



# Using Multi-Zone Engine Modeling with Detailed Chemistry for Accurate Ignition and Emissions Predictions in HCCI Engines

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## Summary

This application note describes how the Multi-Zone Engine Model in CHEMKIN-PRO can be used to simulate HCCI combustion with accurate emissions and ignition predictions. The use of CFD data to set up the zones within the cylinder is also described.

## Benefits of Using Detailed Chemistry in Multi-Zone Engine Simulation of HCCI Combustion

Homogeneous Charge Compression Ignition (HCCI) combustion provides higher efficiency than a spark-ignition gasoline engine, due to operation at a higher compression ratio. This mode of engine combustion also has the potential to reduce particulate and  $\text{NO}_x$  emissions, by using a homogeneous charge and dilute conditions. One of the challenges in implementing HCCI combustion is the difficulty in controlling ignition timing. In HCCI combustion, the ignition timing is not dictated by the timing of the spark as in spark-ignition engines or by the injection of fuel as in diesel engines. Instead, HCCI ignition timing is controlled by compression-induced chemical kinetics. Accurate simulation of HCCI ignition therefore requires detailed kinetic models of the fuel combustion over the wide range of pressures and temperatures that may exist inside the cylinder volume. Further, chemical kinetics details are required to accurately predict emissions of trace species, such as  $\text{NO}_x$ , CO and unburned hydrocarbons (UHC). Reaction mechanisms that can handle both fuel-ignition and emissions phenomena typically include hundreds to thousands of species.

Various modeling approaches can be used for simulating HCCI combustion, and each has its advantages and disadvantages. Use of CFD simulation accounts well for flow and geometry effects, including turbulence and mixing. However, using chemical-kinetics mechanisms that have many more than 50 species in a CFD calculation typically translates to prohibitively long CPU times. Single-Zone Engine modeling with fully detailed chemistry has shown value in accurately predicting the onset of ignition. However, engine characteristics such as combustion duration and emissions are not well captured by a single-zone model. For HCCI engines, relatively large emissions of UHCs can be of particular concern, due to fuel quenching in crevices and at wall boundaries.

The Multi-Zone Engine model that is available in CHEMKIN-PRO addresses several of the deficiencies of a single-zone model, while still allowing inclusion of fully detailed chemical kinetics over reasonable CPU times, and providing accurate ignition and emissions predictions. In Multi-Zone Engine modeling,

the cylinder volume is split into a series of zones that are then treated as homogeneous regions where detailed chemistry can be applied efficiently. The Multi-Zone Engine Model handles stratification of temperature and composition, where different zones can have different starting temperatures and compositions. Also, the Multi-Zone Engine Model can be used in concert with CFD modeling, if appropriate, by incorporating information from a CFD cold-flow simulation prior to a point in the compression cycle where kinetics become important (typically, up to ~-30 CAD ATDC), and then creating zones based upon the stratification information from the CFD solution. The multi-zone model is able to use detailed chemistry with reasonable CPU times.

## Description of Multi-Zone Model Example

The Multi-Zone Engine Model example in this application note is based on a super-charged, natural-gas fired, reciprocating engine designed for power generation. Validation data for this application note has been extracted from the paper by Aceves et al. (2000)<sup>1</sup>. The engine geometry and operating conditions are as described in [Table 1](#).

The cylinder volume has been divided into several zones to account for regions with varying heat transfer to walls and varying fuel/air distribution. The Multi-Zone Engine Model assumes that all zones are at constant pressure and that there is no mass transfer between zones. The pressure work exerted by one zone on neighboring zones, due to reaction-induced expansion of the zone volume, is included in the governing equations. As shown in [Table 2](#), there are several zones allocated within the boundary layer and the crevice to account for the effect of cooler temperatures in these areas that may result in higher CO and UHC predictions.

Table 1. Engine Geometry and Operating Conditions

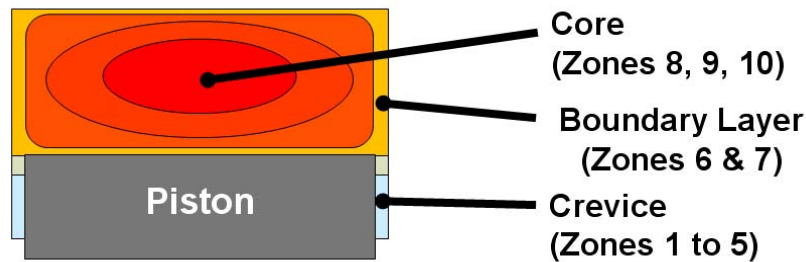
<b>Engine Parameter</b>	<b>Setting</b>
Displacement volume	1600 cm <sup>3</sup>
Bore	12.065 cm
Stroke	14 cm
Connecting rod length	26 cm
Engine speed	1000 rpm
Compression ratio	21

<sup>1</sup> Aceves, S. M., D. L. Flowers, et al. (2000). *A multi-zone model for prediction of HCCI combustion and emissions*. SAE Technical Paper 2000-01-0327.

