



Acceleration of Detailed Chemical Kinetics Using Multi-zone Modeling for CFD in Internal Combustion Engine Simulations

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ABSTRACT

Detailed chemical kinetics, although preferred due to increased accuracy, can significantly slow down CFD combustion simulations. Chemistry solutions are typically the most computationally costly step in engine simulations. The calculation time can be significantly accelerated using a multi-zone combustion model. The multi-zone model is integrated into the CONVERGE CFD code. At each time-step, the CFD cells are grouped into zones based on the cell temperature and equivalence ratio. The chemistry solver is invoked only on each zone. The zonal temperature and mass fractions are remapped onto the CFD cells, such that the temperature and composition non-uniformities are preserved. Two remapping techniques published in the literature are compared for their relative performance. The accuracy and speed-up of the multi-zone model is improved by using variable bin sizes at different temperature and equivalence ratios. In addition, a general n-dimensional zoning strategy is developed to include other cell variables such as pressure, mass fractions of different species, etc. to improve the performance of the zoning strategy. This paper discusses the savings in computational time achieved and the accuracy of the results using the multi-zone model for a range of scenarios. Gasoline and Diesel engine simulations are performed. Test cases are run for single fuel and multi-component fuels. Exhaust gas recirculation (EGR) scenarios are also tested.

INTRODUCTION

The incorporation of detailed chemical kinetics into Computational Fluid Dynamics (CFD) improves the accuracy of prediction of ignition time delay, heat release rate and emissions for engine combustion simulations [1-2] compared to empirical reaction models. However, the use of detailed chemical reaction mechanisms could significantly increase the computational time and could even prohibit its use. Typically, the computational time of the chemistry part is the most time consuming compared to the solution of the transport equations. As combustion science is advancing, researchers are coming up with bigger mechanisms to improve the accuracy of the predictions. As the size of the mechanism increases, the computational time spent in the chemistry part of the engine simulation code increases as the square or cube [3] of the number of species. In a typical engine simulation code, the chemistry calculations have to be done for each cell. Thus, even for a mechanism containing around 50-100 species, the simulation would take a week or more on a single machine depending on the mesh size.

Hence, there is a need to accelerate the chemistry part of the engine simulation code to make it feasible to run large mechanisms in a reasonable amount of time. Several numerical methodologies are available to enhance the speed of chemistry computations. A straight forward method is to use a reduced mechanism [3], consisting of a lesser number of species and reactions compared to the detailed chemical mechanism. The chemistry calculations can be enhanced using sparse matrix techniques [4]. For engine combustion simulations, the multi-zone modeling concept is used to

significantly reduce the computational time. This concept was introduced by Aceves et al. [5]. They used a sequential multi-zone approach for Homogenous Charged Compression Ignition (HCCI). In their approach, fluid mechanics is solved until the start of combustion. Then the entire domain is split into many zones based on the local temperature. Chemistry is then solved on each of the zones. Inter-zone mass transfer and heat transfer is completely neglected. The results show a good prediction of maximum pressure, burn duration and combustion efficiency. However, there are discrepancies in the prediction of HC and CO emissions.

This method was later extended by Flowers et al. [6] and Babajimopoulos et al. [7] to couple the zone-based chemistry solution and the cell-based transport solution via an interactive mapping technique. The cells are divided into a fixed number of zones based on the cell temperature and the cell equivalence ratio. The zoning is controlled to ensure that the mass of each zone does not exceed 1% of the total mass. Remapping of the zonal solution to the individual cells is based on an empirically defined “*ch*” value for each cell. This method has been successfully demonstrated for HCCI and PCCI (Premixed Charge Compression Ignition) problems [7-8]. Liang et al. [9] presented a dynamic multi-zone (DMZ) partitioning scheme, which dynamically determines the optimal number of zones using a rigorous data-clustering technique. In addition, they report a different remapping strategy for mapping the zonal solution on to the individual cells in the zone. This remapping technique has the specific advantage that the cell species density is assured to be nonnegative after remapping. However, the mass of some of the individual cells may change slightly within a zone.

This paper offers refinement to the zoning strategy adopted by Babajimopoulos et al. [7] for better performance of the multi-zone method over a wide range of engine simulation cases. A variable bin strategy is adopted to refine the size of the bins in the region of interest. A general n-dimensional binning strategy is also proposed and implemented to improve the robustness of the zoning. A general n-dimensional binning strategy is demonstrated to be especially important for multi-component fuel simulations. In addition, the paper compares the performance of the remapping strategies of Babajimopoulos et al. [7] and Liang et al. [9] over a range of real engine simulations.

MULTI-ZONE MODEL FORMULATION

MULTIZONE ALGORITHM

This paper presents the implementation of the multi-zone model coupled to the CONVERGE Computational fluid dynamics solver [10-11]. CONVERGE uses a modified cut-cell Cartesian technique and includes state-of-the-art numerical methods and sub-models for simulating the

complex physical and chemical processes that occur in engines. CONVERGE has an integrated chemistry solver, referred to as SAGE, which performs the detailed chemistry calculations on each grid cell. The species composition within a computational cell is treated uniform within the cell. Lucchini et al. [12] reported the relevance of a perfectly stirred reactor model and concluded that the turbulence chemistry interactions may be neglected for modeling purposes. The use of Adaptive Mesh Refinement (AMR) in the flame region obviates the necessity of using a sub-grid model within a cell, while accurately resolving the flame front and the species gradients [2,13]. In contrary to the detailed chemistry solver (SAGE), the multi-zone model solves chemistry only on a relatively small number of zones. The governing equations relevant to the multi-zone model are the continuity equation for each individual species and the internal energy equation

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \bar{u}) = \nabla \cdot \left(\rho D \nabla \left(\frac{\rho_k}{\rho} \right) \right) + \dot{\rho}_k^{chem} + \dot{\rho}_k^{spray} \delta_{kl} \quad (1)$$

where ρ_k is the mass density of the species k , ρ is the total mass density, \bar{u} is the fluid velocity vector, D is the diffusion coefficient, $\dot{\rho}_k^{chem}$ indicates the source term resulting from chemistry, $\dot{\rho}_k^{spray}$ indicates the source term resulting from spray evaporation. Species l is the species of which the spray droplets are composed and δ_{kl} is the Dirac delta function.

$$\begin{aligned} \frac{\partial \rho e}{\partial t} + \frac{\partial u_j \rho e}{\partial x_j} &= -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(K \frac{\partial T}{\partial x_j} \right) \\ &\quad + \frac{\partial}{\partial x_j} \left(\rho D \sum_k h_k \frac{\partial Y_k}{\partial x_j} \right) + S^{chem} + S^{other}, \end{aligned} \quad (2)$$

where ρ is the density, Y_k is the mass fraction of species k , D is the mass diffusion coefficient, S^{chem} is the chemistry source term due to heat release, P is the pressure, e is the specific internal energy, K is the conductivity, h_k is the species enthalpy, σ_{ij} is the stress tensor, and T is the temperature. S^{other} consists of other source terms like spray interaction and turbulent dissipation. The first term on the

$-P \frac{\partial u_j}{\partial x_j}$ RHS is the pressure work term, to account for compression and expansion, the second term is a viscous dissipation term, $\sigma_{ij} \partial u_i / \partial x_j$, which account for kinetic energy viscously dissipating into heat, the third and the fourth terms

represents energy transport due to conduction and species diffusion respectively.

Figure 1 shows the schematic of the multi-zone solver. At each discrete time t , every cell in CONVERGE is at some thermodynamic state. Based on the thermodynamic state of the cells, the cells are grouped in zones. The procedure for grouping into procedure for grouping into zones is described in the next section. In a two-dimensional zoning strategy, the zoning is done based on two variables, the temperature and the equivalence ratio of the cells. For each zone, the average temperature, pressure and the composition are determined to specify the thermodynamic state of the mixture in that zone. The SAGE chemistry solver is invoked on each zone.

