Dynamic Species Reduction for Multi-Cycle Computational Fluid Dynamics (CFD) Simulations (Co-Optima)

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Overview

- **Timeline:**
  - Start – April 17, 2017
  - Finish – June 30, 2020
  - 25% complete
- **Budget:**
  - Total project funding: $480k
    - DOE share: $432k
    - Contractor (UM) share: $48k
  - DOE funding FY2017: $34k
  - DOE funding FY2018: $138k
- **Barriers Addressed:**
  - Improved robust modeling tools to rapidly study cycle-to-cycle variability relevant for Dilute Gasoline Combustion.
  - Improved simulation capability to investigate Low Temperature Combustion strategies which rely on retained residuals.
  - Understand the impact of Ethanol and advanced Bio-Fuels and the coupling of fuel formulation to both Dilute SI and LTC combustion strategies
- **Project Partners:**
  - Argonne National Laboratory
  - Convergent Sciences

Project Objectives – Overall

- Goal: Develop tools to accelerate high fidelity simulations of Advanced Combustion Engines with detailed turbulence and kinetics.
  - Dynamic Species Reduction (DSR) to reduce gas exchange costs
  - Product Directed Remapping to reduce post combustion kinetics costs

- Impact: Enable multi-cycle 3-D CFD engine modeling needed to develop and validate fuel kinetic schemes in an engine relevant environment.
- Efficient multi-cycle simulations will help identify the impact of residuals on subsequent cycle ignition characteristics in a variety of Co-Optima engine configurations.
- Sensitivity analysis will identify the fuel chemical components of importance to combustion behavior.

Project Objectives and Relevance

- Project goals:
  - Improve computational efficiency
  - Enable multi-cycle fidelity
  - Provide insight into important feedback species and processes

- 2017 Goals:
  - Define baseline simulations
  - Implement Dynamic Species Reduction (DSR) in Converge

CYCLE STAGE	CURRENT SPECIES TREATMENT	PROPOSED SPECIES TREAMENT	ESTIMATED TIME SAVING
COMPRESSION	REACTANT DIRECTED REMAPPING		
COMBUSTION			
EXPANSION	NO REMAPPING	PRODUCT DIRECTED REMAPPING	50 %
GAS EXCHANGE	FROZEN	DYNAMIC SPECIES REDUCTION	90 %
ESTIMATED FULL CYCLE SAVING			80 %

Project Milestones – 1

Task #	Milestone Description (Go/No-Go Decision Criteria)	Anticipated Start and Completion Dates (Q)	Actual Start and Completion Dates (Q)	% Complete
1	**Model Development for Dynamic Species Reduction**			
1.1	Obtain engine and operating conditions for simulation, chemical mechanisms and surrogates to be used for project simulations.	1	1-2	100
1.2	Obtain CFR and ACI meshes from National Lab activities.	1	1-2	100
1.3	Complete baseline ACI and CFR multi-cycle simulations with chemistry active throughout cycle.	1-3	1-	10
1.4	Complete implementation of dynamic species reduction routines into CONVERGE.	1-2	1-	50
1.5	CFR and ACI conditions with cyclic coupling identified through dynamic species reduction model, complete additional validation simulations with baseline model.	3-4	3-	25
1.6	Dynamic species reduction criteria refined (as needed).	3-4		
1.7	Validate dynamic species reduction model.	4		
MI-1 (G/N)	Validated dynamic Species Reduction Model	4		
2	**Improved Multi-zone Binning for more efficient post combustion kinetics**			
2.1	Baseline simulations of heavy and moderately stratified charges.	5-6		
2.2	Analysis of Task 1.3 and 2.1 burned gas states. Develop improved burned gas binning.	5-6		
2.3	Implement improved burned gas binning into CONVERGE.	7		15
2.4	Multi-zone model validated with Task 1.3, 1.5 and 2.1 simulations.	7		
MI-2 (G/N)	Validation of Improved Multi-zone model	7		

