Ansys Model Fuel Library Getting Started Guide

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Chapter 1: Introduction

The Ansys Model Fuel Library (MFL) is a library of detailed and validated reaction mechanisms for over 60 fuel components, which are relevant to combustion simulations in a wide variety of industrial and commercial applications. The fuel components can be used to represent gaseous or liquid fuel combustion for petroleum-derived or alternative fuels. Gaseous components address natural gas, synthetic gas, biofuels, and blends. For liquid fuels, the fuel components can be used in formulating surrogates for a wide range of real-world fuels, including gasoline, diesel, jet-fuel, alternative fuels, fuel blends, and additives.

The reaction mechanisms are suitable for many combustion applications, including spark-ignition engines, compression-ignition engines, gas- and liquid-fired turbine combustors, boilers, flares, and furnaces. The mechanisms have been extensively validated for operating conditions covering a wide range of pressures, temperatures, equivalence ratios, and dilutions. The mechanisms are constructed in a self-consistent manner and follow a rate-rule–based approach for liquid components that results in predictive capabilities for the mechanisms. The predictive capabilities of library mechanisms are not limited to combustion characteristics of the fuels, but also include fuel effects on emissions and combustion intermediates, along with soot particle size and number densities. The Model Fuel Library is based on both the outcome of the industry-driven Model Fuel Consortium (2006-2012) project and the ongoing Model Fuel Library Subscription Service that maintains the Library to keep it up-to-date with the state of current combustion science.

The current Model Fuel Library offering is encrypted for use with Ansys software, including Chemkin, Reaction Workbench, Forte, and Fluent (starting with version 16.0). With the Model Fuel Library, it is possible to model most real fuels by either exactly representing the chemical properties of the fuel or by formulating an appropriate surrogate. We recommend using Ansys Chemkin/Reaction Workbench to formulate surrogates for liquid fuels and also for reducing the full reaction mechanism to provide smaller mechanisms that can be tailored for a particular application (for example, for use in Computational Fluid Dynamics engine simulation).

In addition to the "full" mechanisms, the MFL provides a suite of pre-reduced mechanisms that have been reduced for specific applications and specific fuel compositions. These pre-reduced mechanisms can be used without modification for many applications, or can serve as a starting point for further reduction using a narrower range of operating conditions. In addition, PERK mechanisms installed under the MFL folder may be of interest, as these are developed to keep the mechanism size small while enabling the ability to capture a broader range of conditions than with models containing global reaction steps (see MFL Pseudo-Elementary Reaction Kinetics (PERK) Mechanisms (p. 24)).

The `.inp` file associated with an MFL mechanism includes both the species thermodynamic data and the reaction mechanism. Ansys Fluent provides a check box to indicate that the thermodynamic data is included in this way (see The Import CHEMKIN Format Mechanism Dialog Box for Volumetric Kinetics in the *Fluent User's Guide*).

Table 1.1: Components in the Model Fuel Library (p. 2) shows the list of surrogate components available in the MFL database.

Table 1.1: Components in the Model Fuel Library

Fuel Class	Component	Gasoline	Diesel	Jet Fuel or FT fuels	Natural or Synthetic Gas	Biofuels or Additives	Phase
		Relevant for Modeling					
Hydrogen	hydrogen						G
n-Alkanes	*n*-eicosane		✔				L
	n-octadecane		✔				L
	n-hexadecane		✔	✔			L
	n-tetradecane		✔	✔			L
	n-dodecane		✔	✔			L
	n-decane	✔	✔	✔			L
	n-nonane	✔	✔	✔			L
	n-octane	✔	✔	✔			L
	n-heptane	✔	✔	✔			L
	n-hexane*1*	✔	✔	✔			L
	n-pentane*1*	✔	✔		✔		L
	n-butane	✔			✔		G
	propane				✔		G
	ethane				✔		G
	methane				✔		G
iso-Alkanes	Heptamethylnonane		✔	✔			L
	i-dodecane		✔	✔			L
	i-octane	✔	✔	✔			L
	i-hexane	✔	✔	✔			L
	i-butane	✔			✔		G
1-Ring aromatics	Benzene	✔		✔			L
	Toluene	✔	✔	✔			L
	n-propylbenzene	✔	✔	✔			L
	n-butylbenzene	✔	✔	✔			L
	Ethylbenzene	✔	✔	✔			L
	o-xylene	✔	✔	✔			L
	m-xylene	✔	✔	✔			L
	p-xylene	✔	✔	✔			L
	1,2,4-trimethylbenzene	✔	✔	✔			L

