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ORCh: A package to reduce and optimize chemical kinetics. Application to tetrafluoromethane oxidation

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ABSTRACT

ORCh is a set of C++ routines to analyze the response of detailed chemical kinetics and determine the most influential species and elementary reactions for given operating conditions. The objective is to reduce the number of degrees of freedom to be solved in fluid mechanics simulations while still capturing most of the reactive flow physics. From a detailed chemical kinetics, ORCh returns a set of reduced chemical schemes of decreasing complexity. ORCh operates either from canonical laminar diffusion–reaction problems, such as one-dimensional premixed and diffusion flames, or turbulent/chemistry interaction models through the evolution of stochastic particles. The initial conditions of these canonical problems are representative of the inlets of the reactive flow system under study. In case of a significant reduction of the number of degrees of freedom, the control parameters of the reduced chemistry can be further optimized from a genetic algorithm to still match the reference detailed chemistry response. An illustrative application to tetrafluoromethane oxidation chemistry is discussed.

Code metadata

Current code version	V4.0
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-24-00150
Permanent link to Reproducible Capsule	
Legal Code License	BSD 3-Clause License
Code versioning system used	git
Software code languages, tools, and services used	C++
Compilation requirements, operating environments & dependencies	https://cantera.org/blog/cantera-240-released.html
If available Link to developer documentation/manual	http://orch.coria-cfd.fr
Support email for questions	orch.chem@gmail.com

1. Background and objectives

The theoretical and experimental procedures to construct and validate detailed chemical kinetics have benefited from significant and constant progress, leading to a large variety of accurate and reliable detailed schemes [1–6]. These latters incorporate the complexity of the numerous molecules and elementary reactions involved in gaseous reactive flows. Thereby, the resulting number of degrees of freedom can be very large, typically above many hundreds. The most advanced numerical simulations of reactive flows must benefit from the valuable thermochemical information available in these chemical schemes. However, in practice, it is not possible to incorporate all the available details of the chemical information in the computational fluid dynamics (CFD) tools, because of the large number of variables that would need to be solved for and stored on every node of the mesh. Moreover, these chemical schemes are driven by large ranges of characteristic times, imposing the solving of stiff differential equations that require CPU-expensive numerical methods.

Many strategies have been developed to reduce the size of chemical problems for their introduction in flow simulations [7], such as reduced global schemes [8], analytically reduced schemes [9], low-dimensional

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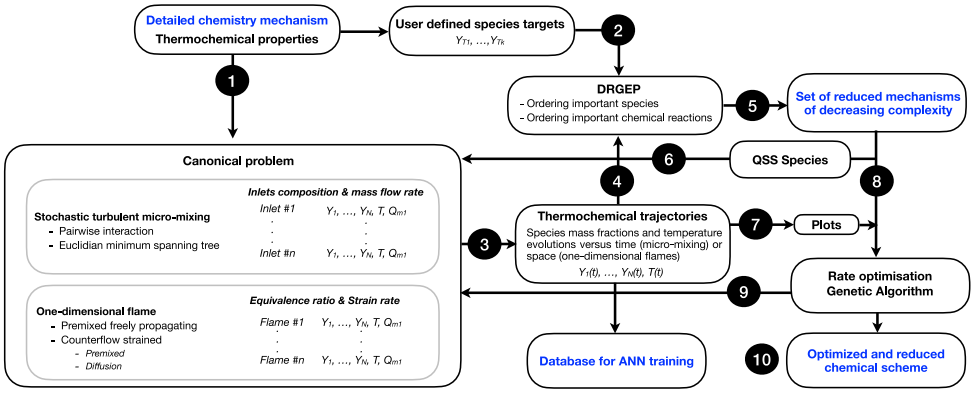

Fig. 1. Flowchart of ORCh.

manifolds and tabulated chemistry [10–12], in-situ tabulated chemistry [13], and the training of neural networks [14] (non-exhaustive list). The set of routines discussed in this paper generates reduced kinetics from well-established automated methods, combining graph analysis and genetic algorithms [15,16], with canonical combustion problems [17].

There are two major steps in the process of reducing a chemical scheme involving a number n_S^o of chemical species and a number n_R^o of elementary reactions. The first step consists of selecting the $n_S^r < n_S^o$ degrees of freedom that must appear in the reduced problem. In this ensemble of n_S^r chemical species, are those whose concentration knowledge is mandatory for the problem analysis (for instance the reactants, major products, and pollutants). To these n_S^T target species, a number $n_S^r - n_S^T$ of additional intermediate species are required to preserve the skeleton of the complex chemical paths securing a reasonable level of accuracy. If the n_S^T target species are easily defined, the choice of the intermediate ones requires a careful analysis of the dynamics of the non-linear system, and this is one of the outputs of the ORCh package.

