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Continued Research in Combustion Chemistry Mechanisms

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ABSTRACT

The objective of this research is to evaluate reaction kinetics inputs involving 1-4 carbon atom species for combustion modeling and optimization. Reactions, products, rate coefficient expressions and values, thermodynamics, and uncertainties must be selected. We updated and revised the first mechanism version covering species of up to two carbon atoms. Improvements included revised CH_4 C_2H_4 and CO_2 decomposition rates. Additional species and reactions were added and involved ethanol and many other R-OH intermediates, and peroxy species and chemistry. A key important change was made to incorporate pressure-dependent kinetics for chemical activation reactions such as $2CH_3$->$H+C_2H_5$. Reactions involving C_2H_4O and $C_2H_3O_2$ intermediates, and a larger number of C3 and C4 hydrocarbon intermediates, were theoretically addressed to accomplish this parameterization and avoid misleading model performance issues at high pressure. A new proposed reaction $CH_3O_2+O_2$->CH_2O+O_2+OH was investigated. Ignition sensitive molecular reactions with HO_2 and O_2 were examined for consistency. Selected chemistry was then added for important three- and four-carbon-containing species kinetics based on existing mechanisms, and was evaluated, updated, and augmented with attention given to providing a proper treatment of pressure dependence. Theoretical investigations on the butene system (and others) proved particularly valuable, as there is little data and many pathways for larger systems. The resulting evaluated thermodynamics and kinetics mechanism made available for use in producing optimized foundational fuel chemistry models has 89 active species and 990 reactions. Adding this model to real fuel pyrolysis parameterizations and limited aromatics chemistry will enable accurate chemical modeling of most fuel combustion.

OBJECTIVES

The objective of this research is to assemble, evaluate, and optimize the reaction kinetics inputs involving 1-4 carbon atom species for combustion modeling of real fuels. Elements include selection and evaluation of reactions, products, thermodynamics, appropriate temperature and pressure-dependent rate expressions, coefficients, and uncertainties. This effort involves a close collaboration and feedback regarding the mechanism optimization process with Prof. Hai Wang and his group at Stanford University.

Specific steps in this iterative process include:

- Completion, documentation, and release of the initial C0-C2 mechanism.
- Revising and expanding this evaluated and optimized combustion kinetics model for unsaturated and other hydrocarbon fuels containing up to two-carbon atoms.
- Updating and expanding this model with additional kinetics and optimization targets to accommodate unsaturated C_3H_X fuel fragments, C_4H_X fuel fragments, and intermediate species arising in their pyrolysis and oxidation chemistry.

RESULTS OF EFFORT

- The first optimized and evaluated C0-C2 Foundational Fuels Chemistry Model (FFCM1) mechanism was completed, documented, and released on the Web [1].
- Review, revision, and expansion of the C1-C2 chemistry mechanism was performed. The C2 alcohols and peroxides are now included. Pressure dependence of chemical activation reaction rate constants is now included.
- Development of the C3Hx component oxidation kinetics mechanism was conducted, starting from Curran's AramcoMech chemistry [2]. Additions, evaluations, alterations, and revisions were undertaken, including some rate theory pressure-dependence calculations.
- A C4Hx oxidation kinetics reaction set was added and updated based on the previous USCMech mechanism [3]. Alterations, additions, and improvements were implemented, including many regarding the pressure dependences of rate constants.
- Final preparations are underway for optimizing and documenting the C0-C4 combustion chemistry to produce the second version of the FFCM model.

ACCOMPLISHMENTS / NEW FINDINGS

After release of the first version of the FFCM1 C0-C2 mechanism, and documentation of the kinetics for the Web site, a re-examination of those rate parameters significantly changed by the optimization or showing high sensitivity to many targets was conducted to refine or reevaluate the values and narrow the uncertainties if possible. New literature was also examined. The FFCM1 Web site discussion also describes the reactions that would benefit from improved experimental or theoretical study. Several important changes resulted. A more precise parameterization of the H + CH_3 recombination pressure dependence has been adopted, which should allow for improved optimization results according to our analysis. A revised and corrected master equation expression for ethylene decomposition was developed; rates are still fast, but no longer inexplicably so from a theoretical point of view. Newly published theoretical work [4] indicates significant prompt dissociation of the HCO product from the H + CH_2O reaction, so this potentially important chain-branching step has been added to the next base mechanism. More accurate theoretical rates [5] for the spin-forbidden dissociation of CO_2 (and its reverse recombination) are now used, a change supported by the FFCM-1 optimization. New theory values are also now used for some methanol abstraction reactions.