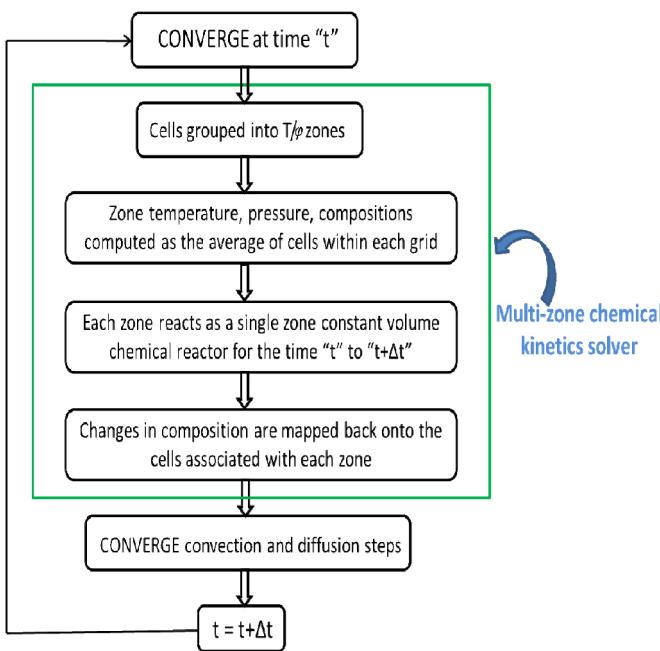


Figure 1. Schematic of the two-dimensional multi-zone algorithm in CONVERGE

The chemical kinetic equations for a closed-volume homogeneous reactor of each zone can be written as

$$\frac{\partial Y_k}{\partial t} \Big|_{\text{zone}} = \frac{\dot{\omega}_k W_k}{\rho} \Big|_{\text{zone}} \quad (k=1,\dots,K) \quad (3)$$

$$\frac{\partial T}{\partial t} \Big|_{\text{zone}} = -\frac{1}{\rho \bar{c}_v} \sum_{k=1}^K \dot{\omega}_k W_k e_k \Big|_{\text{zone}} \quad (4)$$

where $\dot{\omega}_k$ is the production/consumption rate of species k , W_k and e_k are the molecular weight and the specific internal energy of the species k and \bar{c}_v is the constant volume specific

heat of the gas mixture. All of these quantities are zone-based values. Each zone is allowed to react from time t to $t + \Delta t$. Once the new zone composition is obtained, the zonal compositions are mapped back on to the individual cells in the zone. The remapping strategy is critical to ensure the quality of the multi-zone solution. Mapping strategies will be discussed in the following sections. After the species are mapped onto the individual cells, the source terms in Eqs. (1) and (2) are calculated as

$$\dot{\rho}_k = \frac{\Delta Y_k}{\Delta t} \quad (k=1,\dots,K) \quad (5)$$

$$S^{\text{chem}} = -\sum_{k=1}^K \frac{\Delta Y_k}{\Delta t} \frac{(\Delta h_f^0)}{W_k} \quad (6)$$

where Δ represents the change in quantity before and after the multi-zone chemistry integration. The steps shown in Fig. 1 are repeated at every time step.

ZONING STRATEGY

The zoning strategy is that used by Babajimopolous et al. [7]. However, there are some key differences in the zoning strategy used in this paper. The number of zones is not pre-decided. The number of zones dynamically varies with the stratification of the flow field parameters. For a two-dimensional zoning strategy, the zoning is based on temperature and the equivalence ratio of the cells. There are two possible definitions of equivalence ratio. The “global” equivalence ratio ϕ is given as

$$\phi = \frac{2C^\# + \frac{H^\#}{2}}{O^\#} \quad (7)$$

where $C^\#$, $H^\#$ and $O^\#$ are the total number of carbon, hydrogen and oxygen atoms present in the mixture. On the other hand, the “progress” equivalence ratio φ is given as

$$\varphi = \frac{2C_{-\text{CO}_2}^\# + \frac{H_{-\text{H}_2\text{O}}^\#}{2}}{O_{-\text{CO}_2-\text{H}_2\text{O}}^\#} \quad (8)$$

where $C_{-\text{CO}_2}^\#$, $H_{-\text{H}_2\text{O}}^\#$ and $H_{-\text{H}_2\text{O}}^\#$ are the number of carbon atoms (without CO_2), the number of hydrogen atoms (without H_2O) and the number of oxygen atoms (without CO_2 and H_2O). Babajimopolous et al. [7] indicate that the progress equivalence ratio is a better choice for identifying cells with

similar composition. Hence, temperature and the progress equivalence ratio of the cell are used for classifying cells into zones.

Two different input options can be specified.

(a). The first option is a fixed bin size input for the temperature and the equivalence ratio. For example, a fixed temperature bin size of 10 K and a fixed equivalence ratio bin size of 0.1. Then the cells are placed into the appropriate bins (or zones) as shown in Figure 2. The total number of zones will depend on the range of temperature variation and the range of equivalence ratio variation in the whole flow field. In this zoning strategy, the mass of each zone will be distributed non-uniformly. The accuracy of the multi-zone algorithm depends on the user supplied bin sizes. The smaller the bin sizes, the greater the accuracy compared to the detailed chemistry calculations on each cell.

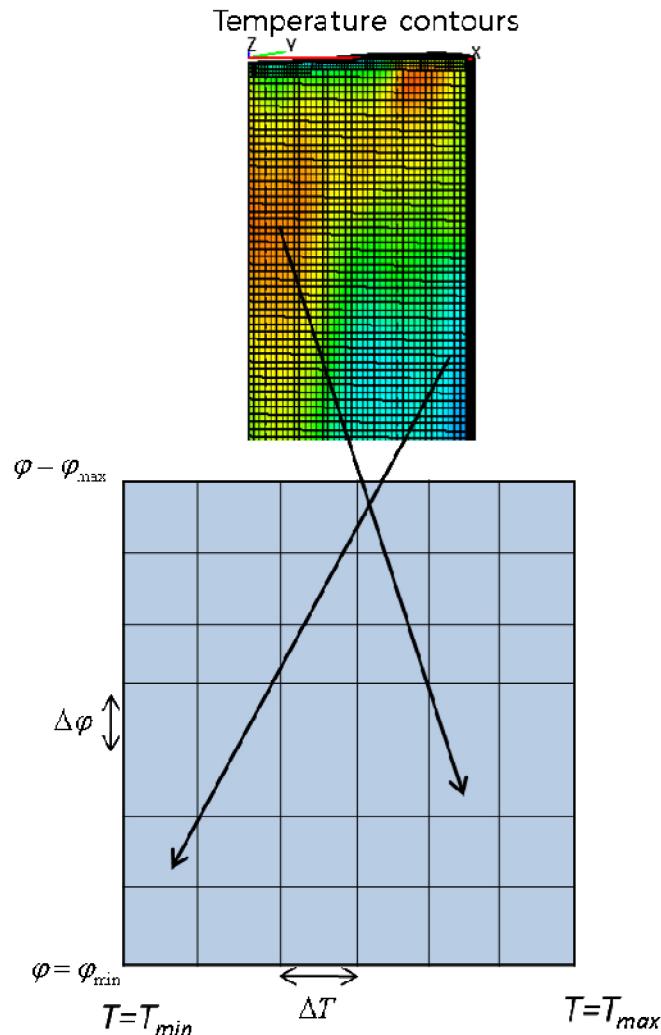


Figure 2. Zoning strategy

(b). The second option a variable bin sizes input, where the bin size can vary as a function of the value of the variable. Table 1 shows an example of a variable bin input for the temperature variable. The table shows the bin size for all of the cells in the range of 0-1000 K is 10 K, 1000-2000 K is 5 K, 2000-3000 K is 20 K and > 3000 K is 50 K. The idea of using a variable bin size to use to refine the zones in the temperature range where combustion is very prominent and use coarser bins where combustion is not very prominent. This option would save computational time as compared to using a fine bin size throughout the range.

Table 1. Variable bin size input for temperature

Temperature (K)	Bin size (K)
0 – 1000	10
1000 – 2000	5
2000 – 3000	20
>3000	50

In addition to the two-dimensional strategy for zoning, a general n-dimensional zoning strategy is developed in this paper, in which the zoning can be done using more than two variables. A subset of different available variables can be chosen by the user to group the cells into zones. The different available variables are (a) temperature, (b) equivalence ratio, (c) pressure, (d) region identity (e.g. cylinder, exhaust port etc.) of the geometry (e) mass fractions of the individual species. It will be shown later that the temperature and equivalence ratio of the cells alone cannot properly classify similarly reacting cells into different zones. The use of other variables will be helpful in improving the accuracy of the multi-zone model.