Project Milestones – 2

Task #	Milestone Description (Go/No-Go Decision Criteria)	Anticipated Start and Completion Dates (Q)	Actual Start and Completion Dates (Q)	% Complete
3	**Coupled Validation of Task 1 and Task 2 Models**			
3.1	Initial validation of Task 1 and 2 models with multi-cycle CFD simulations having full composition and chemistry throughout the cycle completed.	8		
3.2	Any necessary changes identified in Task 3.1 implemented and final Task 1 and Task 2 model validation completed.	8		
MI-3 (G/N)	Validation of Task 1 and Task 2 Models	8		
4	**Understand Cyclic Coupling Effects Using New Models**			
4.1	Analyze species sensitivity to identify key residual species for CFR and ACR engines.	9-10		
4.2	For a given AKI, study to understand the influence of surrogates formulated with similar component reactivities completed.	10-11		
4.3	Study to understand the influence of significantly varying AKI completed.	11-12		
MI-4 (G/N)	Complete cycle-to-cycle studies	12		

Currently Q2:
Oct 1 – Dec 31

Project Technical Tasks

- Task 1: Model Development for Dynamic Species Reduction (**Year 1**)
  - Implement Dynamic Species Reduction (DSR) in Converge.
  - Validate against detailed multi-cycle simulations.

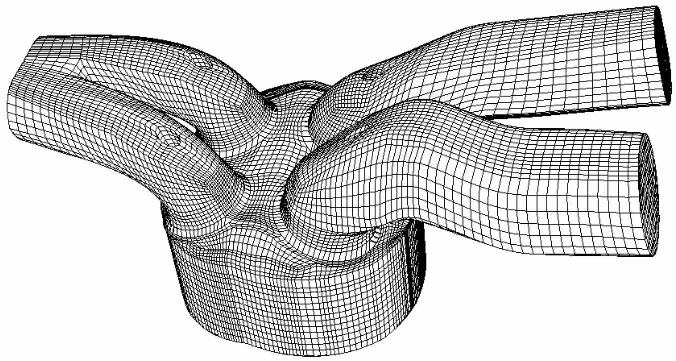
- Task 2: Improved Multi-zone Binning for More Efficient Post Combustion Chemical Kinetics (**Year 2**)
  - Implement Product Directed Remapping (PDR) in Converge.
  - Validate against detailed kinetics simulations.

- Task 3: Coupled Validation of Task 1 and Task 2 Models (**Year 2**)
  - Validate all new computational sub-models under Co-Optima relevant conditions.

- Task 4: Understand Cyclic Coupling Effects Using New Models Developed in Tasks 1 and 2 (**Year 3**)
  - Explore the impact of varying fuel blends on ignition behavior.
  - Carry out sensitivity analysis on fuel component reactivity on subsequent cycle ignition characteristics.

Technical Approach – Converge CFD

- All 3-D CFD modeling will be performed using Convergent Science's Converge CFD software package.
  - Industry standard consistent with other Co-Optima efforts.
  - Previously used at UM for other projects.
  - Support for custom User Subroutines available from vendor.

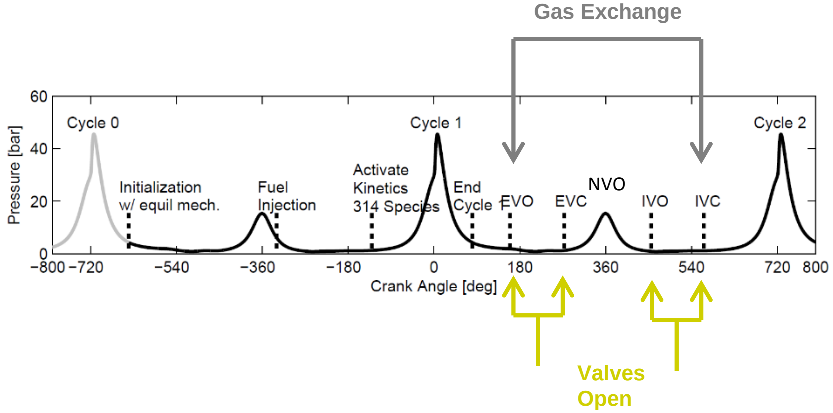


- Simulations will be conducted on UM's High Performance Computing cluster 'Flux'.
  - 27,000 cores on 1400 nodes.
  - Successfully used for several other UM/DOE projects.

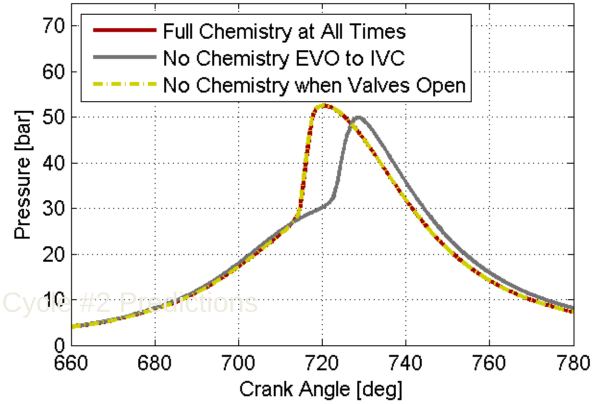
- Detailed simulations will be used as baselines to verify computational efficiency improvement of new models while maintaining fidelity.