Once the n_S^r species are selected, the elementary reactions involving the species that have been removed systematically disappear. In many cases, more reactions can be removed in a second step, without affecting too much the accuracy in the prediction of the target species, leading to a number $n_R^r < n_R^o$ of elementary reactions.

From this point, three options exist for dealing with the obtained reduced scheme of size (n_S^r, n_R^r): (i) The reduction gained in terms of CPU is sufficient and the scheme is ready to be used; (ii) More intermediate species must be removed to render the scheme tractable for computational fluid mechanics (CFD). Then, a quasi-steady state assumption can be invoked for some species whose net rate of variation is small compared to their rate of production or consumption. The net rate of these species is set to zero and the corresponding combination of reactions in which they are present provides algebraic relations to express these species from the kept ones; (iii) Sometimes, to comply with CPU constraints, the number of species has been seriously reduced and a departure is observed between the species response given by the reduced scheme and the detailed one. In most cases, this deviation can be overcome by slightly adjusting the rate parameters of the elementary reactions that have been kept. A genetic algorithm is then applied to adjust the parameter rates so that the response of the reduced scheme matches the detailed one.

The routines available in ORCh are designed to perform these various steps automatically.

2. ORCh description

The inputs (❶ in Fig. 1) are a detailed chemical scheme and the corresponding thermochemical database in the format of the open-source software Cantera (https://cantera.org), whose C++ routines are used to generate and manipulate chemical species properties and perform the time integration of stiff systems of differential equations.

A choice of target chemical species whose concentrations must be predicted with accuracy from the reduced scheme is enforced by the user (❷ Fig. 1). Typically, they are the molecules that are important in the calibration of the reactive flow problem under study. The reactants and the major products are obviously among those targets along with some intermediates essential radicals and eventually pollutants, for hydrocarbon combustion CO, NO, N_2O, NO_2, and soot precursors can be selected as additional targets. Also, if an intermediate species prediction fails after reduction, adding this species to the target list may help. All these target chemical species are fixed at the start of the process and modifying their list means restarting the reduction from scratch.

The chemical reduction is performed for a range of given operating conditions (i.e., temperature levels, concentrations in the feeding streams, and mass flow rates). Ideally, these conditions are those of the reactive flow system to which CFD will be applied. They are prescribed by the user and unchanged during all the reduction and optimization procedures.

For the retained detailed description of the chemical kinetics and the chosen operating conditions, reference evolutions of the chemistry from fresh reactants up to a given level of reaction progress (for instance chemical equilibrium or fully burnt products) are computed. These evolutions are obtained by solving for canonical reactive flow problems, such as reactors subjected to turbulent micro-mixing, and one-dimensional premixed and diffusion flames, the results are stored in the form of thermochemical trajectories, i.e. species and temperature evolutions versus time or a spatial coordinate (❸ Fig. 1).

In the case of turbulent micro-mixing, an unlimited number of inlets can be considered, including some corresponding to the recirculation of non-adiabatic reaction products. In every one of these inlets, stochastic particles carrying the vector of species mass fractions and temperature are injected, whose number is proportional to the relative contribution of this inlet to the total mass flow rate of the real system to be simulated afterward. Both the pairwise interaction Curl [18] and the Euclidean minimum spanning trees (EMST) [19] mixing models are available. (For combustion systems with nonpremixed inlets, it is advised to use EMST to better mimic the flame structure in composition space.) In addition to the stochastic particles, a single deterministic particle is also introduced in every inlet whose evolution is solved following the interaction with the mean (IEM) mixing model [20,21], also called the linear mean square estimation (LMSE) closure [22,23], to which the chemical source is added. These trajectories (❼) are useful to visualize in a compact form the response of chemistry versus time (see for instance Fig. 2).