MAPPING STRATEGY

Two different multi-zone mapping strategies have been reported in the literature. The first mapping technique is reported by Babajimopoulos et al. [7]. This mapping is referred to as **Map-I** in this paper. This mapping is based on the “ch” value of the individual cells in the zone. The “ch” value of an individual cell is defined as

$$ch_{cell} = 2C_{-CO_2}^{\#} + \frac{H_{-H_2O}^{\#}}{2} \quad (9)$$

The “ch” value is calculated for all of the individual cells and the zones before the start of chemistry calculations on the zones. The sum of all the “ch” values of the individual cells (ch_{cell}) in a particular zone will be equal to the zone’s “ch” value (ch_{zone}).

$$m_{k,cell} = \frac{ch_{cell}}{ch_{zone}} m_{k,zone} \quad (10)$$

Equation 10 is used for calculation of all the individual species except CO_2 , H_2O , O_2 and N_2 . An attempt is made to conserve the carbon atoms, hydrogen atoms, oxygen atoms in each cell by readjusting the mass of CO_2 , H_2O , and O_2 as given below

$$\sum_k \frac{m_{k,cell}}{W_k} c_k + \frac{m_{\text{CO}_2,cell}}{W_{\text{CO}_2}} = C_{cell}^{\#} \quad (11)$$

$$\sum_k \frac{m_{k,cell}}{W_k} h_k + 2 \frac{m_{\text{H}_2\text{O},cell}}{W_{\text{H}_2\text{O}}} = H_{cell}^{\#} \quad (12)$$

$$\sum_k \frac{m_{k,cell}}{W_k} o_k + 2 \frac{m_{\text{O}_2,cell}}{W_{\text{O}_2}} = O_{cell}^{\#} \quad (13)$$

where $m_{k,cell}$ is the mass of species k in a cell, c_k , h_k and o_k are the number of carbon atoms, hydrogen atoms and oxygen atoms in species k , $C_{cell}^{\#}$, $H_{cell}^{\#}$ and $O_{cell}^{\#}$ are the number of moles of carbon atoms, hydrogen atoms and oxygen atoms in a given cell.

Equations 11, 12, 13 ensure atomic balance in each cell. The total mass in an individual cell is conserved by readjusting the mass of the remaining N_2 . Addition details about this mapping strategy could be found in Ref. [7-8].

The second mapping technique was proposed by Liang et al. [9], referred to as **Map-II** in this paper. In this mapping, the density of species k in cell i is given as

$$\rho_{k,i}^{t+dt} = \rho_{k,i}^t + \Delta m_{k,zone} \frac{\rho_i^t}{\sum_{l=1}^K (\rho_l^t V_l)} \quad \text{if } \Delta m_{k,zone} \geq 0 \quad (14)$$

$$\rho_{k,i}^{t+dt} = \rho_{k,i}^t + \Delta m_{k,zone} \frac{\rho_{k,i}^t}{\sum_{l=1}^K (\rho_{k,l}^t V_l)} \quad \text{if } \Delta m_{k,zone} < 0 \quad (15)$$

Where $\Delta m_{k,zone}$ is the change of mass of species k in a zone and V_l is the volume of cell l . No attempt is made to conserve the mass of each element in the cell as was done for the Map-

I strategy. This mapping guarantees positive concentrations of all the species being mapped. However, it is to be noted that the individual cell mass is not conserved after mapping although the total mass in the zone is conserved. Addition details about this mapping strategy could be found in Ref. [9].

RESULTS AND DISCUSSION

The purpose of this paper is two-fold. The first is to compare the performance of the two mapping strategies available in the literature under different scenarios. The second purpose is to reveal the importance of using a generalized n-dimensional binning strategy for improving the accuracy of multi-zone simulations especially for multi-fuel combustion calculations.

Test Case 1

The first test case is a Caterpillar Single-Cylinder Oil Test Engine (SCOTE) operating in a Compression Ignition (CI) mode. The engine specifications and modeled operating conditions are shown in Table 2. A 60-degree sector mesh is used in the simulations. Diesel spray is injected at -9 ATDC (After Top Dead Center) for duration of 12 crank degrees. N-heptane is used as a surrogate for Diesel fuel. The Chalmer's mechanism [14] consisting of 42 species and 168 reactions is used to simulate diesel combustion. CONVERGE is used to solve the CFD and the kinetic equations. Chemistry is solved in a cell only if the temperature of the cell is above 600 K. For this test case, three cases are run using (a) SAGE chemistry solver, where chemistry is solved on each grid cell, (b) Multi-zone solver with the Map-I mapping strategy, and (c) Multi-zone solver with the Map-II mapping strategy. A bin size of 10 K is used for temperature and a bin size of 0.1 is used for the equivalence ratio. Figures 3 and 4 show the comparison of the performance of SAGE and the multi-zone solver with the two mapping strategies. Figure 3 shows the average pressure, average temperature and maximum temperature profiles in the cylinder. Results show that the multi-zone simulations match quite close to the SAGE simulations. Note that the distribution of the fuel is highly stratified in this case and yet there is a good match between SAGE and multi-zone. The performance of the Map-I strategy is slightly better than the Map-II strategy. Figure 4 shows the comparison of the heat release rate and the species mass. The heat release rate of the multi-zone simulations is lower compared to that of the SAGE simulations at the start of ignition. The multi-zone simulations exhibit slightly earlier ignition but a lower peak in heat release rate compared to SAGE. All of the species mass are well predicted by the multi-zone simulations Figure 4 shows some deviation in the CO prediction on a log scale plot at the end of the simulation. However, it is misleading since the species mass is negligibly small. Figure 5 shows the comparison of the CO species mass on a normal plot, instead of a log scale plot. Figure 5 clearly shows that the CO species mass is quite accurately predicted by the Map-I strategy as compared to SAGE. Overall, the

prediction of species mass for the Map-I strategy is better than the Map-II strategy.

Table 2. Engine specifications and operating conditions

Bore x stroke (mm)	137.2 x 165.1
Compression ratio	16:1
Engine speed (rev/min)	1600
Start of injection ($^{\circ}$ ATDC)	-9
Temperature at IVC (K)	355
Pressure at IVC (bar)	2
EGR (% by mass)	0%, 20%

The better prediction of Map-I strategy compared to the Map-II strategy is attributed to the fact that in Map-I strategy, special care is taken to ensure atomic mass balance in each cell. In addition, cell mass is conserved in Map-I strategy. In the case of Map-II strategy, although the total mass is conserved over the entire zone, the mass of each individual cell is not conserved. This will lead to artificial diffusion of mass amongst cells in the same zone. Figure 6, 7, 8 show the comparison of temperature, CO mass fraction and CO₂ mass fraction contours along a section at -5, 0 and 15 $^{\circ}$ ATDC. Figure 9 shows the comparison of CPU times in minutes for the combustion part of the simulation. Combustion solver is activated from -10 $^{\circ}$ ATDC to 135 $^{\circ}$ ATDC. The cell count in this time interval lies in the range of 40,000 to 190,000 cells. All the cases are run in parallel on 16 processors. Multi-zone with Map-I strategy gives a speed-up of 8.7 times compared to SAGE and multi-zone with Map-II strategy gives a speed-up of 9.5 times compared to SAGE. There is a slight difference in the CPU times of both the mapping strategies resulting from the different thermodynamic evolution during the simulations. Figure 10 shows the comparison of the multi-zone Map-I results with SAGE for different choices of bin sizes. Figure 7 shows the mean pressure inside the cylinder. The error in the prediction of multi-zone with temperature bin size 30 K and equivalence ratio bin size 0.3 is high. The error in the prediction of multi-zone with temperature bin size 2 K and equivalence ratio bin size of 0.02 is small. As the bin sizes become smaller, the multi-zone prediction becomes closer to the SAGE prediction.

