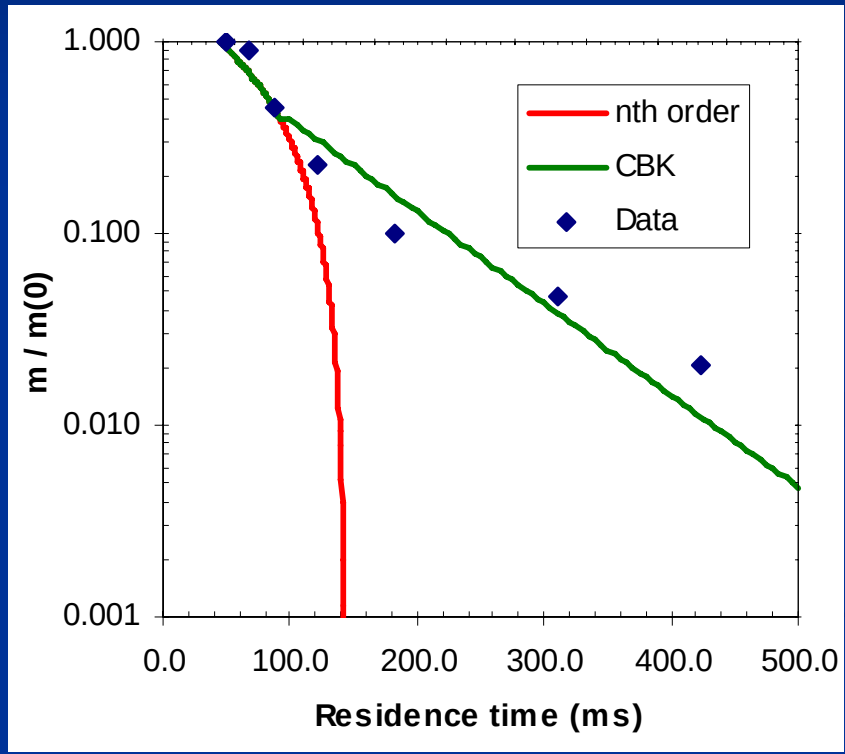


Fraction Volatiles Released for a Heating Rate of 1000 K/s



Fraction Volatiles Released for a Heating Rate of 1 K/s

Verification of Char Oxidation Models



Char Burnout Predictions for the Global nth-order Model and the CBK Model

Model Validation

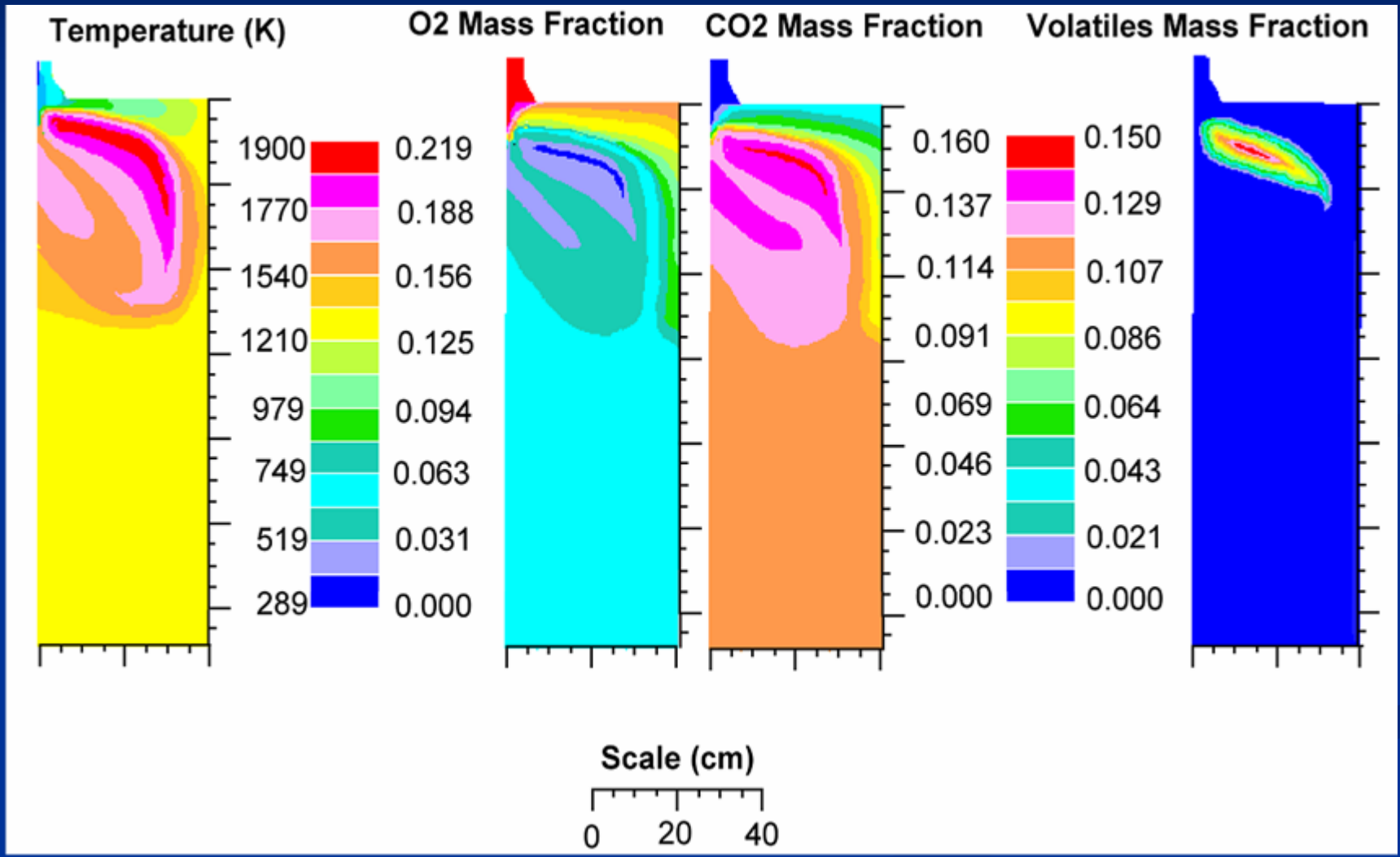
- Validation of the overall coal combustion code involved comparing the predictions made with STAR-CD and experimental data from the BYU Burner Flow Reactor (BFR).
- Four validation cases were performed:
  - Original STAR-CD Models (1-step Devolatilization/1st-order Char Oxidation)