Species Reduction – Exploratory Results (1)

- Exploratory RANS 3-D CFD simulations were previously conducted in KIVA for an HCCI engine configuration.
  - Modeled 2 sequential cycles including fuel injection and gas exchange.
  - 314 species gasoline surrogate mechanism.



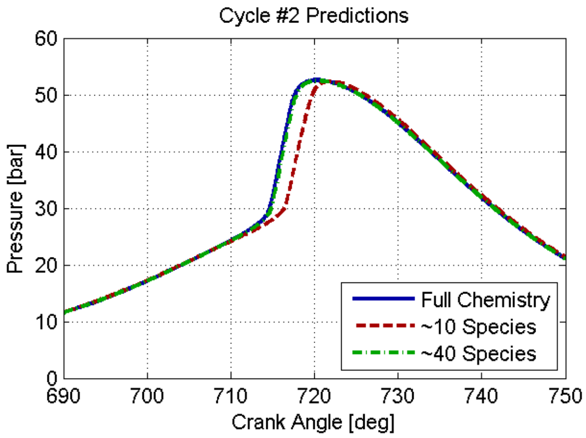
- Chemical kinetics calculations were deactivated during:
  - Gas exchange (EVO to IVC)
  - While valves open (EVO to EVC & IVO to IVC)



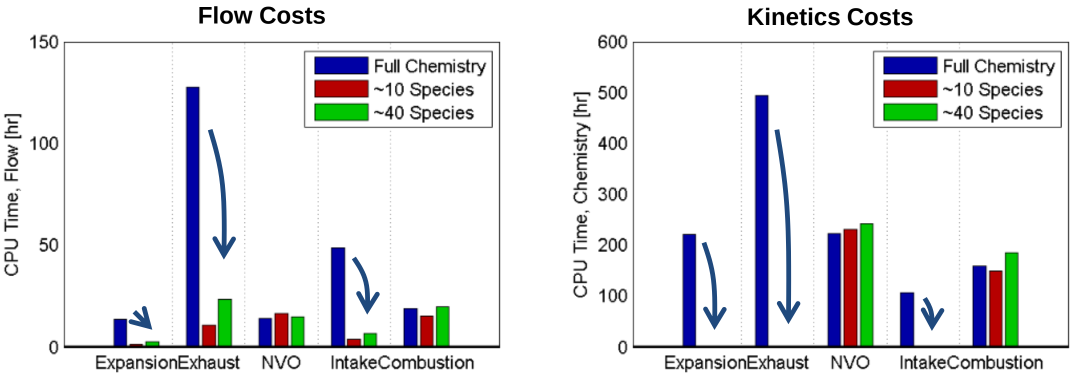
- Results showed no sensitivity to deactivating chemical kinetics when the valves were open.
- Chemical calculations during NVO had a significant impact on subsequent cycle behavior.

Species Reduction – Exploratory Results (2)

- Dynamic species reduction was applied to compare the computational cost and accuracy of several configurations:
  - Full Chemistry – 314 species mechanism with kinetics active at all times.
  - ~10 Species – reduced mechanism when valves are open, no reactions.
  - ~40 Species – less aggressive species reduction configuration.



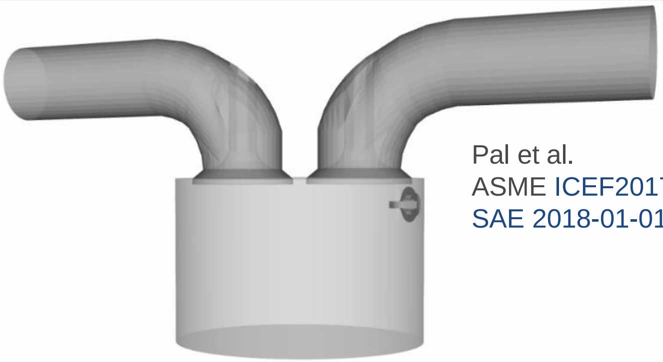
- Species reduction during exhaust and intake:
  - Dramatically reduced flow costs
  - Eliminated kinetics costs
  - Reproduced the detailed results using ~40 species