The preparation of the version 2 starting mechanism also employed several additions of significance, to improve the kinetics and adequately describe the chemistry of the wider range of fuels to be considered in the enlarged optimization target set. The pressure dependence of chemical activation reactions, such as $OH + CH_3 = {}^1CH_2 + H_2O$, is now incorporated. Another important case is the $2CH_3 = C_2H_5 + H$ reaction. If pressure dependence is neglected, the rates may be too fast at high pressures and modest temperatures, and produce inaccurate simulation results at high pressure. More sophisticated multichannel master equation rate theory expressions have also been added to the mechanism for the reaction systems involving CH_3CHO intermediates, C_2H_3 + OH, and $C_2H_3 + O_2$.

New species and their chemistries have been added, including ethanol (C_2H_5OH), vinyl alcohol (C_2H_3OH), and cyclic isomer ethylene oxide (cy-C_2H_4O, oxirane). There are also several more weakly bound species that our investigations showed can play a role in the oxidation kinetics in the 800-1200K temperature range, especially at high pressures. Thus kinetics and thermodynamics were evaluated and added for C_2H_2OH, C_2H_4OH, CH_3CHOH, and methyl and ethyl peroxy radicals and hydroperoxides. Rate constants and uncertainties were evaluated for these additions. We continue to omit less stable isomers of ketene (CH_2CO), namely HCCOH and CHCHO, assuming they isomerize or decompose.

The revised and expanded base C0-C2 mechanism is now ready for use in the next optimization (pending any possible last minute changes). It comprises 43 active species and 414 reactions. It should be applicable for all two carbon fuels except dimethyl ether, which was not included since its chemistry has no effect on the hydrocarbon oxidation.

Assembly and evaluation was conducted for the species, thermodynamics, reactions, products, rate constants, and uncertainties for the three-carbon fuel's oxidation chemistry. Taken from the basis of Curran's Aramco mechanisms [2], the result of this effort covers 17 additional species with 253 reactions. Many revisions were made. (Note this AramcoMech base is poorly or incorrectly documented in places.) Many aldehyde and alcohol intermediates are possible, so we employed compromises involving some exclusions or consolidations by lumping isomers as one representative compound. Possible cyclic compounds were excluded, with linear isomers substituted in reactions with likely cyclic products, the equivalent of assuming rapid isomerization. The two higher-energy isomers of allyl (CH_2CHCH_2), namely CH_3CCH_2 and CH_2CH_2CH, were omitted. Again, product channels to these isomers are included, with a rapid assumed isomerization to the allyl radical as the designated product. (This isomerization can be catalyzed by fast reactions with ever-present H atoms by addition/decomposition sequences.)

As the sheer number of possible reactions becomes larger with three-carbon atoms, the experimental and theoretical databases we can draw from are much sparser, leading to increased reliance on estimating many of these rate constants, with larger uncertainty. Considerably more different reaction products are possible, particularly in chemical activation systems, with the further complication of pressure dependence. Theoretical evaluation is more difficult. We have added pressure-dependent expressions where possible, often drawing on literature computations. As we found new and more reliable literature data, or additional reactions to add from an examination of mechanism consistency, we made revisions. It was also important to look for C_3H_x formation reactions from various C_2H_y species reactions that are not in the C2-only mechanism. Although a complete review would need more resources, a viable starting version is now in place for this chemistry. In addition to the set of C_3H_X hydrocarbons, kinetics involving acetone, C3 aldehydes, C3 peroxides, and C_3H_5OH are now included. This last propenol species is not present in most mechanisms, but appears stable enough and formed in some amount by recombination of stable allyl radical with OH to merit consideration. Note, however, that propanol kinetics are not covered, as a fuel or intermediate, since propanol likely has a small role in C3 hydrocarbon oxidation. (It would be formed in small amounts by C_3H_7 + OH recombination.) The review also prompted several thermodynamics revisions to the original database, particularly for the important propargyl radical C_3H_3 whose role as precursor to benzene has impact on aromatics chemistry. We now use the Active Table [6] values for propargyl and allyl, and have also reevaluated peroxide and C3 aldehyde enthalpies.

