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Validation and application of the ReaxFF reactive force field to hydrocarbon oxidation kinetics

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14. ABSTRACT

The ReaxFF reactive force field method enables large scale (>>1000 atoms), long-time (> 1 ns) fully reactive, fully dynamical simulations of complex chemical reactions. The Chenoweth et al. (JPC-A 2008) ReaxFF C/H/O description has been very popular in the combustion community, providing detailed reaction kinetics for complex fuel molecules that have been validated by experiment. However, this 2008 C/H/O description is not very accurate for C1-chemistry, especially reactions involving carbon monoxide. During the first year of this project, we had successfully extended the 2008 C/H/O description to both C1-chemistry as well as graphitic materials by training against additional reaction energies and reaction barriers - derived from quantum chemical calculations (2015 C/H/O).

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Validation and application of the ReaxFF reactive force field to hydrocarbon oxidation kinetics

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PI: Adri van Duin, Penn State
Work performed by Chowdhury Ashraf (PhD-student).

Introduction.

The ReaxFF 2008 C/H/O force field[1], popularly known as the Chenoweth force field has been successfully applied to study the oxidation of high-molecular weight fuels. However, while this force field has been successfully used for studying the initial stages of pyrolysis and combustion for complex fuels (e.g. [2-10]) the performance of this force field in studying smaller hydrocarbon combustion is not satisfactory, especially for reactions involving carbon monoxide. The main goal of our project is to improve the Chenoweth force field for C1 chemistry so that we can capture all the important species mentioned in literature (Li et al, J. of Chem. Kinet, 2008) and along with the reactions involving those species, while retaining the quality of the force field for larger hydrocarbon pyrolysis and combustion reactions. Furthermore, in order to extend communication between experiment and simulations, we have developed a computational strategy for evaluating flame speed in fuel/oxidant mixtures.

Method development.

In order to improve ReaxFF description for C1-chemistry – more specifically, the CO-chemistry, we modified the ReaxFF angular term that relates to over-coordination effects on the central atom.

$$SBO = \sum_{n=1}^{neighbors(j)} \left(BO_{jn}^{\pi} + BO_{jn}^{\pi\pi}\right) + \left[1 - \prod_{n=1}^{neighbors(j)} \exp\left(-BO_{jn}^{8}\right)\right] . \left(-p_{val8} \cdot n_{lp,j}\right)$$

Equation 1: Modified ReaxFF angular function for central-atom overcoordination.

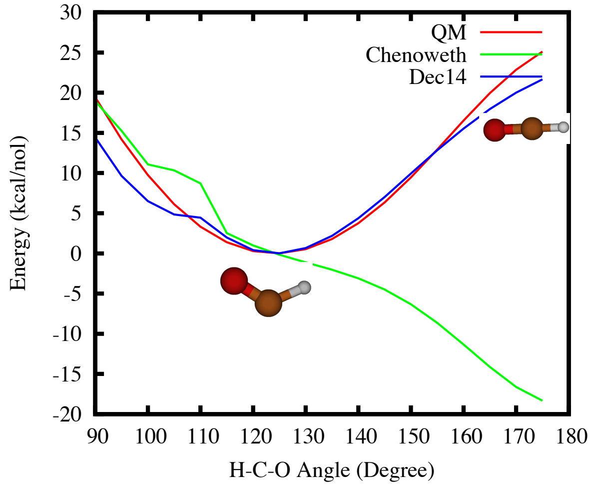


Figure 1: Comparison of the Chenoweth and the C/H/O 2015 ReaxFF description of H-C=O angle bending in a HCO-radical against quantum mechanical (QM)-data. QM calculations were performed at the DFT 6-311G**/B3LYP level.

As Figure 1 indicates – this modification enables our new ReaxFF C/H/O description (C/H/O 2015) to properly capture the H-C=O equilibrium angle in the HCO-radical – which is a key intermediate in C1 chemistry. In the Chenoweth description, this angle is forced to be linear (Figure 1), but, according to quantum mechanical (QM) calculations, it should have an equilibrium angle of around 120 degrees. As Figure 1 indicates, the modification to the ReaxFF angular function enables C/H/O 2015 to properly reproduce the C/H/O equilibrium angle and is distortion energies.

Training of the C/H/O 2015 parameters.

After introducing the new angular term, we re-trained the ReaxFF C/O/H bond, angular and torsion terms against the HCO-chemistry, as revealed from QM (Density Functional Theory (DFT)-calculations by Hsu and co-workers[11]. Figure 2 compares the DFT data from Hsu et al. to the ReaxFF Chenoweth and C/H/O 2015 (Dec.14) results – showing that the new ReaxFF parameters provide a substantially improved description of the HCO-related chemistry.

