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► To cite this version:

Timothée Fages, R Veillet, R Fournet, B. Sirjean, Pierre-Alexandre Glaude. AN AUTOMATIC MERGING PYTHON CODE FOR LARGE MECHANISM: EXAMPLE OF A TRF-IB MECHANISM. Joint Meeting of the Belgian and Italian Sections of The Combustion Institute 45 th Meeting of the Italian Section of The Combustion Institute, May 2023, Florence, Italy. pp.ISBN 978-88-88104-27-0. <hal-05245314>

HAL Id: hal-05245314

<https://hal.science/hal-05245314v1>

Submitted on 10 Sep 2025

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AN AUTOMATIC MERGING PYTHON CODE FOR LARGE MECHANISM: EXAMPLE OF A TRF-IB MECHANISM

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Abstract

TIRAMISU, an automatic merging python code, was developed to generate and compare several kinetic models of combustion of toluene, *n*-heptane, isooctane, blended with isobutanol (toluene reference fuel-isobutanol, TRF-iB), based on detailed mechanisms from the literature. This code consists of a reading and cleaning step, followed by an automatic translation step and a merging and writing final step. Two different fusion tasks are presented: the full fusion of two mechanisms, a TRF and a model for alkyl aromatics (hereafter ALLNL), and the extraction of 3 different isobutanol sub-mechanisms and their integration into ALLNL.

Introduction

Despite the expected increase in the share of electric vehicles in the vehicle fleet over the next few years [1], conventional thermal vehicles, especially gasoline-powered ones, are expected to remain in the majority in 2030 and to become increasingly hybrid. Among gasoline engines, progress in electronic injection control greatly favors direct injection. Nevertheless, these engines suffer from soot emissions especially nano soots, which are going to be regulated in the Euro7 standard.

Biofuels are expected to play an increasing role in decarbonization, growing by about 50% by 2030 [1]. Despite a reduction in soot emissions with the use of alcohols [2], oxygenated fuels raise new problems such as an increase in the production of nitrogen oxides (NO_x), or an increase in aldehydes, which are hazardous to health.

Moreover, ethanol, which is currently used in fuel blends, is one of the lowest energy-density alcohols, supplanting only methanol. The search for new biofuels is shifting to heavier higher carbon content alcohols. Bio isobutanol is one of those that can replace ethanol [3]. Although heavier bio-alcohols are being considered, their production on an industrial scale is non-existent.

To model gasoline combustion with isobutanol addition, a detailed kinetic mechanism based on a gasoline surrogate, such as a toluene reference fuel (TRF) coupled with an isobutanol (iB) sub-mechanism is required. It should also contain a soot precursor and a NO_x sub-mechanism to predict pollutant formation. However, in the literature, such models are quite cumbersome and often lack one of these sub-mechanisms. To complete them, a merging task needs to be done between two or more mechanisms/sub-mechanisms. In these models, species do not have standardized name (like IUPAC names) due to character limitation used in

simulation software such as Chemkin-Pro [4] or Cantera [5]. It is therefore up to the author of the model to establish a convention and to give a name to each species, which makes it difficult and tedious to translate a species from one model to another. According to the author's knowledge, there is currently no software that can automatically perform this translation without the use of a complementary file containing the chemical identifier of the species (such as InChI or SMILES).

The current study introduces TIRAMISU (Thermodynamical Interpretation of Reactions and Automated Merging for Inter-Scheme Union), an automatic merging python code for large mechanisms. It automatically translates most of the species thanks to thermodynamic and reaction data and assists the manual translation for the remaining species. It then merges the two mechanisms.

This code will be illustrated with two different fusion tasks, namely the complete merging of two mechanisms, one devoted to combustion of alkyl aromatics, AlkylaromaticV2.1 (AA) [6] and LLNL [7], in order to complement the aromatic part of LLNL; and the fusion of the newly formed model ALLNL, with 3 isobutanol sub-mechanisms extracted from their models [3,8,9].

Methodology

The goal of the code presented in Figure 1 is to significantly reduce the time required for the merging task, while simultaneously minimizing the potential for human translation error. The TIRAMISU code is divided into three main steps.