The selection of turbulent micro-mixing as a canonical problem offers the possibility to study the concentration evolutions with various levels of turbulence/chemistry interactions. This may be very helpful

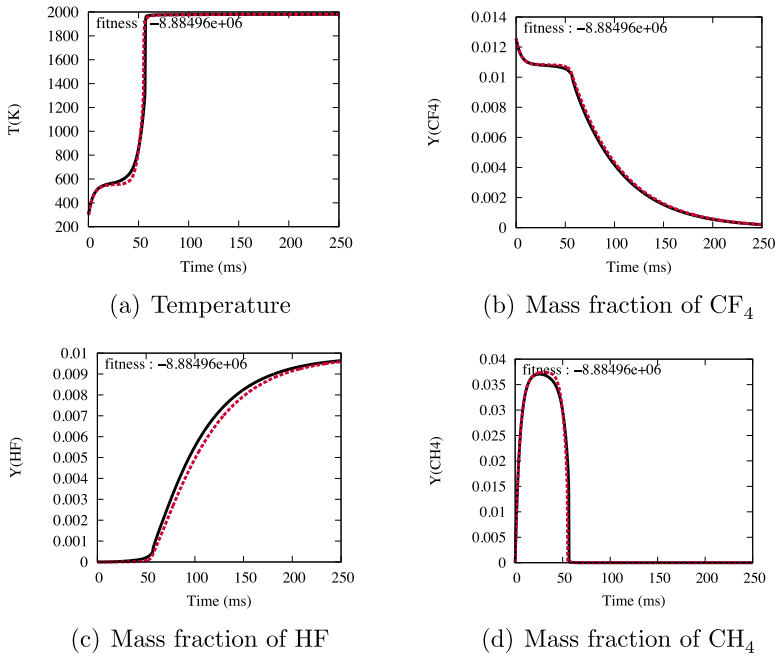

Fig. 2. Temperature, CF_4, HF, CH_4. Time evolutions from CF_4 inlet. Red: reduced mechanism Skeleton-3 (Table 1). Black: reference mechanism. (The shown fitness values correspond to a high level of accuracy.). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
List of reduced and optimized schemes. In skeleton-1, 2, and 3, all chemical rates are also optimized by GA.

Scheme type	*Conditions*	*#Species*	*#Reactions*
Skeleton-1	Case 1 & 2	30	76
Skeleton-2	Case 1	24	60
Skeleton-3	Case 2	30	55
Skeleton-4	Case 1 & 3	27	82

when applying reduced schemes to the simulation of turbulent flames. For instance, staged combustion with a secondary injection of air dilution can easily be mimicked by timing the introduction of additional air stochastic particles. Liquid fuel in the form of atomized spherical droplets can also be injected, the liquid fuel will heat-up and evaporate according to the prescribed liquid fuel properties. A formalism which can be extended to solid fuel particles with devolatilization and eventually char burning stages.

For one-dimensional flames, the fresh gas composition, temperature, and strain rate must be provided. Conditions for a set of flames covering a range of equivalence ratios or/and strain rates can be imposed.

The response collected over the trajectories is analyzed for the user-defined species target (❷) with the well-established Directed Relation Graph with Error Propagation method [15,16] (❹). The details on the exact implementation of DRGEP in ORCh, in terms of choices made to calibrate the criteria to rank species and reactions, and to measure the deviation from the detailed chemical kinetics, are given in [17]. The output of this step is a set of chemical schemes with a decreasing number of species and reactions involved (❺). Quasi-steady state assumption (QSS) can be tested and an algebraic system ready to be implemented in a CFD code is provided to deal with the species assigned to QSS.

Chemical trajectories are recomputed for every one of these schemes (❻) and global measures of the errors between detailed and reduced kinetics are returned [17]. Plots are also provided (❼) to compare with the reference detailed scheme so that the user can decide in fine which of the reduced schemes to select.

At this point, the reduced chemistry that provides satisfactory accuracy may require too many degrees of freedom to be useable in CFD. A more reduced scheme can then be selected to enter the rate optimization loop (❽, ❾, ❸, ❼) in which a genetic algorithm (GA) is cast to adjust (only a few % of variation is allowed) the pre-exponential constant, the temperature exponent, and the activation energy of every elementary reaction, so that the deviation to the reference response becomes minimum [17]. The trajectories are then recomputed for every member (set of parameters) of the population undergoing the evolution through the GA. The code is ready for parallel computing for this part. The output of the optimization loop is the scheme providing the best fit to the detailed chemistry response (❿). The deviation to the optimal parameters of the reference detailed scheme should be kept to very few % to preserve the thermochemical major properties of the kinetics. If significant variations of the parameters would be needed to reach convergence of the genetic algorithm, it is mandatory to return to the DRGEP step (❷) to add more species as targets.