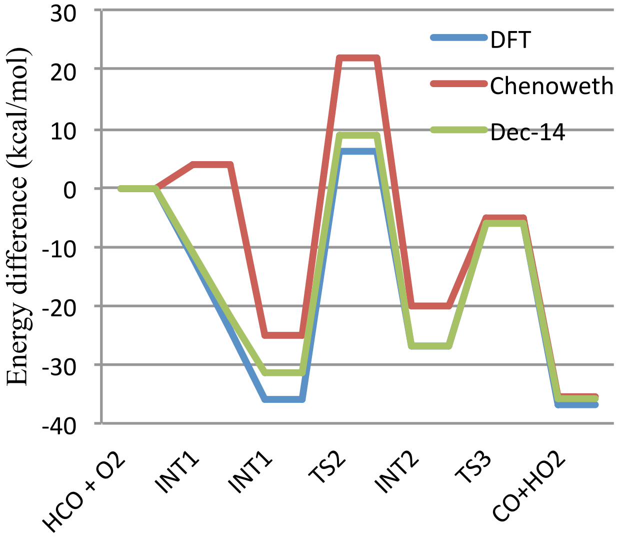


Figure 2: Comparison of the Chenoweth et al. and the C/H/O 2015 (Dec. 2014) ReaxFF descriptions of the HCO + O_2 reaction to CO + HO_2 with the DFT-data from Hsu et al. (1996).

We also included other HCO-reaction channels, including $HCO+O_2 \rightarrow OH + CO_2$ and alternative $HCO+O_2 \rightarrow CO + HO_2$ pathways in our training and found that the C/H/O 2015 parameters are in overall good agreement with DFT for all these reactions. Subsequently, we added the other ReaxFF training items using in the Chenoweth et al. development to the HCO-training set – thus ensuring that the C/H/O 2015 force field retains the Chenoweth et al. quality for more complex fuels.

Validation of the C/H/O 2015 parameters using high-temperature molecular dynamics simulations.

In order to validate the new C/H/O 2015 ReaxFF description we performed a series of high-temperature (3000K) reactive molecular dynamics simulations on $H_2/O_2/CO$

mixtures. From these simulations we could directly evaluate the available reaction channels for conversion of CO to CO_2. Figure 3 shows the reaction channels, as observed from these simulations, using the Chenoweth and the C/H/O 2015 force fields:

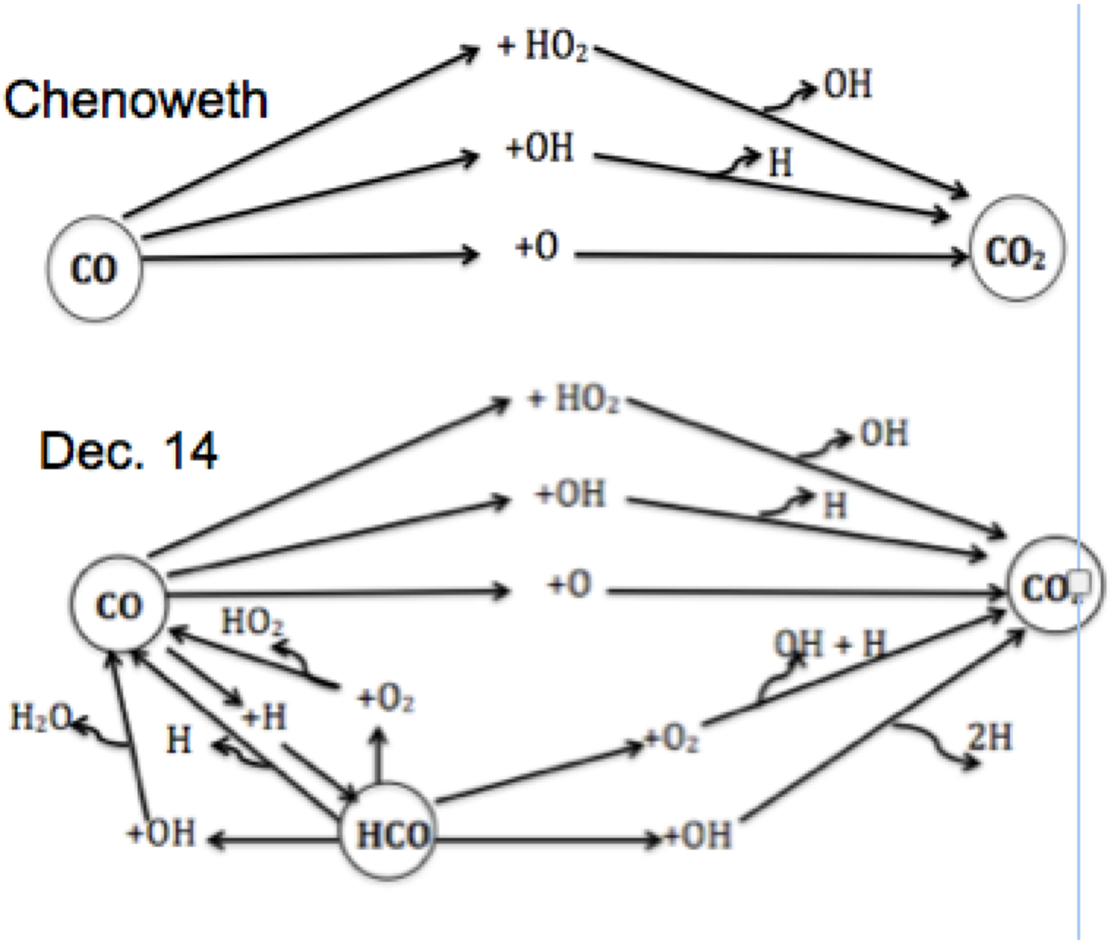


Figure 3: CO to CO_2 reaction channels in a $CO/H_2/O_2$ mixture, as observed from ReaxFF simulations using the Chenoweth (top) and the C/H/O 2015 (bottom) force fields.

The Chenoweth force field only captures a single channel for CO-oxidation – by direct oxidation using either atomic oxygen, HO, or HO_2 as an oxidant. However, the C/H/O 2015 ReaxFF description recognizes additional channels through an HCO intermediate. Table 1 summarizes the species observed in the Chenoweth and C/H/O/2015 simulations, and compares them against the available experimental data, clearly demonstrating that the C/H/O 2015 gives a far more complete description of the CO-reaction channels.

Reaction	Literature[1-3]	Chenoweth	C/H/O 2015
$CO + O = CO_2$	✓	✓	✓
$CO + O_2 = CO_2 + O$	✓	x	x
$CO + OH = CO_2 + H$	✓	✓	✓
$CO + HO_2 = CO_2 + OH$	✓	✓	✓
$HCO = H + CO$	✓	x	✓
$HCO + O_2 = CO + HO_2$	✓	x	✓
$HCO + H = CO + H_2$	✓	x	x
$HCO + O = CO + OH$	✓	x	x
$HCO + OH = CO + H_2O$	✓	x	✓
$HCO + O = CO_2 + H$	✓	x	x
$HCO + HO_2 = CO_2 + OH + H$	✓	x	✓
$HCO + OH = CO_2 + 2H$	x	x	✓

Table 1: Comparison of reactions observed during the ReaxFF simulations using the Chenoweth and the C/H/O 2015 force field and experimental data (1: Li et al., J.Chem.Kinet. 39:3, 2007, 2: Mueller et al. J.Chem.Kinet. 31:113, 1999, 3: Starik et al., Combustion, Explosion and Shock Waves, 46:5, 2010)

Atomistic-scale simulations of flame speed.

In order to develop new concepts for comparing atomistic-scale simulations with experiment we have designed a simulation strategy for measuring flame speeds from ReaxFF-based molecular dynamics simulations. For now, we have been using the Chenoweth et al. ReaxFF description in these simulations – we are planning to transition to the C/H/O 2015 description in the near future.

Initially, we set up the simulations in a relatively small system (Figure 4), where we equilibrate a O_2/fuel mixture (here, the fuel is n-butane) to a temperature of 1800K. At this temperature, on the ReaxFF pico-to nanosecond time scale, this mixture is non-reactive. Subsequently, we replace 2 O_2 molecules with O-radicals and perform a NVE (microcanonical) ensemble simulations. The O-radicals initiate a combustion reaction that spreads through the simulation box – raising temperature (Figure 5) and causing radical species to spread through the system. By monitoring the OH-radical front as a function of time, we can derive a flame speed from our simulations. As indicated in Figure 5 – we successfully identified first-stage combustion – primarily resulting in formaldehyde formation – and second-stage combustion – resulting in complete oxidation to CO_2 and H_2O – during our simulations, where the first-stage is associated with a limited temperature increase, following by a much more substantial temperature increase during the second stage.

