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Automated Kinetic Models to Predict the Flame Speeds of Halocarbons

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Abstract: Previous generations of halocarbon refrigerants and flame suppressants cause intolerable levels of ozone depletion and global warming, motivating the search for environmentally-friendly alternatives, but the complex flammability of proposed halocarbon compounds has proven to be a challenge. Because the combustion chemistry of these greener halocarbon refrigerants and suppressants is very condition-dependent, the flammability of potential alternatives need to be screened under a variety of operational conditions prior to marketing and further product development. To facilitate this screening, kinetic models can be generated automatically in Reaction Mechanism Generator (RMG) to predict the flammability. RMG, a software package that automates the generation of detailed reaction mechanisms, has recently been extended to predict the chemical kinetics involved in halocarbon combustion. Full kinetic mechanisms with kinetic, thermodynamic, and transport properties generated from RMG are then evaluated with Cantera to predict laminar flame speeds under different reacting conditions. Recent work developed an RMG model of flame suppressant 2-BTP (CH_2=$CBrCF_3$) in methane flames. Current work has advanced RMG's 2-BTP model to achieve improved quantitative agreement with experimental flame speeds. We also use RMG to generate models of binary halocarbon blends to determine the importance of "cross reactions" that are not accounted for through simple concatenation of individual combustion mechanisms. Flame speeds of RMG-generated blend models and blend models comprised of concatenated mechanisms are compared, along with experimental flame speeds found in literature. As demonstrated in current and previous work, automating the generation of full halocarbon kinetic models through RMG expedites screening for the next generation of environmentally-friendly refrigerants and suppressants, a task that would be both time- and cost-intensive if conducted without automation.
Keywords: *refrigerants, suppressants, kinetic models*

1. Introduction

1.1 Halocarbons

International treaties like the Montreal Protocol have phased out the use of chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs) in flame suppressants and refrigerant working fluids due to their high ozone depletion potential (ODP) [1]. Hydrofluorocarbons (HFCs) emerged as a zero-ODP replacement for these phased-out chemicals, but possess a high global-warming potential (GWP) and are now among the fastest growing sources of greenhouse gases [2,3]. The 2016 Montreal Protocol addendum aims to phase-out this second generation of chemicals by instituting new restrictions on the use of HFCs [3].

The search for a new generation of low-GWP replacements for use in refrigerants and suppressants is currently underway. The addition of hydrogen atoms and double bonds to compounds of previous generations allow for proper degradation in the atmosphere but increase flammability unpredictably [1]. For example, the proposed compound 2,3,3,3-tetrafluoropropene ($C_3H_2F_4$) of this new generation has proven to be environmentally-friendly, with a GWP100yr < 1

compared to previous HFC refrigerants with a GWP100yr typically in the thousands, but is weakly flammable [3]. Other proposed suppressants of this new generation (C_2HF_5, $C_6F_{12}O$, and CH_2=$CBrCF_3$) were found to unexpectedly increase rather than decrease overpressure in an FAA aerosol can test [4]. Further, studies have shown changes in flammability to be dependent on operating conditions like suppressant concentration [9,4]. This unpredictability in flammability is reported to be partly due to competing H-atom removals to form HF and heat generation during HF formation [9]. The complicated flammability of these newly proposed replacements poses a challenge for both the fire suppression and the Heating, Ventilation, Air Conditioning and Refrigeration (HVACR) industry. For the next generation of replacements to be deemed safe for use in industry, proposed compounds must meet the criteria of low toxicity, zero ODP, low GWP, high efficiency, sufficient volumetric capacity, and reduced flammability [1]. Therefore, a method to screen the flammability of proposed compounds under various operating conditions is necessary. Rather than conducting time- and resource-intensive experimental studies, flame simulations that predict the laminar burning velocity of a compound can be used to determine flammability. Because burning velocity involves the effects of heat and mass transfer, energy release, and overall reaction rate, this value is practical for determining flammability and is considered a standard parameter for analyzing proposed replacement compounds [1].