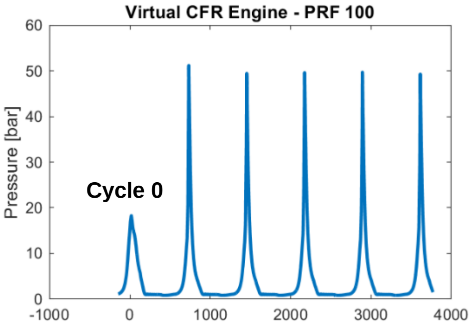
Technical Accomplishments

Task 1: CFR Engine Mesh and Baseline Operating Conditions

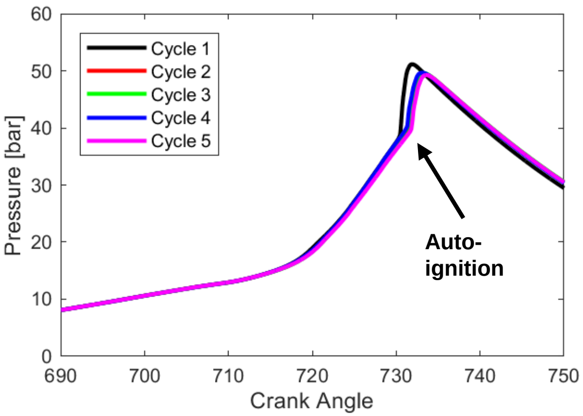
- CFR Engine Mesh and baseline simulation configuration + results obtained from Argonne National Lab
  - RON test (600 rpm, 52C inlet T)
  - PRF 100 (iso-Octane), 121 species mech
  - 7.8 compression ratio
  - 6 consecutive cycles (1 initialization)
  - With and without Converge's "skip species" model (next slide)



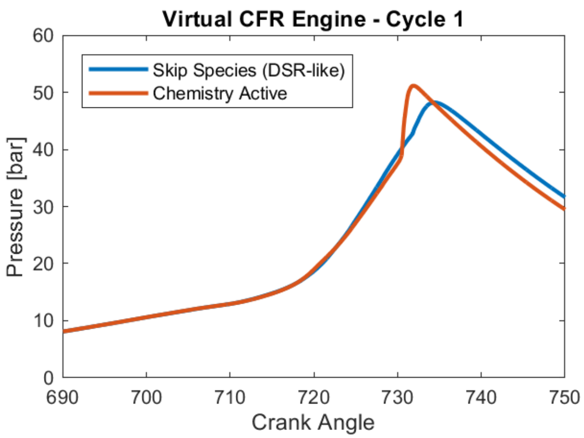
Pal et al.
ASME ICEF2017-3599
SAE 2018-01-0187

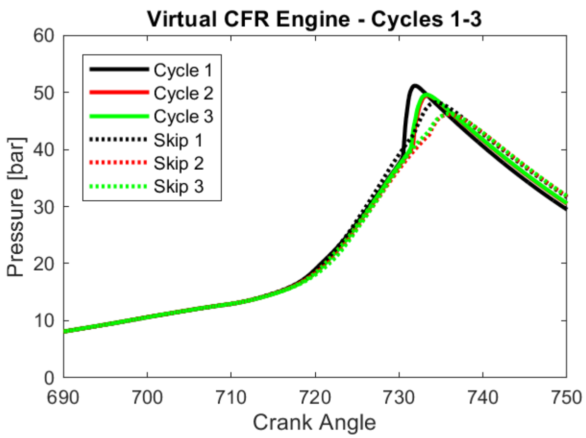


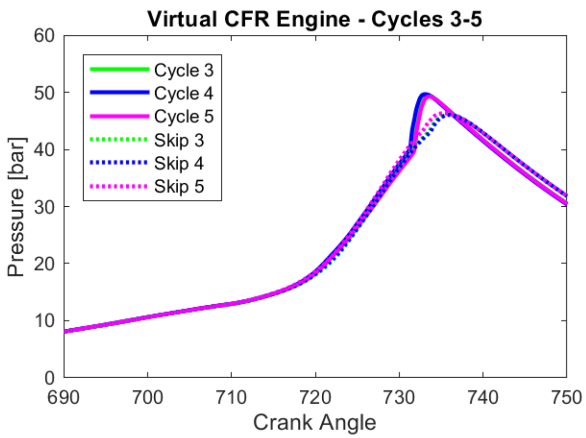
- Results:
  - All cycles show auto-ignition/knock
  - Cycle 1 is more advanced than others
  - Cycles 2-5 reach a steady state phasing