  - 1-step Devolatilization/Global nth-order Char Oxidation
  - 2-step Devolatilization/Global nth-order Char Oxidation
  - CPD/CBK

Validation Set-up

Inlet Parameter	Value
Coal Flow Rate (kg/hr)	11.4
Primary Air Flow Rate (kg/hr)	15
Primary Air Temperature (K)	289
Secondary Air Flow Rate (kg/hr)	127
Secondary Air Temperature (K)	533
Mass-mean particle size (μm)	55
Swirl Number	1.4
Equivalence Ratio	1.15

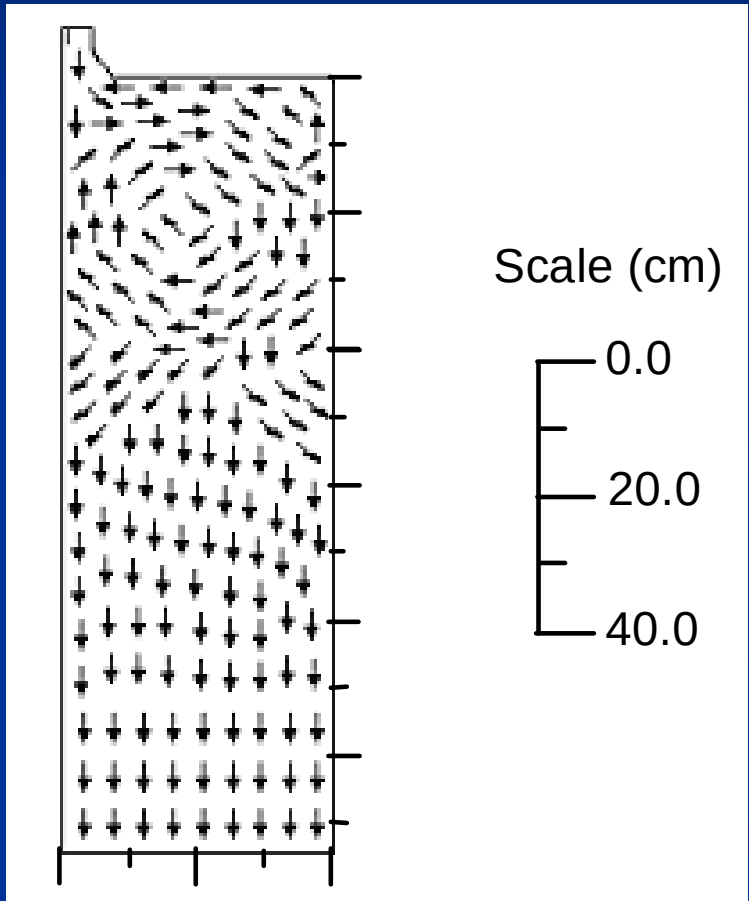
Proximate Analysis (mass %, as received)	
Moisture	8.54
Ash	13.25
Volatile	39.35
Fixed Carbon	38.86
Heating Value (kJ/kg)	5476
Ultimate Analysis (mass %, dry basis)	
Carbon	69.13
Hydrogen	5.18
Oxygen	9.37
Nitrogen	1.34