1.2 Reaction Mechanism Generation

Flame simulations to predict laminar burning velocity require full detailed kinetic models. These models contain hundreds of species, thousands of elementary reactions, and corresponding thermodynamic, transport, and gas-phase reaction rate data. As a result, a detailed kinetic model is often tedious and time-consuming to produce manually. Reaction Mechanism Generator (RMG) is a software package that uses reaction templates, parameter estimation methods, existing thermochemical and kinetic data, and a core-edge model structure to automatically generate detailed chemical kinetic mechanisms. The reader is encouraged to review a full description of RMG provided elsewhere [5, 6]. The RMG database had previously been limited to C, H, O, N, S chemistry, but has recently been expanded to include halogen (fluorine, chlorine, bromine) chemistry, allowing for the prediction of detailed kinetic models for halocarbon combustion [4]. To assess RMG's ability to generate accurate detailed kinetic models involving halocarbon combustion, RMG was previously used to construct a preliminary kinetic model of the fire suppressant 2-bromo-3,3,3-trifluoropropene (2-BTP, CH_2=$CBrCF_3$) [7]. This work has advanced RMG's 2-BTP model to improve quantitative agreement in predicted laminar burning velocities with both the existing NIST 2-BTP kinetic model [8] and experimental burning velocities present in literature [8].

1.3 Blends of Halocarbons

Rather than pure halocarbon compounds, industry often uses optimized blends of compounds as proposed replacements of phased-out refrigerants and suppressants [1]. The efficiency, volumetric capacity, toxicity, GWP, and ODP of proposed blends can all be predicted through analytical methods, while flammability cannot [1]. To predict flammability of these mixtures, computational methods like flame simulations to calculate laminar burning velocity can be applied to blend models. The accuracy of calculated laminar burning velocities, and thus the predicted flammability of a mixture, is dependent on the quality of the blend model. In this work, RMG is used to generate models of binary halocarbon blends to determine the importance of "cross reactions" that are not accounted for through simple concatenation of individual halocarbon combustion mechanisms.

Flame speeds of RMG-generated blend models and blend models comprised of concatenated mechanisms are compared, along with experimental flame speeds found in literature [9].

2. Methods / Experimental

2.1 Blends of Halocarbons

RMG (version 3.1.0) was used to generate full detailed mechanisms of seven halocarbon refrigerants (C_2H_5F, CH_2F_2, CH_2FCH_2F, CH_2FCHF_2, CH_2CF_3, CH_3CHF_2, CH_3F) using the publicly available branches of RMG-Py [10] and RMG-database [11] developed by Dr. David Farina for modeling halogen combustion. RMG input files for halocarbon models included pressure dependence using the 'modified strong collision' method [18]. Specified tolerances and RMG libraries can be found in the sample input file [23].

This work seeks to investigate the importance of "cross reactions" in RMG-built blend models that are not accounted for through simple concatenation of pure combustion mechanisms. "Cross reactions" are defined as reactions involving the unique species of both pure halocarbon sub-mechanisms within the blend model. 50/50 binary mixtures with the seven pure halocarbons were created through two methods: (1) simple concatenation of two pure halocarbon mechanisms and (2) building the binary blend with RMG. The first method uses the RMG tool 'mergemodels' to combine two RMG-generated pure halocarbon mechanisms into a single RMG mechanism, identifying equivalent species (by chemical structure rather than name) and removing duplicate reactions. The resulting single RMG mechanism includes all reactions and species described in the two individual mechanisms but does not include any new chemistry that could result from the combination of the two. For sake of simplicity, models built through this method are termed "concatenated" blend models in this work. The second method involves creating entirely new input files for each binary blend and allowing RMG to determine the chemistry of the binary system as a whole. Due to the complexity of these binary systems, the generation of these blends is time-intensive and often take weeks to satisfy the user-specified completion criteria. As a result, blend models were not able to reach completion within the RMG job and were instead manually terminated after six days of run time. This limited run time raised concerns as to whether RMG could successfully incorporate well-developed combustion sub-mechanisms of the two individual blend species into the final blend model. To address this, species of the combustion mechanisms of individual blend compounds were included in the initial RMG core. This speeds up the discovery of chemistry *within* the two pure compound sub-mechanisms and ensures that most of the run time is allotted for discovering interaction chemistry *between* sub-mechanisms of the blend. Models built using this method will be termed "RMG-built" models. **Figure 1** offers a visual schematic demonstrating the differences between concatenated and RMG-built models.