Numerous chemical responses are generated during the computation of chemical trajectories. The database (Fig. 1) can also serve for the training of neural networks, as a substitute for the integration of stiff-chemical systems in CFD, examples of artificial neural networks trained by ORCh may be found in [14,24,25].

3. Illustrative example

So far the application of ORCh has been reported for various hydrocarbon combustion problems. This include laminar premixed and diffusion flames [17], flames propagating in channels with wall heat-loss [26], high Karlovitz number liquid kerosene turbulent combustion [27], selective non-catalytic reduction (SNCR) of nitrogen oxide emissions [28], sodium emission by solid fuel combustion [29], potassium emission during biomass combustion [30], high-pressure methane-oxygen combustion [31], and flameless combustion of residual steel gases [25].

The illustrative example given below is in a slightly different context that concerns the neutralization of tetrafluoromethane, CF_4. From the

Table 2
Left: Hydro-oxygenated elementary reactions. Right: CH_4 oxydation. Black: Common to cases 1, 2, and 3. Violet: Cases 1 and 2. Brown: Cases 1 and 3. Red: Case 1. Orange: Case 2. Blue: Case 3.

$H + O_2$	⇌	$O + OH$
$O + H_2$	⇌	$H + OH$
$OH + H_2$	⇌	$H + H_2O$
$2\,OH$	⇌	$O + H_2O$
$H_2 + O_2$	⇌	$HO_2 + H$
$H + O_2(^+M)$	⇌	$HO_2(^+M)$
$2OH(^+M)$	⇌	$H_2O_2(^+M)$
$HO_2 + O$	⇌	$OH + O_2$
$HO_2 + H$	⇌	$O + H_2O$
$HO_2 + H$	⇌	$2OH$
$2HO_2$	⇌	$O_2 + H_2O_2$
$OH + HO_2$	⇌	$H_2O + O_2$
$H_2O_2 + OH$	⇌	$HO_2 + H_2O$
$H_2O_2 + H$	⇌	$HO_2 + H_2$
$H_2O_2 + H$	⇌	$OH + H_2O$

$CO + O(^+M)$	⇌	$CO_2(^+M)$
$CO + OH$	⇌	$CO_2 + H$
$CO + HO_2$	⇌	$CO_2 + OH$
$HCO + M$	⇌	$CO + H + M$
$HCO + H_2O$	⇌	$CO + H + H_2O$
$HCO + O_2$	⇌	$CO + HO_2$
$CH_2 + O_2$	⇌	$CO_2 + 2\,H$
$CH_2^* + N_2$	⇌	$CH_2 + N_2$
$CH_2^{*+}O_2$	⇌	$H + OH + CO$
$CH_2O + H(^+M)$	⇌	$CH_3O(^+M)$
$CH_2O + H$	⇌	$HCO + H_2$
$CH_2O + O$	⇌	$HCO + OH$
$CH_2O + OH$	⇌	$HCO + H_2O$
$CH_2O + HO_2$	⇌	$HCO + H_2O_2$
$CH_3 + H(^+M)$	⇌	$CH_4(^+M)$
$CH_3 + O$	⇌	$CH_2O + H$
$CH_3 + OH(^+M)$	⇌	$CH_3OH(^+M)$
$CH_3 + OH$	⇌	$CH_2^* + H_2O$
$CH_3 + O_2$	⇌	$O + CH_3O$
$CH_3 + O_2$	⇌	$OH + CH_2O$
$CH_3 + HO_2$	⇌	$CH_4 + O_2$
$CH_3 + HO_2$	⇌	$CH_3O + OH$
$CH_3 + H_2O_2$	⇌	$CH_4 + HO_2$
$CH_3 + CH_2O$	⇌	$CH_4 + HCO$
$2\,CH_3(^+M)$	⇌	$C_2H_6(^+M)$
$CH_3O + H$	⇌	$CH_3 + OH$
$CH_3O + O_2$	⇌	$CH_2O + HO_2$
$CH_4 + H$	⇌	$CH_3 + H_2$
$CH_4 + O$	⇌	$CH_3 + OH$
$CH_4 + OH$	⇌	$CH_3 + H_2O$
$CH_3OH + OH$	⇌	$CH_3O^+H_2O$
$CH_3OH + CH_3$	⇌	$CH_3O + CH_4$

Table 3
Fluorocarbon elementary reactions. Black: Common to cases 1, 2, and 3. Violet: Cases 1 and 2. Brown: Cases 1 and 3. Red: Case 1. Orange: Case 2. Blue: Case 3.