2-Ring aromatics	naphthalene		✔	✔			L
	1-methylnaphthalene	✔	✔	✔			L
	Cyclopentane	✔					L
Cycloalkanes/ Naphthenes	Cyclohexane	✔	✔	✔			L
	Methylcyclohexane	✔	✔	✔			L
	Decalin	✔	✔	✔			L
Olefins	2-methyl-2-butene	✔	✔	✔			L
	1-hexene	✔	✔	✔			L
	2-hexene	✔	✔	✔			L
	3-hexene	✔	✔	✔			L
	1-pentene	✔	✔	✔			L
	2-pentene	✔	✔	✔			L
Oxygenated fuels	Carbon Monoxide				✔		G
	Methanol				✔	✔	L
	Ethanol	✔				✔	L
	n-Butanol	✔	✔			✔	L
	Tetrahydro furan	✔	✔	✔		✔	L
	ETFE (ethyltetrahydrofurfurylether)	✔	✔	✔		✔	L
	Methyl butanoate	✔	✔	✔		✔	L
	Methyl palmitate	✔	✔	✔		✔	L
	Methyl stearate	✔	✔	✔		✔	L
	Methyl oleate	✔	✔	✔		✔	L
	Methyl linoleate	✔	✔	✔		✔	L
	Methyl linolenate	✔	✔	✔		✔	L
Additives	DME (dimethyl ether)						L
	ETBE (ethyl tert-butyl ether)						L
	MTBE (methyl tert-butyl ether)						L
	H2S		✔				G
	Calcium Carbonate	✔					S
Soot precursors and emissions pathways	1,3-butadiene						G
	Propene						G
	Allene						G
	Acetylene						G
	Ethylene				✔		G
	Propyne						G
	Formaldehyde						L
	PAH formation						-
	Soot		✔				S

	NOx						G

Ratings of each of the available component mechanisms are listed in the following section. These ratings are qualitative. They summarize both the accuracy of the mechanism based on validation against fundamental kinetics data and our assessment of the expected predictive capabilities of that component mechanism. In some cases, the assessment is limited by availability of appropriate experimental data for validation. Also discussed in the next chapter is the applicability of those components in formulating surrogates for various fuels.

The documentation is now separate for:

- Descriptions of the component mechanisms for each fuel class
- Summaries of the validation for the components and blends

  The **Model Fuel Library Validation Manual** (formerly named *Model Fuel Library Manual*) is a PDF file that is located in the `docs` subfolder under the main Ansys Chemkin installation location. You can access it via the Windows **Start** menu.

An appropriate MFL full or a pre-reduced mechanism for the tailored fuel model can further be reduced using the targeted mechanism reduction capability in Ansys Chemkin Reaction Workbench. Refer to the Reaction Workbench Tutorial Guide and Mechanism Reduction Best Practices for more information.

1.1. Location of the MFL Mechanisms

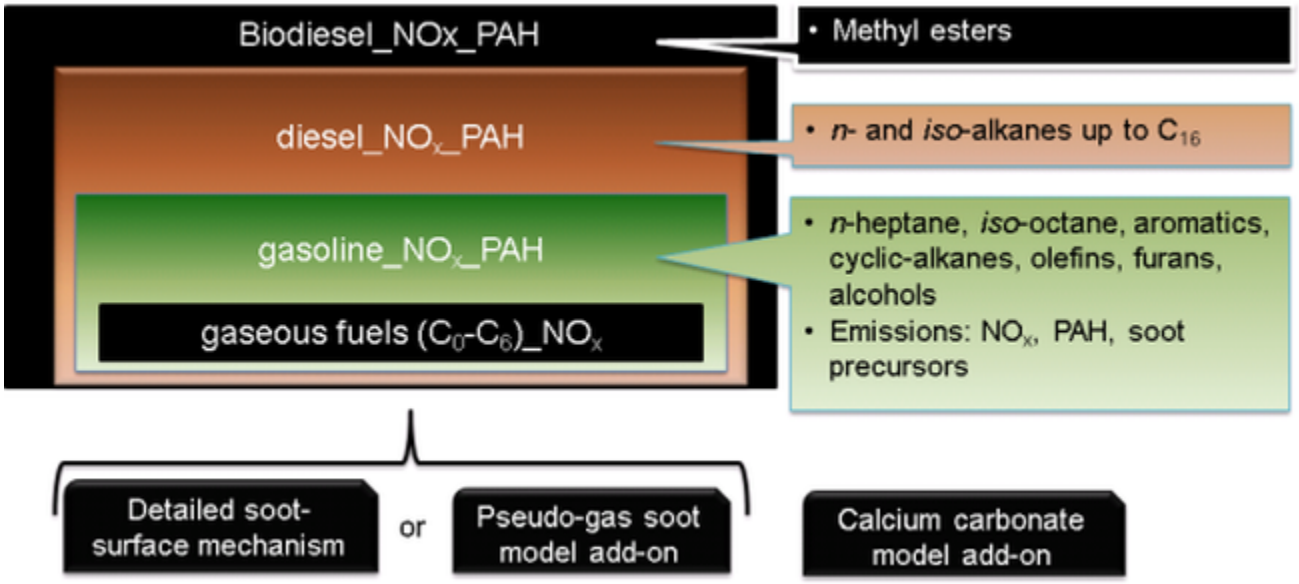
The Ansys MFL mechanisms are installed under the main Ansys install location, in the `reaction\data\ModelFuelLibrary` subfolder. Under the `ModelFuelLibrary` subfolder, all the full mechanisms are located in the subfolder named `Master`, and all the pre-reduced mechanisms are in the subfolder `Reduced`. For assistance with installation, log in to the Ansys Help site and search for or select "Installation and Licensing".