The laminar flame speeds of generated models were calculated using a freely-propagating, adiabatic premixed flame simulation in Cantera software (version 2.5.1). Laminar flame speeds for the combustion of individual halocarbon refrigerants with normal air across increasing refrigerant volume fractions were plotted and compared to experimental flame speeds reported by Takizawa et al [12,13,14]. Flame speeds for both concatenated and RMG-built 50/50 refrigerant blends were computed across increasing total refrigerant fraction.

Lastly, individual combustion mechanisms for 2,3,3,3-tetrafluoropropene ($C_3H_2F_4$), difluoromethane (CH_2F_2), and propane (C_3H_8) were generated , as well as concatenated and RMG-built binary models of $C_3H_2F_4/C_3H_8$ and $C_3H_2F_4/CH_2F_2$. Flame speeds for pure models were calculated across equivalence ratios, while stoichiometric flame speeds for $C_3H_2F_4/C_3H_8$ and $C_3H_2F_4/CH_2F_2$ were computed across increasing mole fraction of $C_3H_2F_4$. The stoichiometry of

the HFC-air systems at equivalence ratio = 1 was determined using the equation balancing rules described in [9]. Computed flame speed values were then compared to those reported in literature.

To compare the major pathways among the concatenated blend models and their RMG-built equivalents, sensitivity analyses were conducted in Cantera. Within each model, the normalized sensitivities, s_i, of the laminar flame speed S_u with respect to the reaction rate constant k_i were computed via the following equation to determine which reactions had the most significant effect on flame speed.

$$s_i = \frac{k_i}{S_u}\frac{dS_u}{dk_i} \quad (1)$$

The laminar flame speeds and sensitivities for a concatenated blend model and the corresponding RMG-built blend model are compared to determine the importance of "cross reactions" that are not accounted for through simple concatenation of individual pure compound combustion mechanisms.

2.2 Optimizing RMG Model of 2-BTP

The previously published RMG-generated 2-BTP model [7] lacked pressure-dependent chemistry. As a result, the laminar flame speeds calculated using this model demonstrated poor quantitative agreement with experimental flame speeds of methane-air with added 2-BTP. This work offers an improved RMG-generated 2-BTP model that includes pressure-dependent chemistry and updated kinetics for two reactions involved in flame suppression. The 2-BTP input file with specified pressure dependence is provided in supplementary material on Zenodo [23].

A kinetic mechanism for 2-BTP flame inhibition published by Burgess et al. [8] in 2015 demonstrates excellent agreement with reported experimental burning velocities for laminar, premixed methane-air flames with added 2-BTP obtained using a constant-volume combustion sphere [8]. Comparison of the Burgess et al. model (further referred to in this work as the "NIST model") and the RMG-generated model were conducted to identify possible areas of improvement within the RMG model. A modified sensitivity analysis was used to account for the highly sensitive reactions of the methane sub-mechanism. In order to shift the focus away from these pure methane reactions and towards the reactions that are most sensitive in 2-BTP flame suppression, the sensitivities of the pure methane reactions were subtracted from the sensitivities of the mechanism at different volume fractions of added 2-BTP. Analysis of the NIST model revealed the reaction BrOH (+M) ⇌ Br + OH (+M) to be among the top 20 most sensitive reactions affecting the burning velocity between the added 2-BTP volume fractions of ~0.68% and ~1.0 %. As BrOH was previously missing from the original RMG model, this species was manually included into the core of the new RMG model at the start of model generation.