$CHF_3 + H$	⇌	$CF_3 + H_2$
$CH_2F + H$	⇌	$CH_2^* + HF$
$CH_2F + OH$	⇌	$CH_2O + HF$
$CF_3 + O$	⇌	$CF_2{-}O + F$
$CF_3 + OH$	⇌	$CF_2{-}O + HF$
$HF + M$	⇌	$H + F + M$
$H_2 + F$	⇌	$H + HF$
$OH + F$	⇌	$O + HF$
$HO_2 + F$	⇌	$O_2 + HF$
$H_2O + F$	⇌	$OH + HF$
$H_2O_2 + F$	⇌	$HO_2 + HF$
$CH_3F(^+M)$	⇌	$CH_2^* + HF(^+M)$
$CF_4 + M$	⇌	$CF_3 + F + M$
$CH_3F + H$	⇌	$CH_3 + HF$
$CH_3F + H$	⇌	$CH_2F + H_2$
$CF_4 + H$	⇌	$CF_3 + HF$
$CHF_3 + O$	⇌	$CF_3 + OH$
$CHF_3 + OH$	⇌	$CF_3 + H_2O$
$CH_3F + OH$	⇌	$CH_2F + H_2O$
$CF_3 + H_2O_2$	⇌	$CHF_3 + HO_2$
$CF_3 + CH_4$	⇌	$CHF_3 + CH_3$
$CH_2O + CF_3$	⇌	$HCO + CHF_3$
$HCO + CF_3$	⇌	$CO + CHF_3$
$HCO + CF_3$	⇌	$CF_2CO + HF$
$CF_3 + O_2$	⇌	$CF_3O + O$
$CF_3 + HO_2$	⇌	$CF_3O + OH$
$CF_3 + HO_2$	⇌	$CHF_3 + O_2$
$CH_2F + HO_2$	⇌	$CH_3F + O_2$
$CF_3O + M$	⇌	$CF_2{-}O + F + M$
$CF_3O + H$	⇌	$CF_2{-}O + HF$
$CF_3O + H_2$	⟶	$CF_2{-}O + HF + H$
$CF_3O + H_2O$	⇌	$CF_2{-}O + HF + OH$
$CF_3O + CH_4$	⇌	$CF_2{-}O + HF + CH_3$
$CF_2{-}O + H_2O$	⟶	$CO_2 + HF + HF$
$CF_2{-}O + OH$	⟶	$CO_2 + F + HF$
$CF_3 + CF_3(^+M)$	⇌	$CF_3{-}CF_3(^+M)$
$CH_3 + CF_3$	⇌	$CH_2{-}CF_2 + HF$
$CF_3 + CH_2$	⇌	$CH_2{-}CF_2 + F$
$CF_2CO + O$	⇌	$CF_2{-}O + CO$
$CH_4 + F$	⇌	$CH_3 + HF$
$CF_3CHO(^+M)$	⇌	$CF_2CO + HF(^+M)$
$CF_3O + CO$	⟶	$CO_2 + CF_3$
$CH_3F + F$	⇌	$CH_2F + HF$
$CH_2O + F$	⇌	$HCO + HF$
$CF_4 + CH_3$	⇌	$CH_3F + CF_3$

detailed mechanism by Burgess et al. [32] (188 species and 1489 reactions), reduced schemes specialized to different operating conditions are obtained (Table 1).

At room temperature, the free decomposition of fluorinated gases (or F-gases: perfluorocarbons PFCs, hydrofluorocarbons HFCs, and sulfur hexafluoride SF_6) is extremely slow due to their tetrahedral structure and strong C-F bond [33], especially the tetrafluoromethane (CF_4), featuring about 50 000 years of atmospheric lifetime. These F-gases, such as CF_4, C_2F_6, and C_3F_8, possess an intense global warming potential (GWP), which is several thousand times higher than the GWP of CO_2, mostly because of this long atmospheric lifetime and strong absorption coefficient in the infrared spectrum.

Injecting CF_4 in burning natural gas is a well-established process to secure its transformation with a removal efficiency reaching up to 90% [34]. The numerical simulation of these specialized combustion systems implies accounting for the complexity of the simultaneous oxidation chemistry of methane (CH_4) and CF_4. These systems operate in the nonpremixed combustion regime, usually with a swirling flame, the reduction is then performed in the non-premixed context, with the EMST [19] stochastic micro-mixing to mimic the effect of turbulence on the reacting mixture.