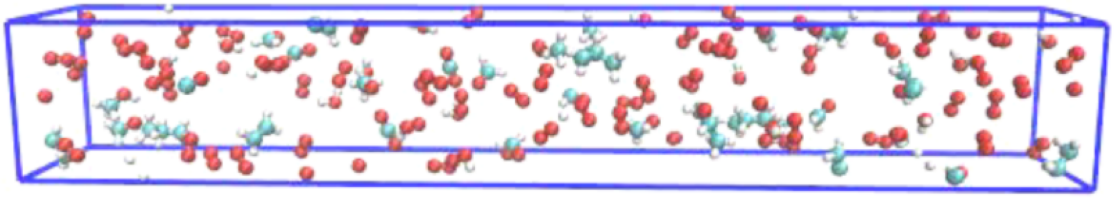


Figure 4. Mixture of 12 Butane/78 O_2 in a 12x12x80 Angstrom periodic box, as used in the small-scale flame-speed ReaxFF simulations. The O-atoms, intiating the combustion, were added on the extreme left side of the box.

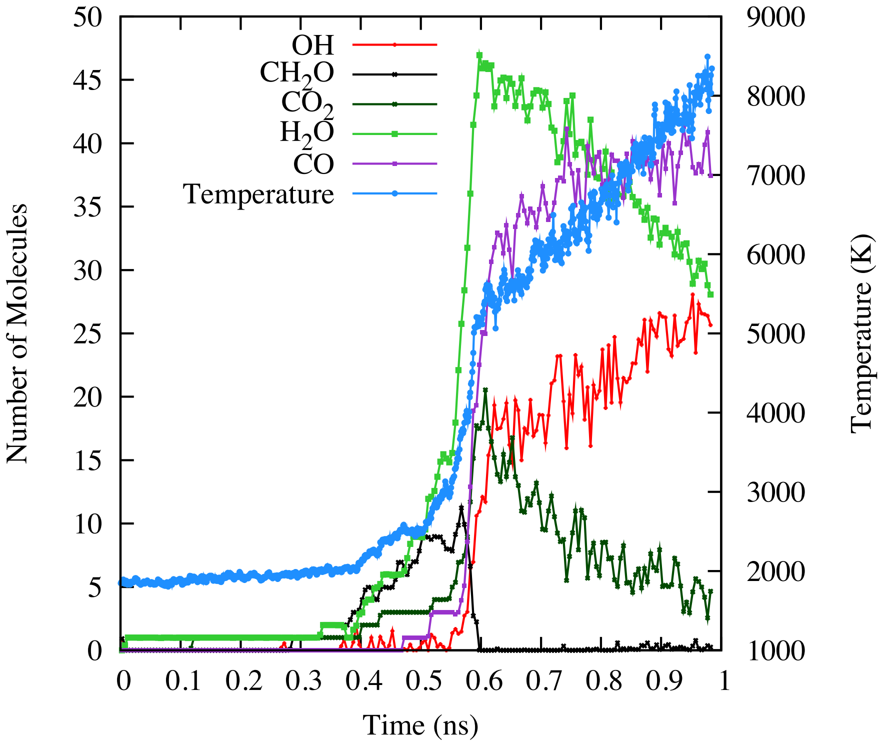


Figure 5: Main species and system temperature observed during the small-scale (Figure 4) ReaxFF NVE-simulations on combustion initiations. We observe a distinct maximum in formaldehyde concentration, connected to a modest temperature increase, around t=0.6 ns., followed by a complete combustion and a far more significant temperature rise during the later stages of the simulation.

Our analyses from the small-scale simulations (Figure 4) showed a very fast OH-radical diffusion, making flame speed measurements highly uncertain. For that reason, we increased the box by a factor 25 in the z-direction (12x12x2000 Angstrom) allowing more straightforward observation of the OH-radical profiles as a function of time.

Figure 6 shows the OH-concentration profiles as a function of time for the 2000 Angstrom box – showing a distinct OH-profile, from which a flame speed can be derived.