In addition, reaction rates in the NIST model were compared to rates of corresponding reactions in the RMG model. To determine how each reaction rate within the RMG model influenced the Cantera-simulated laminar burning velocity, the kinetics of reactions within the full RMG model (with BrOH added into the core) were altered one-at-time to match the kinetics reported in the NIST model. When altered to match NIST kinetics, the kinetics of two reactions (**Table 1**) were identified to produce significant decreases in simulated burning velocity. Because the NIST kinetics of reactions 1 and 2 of **Table 1** were both experimentally derived using analytical methods and published in existing literature [16, 17], these rates were assumed to be more reliable than the corresponding estimated RMG rates. In the final version of the improved RMG model, the kinetics of these two reactions were altered to match the NIST rates, pressure dependent chemistry was specified, and BrOH was manually added into the core.

Table 1: Kinetics of Selected Reactions in NIST and RMG Model.

	Reaction	Source for RMG Rate	Source for NIST Rate
1	$Br + CH3 \rightleftharpoons CH_3Br$	Estimated from 'R-Recombination' reaction family	Shock tube [16]
2	$CHF_3 \rightleftharpoons HF + CF_2$	Library reaction in 'halogen_pdep' [1][1]	Vis-UV absorption [17]

[1] source provides a rate that is estimated to improve agreement with experimental values.

3. Results and Discussion

3.1 Blends of Halocarbons

The computed laminar burning velocity at various refrigerant volume fractions were computed for both concatenated and RMG-built 50/50 binary halocarbon blend models. Prior to analyzing the computed flame speeds of binary blends, it is important to first determine the accuracy of the pure halocarbon mechanisms comprising the blends. **Figure 1** features experimental and recalculated laminar burning velocities of seven pure halocarbon refrigerants in normal air at increasing refrigerant volume fractions, first calculated in [7] using similar RMG-generated models. Although RMG models of pure refrigerants slightly overestimate the laminar burning velocity across most refrigerant volume fractions, experimental and computed laminar burning velocities are in good agreement with the exception of CH_3F. Discussion on these results can be found in [7] and is omitted here. **Figure 2** reports computed laminar burning velocities of RMG-generated pure halocarbon models alongside velocities obtained using concatenated and RMG-built models of a 50/50 binary halocarbon mixture by volume fraction.

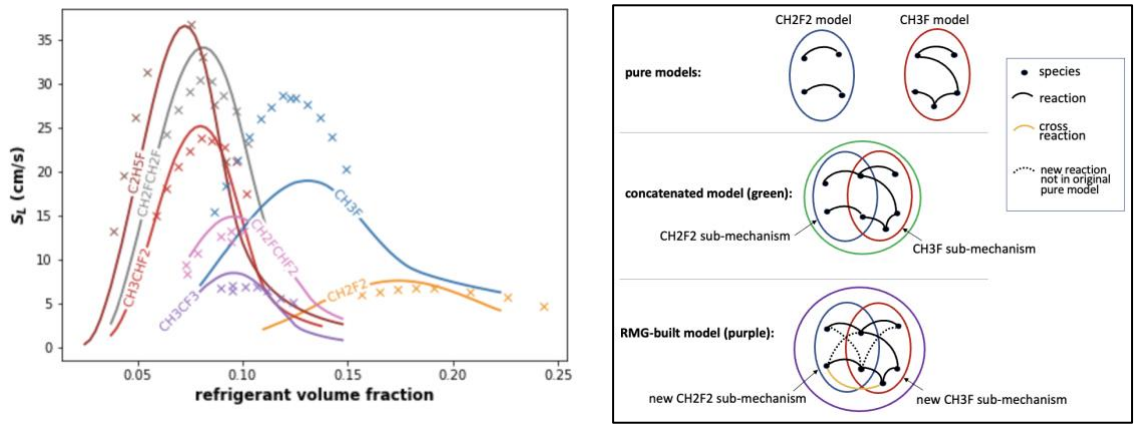

Figure 1: (left) (x) Experimental [12,13] and (—) recalculated laminar burning velocities of pure halocarbon refrigerants in normal air at increasing refrigerant volume fractions (first calculated in [7]). (right) Visual of differences in CH_2F_2/CH_3F blend models.