Chapter 2: Overview of the MFL Mechanisms

The Model Fuel Library (MFL) includes "full" mechanisms that contain comprehensive details of the fuel combustion chemistry for the fuel components. These typically need to be reduced before applying to engine CFD simulations. In addition, several pre-reduced mechanisms for common fuel types are included that allow direct use in CFD. The pre-reduced mechanisms may be further reduced for narrower ranges of conditions or simulation targets, if desired.

2.1. MFL Full Mechanisms

Figure 2.1: Hierarchy of the full mechanisms in the Model Fuel Library



The hierarchical structure of the full mechanisms is depicted in Figure 2.1: Hierarchy of the full mechanisms in the Model Fuel Library (p. 5). The full mechanisms for the gas-phase reactions are described below.

1. **GaseousFuels_C0-C6_NOx**: This mechanism is designed for combustion simulations involving gaseous fuels, such as syngas, natural gas, etc. The mechanism includes the essential "core" chemistry that involves reactions of species with carbon number 4 (C4) and smaller. The core mechanism is the most critical component of all the mechanisms, because most components, even the large heavy components, break down during combustion and create smaller species that then undergo reactions included in the core mechanism. This mechanism can predict CO and hydrocarbon emissions up to benzene. The component mechanism for soot-precursor species, except for PAH, are included. The submechanisms for NO_x emissions and sulfur emissions are also included. This mechanism also contains reactions of the additives methanol, ethanol, *n*-butanol, tetrahydrofuran, DME, and MTBE. This mechanism has 1532 species and 10469 reactions.

2. **Gasoline_NOx_PAH**: This mechanism is a superset of and therefore inherits all the capabilities of the GaseousFuels_C0-C6_NOx mechanism. In addition, it has reactions for components for gasoline surrogates. These include *n*-alkanes components up to 'C7,' *iso*-alkanes up to C8, olefins up to C6, all aromatic components, all cycloalkane components, and other components for formulating a gasoline surrogate, as listed in the mechanism ratings in the *Model Fuel Library Validation Manual*. The submechanism for ETFE is included. This mechanism also includes the PAH chemistry that is necessary for use with soot models. This mechanism has 3173 species and 22,857 reactions.

3. **Diesel_NOx_PAH**: In addition to the capabilities of the Gasoline_NOx_PAH mechanism, larger alkanes useful for formulating surrogates for diesel and jet fuels are included in this mechanism. These include *n*-Alkanes up to C20 and the *iso*-alkanes: *iso*-dodecane (C12H26) and heptamethylnonane (C16H34). This mechanism has species 6297 and 72,685 reactions.

4. **Biodiesel_NOx_PAH**: This is the superset of all the mechanisms in the MFL database. This mechanism extends the capabilities of the Diesel_NOx_PAH mechanism to modeling biodiesel and biodiesel/diesel blends. The components included are methyl esters that range from the small component, methyl-butanoate, to heavy components, such as methyl linolenate, as listed in the mechanism ratings in the *Model Fuel Library Validation Manual*. This mechanism has 10,436 species and 88,327 reactions.

5. **Electrolyte**: This mechanism is designed for lithium-ion battery thermal runaway applications. It includes the gas-phase combustion chemistry of the electrolytes ethylene carbonate (EC), dimethyl carbonate (DMC), diethyl carbonate (DEC), and ethyl methyl carbonate (EMC). The mechanism has 227 species participating in 1551 reactions.

2.2. MFL Pre-Reduced Mechanisms

MFL mechanisms provide detailed descriptions of various combustion and emissions processes. They are applicable over a broad range of conditions and include chemistry for many fuel components and their blends. The full MFL mechanisms can be used directly for many reactor models in Ansys Chemkin.

Tip:

For flame simulations in Chemkin, a high-temperature version of the full mechanism can be easily extracted in one step using Reaction Workbench.