Chemical schemes of decreasing complexity are derived and optimized for three cases featuring a variety of gas compositions that will mix and react:

- In case 1, a CF_4 effluent is studied and the reaction zones are fed by three fluxes containing respectively: (i) Air enriched in O_2 and carrying CF_4 at 300 K for 88.98% of the total mass flow rate $\dot{Q}_m$, and with the mass fractions $Y_{O_2} = 0.4080$, $Y_{N_2} = 0.5822$ and $Y_{CF_4} = 0.0098$. (ii) Pure CH_4 at 300 K for 5.85% of $\dot{Q}_m$. (iii) Pilot flame gases at the equilibrium temperature of the fully burnt composition of a stoichiometric CH_4/Air flame for 5.17% of $\dot{Q}_m$.
- Case 2, is similar to case 1 but with different concentrations and mass flow rates: (i) 300 K for 86.21% of $\dot{Q}_m$ with $Y_{O_2} = 0.3441$, $Y_{N_2} = 0.6432$ and $Y_{CF_4} = 0.0127$. (ii) CH_4 for 3.79% of $\dot{Q}_m$. (iii) Pilot flame for 10% of $\dot{Q}_m$.
- Case 3 is representative of a four fluxes composition: (i) Air enriched in O_2 with H_2O, $Y_{O_2} = 0.4157$, $Y_{N_2} = 0.4908$, $Y_{H_2O} = 0.0935$ at 373 K for 64.38% of $\dot{Q}_m$. (ii) CH_4 at 300 K for 3.43% of $\dot{Q}_m$. (iii) Pilot flame for 10.71% of $\dot{Q}_m$. (iv) C_xF_y flux at 300 K for 21.48% of $\dot{Q}_m$, with $Y_{N_2} = 0.0234$, $Y_{CF_2O} = 0.0606$, $Y_{C_2F_6} = 0.6034$, $Y_{CF_4} = 0.1386$, $Y_{CHF_3} = 0.0040$ and $Y_{CO} = 0.1700$.

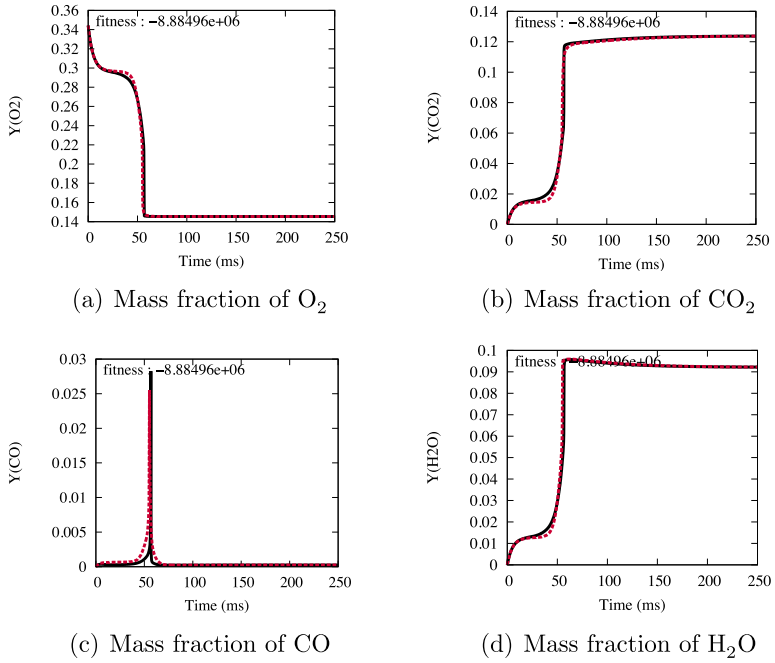

Fig. 3. O_2, CO_2, CO, H_2O. Time evolutions from CF_4 inlet. Red: reduced mechanism Skeleton-3 (Table 1). Black: reference mechanism. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1 summarizes the obtained chemical schemes available in the supplementary material.

In the building of the skeleton schemes, the dominant paths as returned by ORCh are organized into three groups: (a) hydro-oxygenated (H_2,O_2) and (b) hydrocarbon (C_xH_y,O_2) shown in Table 2; (c) fluorocarbon (C_xF_y,C_xH_y,O_2) in Table 3. To illustrate the automated schemes adaptation to given operating conditions, the elementary reactions in black are those common to Case 1, 2 and 3; in violet those specific to Case 1 and 2, and in brown to case 1 and 3. The elementary reactions in red are specific to Case 1 (synthetic effluent), the reactions in orange are specific to Case 2 (synthetic effluent), and the reactions in blue are specific to Case 3 (representative industrial composition).