Table 2. Zone Configuration

Zone#	1	2	3	4	5	6	7	8	9	10
Region	Crevice					Boundary Layer		Core		
Mass %	2	1	1	1	2	5	10	18	25	35
Wall Area %	7	2	2	2	3	6	9	16	22	31

Figure 1. Multi-Zone Engine Model Zone Definitions



## Setting Up a Multi-Zone Engine Model

The fuel/air mixture is divided into zones in order to capture the specific heat transfer, chemical reaction and mechanical work that are developed during the engine cycle. In this example, 10 zones are defined by [Table 2](#) and the engine geometry and operating conditions are provided in the CHEMKIN-PRO Input Panel in [Figure 2](#). Here the basic engine geometry, operating conditions and some key heat transfer parameters are entered for the simulation. A list of the parameters for each engine zone is given in [Figure 3](#).

Figure 2. Multi-Zone Engine Model Input Panel

**Reactor Physical Properties**

- End Time: [ ] sec
- Engine Crank Revolutions: Keyword: TIME
- Engine Crank Angle: Ending time for the transient simulation. [ ] degrees
- Engine Compression Ratio: 21.0
- Engine Cylinder Clearance Volume: [ ] cm3
- Engine Cylinder Displacement Volume: 1600.0 cm3
- Engine Connecting Rod to Crank Radius Ratio: 3.714
- Engine Speed: 1000.0 rpm
- Starting Crank Angle (ATDC): 310.0 degrees

**Temperature**: [ ] K, Constant

**Pressure**: 18.8 atm

**Energy Calculation**

- Energy Calculation Switch Time: [ ] sec
- Energy Calculation Switch Crank Angle: 357.0 degrees

**Heat Transfer Correlation**

- Adiabatic:
- Heat Transfer Correlation: 
  - Coefficient a: 0.035
  - Coefficient b: 0.8
  - Coefficient c: 0.0
  - Chamber Bore Diameter: 12.065 cm
  - Wall Temperature: 424.0 K

**Prandtl Number**: 0.71

**Woschni Correlation of Average Cylinder Gas Velocity**

- Coefficient C11: 2.28
- Coefficient C12: 0.0
- Coefficient C2: 0.324 cm/sec-K
- Ratio of Swirl Velocity to Mean Piston Speed: 0.0