However, most CFD applications require that the full mechanisms be reduced. Mechanism reduction can be performed using Reaction Workbench, which contains various reduction methods, such as DRG, DRGEP, DFGPFA, sensitivity analysis combined with DRG or DRGEP or DFGPFA, automatic isomer lumping, full sensitivity analysis, and more. Using these methods iteratively with the Mechanism Reduction Sessions facility in Reaction Workbench can effectively reduce a mechanism so that it can be used in many CFD applications, including Ansys Forte and Ansys Fluent.

Mechanism reduction is performed for a specific fuel surrogate of interest and for specific conditions of interest to the CFD application. Therefore, a reduced mechanism is accurate only for the fuels and conditions used for the reduction. We have pre-selected components for different conventional fuels

and reduced their mechanisms for typical operating conditions. Table 2.1: Reduced mechanisms provided with the MFL (p. 7) shows the details of these pre-reduced mechanisms.

Table 2.1: Reduced mechanisms provided with the MFL

Fuel	Surrogate Components	Species name	Low-T auto-ignition	CO, HC, NOx emissions	Num. of species	Soot models that can be used with reduced mechanism
Hydrogen	hydrogen	h2			11	N/A
Hydrogen + Ammonia	hydrogen, ammonia	h2, nh3		NOx	33	N/A
Natural gas[a]	methane	ch4	x	✓	35	Acetylene-based empirical
	93 vol% methane/ 5% ethane/ 2% *n*-butane	93 vol% ch4/ 5% c2h6/ 2% c4h10	✓	✓	70	(a) Acetylene-based empirical
					76	(b) Pseudo-gas
					113	(c) Detailed soot-surface model
Propane	propane	c3h8	✓	✓	63	(a) Acetylene-based empirical
					114	(b) Pseudo-gas
Methanol	methanol	ch3oh	✓	✓	33	Acetylene-based empirical
Ethanol	ethanol	c2h5oh	✓	✓	48	Acetylene-based empirical
Gasoline	*iso*-octane	ic8h18	x	✓	61	Acetylene-based empirical
	22.4 wt% *iso*-octane/ 30.4% toluene/ 19.1% *n*-pentane/ 11.2% MCH/ 7.5% 1-hexene/ 7.3% 1,2,4-trimethyl benzene/ 2.1% *n*-butane	22.4 wt% ic8h18/ 30.4% c6h5ch3/ 19.1% nc5h12/ 11.2% mch/ 7.5% c6h12-1/ 7.3% tmb124/	✓	✓	192	(a) Acetylene-based empirical
					194	(b) Pseudo-gas
					259	(c) Detailed soot-surface model

		2.1% c4h10				
Diesel	*n*-heptane	nc7h16	✓	✓	119	(a) Acetylene-based empirical
					133	(b) Pseudo-gas
	36 wt% *n*-hexadecane/ 9.7% AMN/ 16.4% HMN/ 38.9% decalin	36 wt% nc16h34/ 9.7% a2ch3/ 15.4% hmn/ 38.9% decalin	✓	✓	233	(a) Acetylene-based empirical
					291	(b) Pseudo-gas
					329	(c) Detailed soot-surface model
Jet fuel	*n*-dodecane	nc12h26	x	✓	82	Acetylene-based empirical
	36.6 wt% *n*-dodecane/ 32.2% heptamethylnonane/ 10.3% methylcyclohexane/ 20.9% 1,2,4-trimethylbenzene	36.6 wt% nc12h26/ 32.2% hmn/ 10.3% mch/ 20.9% tmb124	✓	✓	196	(a) Acetylene-based empirical
					222	(b) Pseudo-gas
					296	(c) Detailed soot-surface model
SAF	*iso*-undecane	c11h24-2		✓	96	Acetylene-based empirical
Battery electrolytes EC, DMC, DEC	25 mol% dimethyl carbonate / 25 mol% ethylene carbonate / 25 mol% diethyl carbonate / 25 mol% ethyl methyl carbonate	25 mol% dmc / 25 mol% ec / 25 mol% dec / 25 mol% emc	✓	✓	86	

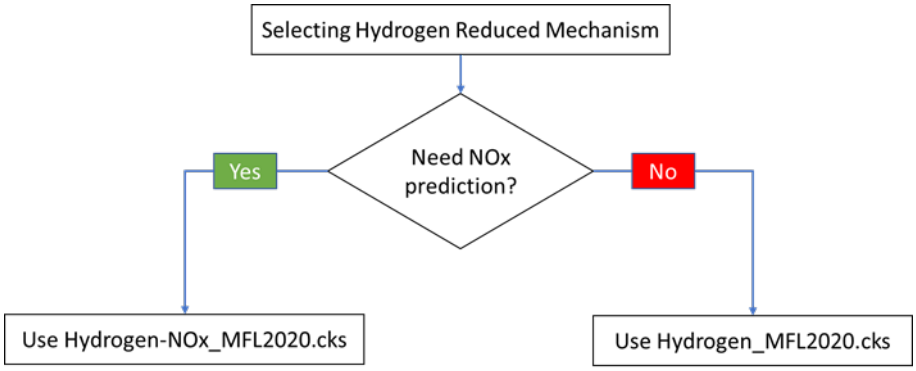
[a] May be used for blends with hydrogen.