Validation Results



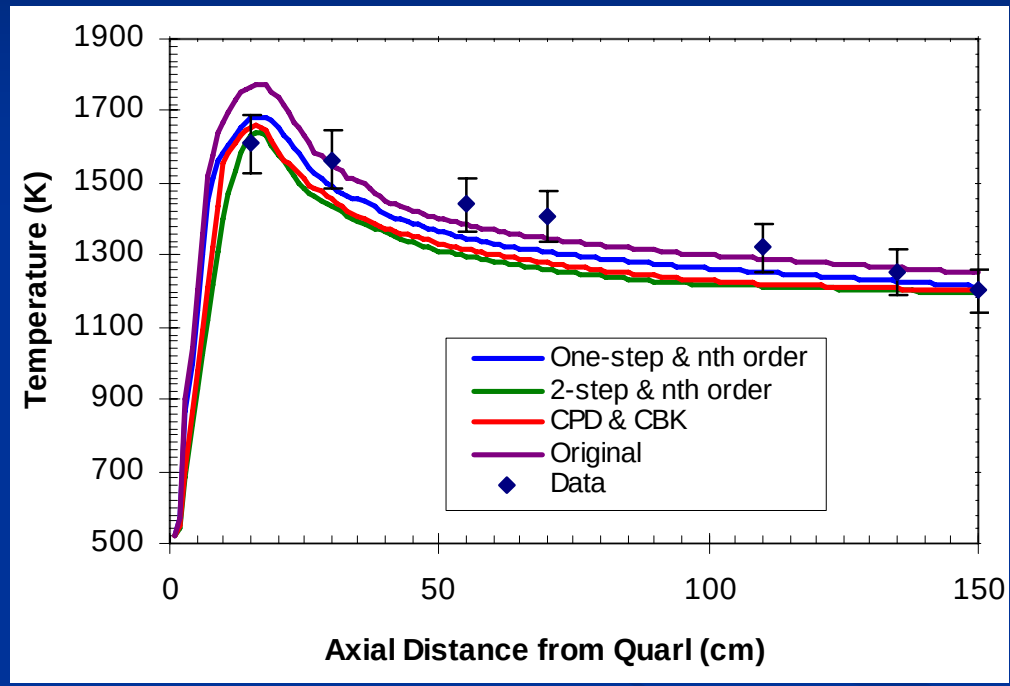
Predictions using the CPD and CBK Models