Fig. 2 and Fig. 3 illustrate results obtained with the Skeleton-3 mechanism of Table 1. The deterministic trajectory (IEM/LMSE model plus reaction) issued from the CF_4 inlet is shown. The mixing with burnt gases, CH_4 (Fig. 2(d)) and O_2 (Fig. 3(a)) promotes ignition of the mixture at about 50 ms (Fig. 2(a)), that is followed by the decomposition of CF_4 (Fig. 2(b)) into HF (Fig. 2(c)). The results obtained with the reduced mechanism are quite close to those of the reference detailed one, also for CO, CO_2 and H_2O (Fig. 3).

The careful reproduction of the ignition delay observed here is mandatory in many combustion systems, as it also opens perspectives on the modeling of related phenomena, such as the minimum spark ignition energy. Then, the generated skeletal mechanisms are likely to perform well in other combustion configurations/scenarios. The precise reproduction of the ignition delay is secured after applying the genetic algorithm for optimization of the kinetics parameters. The genetic algorithm is in particular useful to match multiple canonical problems with a single reduced chemical scheme [17].

4. Conclusion

C++ routines are proposed to analyze the response of detailed chemical kinetics through various canonical flow problems. The objective is to determine the most influential species and elementary reactions for given operating conditions, to reduce the chemistry for its subsequent use in Computational Fluid Dynamics. The code returns a set of chemical schemes of decreasing complexity, optionally with quasi-steady state analytical relations for some intermediate species. If needed, a genetic algorithm optimizes the rates of the elementary reactions of the reduced scheme.

CRediT authorship contribution statement

Nicolas Jaouen: Writing – review & editing, Validation, Software, Project administration, Methodology, Conceptualization. **Huu-Tri Nguyen:** Writing – review & editing, Visualization, Validation, Software, Methodology, Investigation. **Pascale Domingo:** Writing – review & editing, Supervision, Project administration, Methodology, Conceptualization. **Luc Vervisch:** Writing – review & editing, Writing – original draft, Supervision, Project administration, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.softx.2024.101819.

References

[1] Turanyi T, Tomlin AS. Analysis of kinetic reaction mechanisms. Berlin: Springer; 2014, p. 357.
[2] Zhu L, Panigrahy S, Elliott SN, Klippenstein SJ, Baigmohammadi M, Mohamed AAE-S, et al. A wide range experimental study and further development of a kinetic model describing propane oxidation. Combust Flame 2023;248:112562.