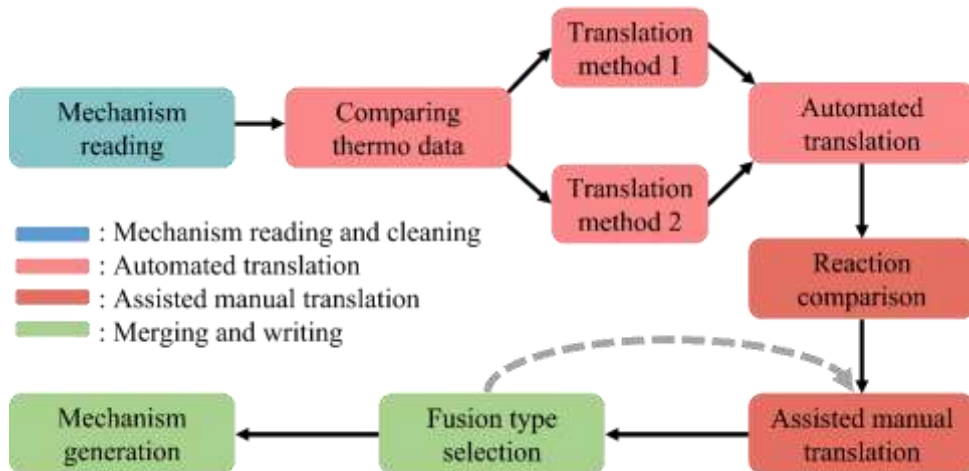


Figure 1. TIRAMISU, an automatic merging python code for large mechanism

Mechanism reading and cleaning: This step reads the mechanism and suppress comments, unnecessary blanks, and empty lines. It also removes duplicate species or species never used in reactions. The entire code relies heavily on this step because it involves storing the data for each species and modifying each reaction to display the stoichiometric numbers for each species, while accounting for the possibility of

reverse reactions. This enables the identification of equivalent reactions such as $\text{CH}_3+\text{CH}_3=\text{C}_2\text{H}_6$ and $\text{C}_2\text{H}_6=2\text{CH}_3$.

Automated and assisted translation: To guess the translation differences of the species between two models, species are first separated into isomers group (one isomer group will be called M1 for model 1 and M2 for model 2). The NASA polynomial of each species is then used to compute $h_l^0 - T s_l^0$ over the temperature range, following the expression in equations (1) and (2):

$$h_l^0(T) = (a_{1l} + \frac{a_{2l}T}{2} + \frac{a_{3l}T^2}{3} + \frac{a_{4l}T^3}{4} + \frac{a_{5l}T^4}{5} + \frac{a_{6l}}{T})RT \quad (1)$$

$$s_l^0(T) = (a_{1l} \ln T + a_{2l}T + \frac{a_{3l}T^2}{2} + \frac{a_{4l}T^3}{3} + \frac{a_{5l}T^4}{4} + a_{7l})R \quad (2)$$

where a_{il} is the i^{th} coefficient (or the $i+7^{\text{th}}$ if T is in the lower bound of the temperature range) of the corresponding NASA polynomial for the species l. The curve H-TS of each species from M1 is then compared to the one of each species from M2 by calculating the normalized mean absolute difference between the two curves. From those results, two different translation methods are used to ensure minimal translation error. The first method consists of computing these values for all translation matches possible between M1 and M2. Then, the pair of names that has the lowest difference is selected. The two species are removed, and this task is repeated until the number of species in M1 or M2 reaches 0. This method is often very effective and scales well with the number of isomers. It also gives the difference between the two species. This difference indicates if the species are well translated or if they are different and have no translation at all. However, in some cases, the thermodynamic data between two isomer groups are slightly shifted; if the difference between species belonging to the same isomers group are of the same order of magnitude, the method could invert species, making a translation error. Indeed, as the method only looks at the lowest difference match at each step, it does not try to achieve the minimal mean difference of all matches. To address this problem, the second method was introduced to help identify and solving those cases. It consists in generating all permutations of combinations between M1 and M2, and choosing the permutation that minimize the global error. It allows finding the best fit of isomer translation in an isomer group, that minimize the error, but also to look at the second-best fit, to see if the difference between the two is relevant. If it is the case, the best fit is probably correct, but should be confirmed with the value given by the first method, to identify species that cannot be translated. Also, this method is very sensitive to the number of species in M1 and M2. The number of permutations is increasing following the equation (3) where $|x|$ is the length of the list x.

$$\text{nb permutations} = \frac{|M1|!}{|M1|! - |M2|!} \quad (3)$$

When the number of permutations is too high, we cannot use this method for the isomers group.

Overall, the automatic translation of species is restricted to certain requirements that need to be achieved thanks to the two methods. Otherwise, a manual translation needs to be used. It is noteworthy that the number of translation method and requirement that need to be satisfied to make an automatic translation is arbitrary. Too low requirement will translate more species, but at a higher risk of error, while too high requirement will reduce this risk, but increase the number of manual translations.