**Reference Viscosity**: [ ] g/cm-sec

**Reference Temperature for Viscosity**: [ ] K

**Exponent for Viscosity**: [ ]

**Reference Thermal Conductivity**: [ ] erg/cm-K-sec

**Reference Temperature for Thermal Conductivity**: [ ] K

**Exponent for Thermal Conductivity**: [ ]

Use Initial Conditions as Reference

**Gas Reaction Rate Multiplier**: 1.0

Figure 3. Description of Multi-Zone Engine Zone Parameters

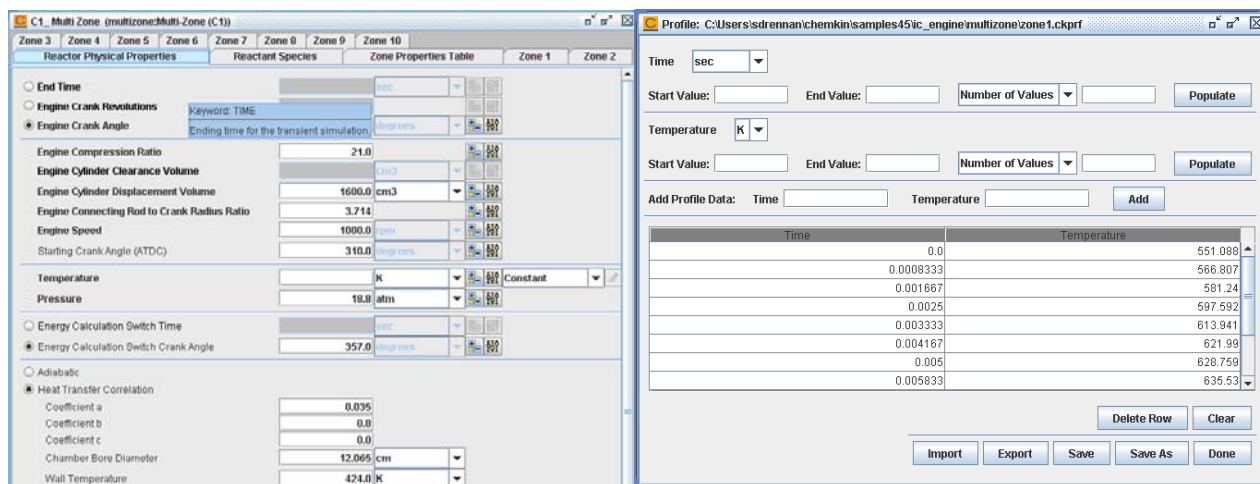
Zone Property	Units	Fill R...	Clear...	Zone 1	Zone 2	Zone 3	Zone 4	Zone 5	Zone 6	Zone 7	Zone 8	Zone 9	Zone 10
Temperature	K	Fill	Clear										
Zone Volume Fra...	none	Fill	Clear										
Zone Mass Fracti...	none	Fill	Clear	2.0	1.0	1.0	1.0	2.0	5.0	10.0	18.0	25.0	35.0
External Heat Tra...	none	Fill	Clear	0.05	0.05	0.05	0.1	0.1	0.15	0.15	0.15	0.1	0.1

## Using CFD Results to Initialize the Multi-Zone Engine Simulation

The setup of a Multi-Zone Engine Model requires understanding of the fluid dynamics and fuel/air mixing to help guide the assignment of zones. Computational Fluid Dynamics (CFD) can provide this non-reacting flow information up until the onset of ignition. Once the ignition process starts, more kinetics detail is needed than CFD can provide. However, using information from the “cold-flow” CFD simulation up to a pre-ignition point allows a more accurate estimate of initial conditions for the Multi-Zone Engine Model, giving a good starting point for using detailed chemistry to calculate ignition and combustion more effectively.

*Figure 4* demonstrates how CFD-generated data can be transferred from a CFD solution to the Multi-Zone Engine Model’s initial conditions. Here, a temperature profile vs. time from a CFD solution with no chemistry or with global chemistry is used directly by the Multi-Zone Engine Model, instead of solving the energy equation with full kinetics, for the beginning portion of the engine-compression stroke. At the specified Energy Equation Calculation Switch Time (Crank Angle), the Multi-Zone Engine Model takes control of the temperature calculation with fully coupled kinetics.

Figure 4. Using CFD Results to Initialize the Multi-Zone Engine Model



### Choosing to Use the Energy Equation

Alternatively, instead of using CFD results to set the stage for the ignition, you can turn on the energy equation from the beginning to solve for zone temperatures.

## Reviewing Results of Multi-Zone Engine Simulation

The different heat transfer areas and reaction volumes for each of the zones result in large variations of combustion effectiveness across the engine-cylinder volume. The CFD solution is used in this example to provide accurate delineation of the zone conditions prior to letting detailed fuel chemistry drive the ignition and combustion within the cylinder. *Figure 5* shows how the temperature of each zone is affected throughout the cycle. Here, the larger zones in the center of the cylinder volume clearly

ignited, while the zones in the boundary layer and the crevice region showed a lack of ignition. The zone-to-zone ignition is also shown with the sequencing of the ignition from zone 10 through zone 5. It is interesting to note that no ignition is seen in zones 1-4. This lack of local ignition contributes the bulk of the engine emissions of incomplete combustion products CO and UHC (Figure 6).