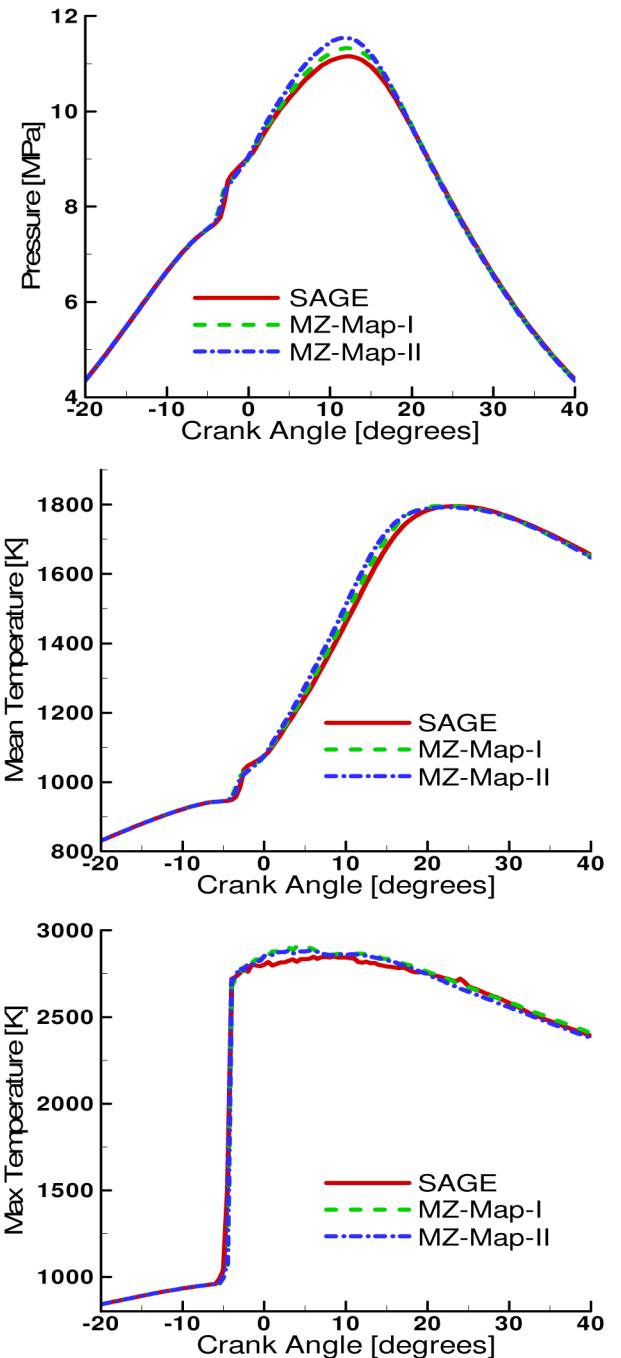


Figure 3. Comparison of multi-zone solution with the detailed solution for test case 1