Laminar burning velocity predicted by concatenated and RMG-built models are compared to investigate the effect of 'cross reactions' present in the RMG-built mechanism. Nearly all blend compositions included in **Figure 2** demonstrate a noticeable change in laminar burning velocity predicted using concatenated versus RMG-built blend mechanisms, with the most significant difference in flame speed occurring at the refrigerant volume fraction where laminar burning velocity is at a maximum. This change in predicted flame speeds indicates differing blend chemistry between concatenated and RMG-built mechanisms. It is anticipated that the difference in blend chemistries is due to additional "cross reactions" present in the RMG-built model. To confirm if this is the case, an in-depth analysis of the blends and their corresponding pure halocarbon sub-mechanisms is necessary and provided in proceeding discussion.

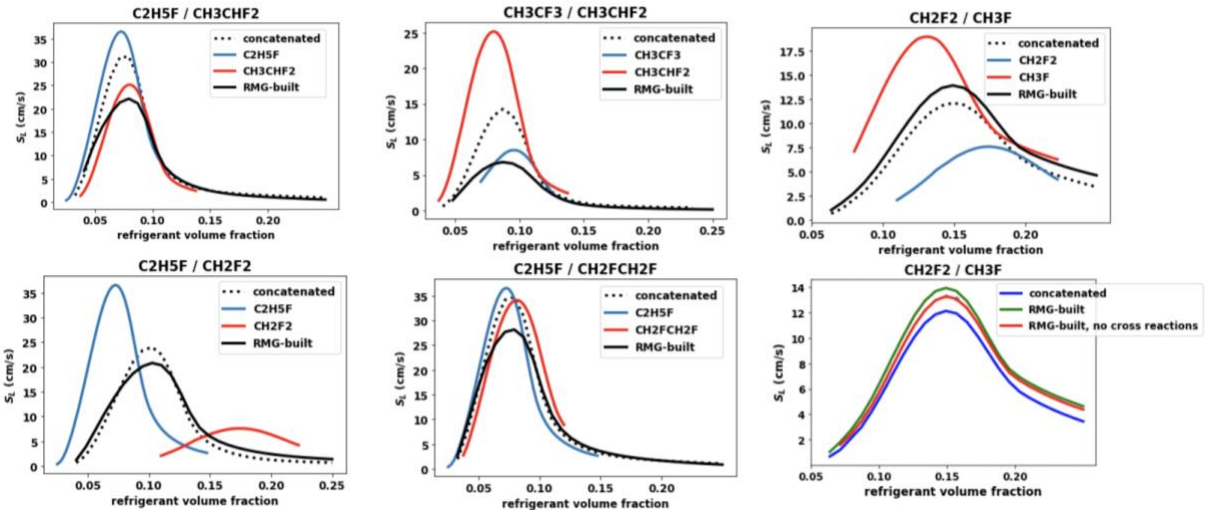

Figure 2: Laminar burning velocities of pure and 50/50 binary refrigerant mixtures by volume fraction combusted in normal air, with the x-axis representing total refrigerant volume fraction.

Accuracy in the prediction of laminar burning velocities of constructed binary models is directly related to the quality of their pure halocarbon sub-mechanisms; accuracy is compromised if pure sub-mechanisms within the blend are (1) incomplete, (2) demonstrate strong disagreement with experimental values, or (3) includes an abundance of rates and thermochemical data that are simply estimated to better fit measured values and have no basis in analytical experiments. Of the seven pure halocarbon mechanism generated in RMG, five models (C_2H_5F, CH_2FCH_2F, CH_2FCHF_2, CH_2CF_3, CH_3CHF_2) were not able to reach completion as defined by the user-specified completion criteria. Due to time limitations, the generation of these models were manually halted when species addition into the core began to plateau, indicating that incomplete pure models were close to user-defined completion. Although these five pure models were not technically complete, the fact that each displays satisfactory agreement with experimental data suggests that these models were still successful in incorporating the major, most important pathways in their combustion. While it is likely that a portion of the difference in flame speeds between concatenated versus RMG-built blends involving these five pure halocarbons is due to truncation errors present in the pure sub-mechanisms of the concatenated model, it is also possible that a portion of the difference is due to the addition of "cross reactions" to which flame speed is sensitive to. Because generation of these five pure mechanisms was truncated, it is difficult to determine which of the newly added reactions is a "cross reaction" or instead belongs to a more-complete pure sub-mechanism within the RMG-built blend. Further work should focus on repeating this computational experiment with blends consisting of simpler pure halocarbon models that can be fully-generated in RMG. While it is important to note that truncation error is not eliminated even in completed models (unless, of course, a user-defined 'movetoCore' tolerance in the limit of zero is specified and model size approaches infinity), truncation error among pure sub-mechanisms can be lessened by using "tight" models that have reached a strict user-defined completion versus models that have not reached completion.