Figure 5. Temperature Profile From Multi-Zone Engine Simulation

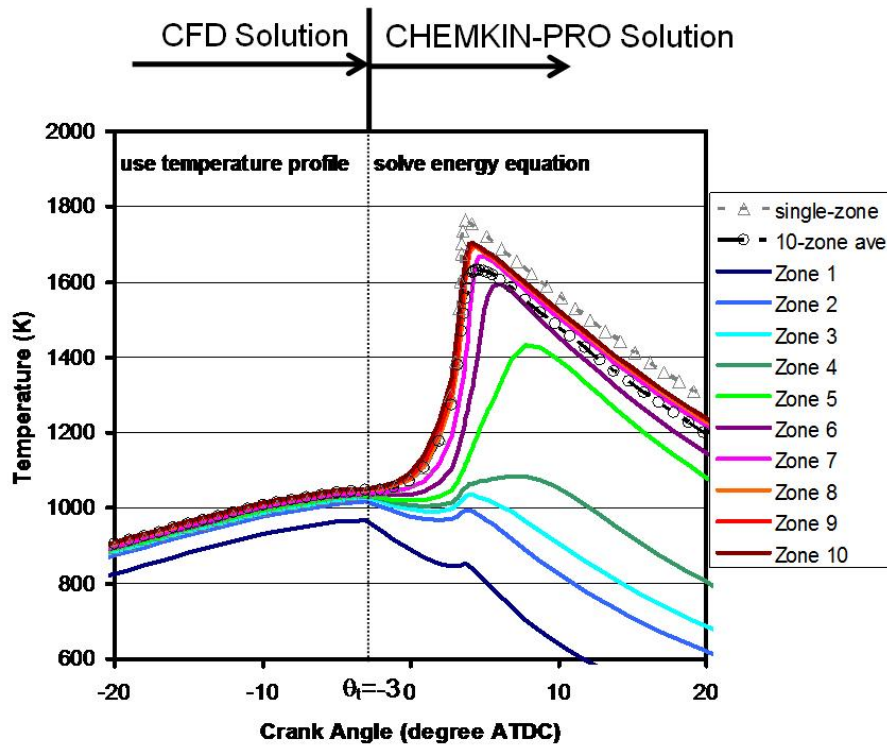
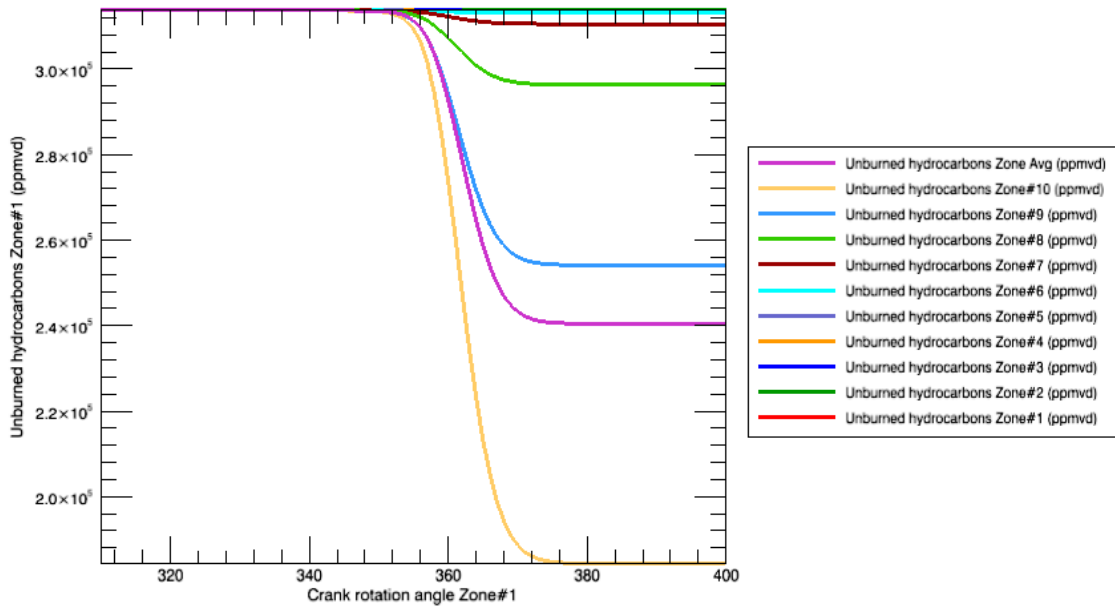
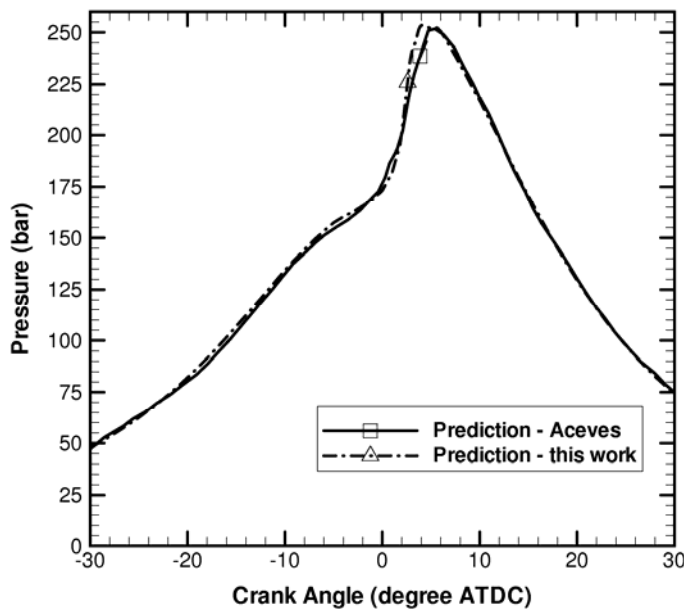