Task 1: CFR Baseline Simulations







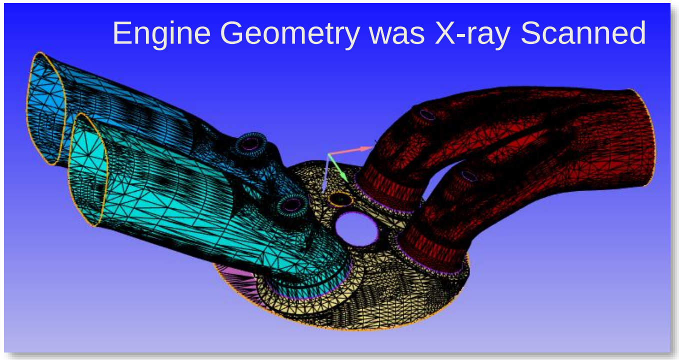
- Converge's "skip-species" option:
  - Removes species and disables kinetics calculations during gas exchange
  - Similar in principle to UM's Dynamic Species Reduction (DSR) method
- "Skip-species" changes combustion behavior:
  - Delayed peak pressure
  - Reduced reactivity and occurrence of knock

- Represents behavior UM model will improve on with DSR

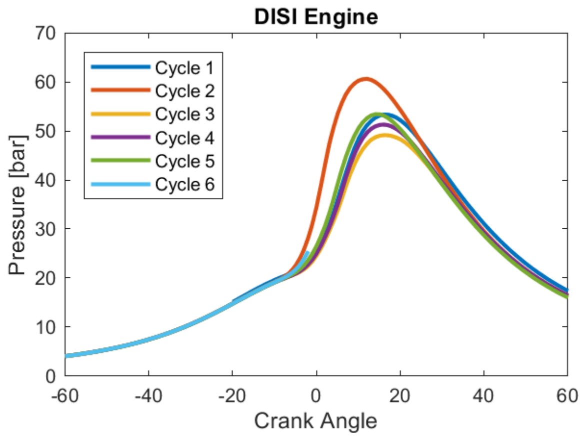
Task 1: Provisional ACI Engine Mesh and Gasoline SI Baseline Operating Conditions

- DISI Engine Mesh and model configuration obtained from Argonne National Lab:
  - ACI merit function and conditions still under review by Co-Optima team
  - Knock limited operation at 2000 rpm
  - 11.5 bar IMEP: 100 ft-lbs torque (136 Nm)
  - Spark timing: 14.23 deg bTDC

- Model predictions:
  - First cycle not the most advanced
  - Range of variability suggests some cyclic coupling to validate DSR



Engine	Ford 1.6 L, 4-valve pent-roof
Mesh Spacing	0.5 mm (min.)
Cell Count	~1.3 million (peak)
Chemical Mech.	ERC PRF (109 sp., 543 rxn.)
Fuel Properties (Phys./Chem.)	Alkylate/PRF97



Tasks 1.4 and 2.3 – Code Conversion

Existing Implementation: KIVA

Written in Fortran.
Complete access to all variables and subroutines.

Provisional DSR and PDR subroutines implemented.

Used external support code.

Current Effort →

New Implementation: CONVERGE

Written in C++
Modification restricted/limited to user defined subroutines and interfaces.

New DSR and PDR subroutines under development.
Not a direct 1:1 conversion.

- Converting existing code and algorithms from KIVA to Converge has been a slower process than anticipated.
- Partially due to the differences in the language and code structure.
- Partially due staffing turnover – looking to hire a graduate student to support this effort and further develop model algorithms.

Response to Previous Year Reviewer's Comments

N/A

This is the first year of this project.

It was not reviewed last year.

Collaborations and Coordination

- Argonne National Lab
  - Working with ANL to define baseline conditions to verify new DSR and PDR model speed improvements and accuracy.
  - Initial simulation configurations and predictions provided by Sibendu Som, Pinaki Pal (CFR engine), and Zongyu Yue (GDI engine).

- Convergent Sciences
  - Industry partner providing software licenses and technical support to integrate new models into Converge via User Functions.