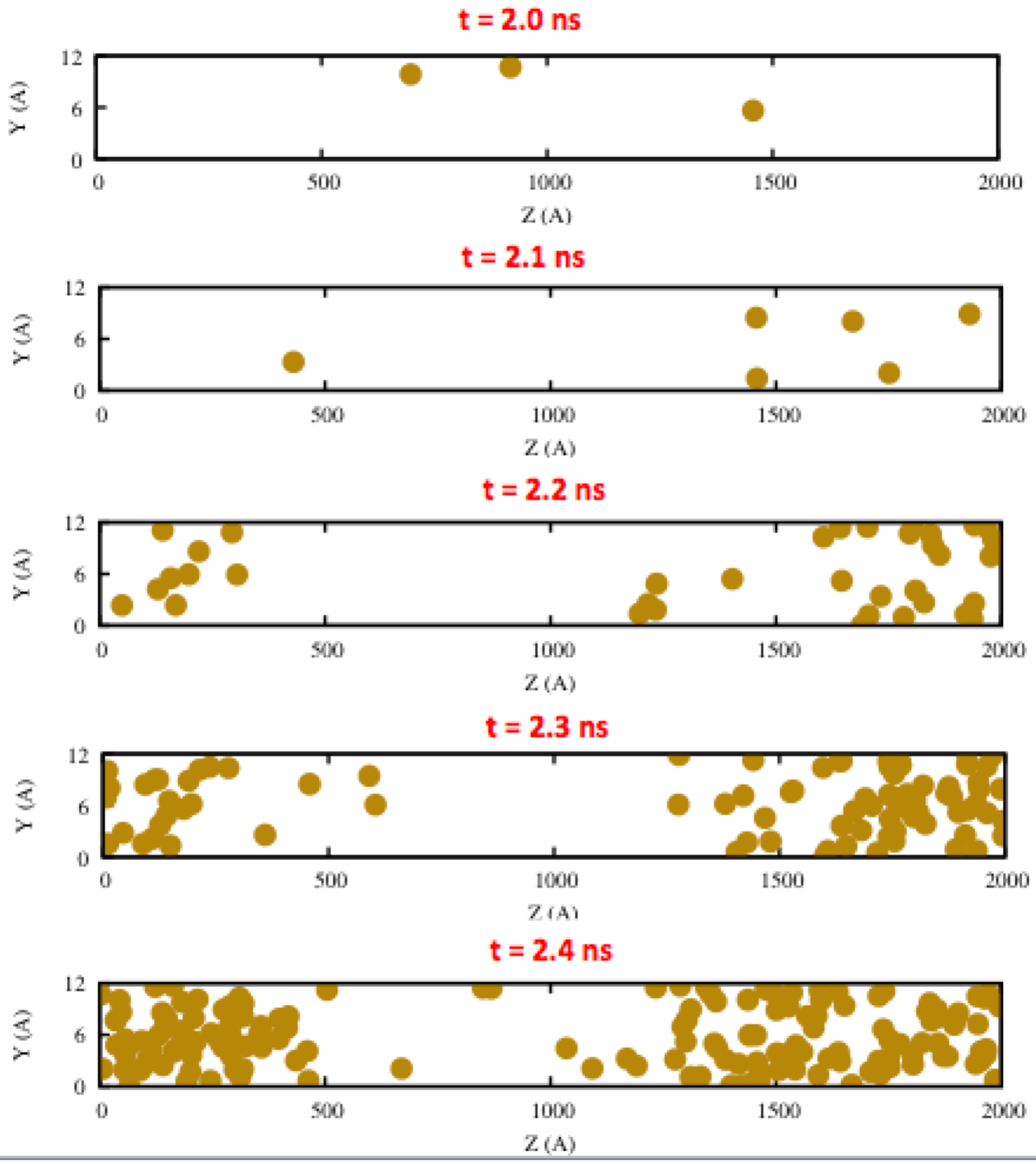


Figure 6: OH-concentration profiles as a function of time for the 12x12x2000 Angstrom box – all orange dots indicate the presence of an OH-radical. Note that, due to the periodicity, the OH-front advances on both sides of the periodic box.

From the OH-profiles we could estimate a flame speed of around 125 m/s. This is significantly faster than the experimental flame speeds for similar hydrocarbon/oxidizer mixtures (0.4 m/s), however, both the ReaxF initial temperatures (1800K) and pressures (55MPa) are substantially higher that experiment (T=300K, P=1atm). Larger-scale and longer-timescale ReaxFF simulations will allow us to lower the initial pressure and get closer to the experimental conditions. However, even with the differences between simulation and experiment, we can already use this tool to evaluate fuel/oxidizer ratio and fuel structure impact on flame speed – and connect this with experimental trends. Furthermore, the high-pressure ReaxFF simulations may provide important information for future experiments on high-pressure combustion.