Figure 6. Unburned Hydrocarbons Profile From Multi-Zone Engine Simulation



The accurate simulation of ignition and heat release are driven by detailed chemical kinetics, and these factors impact the shape of the pressure trace for the cylinder. *Figure 7* shows how the CHEMKIN-PRO Multi-Zone Engine Model has been validated against a published set of modeling results from Aceves et al. for the case considered here (Aceves et al. 2000).

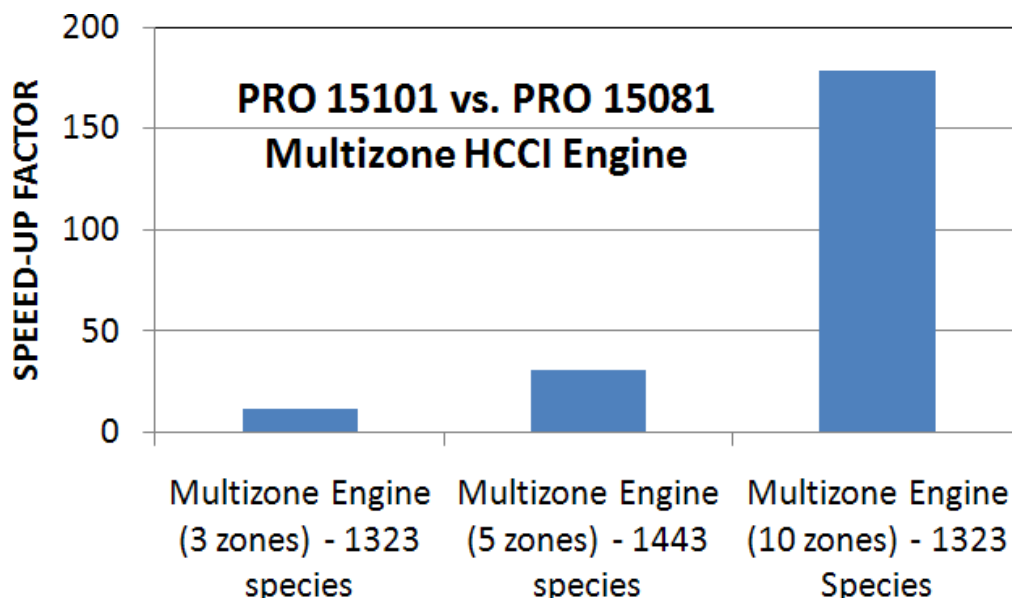
Figure 7. Comparison Between Experimental and Predicted Cylinder Pressure Profiles



In CHEMKIN-PRO version 15101, the performance of the multi-zone engine model has been dramatically improved compared to previous versions, as shown in Figure 8. These speed improvements provide capabilities for the use of more detailed fuel surrogates for HCCI engine modeling, which may not have been possible in previous versions.

In addition to the speed improvements, the multi-zone engine model can now be used in EGR calculations using recycle streams. In previous versions, only the single zone engine model could be used in EGR calculations. The addition of this capability for multi-zone engine cases will allow more accurate estimation of EGR compositions for HCCI engine simulations. A tutorial is provided with the CHEMKIN-PRO 15101 installation that demonstrates this new EGR capability.

Figure 8. Comparison of solution times for CHEMKIN-PRO 15101 vs. CHEMKIN-PRO 15082 for the multi-zone engine model.



## About Reaction Design

Reaction Design helps transportation manufacturers and energy companies rapidly achieve their Clean Technology goals by automating the analysis of chemical processes via simulation and modeling solutions. Reaction Design is the exclusive developer and distributor of CHEMKIN, the *de facto* standard for modeling gas-phase and surface chemistry, providing engineers ultra-fast access to reliable answers that save time and money in the development process. Reaction Design's ENERGICO product brings accurate chemistry simulation to combustion systems using automated reactor network analysis. Reaction Design also offers the CHEMKIN-CFD software module, which brings detailed kinetics modeling to other engineering applications, such as Computational Fluid Dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that

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