Velocity Predictions



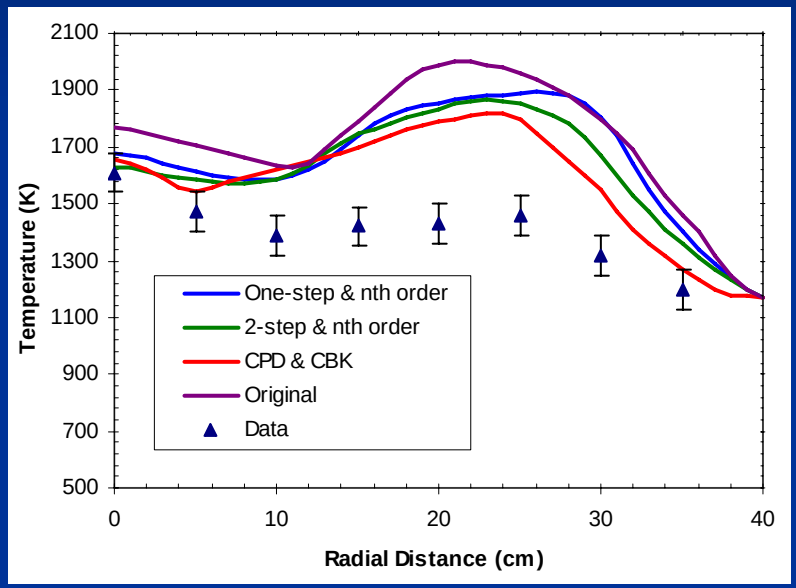
Temperature Predictions

- Centerline temperature increase rapidly between 0-25 cm.
- All predictions are within 5% of the measured data.
- It appears that all models predict a larger temperature decrease following the peak centerline temperature.