H-abstraction by O_2 from Alkane

H-abstraction from alkanes by O_2 molecule is a very important reaction in combustion, especially for smaller hydrocarbons. Smaller hydrocarbons do not pyrolyze, therefore H-abstraction by a nearby O_2 molecule is the most probable initiation reaction. It has been previously reported that the reaction $CH_4 + O_2 = CH_3 + HO_2$ has a reaction barrier of ~50 kcal/mol (Fig 1(a)) in the C/H/O 2008 description. The experimental barrier for this reaction is 52 kcal/mol[12]. However, it has been observed that this reaction takes place very easily while simulating methane/O_2 system at 2500K in spite of having a very high reaction barrier. From the simulation trajectory, a transition state for this reaction is captured (Fig 1(b)), which gives a reaction barrier of only ~31 kcal/mol. This structure was not possible to capture through the bond restraint method as both the O-atoms of the O_2 molecule makes weak bonds with the nearby hydrogen, which is about to be abstracted.

However, our newly developed force field C/H/O 2016 estimates an energy barrier of ~48 kcal/mol (TS structure shown in Fig 1(c)). In order to verify the nonexistence of any other lower energy transition state structure - we ran sample simulations of the same methane/O_2 system at 2500K. During the simulation, lesser amount of H-abstraction by O_2 is observed. Thus, now we have to simulate our system at a higher temperature (2500-3000K) to capture methane chemistry at a shorter time scale, as the initiation is much slower now. Previous ReaxFF study shows that, after this initiation reaction, the two products of this reaction recombine and generates CH_3OOH, which then produces CH_2O. The recombination of CH_3 and HO_2 is only possible at lower temperature as these two will stay close to one another. However, C/H/O 2016 gives a slightly different pathway of CH_2O generation at higher temperature. At that temperature, OH and O radicals are generated by the O-O bond dissociation of HO_2. This O radical attacks the methyl radical and produces CH_3O, which then leads to CH_2O formation. Thus, a different pathway of CH_2O from methane combustion is captured using C/H/O 2016 force field.

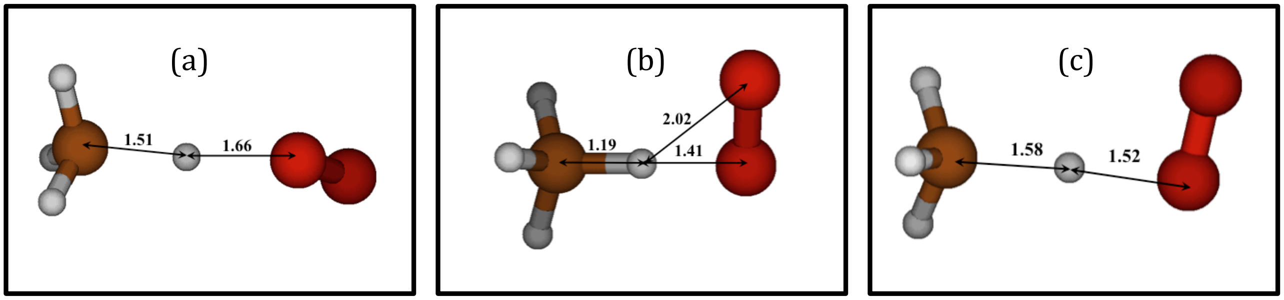


Fig 1: The transition state structure of the reaction $CH_4 + O_2 = CH_3 + HO_2$ using C/H/O 2008 description (a) through bond restrain (b) through simulation, and (c) through bond restrain using C/H/O 2016 force field