Remaining Challenges and Barriers

- Successfully implement Dynamic Species Reduction in Converge
  - Differences in code structure and access may limit our ability to convert and develop our existing algorithms in the Converge framework
  - Improved models may not provide speedup similar to in KIVA

- Cover sufficient range of operating conditions to demonstrate benefits of new DSR and PDR models
  - Additional baseline simulations may need to be conducted
  - Co-Optima team still developing Merit Function and conditions for ACI
  - Speedup may depend on operating condition as well as model configuration (kinetic mechanism and mesh sizing) choices

Future Work for FY18-FY19

- Task 1 (FY18 , Milestone MI-1):
  - Complete implementation and validation of Dynamic Species Reduction in Converge
  - Conduct new simulations to assess DSR performance

- Task 2 (FY18-FY19 , Milestone MI-2):
  - Complete implementation of Product Directed Remapping in Converge
  - Identify variables needed to define reactivity space in a product heavy mixture
  - Validate PDR accuracy and speedup with new simulations

- Task 3 (FY19, Milestone MI-3):
  - Validate coupled DSR and PDR models in Converge using new simulations

- Task 4 (Start FY19, Milestone MI-4):
  - Use DSR model to investigate sensitivity of advanced combustion strategies and ignition behavior to fuel surrogate components and blends identified as relevant for the overall Co-Optima effort

Any proposed future work is subject to change based on funding levels

Summary

- Overall Project:
  - Targeting an 80% reduction in computational cost for a full engine cycle simulation using combination of new Dynamic Species Reduction and Product Directed Remapping models
  - Personnel turnover pushed the work start date back, currently re-staffing

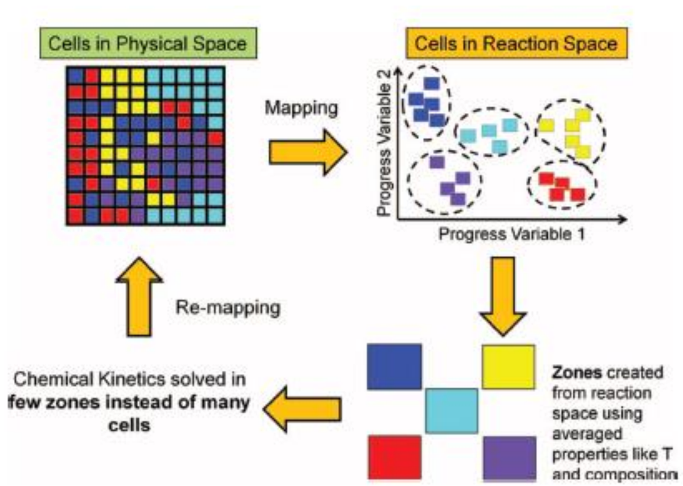
- Task 1:
  - Acquired engine meshes, baseline simulation configurations, and kinetics mechanisms from ANL for CFR and ACI engine operation
  - DSR model development is underway

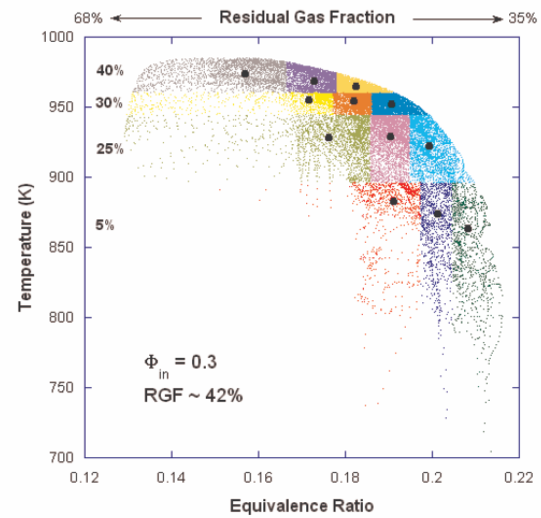
- Task 2:
  - Began implementation of PDR model ahead of schedule to coincide with implementation of DSR model in Task 1

Thank You

Divider for Technical Back Up Slides

Product Directed Remapping – Previous Multi-Zone HCCI Modeling Efforts





- Multiple CFD cells with similar properties are grouped together into ‘Chemistry’ cells
- Reduces the computational expense significantly
  - Typically use 100’s of chemistry cells for 10,000’s CFD cells
- Chemistry results are then mapped back to the original CFD cells

- Reactant directed remapping model configuration developed by Babajimopoulous, extended by Kodavasal at UM.