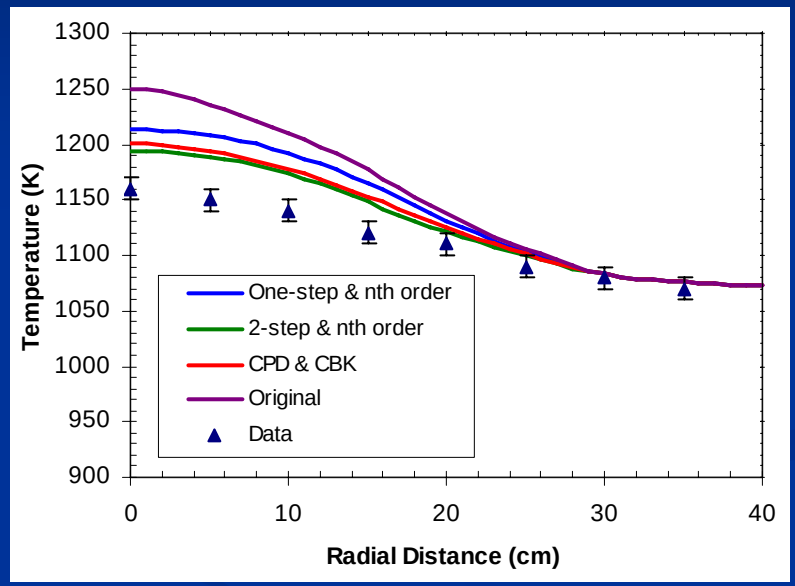


Centerline Temperature Predictions and Experimental Data

Temperature Predictions



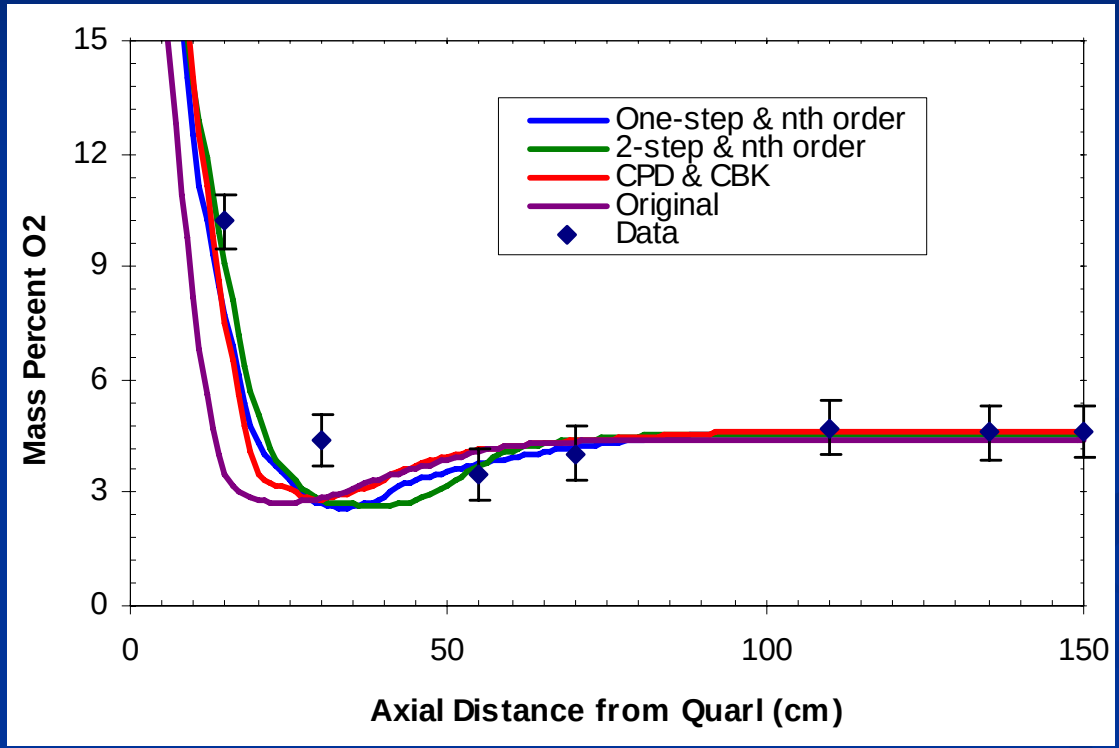
15 cm



150 cm

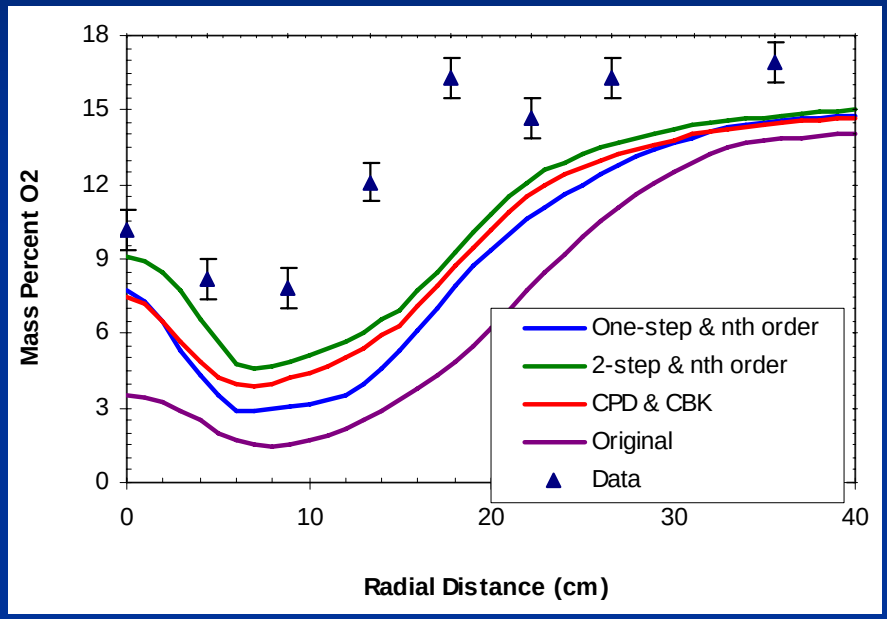
Radial Temperature Profiles at Two Axial Locations