Product Distribution from n-Butane oxidation

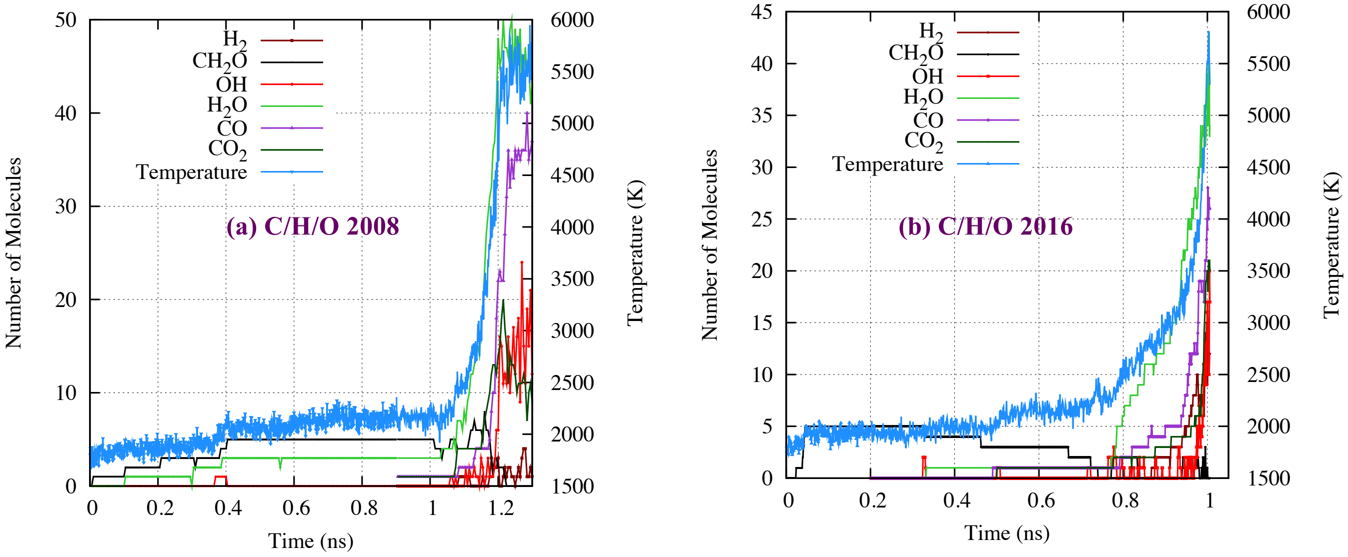


Figure 2: Time distribution of temperature and mass fraction of fuel (C_4H_{10}), important intermediate species (OH and CH_2O) and combustion products (CO_2 and H_2O) using (a) C/H/O 2008 and (b) C/H/O 2016 force field.

Previously, we mentioned that we have developed a mechanism to quantify laminar flame speed related quantity like ignition front speed using ReaxFF. At that time, we used C/H/O 2008 description in the simulations with a future goal to transfer to the newly developed version. Figure 2 shows a comparison of temperature and species distribution from simulations using C/H/O 2008 and 2016 description – same procedure was followed for both the cases. We initially put 12 n-Butane and 78 O_2 molecules in a box of 12A x 12 A x 80 A. The system is them minimized, equilibrated at 1800K using NVT-MD. Next NVE-MD simulation is performed at 1800K,which will allow us to observe a temperature jump indicating combustion. The system is initialized with two O atoms to bypass the high ignition delay time. Figure 2 shows that the temperature and species distribution profile for both the description are similar, except the distribution of formaldehyde (CH_2O). In C/H/O 2008 force field, a clear formaldehyde peak is visible before the OH radical build up. We know that this is a characteristic of low temperature combustion and should not happen at our simulation temperature (1800K). However, in C/H/O 2016 description, no clear peak of CH_2O is observed before the ignition takes places, also the maximum amount of CH_2O is almost 50% of the C/H/O 2008 case. As discussed previously, C/H/O 2008 has much lower reaction barrier of H-abstraction by O_2, which is one of the primary paths of CH_2O formation. This problem is now addressed in the new force field, which gives a lower CH_2O yield. Also, no relation is observed between CH_2O production and system temperature indicating no effect of low temperature chemistry.

Initiation Mechanism for Pyrolysis and Oxidation of Large Hydrocarbons

In order to verify our newly develop force field is performing well for large hydrocarbons; we run some simulations to study the pyrolysis and oxidation of n-pentane. To get some statistically meaningful results, we perform 10 independent simulations of n-pentane/O_2 system. At first, we put 10 n-pentane and 80 O_2 molecules in a cubic box of 25A side length. The simulation box is first energy minimized and then equilibrated at 1500K with reactions between C-O and H-O turned off in order to prevent any reaction. Then 10 different starting points are chosen and simulations are run at 2500K with full reactivity.

In all the 10 simulations we perform, the system initiated through pyrolysis only, not a single initiation reaction involving H-abstraction by O_2 is observed. This observation is consistent with our previous discussion as now the barrier for H-abstraction reaction by O_2 has a much higher value, close to the experimental one. The initial decomposition of n-pentane took place mainly in the following two pathways:

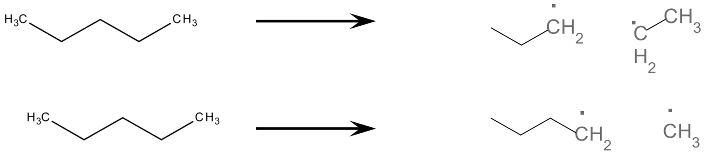


Table 1 lists the percentage of each reaction observed. Reaction (1) dominates over reaction (2)-this trend also supports a previous study[10].