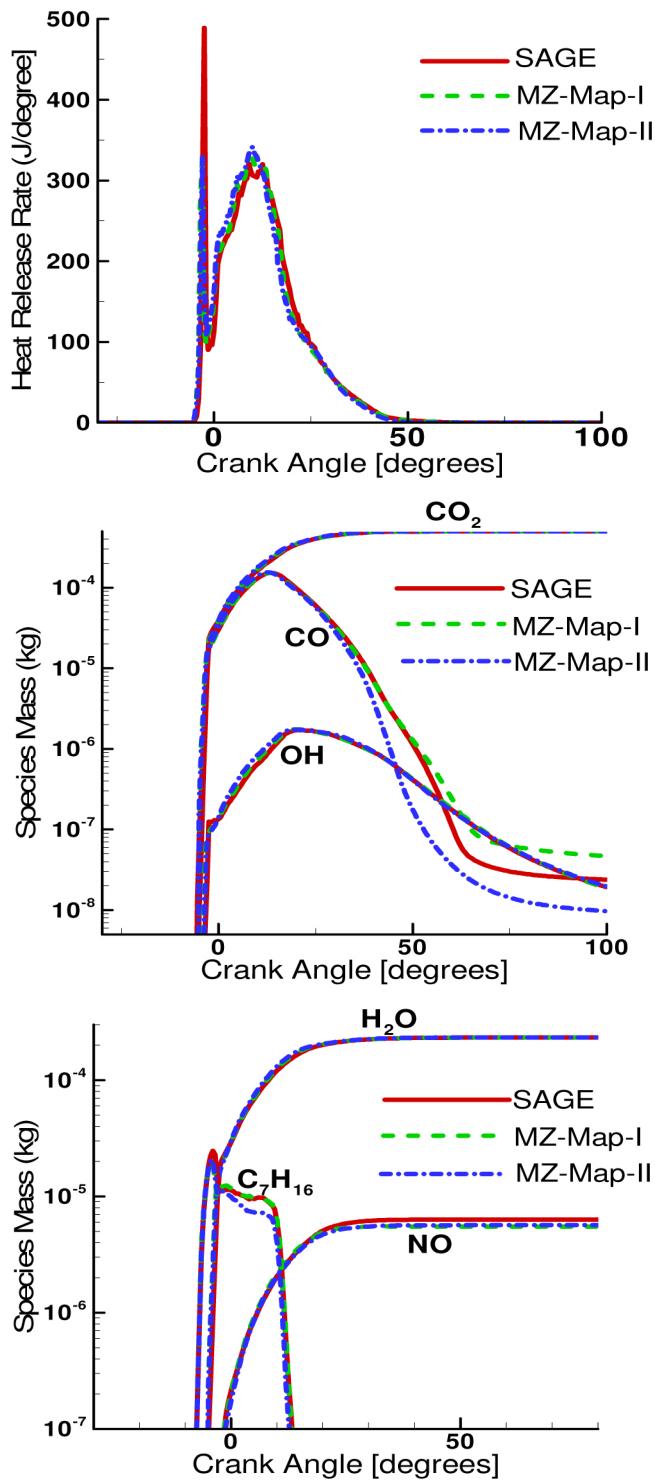


Figure 4. Comparison of heat release rate and species mass for test case 1

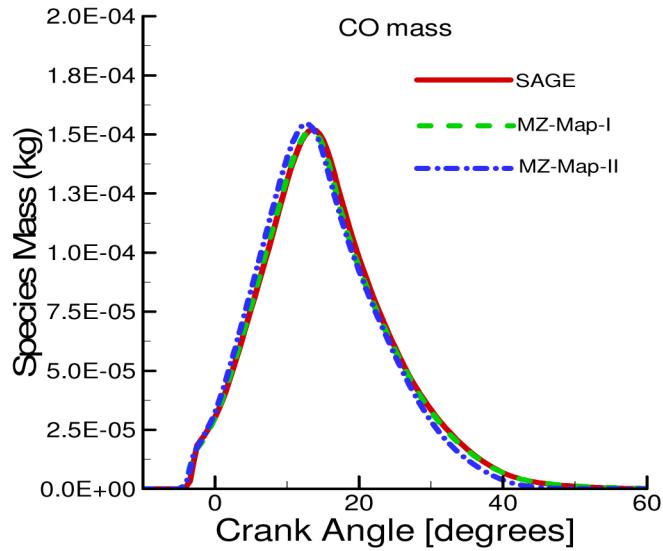


Figure 5. Comparison of CO species mass for test case 1

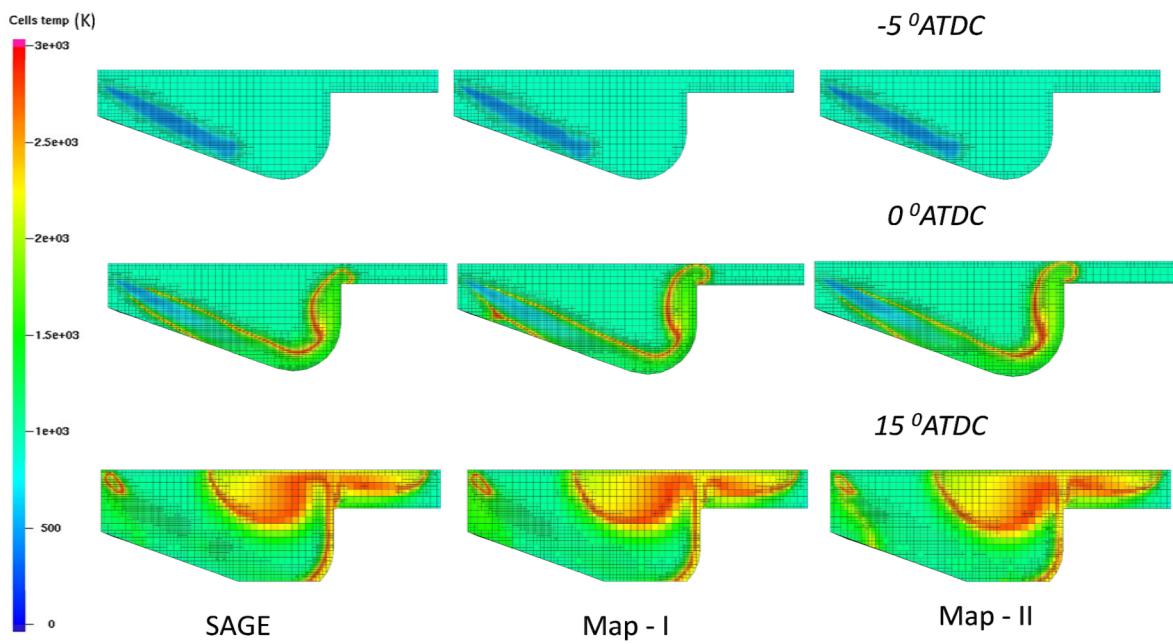


Figure 6. Comparison of temperature contours along a section for test case 1

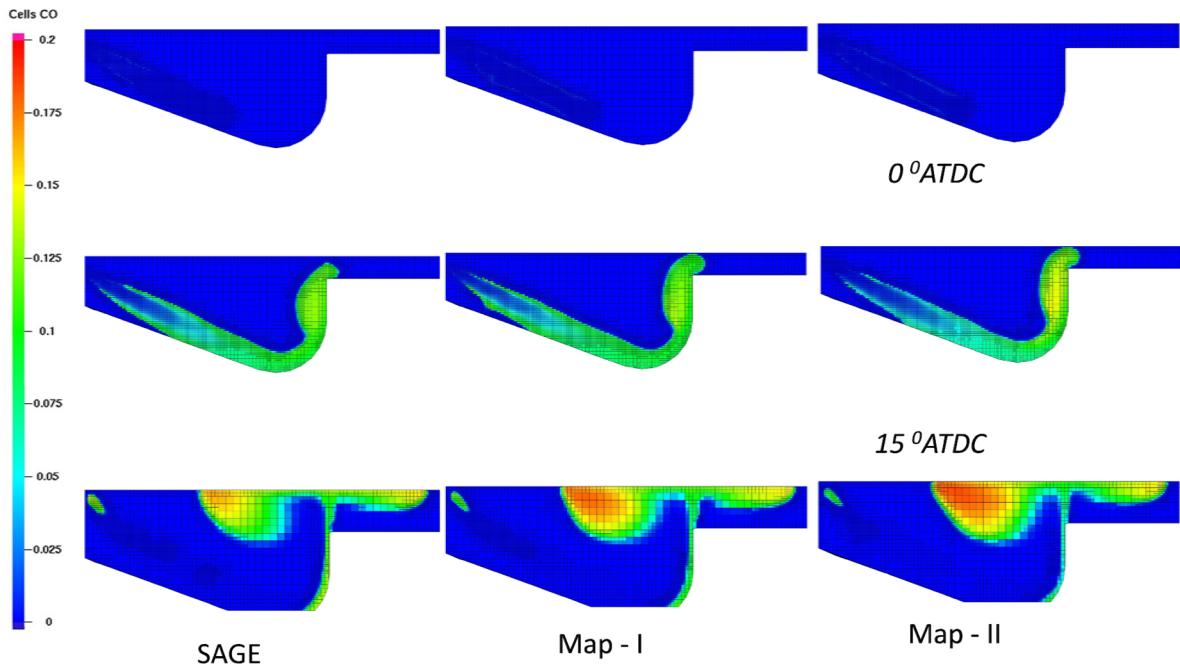


Figure 7. Comparison of CO mass fraction contours along a section for test case 1

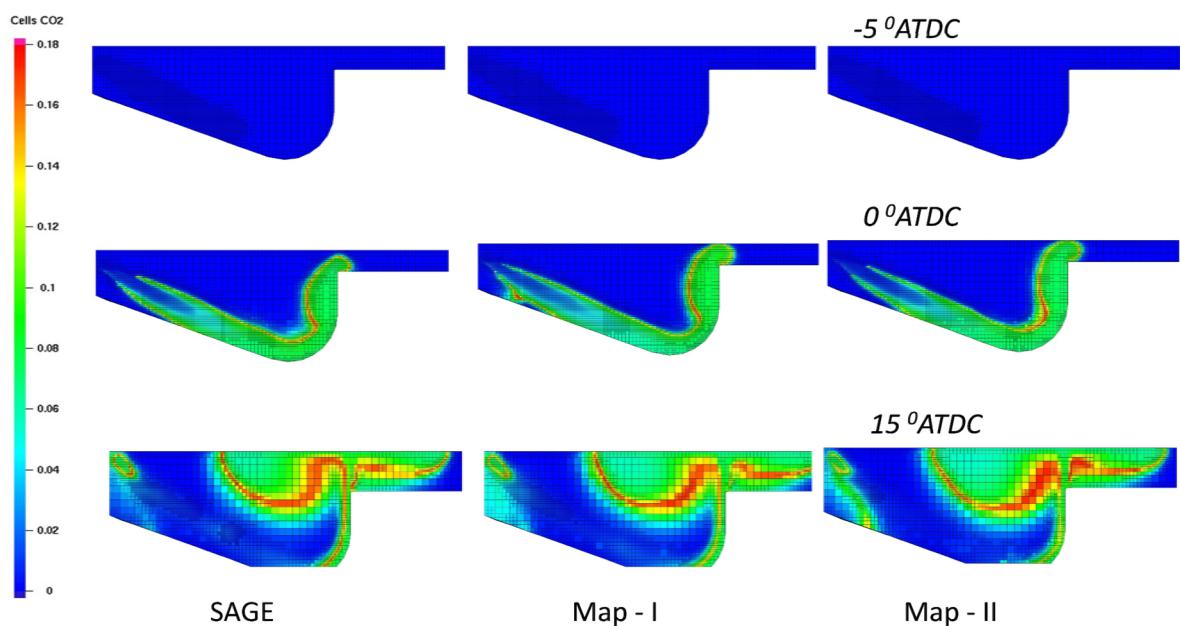


Figure 8. Comparison of CO₂ mass fraction contours along a section for test case 1

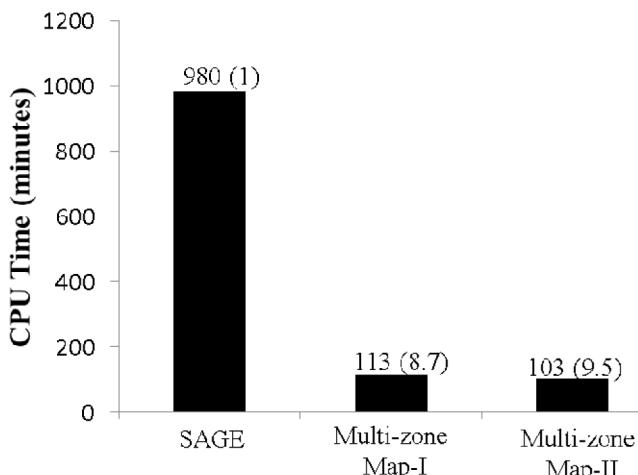


Figure 9. CPU times (minutes) of combustion simulations for test case 1

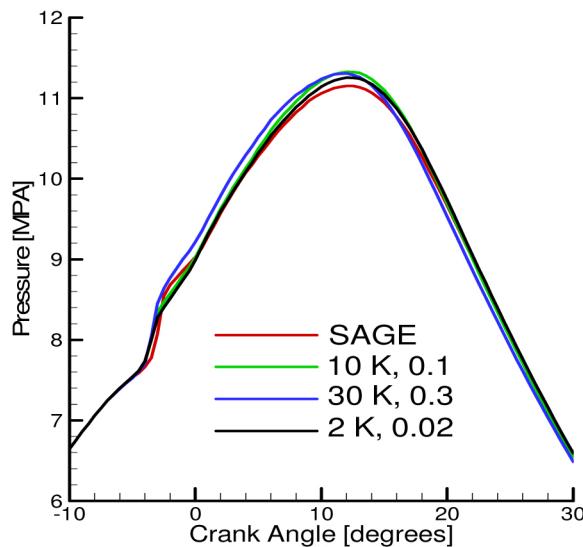


Figure 10. Comparison of pressure prediction for different multizone bin sizes

better prediction compared to the Map-II strategy. The heat release rate is much better predicted by the Map-I strategy with EGR.