Finally, additions to the mechanism were made to accommodate C4 component chemistry, starting from the older relevant USCMech [3] species and reactions, and also consulting any AramcoMech 2 kinetics choices [2], and any relevant literature we located. Updates were made where found, and some missing reactions were added, The most extensive changes were made to reactions of the butene isomers, although considerable uncertainty remains. Pressure-dependent rate theory calculations and expressions were developed for the butadiene system C_4H_6, and extended to some work on the C_4H_4 intermediate. Continued work and revision have extended refined pressure dependence treatments to most of the other hydrocarbon intermediate C_4H_x systems. Chemistries were added for several stable carbonyl intermediate compounds, $C_2H_3COCH_3$, C_3H_7CHO, and $C_2H_3COCH_3$.

As was the case for C3 kinetics, the C4 mechanism effort concentrated on important species and reactions, and is not a complete comprehensive set. Some species and their reactions are omitted. A preliminary set of analogous C4-peroxy kinetics was also produced, but its inclusion in ignition simulations for conditions similar to those C1-C3 test cases in which peroxy kinetics proved important showed this chemistry had a negligible effect. Thus, we believe we are justified in excluding these extra species and reactions from the initial C4 mechanism. Again, we have neglected C4 alcohols and cyclic compounds. Many alkoxy radical products are assumed to rapidly decompose and thus are excluded, with the appropriate decomposition products given as initial products. We do not differentiate between cis and trans isomers of 2-butene, so we adjusted our thermodynamics to reflect an equilibrium mixture. This is a considerably abridged kinetics set, in view of the expansion of species and reaction quantities associated with increased carbon length; however, any alternate starting points for C4 mechanism development would require a much larger effort and yield greater complexity with likely minimal reward. The exclusions make evaluation and computation manageable. This work adds 29 more species and 323 reactions to the mechanism, and should prove adequate to model this oxidation.

After our initial assembly, evaluation, and revision of the full C0-C4 FFCM2 base mechanisms, we continued to make changes based on reexamination of some key kinetics issues and utilization of the results of several theoretical collaborations. We made specific changes based on further reviews and developed a consistent set of C_3H_X and C_4H_X rate constants for H abstraction by O_2 and HO_2; these are potentially important for ignition. We extended work on pressure-dependent C4 rate parameters to the C_4H_9 and C_4H_{10} systems. With advice from Dr. Kun Wang at Stanford, many new and more accurate quantum calculation rate-constant expressions were substituted for abstraction and other reactions in the C4 mechanism. Further study of the important ethylene decomposition reaction provided a new starting recommendation, and remaining uncertainties will be resolved by optimization. Impurity effects and secondary reactions may contaminate almost all experimental determinations. We also checked and corrected some thermodynamics issues.

New theory can provide good constraints to some key optimization kinetics rate parameters. One illustrative collaboration involves work now concluding in Prof. William Hase's group at Texas Tech University on the $CH_2 + O_2$ reaction and its various product channels [7]. Some pathways produced two or three radicals and thus accelerated ignition, but only limited room-temperature data exists. The new potential surface trajectory computations will reconcile and explain this data and now provide sound values at 1000 K and above. We will incorporate this new information into our final pre-optimization base mechanism.

In reviewing the kinetics relevant to high-pressure, modest-temperature, and high-oxygen scenarios, we have considered the possibility of a new reaction between CH_3O_2 and O_2 that might accelerate combustion. At our urging, Prof. Hase's group undertook potential energy surface calculations for this unexplored system and uncovered two possible reactive mechanisms. We used rate theory with his transition state parameters to add parameters for this reaction to the mechanism. An unexpected addition/rearrangement path forming $CH_2O + O_2 + OH$ is the most important. This is a new reaction not in current mechanisms, and the optimization will show how important it turns out to be—likely in lean, high-pressure, moderate-temperature environments.

We will soon conclude work on valuable theoretical collaborations and furnish a final set of key pressure-dependent rate parameters for the base mechanism. Pressure dependencies of various C_4H_X systems, as mentioned previously, have been incorporated or revised for the mechanism. Given the importance of alkenes that fuel pyrolysis produces, it was particularly important to rigorously examine the butene system (C_4H_8). Any different behavior of the isomers (we consider three) and their interconversions are of interest. We collaborated with Dr. Robin Shannon of Bristol University to derive a set of about a dozen pressure-dependent rates based in part on his potential surface calculations, consistent with known experimental and thermodynamic data. One interesting kinetics question is the high-temperature interconversion of butene isomers from the linear to iso forms, which requires carbon rearrangement to a "T" form. We found literature results [8] for methylcyclopropane isomerization (to butenes) and developed a theoretical framework for the butene isomerizations through this cyclic intermediate. These rates are now in the mechanism.