O_2 Predictions

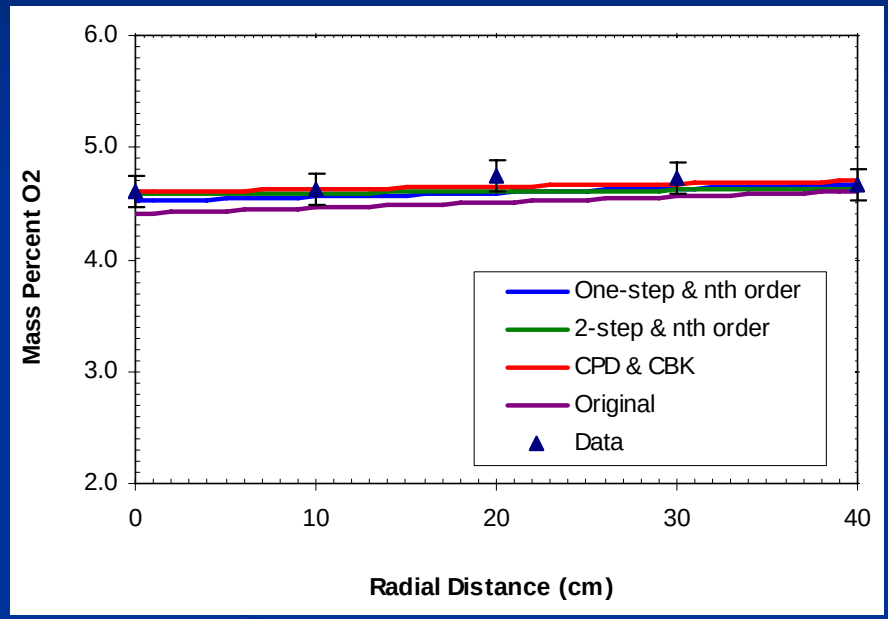


Predictions and Experimental Data of O_2 at the Centerline

O_2 Predictions



15 cm

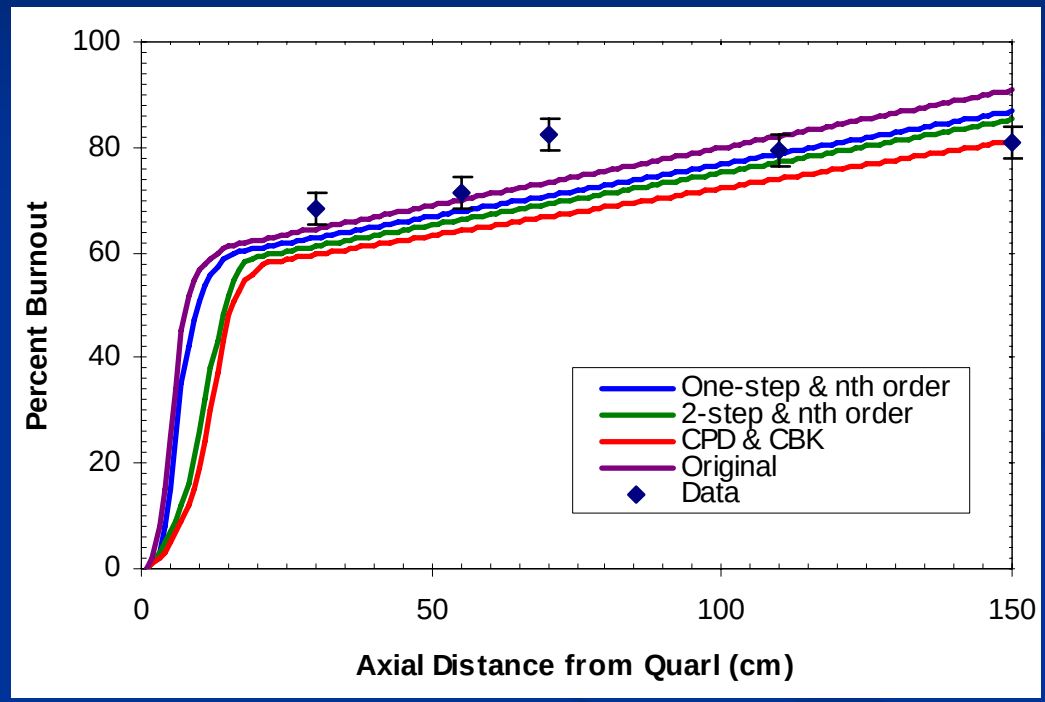


150 cm

Radial O_2 Profiles at Two Axial Locations

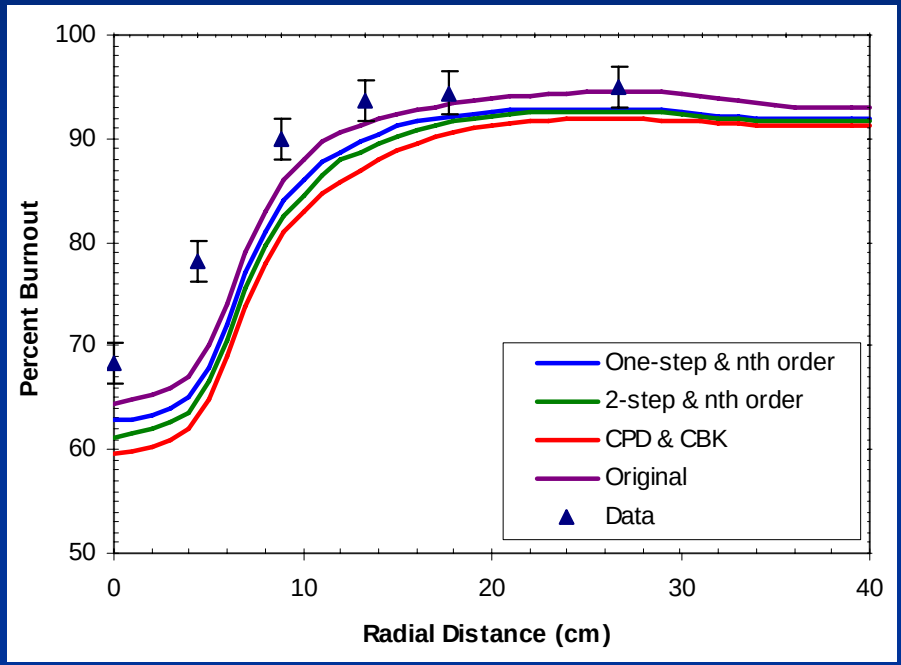
Burnout Predictions

- Burnout predictions show the three distinct coal reaction pathways: moisture vaporization (0-5 cm), devolatilization (5-20 cm), and char oxidation (20-end).
- Differences between predictions and data may be due to data sampling techniques.

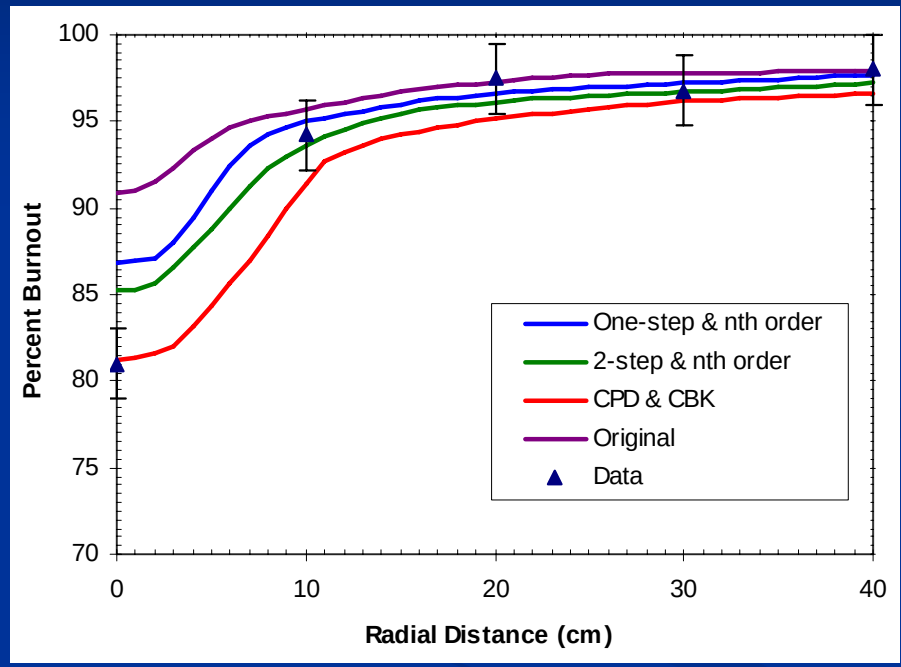


Predictions and Experimental Data of Burnout at the Centerline

Burnout Predictions



15 cm



150 cm

Radial Burnout Profiles at Two Axial Locations

Conclusions

- The modified individual coal submodels have proven accurate by verification of model predictions and experimental data.
- The overall coal combustion code has been validated by comparison between overall predictions and experimental data.
- The modified coal combustion submodels provide improvement over coal combustion submodels previously available in STAR-CD.

Acknowledgments

- STAR-CD and CD-adapco
- Thomas Fletcher – Advisor at BYU
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- All those who helped in the development of the PCGC-3 coal submodels

Questions