Test Case 3

The third case corresponds to a typical spark ignited gasoline engine running in a premixed mode. Premixed gasoline/air is injected through the inlet port. Iso-octane is used as a surrogate for gasoline. A reduced mechanism [15] consisting of 38 species and 59 reactions is used in the simulations. [Table 3](#) shows the engine specifications and the operating conditions. Simulations are run for a full cycle. Bin sizes are chosen as 10 K for temperature and 0.1 for equivalence ratio. [Figure 13](#) shows the average pressure, average temperature and maximum temperature profiles. Multi-zone simulation gives an overall good match with SAGE. There is a slight under-prediction of the peak average pressure in the cylinder. Note the maximum temperature in [Fig. 13](#) reaches 50000 K due to a spark source. Map-I strategy gives a better match with SAGE compared to the Map-II strategy. [Figure 14](#) shows the heat release rate and the species mass profiles. Multi-zone gives a slight under-prediction of the heat release rate. The species mass match quite well with SAGE, especially for the Map-I strategy. The Map-II strategy gives an over-prediction of the residual iso-octane fuel after combustion.

Table 3. Engine specifications and operating conditions

Bore x stroke (mm)	86 x 90
Compression ratio	10:1
Engine speed (rev/min)	3000
Start of spark source(^o ATDC)	-15
Intake port mass fractions	IC8H18:0.1, O2:0.18, N2:0.72

Test Case 2

The second test case is the same as the first test case with an exhaust gas recirculation (EGR) of 20% by mass. EGR is simulated by specifying mass fractions of CO₂ and H₂O in the initial conditions corresponding to an external exhaust gas recirculation of 20% by mass assuming complete combustion in the exhaust gases. [Figure 11](#) shows the comparison of the average pressure, average temperature and maximum temperature for multi-zone and SAGE simulations. [Figure 12](#) shows the heat release rate and the species mass comparisons. Results indicate that the multi-zone model gives a good prediction even for EGR cases. Results also show that the Map-I strategy gives a much closer agreement with the SAGE simulations for the EGR case as compared to test case 1 where there is no EGR. In addition, the Map-I strategy give