The two pure halocarbon models of CH_3F and CH_2F_2 were generated to user-defined completion within RMG. As a result, truncation error of the two sub-mechanisms within the CH_2F_2/CH_3F concatenated model is less of a concern compared to that for concatenated mechanisms of other blends, though is still dependent on the specified tolerance. The CH_2F_2/CH_3F

concatenated model includes 2157 reactions and 118 species, while the CH_2F_2/CH_3F RMG-built model contains 3367 reactions and 141 species. Both models shared 2000 reactions in common, with the common reactions possessing approximately 67% identical, 23% similar, and 10% different kinetics. These statistics indicate differences in the pure sub-mechanisms of the concatenated and RMG-built models, raising the possibility that changes in flame speeds between the blend models could be partly (or even entirely) due to differences in their pure sub-mechanisms. About 40% percent of the reactions in the RMG-built blend were not present in the concatenated model, with 409 of these unique reactions (12% of the total reactions) identified as cross reactions and the remaining 958 unique reactions (28% of the total reactions) identified as reactions belonging to one of the two pure sub-mechanisms. **Figure 1** includes a simplified schematic of the CH_2F_2/CH_3F blend models and their comparison. A normalized sensitivity analysis of flame speed with respect to each cross reaction rate revealed that flame speed was not significantly sensitive to any one cross reaction rate. After removing the identified cross reactions from the RMG-built CH_2F_2/CH_3F blend model and recalculating the predicted laminar burning velocities, the change in flame speeds reduced from ~1.8 cm/s to ~1.1 cm/s (lower, right-most plot in **Figure 2**). Although no single cross reaction had a particularly noteworthy influence on flame speed, deletion of these reactions indicate that the cross reactions as an entire set produce a measurable change in flame speed. This recalculation of laminar burning velocity also suggests that ~60% of the flame speed difference between CH_2F_2/CH_3F concatenated and RMG-built models is attributed to variations in the pure sub-mechanisms across the blends. It is important to note that, although cross reactions in this model did not have as significant an effect on flame speed compared to variations in pure sub-mechanisms, this conclusion only pertains to the CH_2F_2/CH_3F blend at the reported refrigerant volume fractions, and cannot be extrapolated to define the importance of cross reactions among other blends (as each blend possesses unique sets of cross reactions with distinct combustion chemistries).

Figure 3 reports the laminar burning velocities of $C_3H_2F_4/CH_2F_2$ and $C_3H_2F_4/C_3H_8$ blend models along with pure models. While model generation of pure CH_2F_2 and pure C_3H_8 reached user-specified completion criteria, the pure $C_3H_2F_4$ mechanism and all RMG-built blend mechanisms did not. Inconsistency between experimental values and predicted laminar burning velocities using the pure $C_3H_2F_4$ model is believed to be at least partly due to truncation error. As a result, the concatenated mechanisms built using this pure mechanism are prone to erroneous flame speed predictions, and concatenated and RMG-built blend models are not easily comparable. In the case of $C_3H_2F_4$/ CH_2F_2, the concatenated and RMG-built models contain very similar CH_2F_2 sub-mechanism, as both blend models predict nearly the same flame speed at zero mole fraction of $C_3H_2F_4$ (all CH_2F_2). At $C_3H_2F_4$ mole fraction of 1.0 (all $C_3H_2F_4$), the blend models demonstrate strong disagreement in predicted flame speed, pointing to significant dissimilarities in pure $C_3H_2F_4$ sub-mechanisms. It is inconclusive whether improved agreement between experimental and predicted flame speeds using the RMG-built blend model is due to (1) the inclusion of cross reactions not present in the concatenated model, (2) the incorporation of a different but more accurate $C_3H_2F_4$ sub-mechanism, or (3) the incorporation of a $C_3H_2F_4$ sub-mechanism that would have looked similar to the pure $C_3H_2F_4$ mechanism had the model run to completion. Although not as drastic, the case is the same for the $C_3H_2F_4$ /C_3H_8 blend models.