Many empirical soot models use only acetylene as the soot precursor. The MFL pseudo-gas soot model is expected to be more accurate than a 2-step empirical model, as it employs acetylene, benzene, and phenyl as soot precursors and has been shown to be predictive over a wide range of fuels and operating conditions. The pseudo-gas soot model can predict soot mass but not particle sizes. The detailed soot-surface chemistry employs more soot precursors and when used with the Method of Moments or Sectional Method can predict soot particle sizes.

The reduced mechanisms for the pre-selected fuels and conditions are applicable for the conditions specified in the table. They should not be used for conditions outside of their range. However, for the multi-component fuels, it should be acceptable to modify the blend as described in the *Model Fuel Library Validation Manual*.

2.2.1. Hydrogen and Ammonia Mechanisms

Figure 2.2: Decision flowchart for selecting MFL hydrogen mechanism



Two chemistry sets for hydrogen fuel (mechanism name: h2) have been included. The second, `Hydrogen-Ammonia-NOx_MFL2021.cks` , can also be used for ammonia:

1. `Hydrogen_MFL2021.cks`
2. `Hydrogen-Ammonia-NOx_MFL2021.cks`

The focus of both the chemistry sets is on modeling combustion. They can be used to simulate characteristics such as autoignition, flames, and NO_x emissions. The chemistry sets include full detailed kinetics and are applicable over a broad range of conditions. They also include the 3rd-body effects of argon and helium.

This hydrogen chemistry set forms the core of the other full MFL mechanisms. It has been thoroughly validated against fundamental experimental data for the operating conditions of interest for gas turbines.

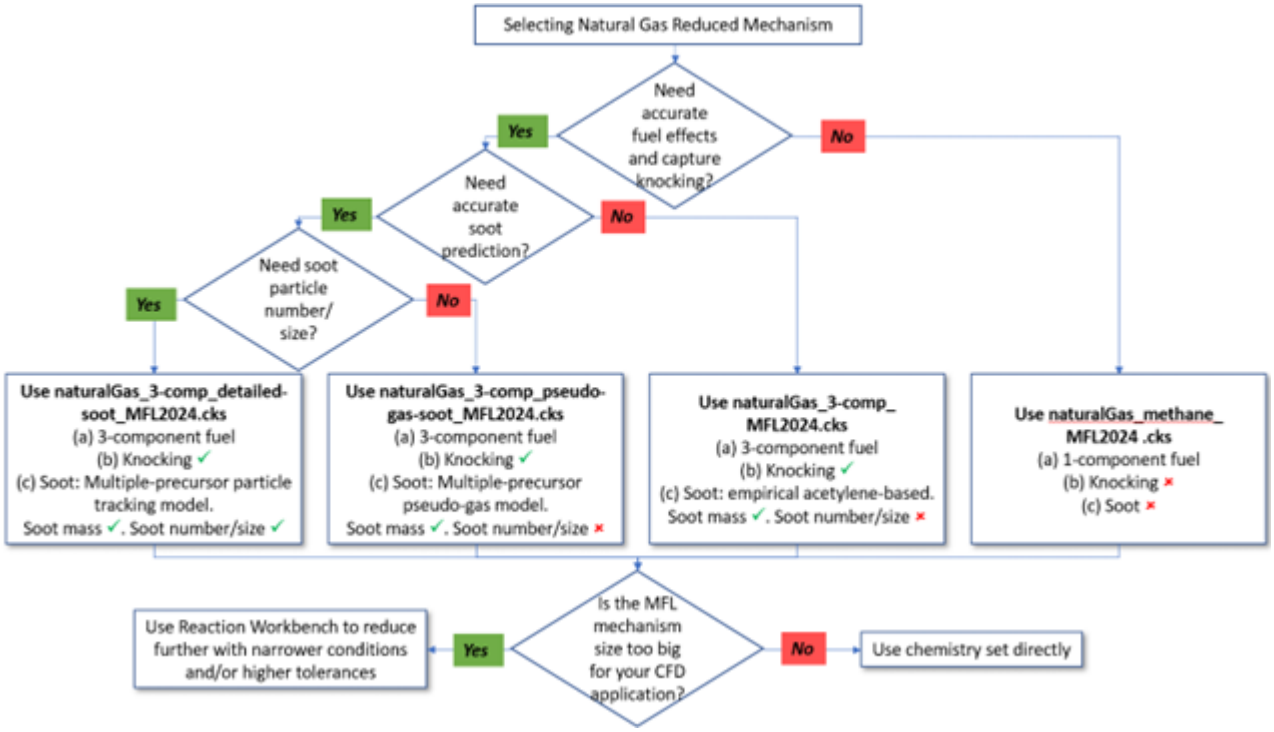
Note:

The hydrogen mechanisms are provided in an open form that can be used in any software. If used in your publication, cite "Ansys, Model Fuel Library. 2024."