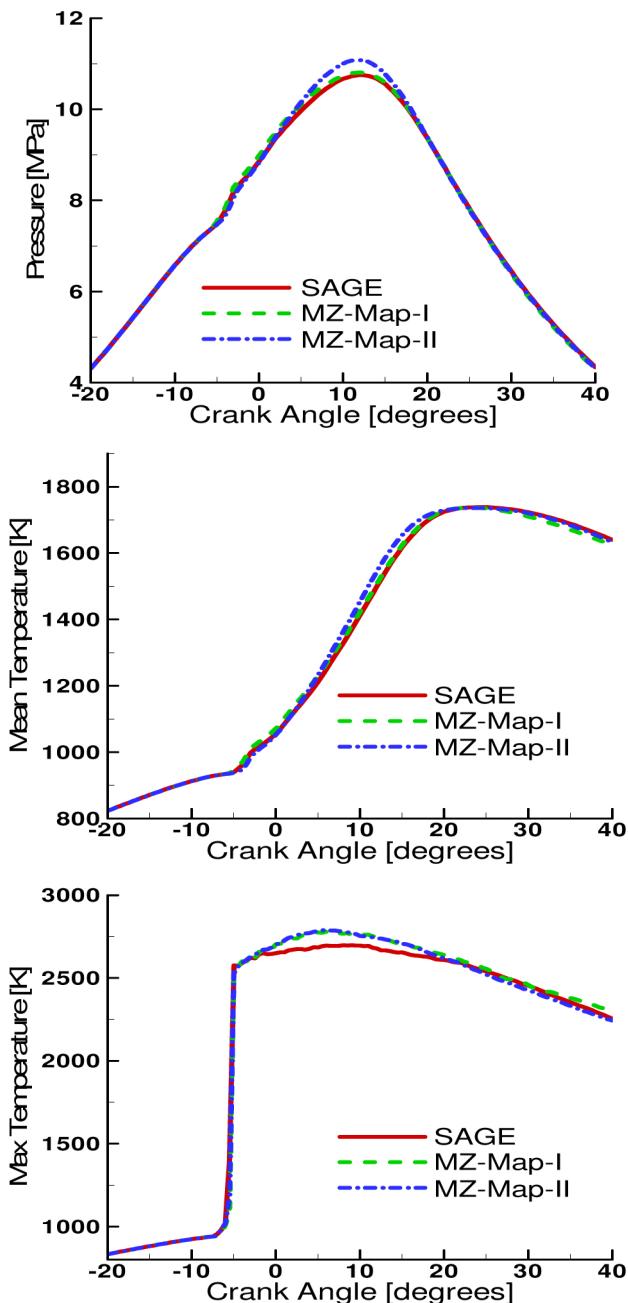


Figure 11. Comparison of pressure and temperature profiles for test case 2

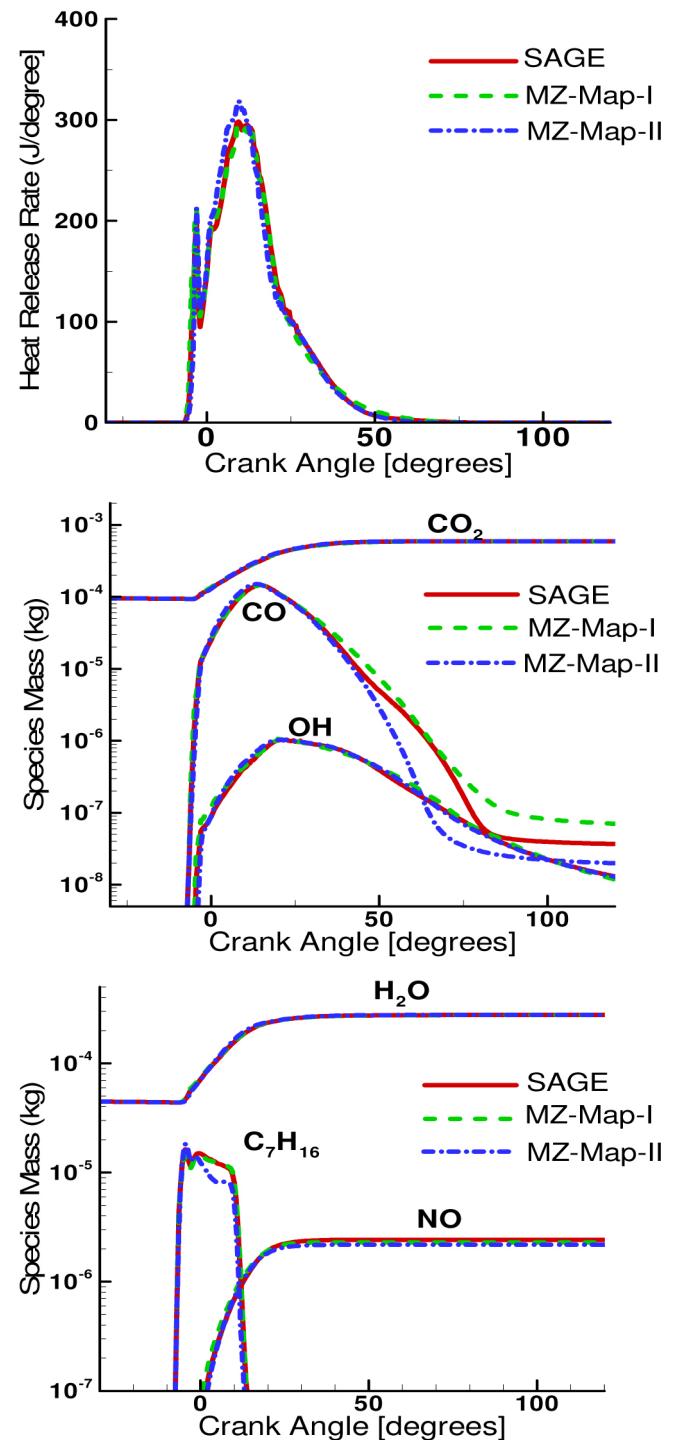


Figure 12. Comparison of heat release rate and species mass for test case 2

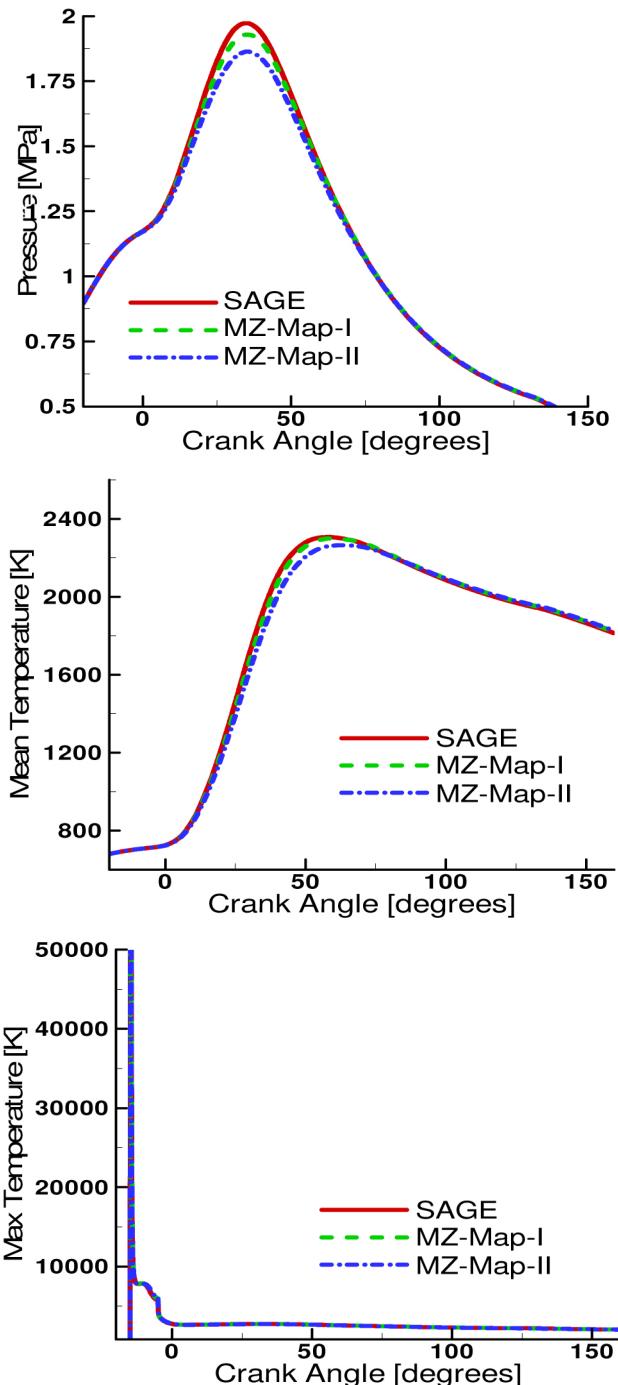


Figure 13. Comparison of pressure and temperature profiles for test case 3

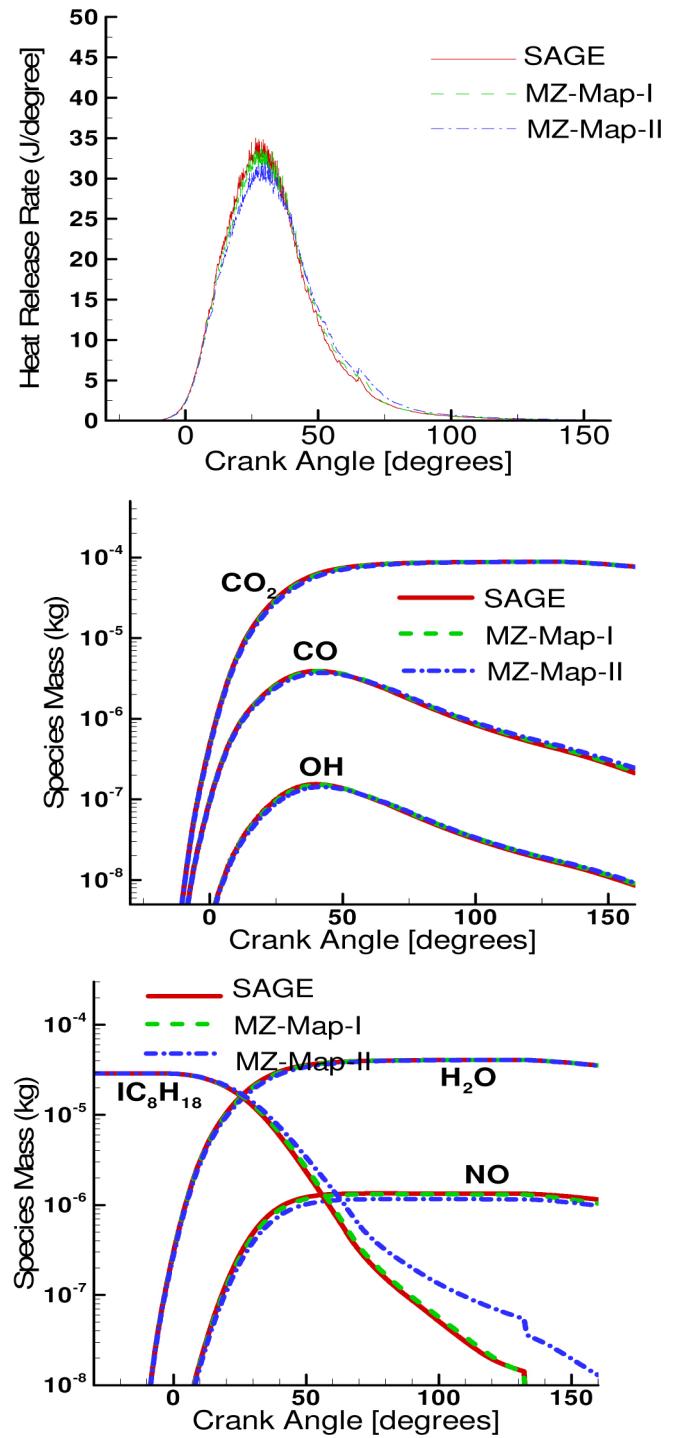


Figure 14. Comparison of heat release rate and species mass for test case 3

Test Case 4

The third test case is designed to examine the performance of the multi-zone for multi-fuel engine simulations. In the case of multi-fuel simulations, each fuel is undergoing chemical reactions via different reaction paths. Two different cells can have apparently the same equivalence ratio but may have different chemical reactivity. For example, a cell may contain a stoichiometric amount of fuel1/air mixture and another cell may contain a stoichiometric amount of fuel2/air mixture. Both have an equivalence ratio of 1 and hence they will be classified into the same bin as per the zoning strategy. This could potentially lead to large deviations in the multi-zone predictions. An extreme test case is designed to demonstrate this effect. The test case geometry consists of a closed cylinder with a flat piston. The compression ratio is chosen as 16:1. Two fuel sprays of equal mass are injected as shown in Figure 15 at diametrically opposite ends. Heptane fuel (surrogate for Diesel) is injected at the left hand side and iso-octane (surrogate for gasoline) is injected at the right hand side. The global equivalence ratio is chosen as 0.1. Fuel is injected at -10 ATDC for a duration of 20 degrees. The geometry specifications and the operating conditions are specified in Table 4. An iso-octane/n-heptane hybrid mechanism consisting of 45 species and 78 reactions is used.

Table 4. Geometry specifications and operating conditions

Bore x stroke (mm)	120 x 150
Compression ratio	16:1
Engine speed (rev/min)	2000
Start of injection ($^{\circ}$ ATDC)	-10
Global equivalence ratio	0.1