With identical tolerances and completion criteria specified, the pure model of $C_3H_2F_4$ requires a longer time for model generation compared to pure CH_2F_2. As a result, it is likely possible that the $C_3H_2F_4$ sub-mechanism present in the RMG-built model, although improved compared to that of the concatenated model, requires more time for full development compared to

the CH_2F_2 sub-mechanism. It is worthy to note that the RMG-built $C_3H_2F_4$/ CH_2F_2 model predicts flame speeds that demonstrate reasonable agreement with experimental data up until the $C_3H_2F_4$ mole fraction of ~0.2, with disagreement heightening as an increasing amount of $C_3H_2F_4$ is added to the blend. Results suggest that the accuracy of predicted flame speeds is correlated with the quality of the sub-mechanisms of the RMG-built blend model. If model generation time for the RMG-built $C_3H_2F_4$/ CH_2F_2 model was extended to allow for the $C_3H_2F_4$ sub-mechanism to reach the same level of completeness as that of the CH_2F_2 sub-mechanism, one can reasonably expect to see increased consistency between experimental and predicted flame speeds in greater $C_3H_2F_4$ mole fractions much like the agreement at lesser mole fractions.

3.2 Improved RMG-generated 2-BTP model

The improved RMG-generated 2-BTP model presented in this work includes 1777 reactions and 204 species, slightly larger than the NIST mechanism consisting of 1591 reactions and 188 species. Comparison of the two models reveals 324 common reactions, with 157 of those common reactions possessing significantly different kinetics. 28 of the reactions in the RMG model were estimated using the rate rules outlined within the recently added halogen reaction families [7,11], while 8 reaction rates in the model were matched to reactions in the new 'halogens_pdep' library. Of the two reactions whose kinetics were altered, only the second reaction of Table 1 featured an RMG rate that was directly derived from the recent halogen chemistry additions to the software. While approximately 90% of the reactions in the improved RMG model either lacked a corresponding match within the NIST model or reported a dissimilar reaction rate, the models demonstrated good agreement after altering only two RMG reaction kinetics to match that of NIST's. **Figure 4** illustrates the calculated laminar burning velocities of methane-air flames with varying volume fractions of added 2-BTP, simulated using the NIST model, the previous RMG model and the improved RMG model. These calculated burning velocities were compared to experimental data present in the literature [8] and indicate improved agreement between experimental values and values calculated using the improved RMG model. Although comparison between experimental and simulated laminar burning velocities demonstrate good agreement, the improved RMG model should be considered a working model in need of further analysis and refinement. Due to the scale of the finalized kinetic model and the complex chemistry present, further work should focus on validation of the included thermochemical data and reaction rates, especially those that are estimated in RMG rather than sourced from reported analytical methods.

4. Conclusion

Because the RMG-generated pure halocarbon model of CH_3F demonstrated a poor fit to experimental data (**Figure 1**), blend models involving CH_3F are most likely unreliable for accurate prediction of laminar burning velocity and associated flammability risk. Although the predicted laminar flame speeds of the CH_2F_2/CH_3F blend may not be accurate compared to experimental values due to inclusion of a poorly-developed CH_3F sub-mechanism, comparison of the CH_2F_2/CH_3F concatenated and RMG-built model reveal that RMG is able to discover cross reactions present in the blend that would have been missed through simple concatenation of pure mechanisms. Further, data suggests that newly discovered cross reactions produce a measurable change in predicted flame speed and should not be ignored when assessing flammability risk of halocarbon blends. Blend models involving pure sub-mechanisms that are in reasonable agreement with experimental values most likely possess increased accuracy in predicting flame speeds, as shown with CH_2F_2 in the $C_3H_2F_4$/CH_2F_2 model. For these blends with well-developed sub-