2.2.2. Natural Gas Mechanisms

Four natural gas reduced mechanisms are available. The flowchart shown in Figure 2.3: Decision flowchart for selecting MFL natural gas mechanism (p. 10) summarizes the applicability of the four mechanisms. More details of these four mechanisms are presented in the subsections below.

Figure 2.3: Decision flowchart for selecting MFL natural gas mechanism



2.2.2.1. Single-component Natural Gas

The **naturalGas_methane_MFL2024.cks** chemistry set represents natural gas with methane (mechanism name: **ch4**) as a surrogate. The focus of this chemistry set is on modeling combustion at high-temperatures in gas turbines. This chemistry can be used to predict CO, HC (hydrocarbons), and NO_x emissions from turbines. The mechanism has been reduced for the following range of conditions:

1. Pressure: 10–100 bar
2. Temperature: 1000–2000 K
3. Equivalence ratio: 0.4–2
4. EGR: 0–20%

This mechanism has been reduced from the full mechanism "GaseousFuels_C0-C6_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for gas turbines. The mechanism was reduced from this comprehensive full mechanism using the Reaction Workbench software, for the conditions listed above. A high-temperature kinetics filter was used as a first-step for mechanism reduction prior to using other reduction methods in Ansys Reaction Workbench.

2.2.2.1.1. Multi-component Natural Gas

For multi-component natural gas, the surrogate used is 93/ 5/ 2 vol% Methane/ ethane/ *n*-butane. There are three chemistry sets for natural gas with this 3-component surrogate:

1. `naturalGas_3-comp_MFL2024.cks`

2. `naturalGas_3-comp_pseudo-gas-soot_MFL2024.cks`

3. `naturalGas_3-comp_detailed-soot_MFL2024.cks`

The difference between the three chemistry sets is the soot model they can be used with; they are any acetylene-based empirical soot model, the pseudo-gas soot model, and the Method of Moments soot model, respectively. The chemistry set may be applied to compositions that are different from this, provided that methane is the dominant component. We recommend lumping other C2 content into the fraction represented by ethane and lumping heavier-than-C2 hydrocarbons into the fraction for *n*-butane. The focus of this chemistry set is on modeling combustion at low- to high-temperatures in gas turbines and on soot emissions. It can be used to track soot particle mass, number and size in Ansys Chemkin and using the Method of Moments in Ansys Forte.

The mechanism has been reduced for the following range of conditions:

1. Pressure: 10–100 bar
2. Temperature: 800–2000 K
3. Equivalence ratio: 0.4–3
4. EGR: 0–20%

This mechanism has been reduced from the full mechanism "Gasoline_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for gas turbines. The mechanism was reduced from this comprehensive full mechanism using Ansys Reaction Workbench software, for the conditions listed above.

For the emissions, the following species predictions are expected to be accurately predicted:

1. Soot-precursor species:

   a. Detailed soot model: Soot can be modeled using the soot-surface mechanism and the Method of Moments soot model.
   - acetylene (c2h2)
   - butadiyne (c4h2)
   - propargyl (c3h3)
   - benzene (c6h6)
   - phenyl (c6h5)
   - toluene (c6h5ch3)
   - naphthalene (naph)
   - acenaphthalene (a2r5)
   - pyrene (a4)
   - coronene (coronene)

   b. Pseudo-gas soot model:
   - acetylene (c2h2)
   - benzene (c6h6)
   - phenyl (c6h5)

c. Acetylene-based empirical soot model:
- acetylene (**c2h2**)

2. CO (**co**)
3. NO_x (**no** and **no2**)
4. Unburned hydrocarbons

The species names in the chemistry file for the fuel species are:

1. Methane is **ch4**.
2. Ethane is **c2h6**.
3. *n*-Butane is **c4h10**.

2.2.3. Propane Mechanism

Two chemistry sets for propane fuels (mechanism name: c3h8) have been included:

1. `propane_MFL2024.cks`
2. `propane_pseudo-gas-soot_MFL2024.cks`

The first chemistry set can be used with any acetylene-based empirical soot model, and the second set includes the pseudo-gas soot model. The focus of both the chemistry sets are on modeling combustion at in gas turbines. They can be used to predict CO, HC (hydrocarbons), and NO_x emissions from turbines. The mechanism has been reduced for the following range of conditions:

1. Pressure: 1–20 bar
2. Temperature: 800–2000 K
3. Equivalence ratio: 0.5–3
4. EGR: 0–20%

This mechanism has been reduced from the full mechanism "GaseousFuels_C0-C6_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for gas turbines. The mechanism was reduced from this comprehensive full mechanism using Ansys Reaction Workbench software, for the conditions listed above.