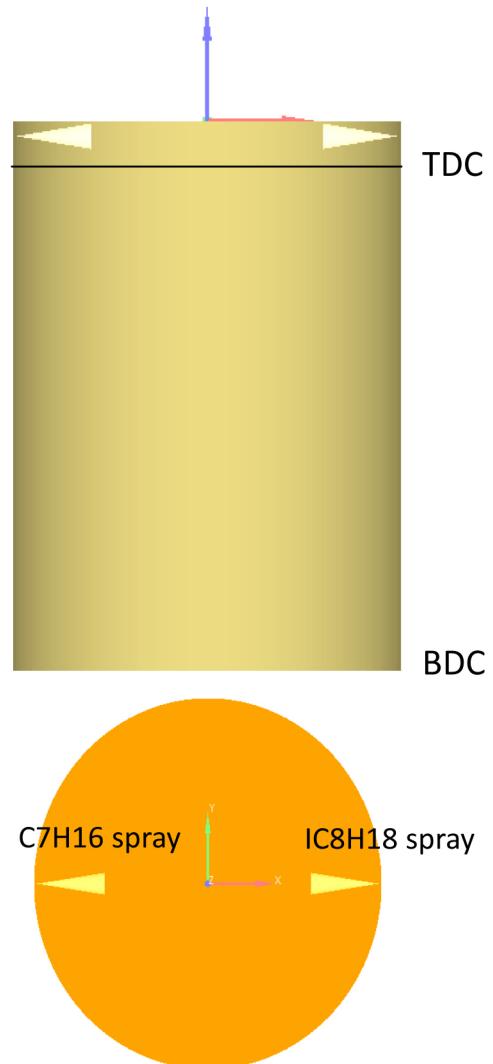


Figure 15. Schematic of geometry (a) front view and (b) top view of test case 4

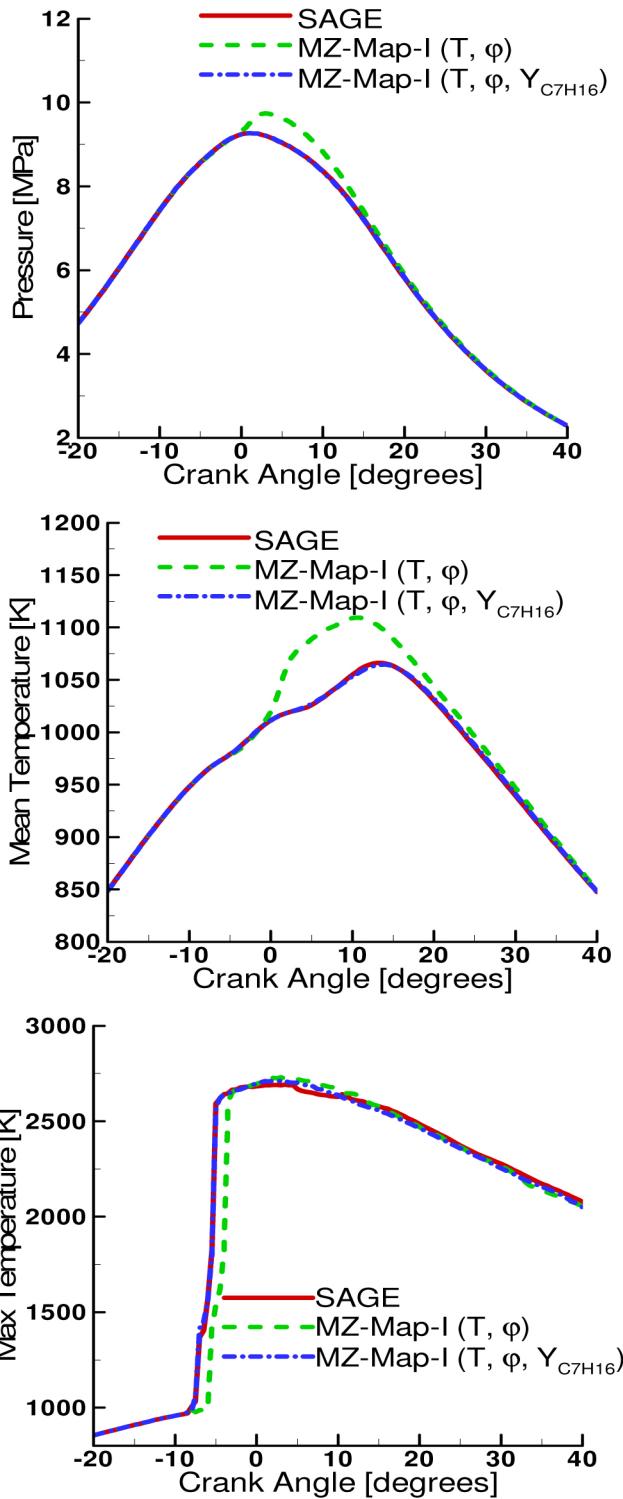


Figure 16. Comparison of pressure and temperature profiles for test case 4

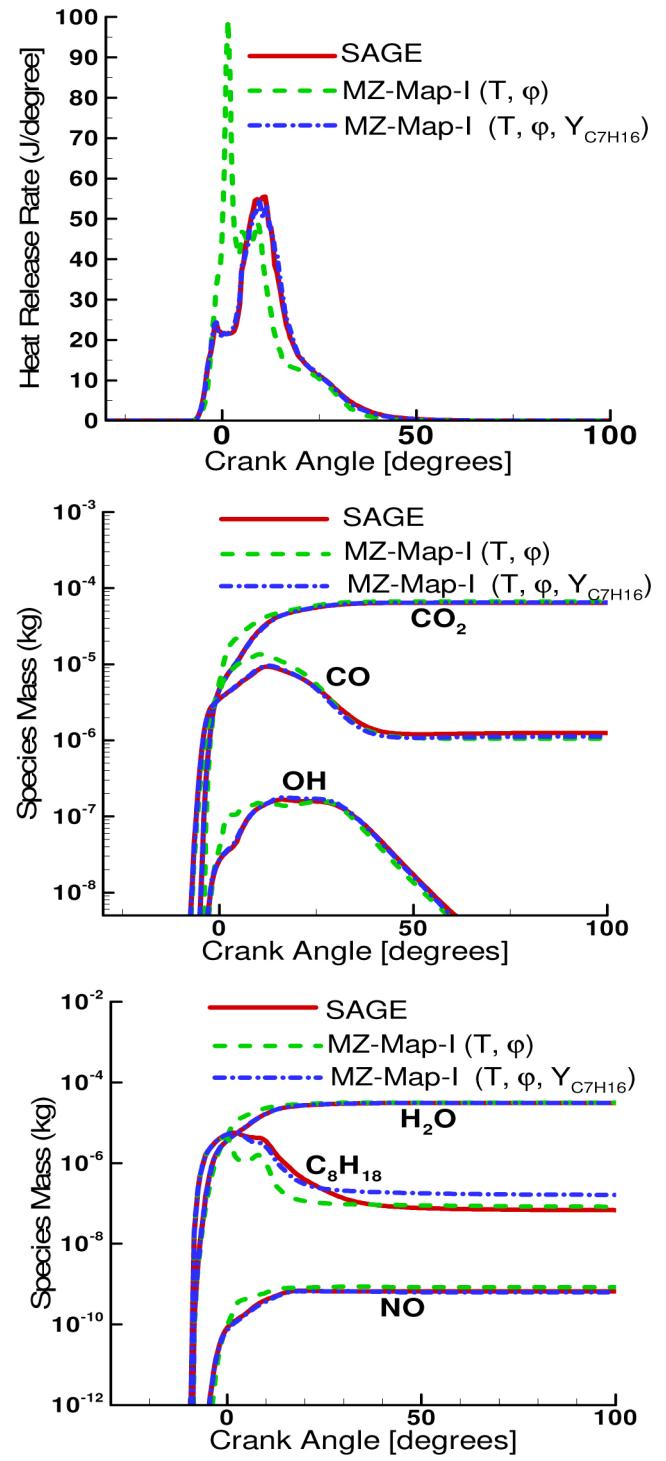


Figure 17. Comparison of heat release rate and species mass for test case 4

Figures 16 and 17 show the comparison of the multi-zone simulation (green line) and sage simulation (red line). The Map-I strategy is used for the multi-zone simulation as it was shown to do better in the previous test cases. The zoning is done using two variables: temperature (10 K bin size) and the progress equivalence ratio (0.1 bin size). Results clearly show the multi-zone simulation is quite different from the SAGE simulation. The heat release rate shows a huge difference indicating that the zoning of the cells is not done effectively. The progress equivalence ratio by itself is not a good indicator of the chemical reactivity when multi-fuels are used in the simulation. A more effective strategy is to increase the dimension of the zoning by using another variable (in general, any number of dimensions could be chosen from a given set of field variables list) in addition to the temperature and equivalence ratio variables. This strategy is referred to as the n-dimensional zoning strategy. The mass fraction of n-heptane (1.e-7 bin size) is chosen as a third dimension in this case. The blue line in Figs. 16 and 17 shows the multi-zone simulation result for the three dimensional bins. The results show a good match with the SAGE simulations. This shows the importance of using an n-dimensional binning strategy for multi-fuel simulations.

SUMMARY/CONCLUSIONS

The Multi-zone scheme is implemented into the CONVERGE engine simulation code. The performance of multi-zone is tested for different scenarios. Two different mapping strategies available in the literature are implemented and the relative performance of both these mapping strategies is compared. The results indicate that the first mapping strategy consistently performs better than the second mapping strategy. The multi-zone scheme performs well even for EGR cases. Results are also compared for a gasoline engine running in premixed mode. A two-dimensional zoning strategy in general performs well for single fuels but does not perform well for multi-fuel applications. A general n-dimensional zoning strategy is implemented. A test case for multi-fuel simulation shows that the n-dimensional zoning significantly improves the performance of the multi-zone simulations.

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