[3] Mao Q, Pratali Maffei L, Pitsch H, Faravelli T. Theoretical study of important phenylacetylene reactions in polycyclic aromatic hydrocarbon growth. Combust Flame 2024;261:113300.
[4] Warth V, Stef N, Glaude P-A, Battin-Leclerc F, Scacchi G, Côme G-M. Computer-aided derivation of gas-phase oxidation mechanisms: application to the modeling of the oxidation of n-butane. Combust Flame 1998;114(1–2):81–102.
[5] Liu B, Di Q, Lailliau M, Belhadj N, Dagaut P, Wang Z. Experimental and kinetic modeling study of low-temperature oxidation of n-pentane. Combust Flame 2023;254:112813.
[6] Zhang P, Zsély IG, Samu V, Nagy T, Turányi T. Comparison of methane combustion mechanisms using shock tube and rapid compression machine ignition delay time measurements. Energy & Fuels 2021;35(15):12329–51.
[7] Goussis DA, Maas U. Model reduction for combustion chemistry. In: Echekki T, Mastorakos E, editors. Turbulent combustion modeling: advances, new trends and perspectives. Dordrecht: Springer Netherlands; 2011, p. 193–220.
[8] Jones WP, Lindstedt RP. Global reaction schemes for hydrocarbon combustion. Combust Flame 1988;73:233–49.
[9] Peters N. Systematic reduction of flame kinetics: Principles and details. In: Kulh AL, Bowen JR, Leyer J-C, Boris A, editors. Dynamics of reactive systems. no. 113, Washington, DC; 1988, p. 67–86.
[10] Maas U, Pope S. Simplifying chemical kinetics: Intrinsic low-dimensional manifolds in composition space. Combust Flame 1992;88:239–64.
[11] Gicquel O, Darabiha N, Thevenin D. Laminar premixed hydrogen / air counterflow flame simulations using flame prolongation of ILDM with differential diffusion. Proc Combust Inst 2000;28:1901–8.
[12] van Oijen JA, Donini A, Bastiaans RJM, ten Thije Boonkkamp JHM, de Goey LPH. State-of-the-art in premixed combustion modeling using flamelet generated manifolds. Progr Energy Combust Sci 2016;57:30–74.
[13] Pope SB. Computationally efficient implementation of combustion chemistry using in situ adaptive tabulation. Combust Theory Model 1997;1:41–63.
[14] Wan K, Barnaud C, Vervisch L, Domingo P. Chemistry reduction using machine learning trained from non-premixed micro-mixing modeling: Application to DNS of a syngas turbulent oxy-flame with side-wall effects. Combust Flame 2020;220:119–29.
[15] Lu T, Law CK. A directed relation graph method for mechanism reduction. Proc Combust Inst 2005;30(1):1333–41.
[16] Pepiot P, Pitsch H. An efficient error propagation based reduction method for large chemical kinetic mechanisms. Combust Flame 2008;154(1–2):67–81.
[17] Jaouen N, Vervisch L, Domingo P, Ribert G. Automatic reduction and optimisation of chemistry for turbulent combustion modeling: Impact of the canonical problem. Combust Flame 2017;175:60–79.
[18] Curl RI. Dispersed phase mixing. Theory and effects in simple reactors. AIChE 1963;9(2):175–81.
[19] Subramaniam S, Pope SB. A mixing model for turbulent reactive flows based on euclidean minimum spanning trees. Combust Flame 1998;115(4):487–514.
[20] Villermaux J. Micromixing phenomena in stirred reactors. Encycl Fluid Mech 1986;707.
[21] Aubry C, Villermaux J. Représensation du mélange imparfait de deux courants de réactifs dans un réacteur agité continu. J Chem Eng Sci 1975;30(5–6):457–64.
[22] Dopazo C. Relaxation of initial probability density functions in the turbulent convection of scalar fields. Phys Fluids 1979;22(1):20–30.
[23] Dopazo C. Non-isothermal turbulent reactive flows: stochastic approaches (Ph.D. thesis), University of New York, Stony Brook; 1973.
[24] Nguyen H-T, Domingo P, Vervisch L, Nguyen P-D. Machine learning for integrating combustion chemistry in numerical simulations. Energy & AI 2021;5(100082).
[25] Nguyen H-T, Barnaud C, Domingo P, Nguyen P-D, Vervisch L. Large-eddy simulation of flameless combustion with neural-network driven chemistry. Appl Energy Combust Sci 2023;(14):100126.
[26] Bioche K, Ribert G, Vervisch L. Simulating upstream flame propagation in a narrow channel after wall preheating: Flame analysis and chemistry reduction strategy. Combust Flame 2019;200:219–31.
[27] Bouaniche A, Jaouen N, Domingo P, Vervisch L. Vitiated high karlovitz n-decane/air turbulent flames: Scaling laws and micro-mixing modeling analysis. Flow Turbul Combust 2019;102(1):235–52.
[28] Locci C, Vervisch L, Farcy B, Perret N. Selective non-catalytic reduction (SNCR) of nitrogen oxide emissions: A perspective from numerical modeling. Flow Turbul Combust 2018;100(2):301–40.
[29] Wan K, Vervisch L, Gao Z, Domingo P, Jiang C, Wang Z, et al. Reduced chemical reaction mechanisms for simulating sodium emissions by solid-fuel combustion. Appl Energy Combust Sci 2020;(1–4):100009.
[30] Wan K, Vervisch L, Jianga C, Domingo P, Gao Z, Xia J, et al. Development of reduced and optimized reaction mechanism for potassium emissions during biomass combustion based on genetic algorithms. Energy 2020;(211):118565.
[31] Monnier F, Ribert G. Simulation of high-pressure methane-oxygen combustion with a new reduced chemical mechanism. Combust Flame 2022;235:111735.
[32] Burgess DR, Babushok VI, Linteris GT, Manion JA. A chemical kinetic mechanism for 2-bromo-3, 3, 3-trifluoropropene (2-BTP) flame inhibition. Int J Chem Kinetics 2015;47(9):533–63.
[33] Qin L, Han J, Wang G, Kim H, Kawaguchi I. Highly efficient decomposition of CF_4 gases by combustion. 2010.
[34] Chang MB, Chang J-S. Abatement of PFCs from semiconductor manufacturing processes by nonthermal plasma technologies: A critical review. Ind Eng Chem Res 2006;45(12):4101–9.