2.2.4. Methanol Mechanism

A chemistry set for methanol fuel (mechanism name: ch3oh) has been included: *Methanol_MFL2024.cks*.

This chemistry set can be used for combustion modeling of methanol fuel with any acetylene-based empirical soot model. It can be used to predict CO, HC (hydrocarbons), soot, and NOx emissions. The mechanism has been reduced for the following range of conditions:

1. Pressure: 1–100 bar

2. Temperature: 800–2000 K
3. Equivalence ratio: 0.5–3
4. EGR: 0–20%

This mechanism has been reduced from the full mechanism "Gasoline_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for engines. The mechanism was reduced from this comprehensive full mechanism using Ansys Reaction Workbench software, for the conditions listed above.

2.2.5. Ethanol Mechanism

A chemistry set for methanol fuel (mechanism name: c2h5oh) has been included: *Ethanol_MFL2024.cks*.

This chemistry set can be used for combustion modeling of ethanol fuel with any acetylene-based empirical soot model. It can be used to predict CO, HC (hydrocarbons), soot, and NOx emissions. The mechanism has been reduced for the following range of conditions:

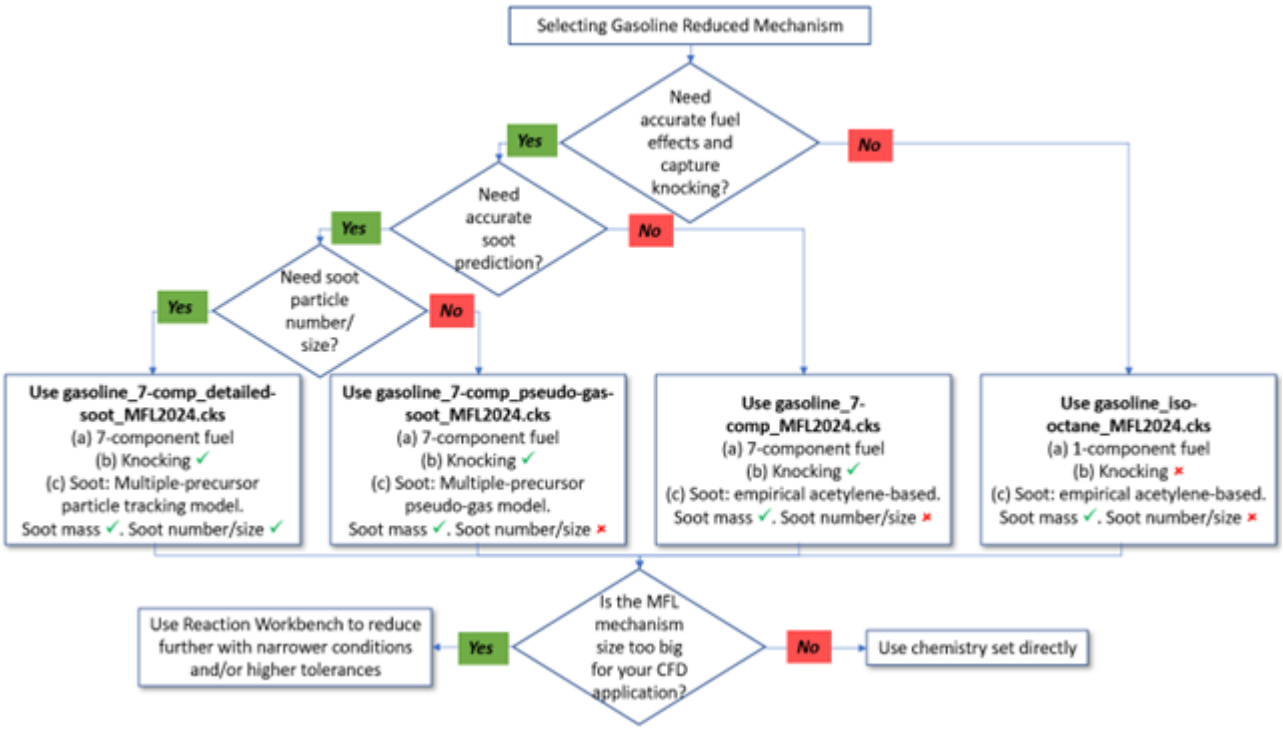
1. Pressure: 1–100 bar
2. Temperature: 800–2000 K
3. Equivalence ratio: 0.5–3
4. EGR: 0–20%

This mechanism has been reduced from the full mechanism "Gasoline_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for engines. The mechanism was reduced from this comprehensive full mechanism using Reaction Workbench software, for the conditions listed above.