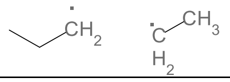
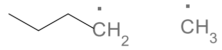
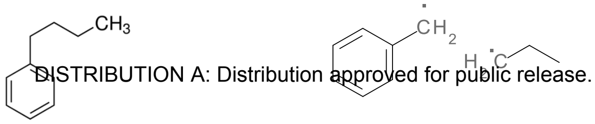
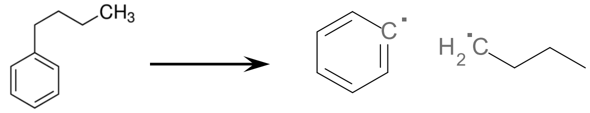
Number	Products	% of Reaction	
		ReaxFF C/H/O 2016	Allara et al.[13]
1		60	62.6
2		40	22.3

Table 1: Percentage of the different reactions observed

Similarly, we performed 10 independent simulations with alkyl benzene (butyl benzene) to see how the new force field performs. Experimentally it is observed that pyrolysis of alkyl benzenes initiate trough beta cleavage, so we expect to see high percentage of the following reaction



In stead we are observing a high percentage (50%) of the alpha cleavage breaking in our simulation.



Thus, the newly developed force field has failed to capture the kinetics of alkyl benzene pyrolysis; further training is required to address this issue.

Conclusions.

We have successfully improved the 2008 ReaxFF Chenoweth-combustion description[1] for CO-chemistry by modifying the ReaxFF angular terms and re-parameterizing the ReaxFF C/H/O parameters against DFT-data from literature. High-temperature ReaxFF simulation using the new C/H/O description confirm a much better agreement between intermediates observed for the $CO/H_2/O_2$ system between ReaxFF and experiments. Also, the problem related to H-abstraction by O_2, which is an important initiation reaction for oxidation of n-alkanes have been fixed. The newly developed force field has retained its quality for larger hydrocarbon combustions. However, the kinetics of alkyl benzene pyrolysis has not been successfully captured by this force field, which will be subjected to further training.

Furthermore, we have designed a computational methodology for calculating flame speeds – providing a new concept for comparing atomistic-scale simulations and experiment.

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Abstract

The ReaxFF reactive force field method enables large scale (>>1000 atoms), long-time (> 1 ns) fully reactive, fully dynamical simulations of complex chemical reactions. The Chenoweth et al. (JPC-A 2008) ReaxFF C/H/O description has been very popular in the combustion community, providing detailed reaction kinetics for complex fuel molecules that have been validated by experiment. However, this 2008 C/H/O description is not very accurate for C1-chemistry, especially reactions involving carbon monoxide. During the first year of this project, we had successfully extended the 2008 C/H/O description to both C1-chemistry as well as graphitic materials by training against additional reaction energies and reaction barriers - derived from quantum chemical calculations (2015 C/H/O). This has resulted in a far more accurate ReaxFF description of syngas chemical kinetics - the 2015 C/H/O description reproduces all the experimentally observed pathways for CO conversion to CO2, while the 2008 C/H/O description only follows a single trajectory - direct oxidation of CO - while ignoring H-radical recombination reactions with CO.
Furthermore, using the 2008 C/H/O description, we have successfully simulated flame speed for butane/O2 mixtures - thus providing a new connection between atomistic-scale simulations and experiment. We established that the 2008 C/H/O description can successfully identify first-stage (formaldehyde production)

and second stage (CO2/H2O formation) combustion events - reproducing experimental trends. The ReaxFF flame speed simulations are typically performed at pressures and temperatures that are beyond experimentally accessible conditions, and as such, direct comparison of simulation and experiments are not straightforward. However, we can compare fuel-trends and oxidizer/fuel ratio trends on flame speed between simulation and experiment. Furthermore, our simulations can provide useful insights in high-pressure combustion, thus benefiting future experimental efforts in that area.
In the second year of the project we have extended our analysis to the methane/O2 system and managed to resolve H-transfer issues with the 2008-force field, providing a more accurate separation between pyrolysis and oxidation reactions. Furthermore, we identified issues with the 2015 C/H/O force field related to alkylbenzene pyrolysis – and are in the process of resolving these issues.

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Mao, Q., van Duin, A., and Luo, K., 2016. Investigation of Methane Oxidation by Palladium-Based Catalyst via ReaxFF Molecular Dynamics Simulation. Proceedings of the Combustion Institute accepted for publication.

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Research Objectives

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Total			

Report Document

Report Document - Text Analysis

Report Document - Text Analysis

Appendix Documents

2. Thank You

E-mail user

Jun 09, 2016 11:50:20 Success: Email Sent to: acv13@psu.edu