In these evaluations and during further revisions, we focused on improving the description of the pressure dependencies of rate constants for recombination, decomposition, and chemical activation reactions, mainly by using rate-theory calculations and approximations. The current version-2 base mechanism contains evaluated thermodynamic and kinetic parameters for 89 active (and three inert) species and 990 reactions. This is of manageable size for computation and analysis. Appendix 1 presents this mechanism in Chemkin format, and includes the uncertainty factors (F) for use in the optimization. Appendix 2 gives brief descriptions of rate constant sources and references.

Since mechanism development is an iterative process, one may look ahead at potential improvements, beyond that produced by the optimization process itself. This is, after all, effectively just the second major C0-C4 FFCM (after AramcoMech 2). Certainly the optimization process will improve the mechanism and illuminate the reactions that require more examination or calculation, as indicated from both the target sensitivities and the optimization modifications. There are reactions and perhaps species in this mechanism that have negligible effect on the relevant chemistry simulations and could be omitted. But similarly there could be reactions or species whose addition needs further examination, if only from a consistency point of view. We may consider incorporating alcohols and the more stable cyclic species into the C3-C4 kinetics to be more comprehensive (also perhaps dimethylether). The final piece of FFCM chemistry, to mate with all parts of the HyChem [9] fuel pyrolysis model, would involve selected aromatic chemistry, particularly that involving benzene and toluene. There would initially be a select set of kinetics (~140) and species (~24) from USCMech to add, evaluate, revise, and perhaps optimize for this supplemental module.

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PERSONNEL

The following personnel participated in the research supported by this contract during this project:

- Gregory P. Smith, Senior Research Chemist, Principal Investigator

PUBLICATIONS

- Y. Tao, G. P. Smith, H. Wang, "Critical kinetic uncertainties in modeling hydrogen/carbon monoxide, methane, methanol, formaldehyde, and ethylene combustion," Combust. Flame. 195, 18-29 (2018).
- Manuscript in preparation (drafted): Y. Tao, G. P. Smith, H. Wang, "Optimization and uncertainty quantification of a foundational fuel chemistry model," Prog. Energy Combust. Sci., to be submitted, 2019.

PRESENTATIONS

- Poster presentation and attendance at the 37th International Symposium on Combustion, Dublin, Ireland, July 30-Aug. 3, 2018. Y. Zhang, Y. Tao, G. P. Smith, H. Wang, "Optimizing a C0-C4 foundational fuel chemistry model II for hydrocarbon combustion," poster 4P020.
- Material on the kinetics and optimization for the Foundational Fuel Chemistry Model version 1 along with the mechanism itself remain available on the Web, for use by other AF researchers and the combustion community. The copyrighted material may be found at the URL http://web.stanford.edu/group/haiwanglab/FFCM1/pages.

INTERACTIONS/TRANSITIONS

- MACCR meeting: Multi-Agency Coordination Committee for Combustion Research (MACCCR) Annual Fuel and Combustion Research Review, Argonne National Laboratory, IL, October 17-20, 2016
- AFOSR/ARO Basic Combustion Research Review Contractors' Meeting, Arlington Virginia, June 7-10, 2016: oral presentation of FFCM1 mechanism results
- AFOSR/ARO Basic Combustion Research Review Contractors' Meeting, Arlington Virginia, August 28-30, 2018.
- MACCCR Fuel and Combustion Research Review Meeting, Livermore CA, April 9-11, 2018.
- Collaboration with Prof. Hai Wang, Dr. Yujie Tao, Mr. Yue Zhang, and Dr. Kun Wang at Stanford in the kinetics evaluations and optimization for the foundational fuels combustion mechanism. This effort is supported by AFOSR.
- Collaborations with Prof. William Hase and his group at Texas Tech University and Dr. Robin Shannon at Bristol University (UK) to provide improved theoretical rate parameter mechanism inputs for key reactions, with AFOSR support.
- AFOSR/ARO Basic Combustion Research Review Contractors' Meeting, Arlington Virginia, June 7-9, 2017.

INVENTIONS/DISCOVERIES

No invention disclosures or patent applications were filed.

APPENDICES

1. Reactions, rate constants and uncertainties in the FFCM2 C0-C4 base mechanism. Version as of 5/15/2019.
File FFCMbaseY-8r.pdf

2. Reactions, source comments, and references for the FFCM2 base mechanism.
File RxnSource-Refs.pdf