Those mandatory manual translation are assisted by prediction of method 1 and 2 but also by a comparison between reactions in the two models. An untranslated species from M1 will be translated into a species from M2 and the code will count how many reactions are identical between the two species. As all species have not been translated prior to this task, other species than the one of M1 and M2 will only be represented by their chemical formula. That will therefore produce more matching reactions between models than it should but this step is sufficiently accurate to help the user.

Merging and writing: Two different fusion tasks can be distinguished. The first is the merging of model 1 with a sub-mechanism from model 2 or *vice-versa*. It doesn't require the entire manual translation to be done, as only species encountered in the sub-mechanism need to be translated. To extract this sub-mechanism, the code starts from one or a list of species given by the user. It will then add a list of all reactions containing these species. Then, it will list all new species encountered in those reactions and replace the starting list. Each time the code makes a new loop, it will be called D_n (for "depth" n) with n being the number of loops, D_1 being the first one. The code will continue until there is no new species encountered or a user provided D_{limit} is reached. The second fusion task is the full merging of model 1 with model 2 and will need all translation to be done. It is based on a "master" mechanism and a "servant" mechanism. Reactions and species in the servant that are not contained in the master will be added to the master model. In this way, the master will have a priority for his own reaction rate constant or NASA polynomials and master and servant can easily be exchanged to compare the impact of these data on the produced mechanism. It is noteworthy that the master for the kinetic does not have to be the master for the thermodynamic.

Merging examples

Full merging: With the aim of improving toluene accuracy on simulations of ignition delay times (IDT) for the LLNL model (1372 species) [7], it was merged with another model from the same team, AA (506 species) [6]. This model is specifically designed for alkyl aromatics compound, and almost the entire model (except species too big, such as propyl-benzenes or butyl-benzenes) was used as servant or master mechanism. As they come from the same team, their core is quite similar, but their

sub-mechanisms follow different conventions. Once automatically translated, only 50 out of the 506 species cannot be translated by method 1 and 2 and were translated manually. Four different mechanisms have been made from this translation, by varying if the LLNL model were master (M) or servant (S) on kinetic or thermodynamic data. This gives the models MM, MS, SM and SS. These models were tested over a large range of TRF IDT, burning velocities and species profiles. Overall, the MM model was better for IDT and SS for burning velocities and species profiles. The two other mechanisms were neither the worse nor the best for any kind of data, but as they have mixed thermodynamic and reaction rate, they are probably less coherent.

Sub-mechanism integration: Following the full merging, the SS and MM model were named ALLNL-1 and ALLNL-2 and merged with 3 isobutanol sub-mechanisms; Sarathy-2012 (279 species, 1892 reactions) [3], Moss-2008 (161 species, 1256 reactions) [9] and Merchant-2016 (376 species, 8324 reactions) [8]. In this example, we will only talk about the merging with ALLNL-1. About the translation, the efficiency depends on the model. For Sarathy-2012, it was very efficient with only 12 species manually translated, but for Moss-2008 and Merchant-2016 there was still 40 % species not translated. For the merging step, different D_{limit} were tested to see its impact on the accuracy on IDT of isobutanol. With the models Sarathy-2012 and Moss-2008, due to the low number of species and reaction added to ALLNL-1 (respectively 26/321 and 13/169 species/reactions), reducing D_{limit} under D_{max} (respectively D_{10} and D_6) has a significant impact on the accuracy of the models, without changing much to his size. However, for the Merchant-2016 model, which has a D_{max} of D_7 , a reduction up to D_2 can be made without increasing the relative mean absolute error on IDT by 0.5%. This reduction is highly valuable because it reduces the number of species/reactions added from 191/5857 to 81/1036. The overall result of this merging can be seen in Table 1. For the Sarathy-2012 merging, the model did not perform as well as the base model. It could be due to lacking reactions with species already present in the ALLNL-1 model or a very different thermodynamic for the core mechanism. For the Moss-2008 and Merchant-2016 merging, the results were equivalent (or better for Merchant-2016) than the base model. That mean that the extraction task was sufficient to extract the most important element of the sub-mechanism.

Table 1. Mean absolute error relative to IDT experimental data [9,10].

Sar.2012	ALLNL-1+ Sar.2012	Moss-2008	ALLNL-1+ Moss-2008	Mer.2016	ALLNL-1+ Mer.2016
66.20%	91.22%	155.46%	156.28%	48.33%	39.52%

Conclusion

The new TIRAMISU automatic merging python code for large models was described and tested over two types of merging: full merging and sub-mechanism integration. This code translates most of the species between two mechanisms thanks to the thermodynamic and reaction data and then merge the first completely with the second, or only one sub-mechanism. The examples show that TIRAMISU could greatly reduce the time needed for translation by automatically making most of them and helping the user for the remaining species. It also shows that the extraction task was sufficiently accurate for at least two of the three models.

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