mechanisms, RMG models constructed with initial addition of pure model species into the core is believed to yield good prediction of laminar burning velocity. In this way, RMG software can be used to screen various blend mixtures for heightened flammability risk and narrow in on optimized blends. Finally, the pre-existing RMG model of 2-BTP [7] was improved upon and now displays increased agreement with experimental data [8] and the published NIST model [8]. The improved RMG model now features pressure dependent chemistry, a manual addition of BrOH into the core, and the kinetic alteration of two reactions to match the NIST rates.

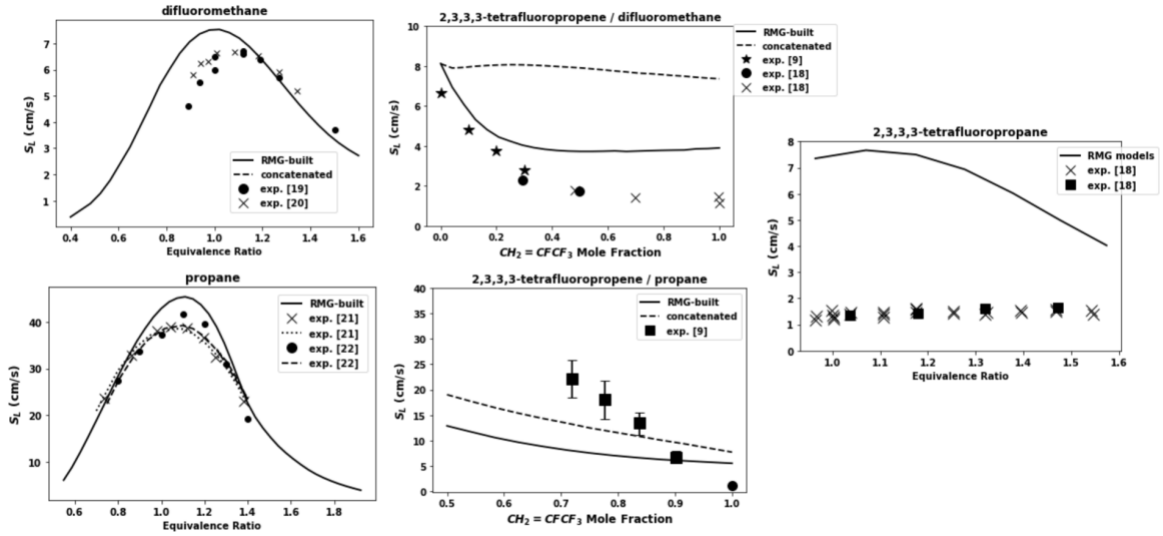

Figure 3: Laminar burning velocities of 2,3,3,3-tetrafluoropropene/difluoromethane and 2,3,3,3-tetrafluoropropene/propane blends and their pure components.

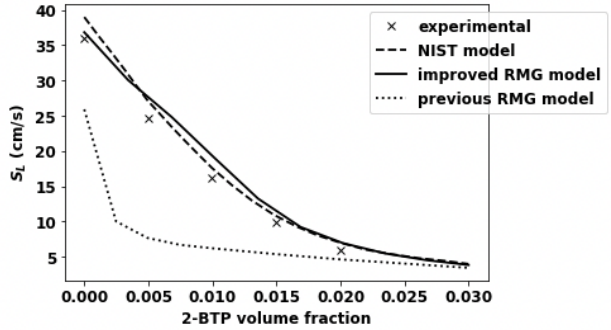

Figure 4: Calculated and experimental [8] laminar burning velocities of methane-air flames with varying volume fractions of added 2-BTP, simulated using the NIST model [8], the previous RMG model [7] and the improved RMG (current work).

5. Acknowledgements

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