2.2.6. Gasoline Mechanisms

Four gasoline reduced mechanisms are available. The flowchart shown in Figure 2.4: Decision flowchart for selecting MFL gasoline mechanism (p. 14) summarizes the applicability of the four mechanisms. More details of these four mechanisms are presented in the subsections below.

Figure 2.4: Decision flowchart for selecting MFL gasoline mechanism



2.2.6.1. Single-component Gasoline

The **gasoline_iso-octane_MFL2024.cks** chemistry set represents gasoline with *iso*-octane (mechanism name: **ic8h18**) as the surrogate. The focus of this chemistry set is on modeling ignition, heat release, and emissions at high temperatures in gasoline engines. For the emissions, the following species predictions are expected to be accurately predicted:

1. Soot-precursor species (two-step soot model only):
   - acetylene (**c2h2**)
2. CO (**co**)
3. NO_x (**no** and **no2**)
4. Unburned hydrocarbons

With acetylene as the soot-precursor, this mechanism can be used with the two-step soot model.

The mechanism has been reduced for the following range of conditions:

1. Pressure: 1–100 bar
2. Temperature: 1200 K and above
3. Equivalence ratio: 0.4–3
4. EGR: 0–40%

This mechanism has been reduced from the full mechanism "Gasoline_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for gasoline engines. The mechanism was reduced from this comprehensive full mechanism using the Reaction Workbench software, for the conditions listed above. The *Model Fuel Library Validation Manual* provides the mechanism validation plots.

2.2.6.2. Multi-component Gasoline

The 7-component gasoline surrogate composition used is: 22.4 wt% *iso*-octane/30.4 wt% toluene/19.1 wt% *n*-pentane/11.2 wt% MCH/7.5 wt% 1-hexene/7.3 wt% 1,2,4-trimethyl benzene/2.1 wt% *n*-butane. There are three chemistry sets for this surrogate:

1. `gasoline_7-comp_MFL2024.cks`
2. `gasoline_7-comp_pseudo-gas-soot_MFL2024.cks`
3. `gasoline_7-comp_detailed-soot_MFL2024.cks`

The difference between the three chemistry sets is the soot model they can be used with; they are any acetylene-based empirical soot model, the pseudo-gas soot model, and the Method of Moments soot model, respectively. The same reduced chemistry set may be used for a surrogate whose composition is different, as long as it consists of the same fuel components (or a subset) and includes a similar amount of the fastest-burning component (in this case mainly *n*-pentane). The focus of this chemistry set is on modeling ignition, heat release, and emissions at low- to high-temperatures in gasoline engines, from HCCI to GDI conditions. The mechanism can be used to model knocking in gasoline engines. It can be used to track soot particle mass, number, and sizes in Ansys Chemkin and employs the Method of Moments in Ansys Forte. This chemistry can be used to predict CO, HC (hydrocarbons), and NO_x emissions from gasoline engines.

For the composition used in the reduction, the surrogate has the following liquid-fuel properties:

Aromatics, vol%	37.7
Research Octane Number	95.9
Motored Octane Number	87
Molar H/C ratio	1.81
Liq. Density, g/cm3	0.73
Distillation curve	
T10, K	340
T30, K	354
T50, K	368.5
T70, K	378.7
T90, K	392.7

The mechanism has been reduced for the following range of conditions:

1. Pressure: 1–100 bar

2. Temperature: 700–2000 K
3. Equivalence ratio: 0.4–3
4. EGR: 0–30%

This mechanism has been reduced from the full mechanism "Gasoline_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for gasoline engines. The *Model Fuel Library Validation Manual* includes the mechanism validation plots. The mechanism was reduced from this comprehensive full mechanism using AnsysReaction Workbench software, for the conditions listed above.

For the emissions, the following species predictions are expected to be accurately predicted:

1. Soot-precursor species:

   a. Detailed soot model: Soot can be modeled using the soot-surface mechanism and the Method of Moments soot model.

   - acetylene (**c2h2**)
   - butadiyne (**c4h2**)
   - propargyl (**c3h3**)
   - benzene (**c6h6**)
   - phenyl (**c6h5**)
   - toluene (**c6h5ch3**)
   - naphthalene (**naph**)
   - acenaphthalene (**a2r5**)
   - pyrene (**a4**)
   - coronene (**coronene**)

   b. Pseudo-gas soot model:

   - acetylene (**c2h2**)
   - benzene (**c6h6**)
   - phenyl (**c6h5**)

   c. Acetylene-based empirical soot model:

   - acetylene (**c2h2**)

2. CO (**co**)
3. NO_x (**no** and **no2**)

4. Unburned hydrocarbons

Soot can be modeled using the soot-surface mechanism and the Method of Moments soot model.

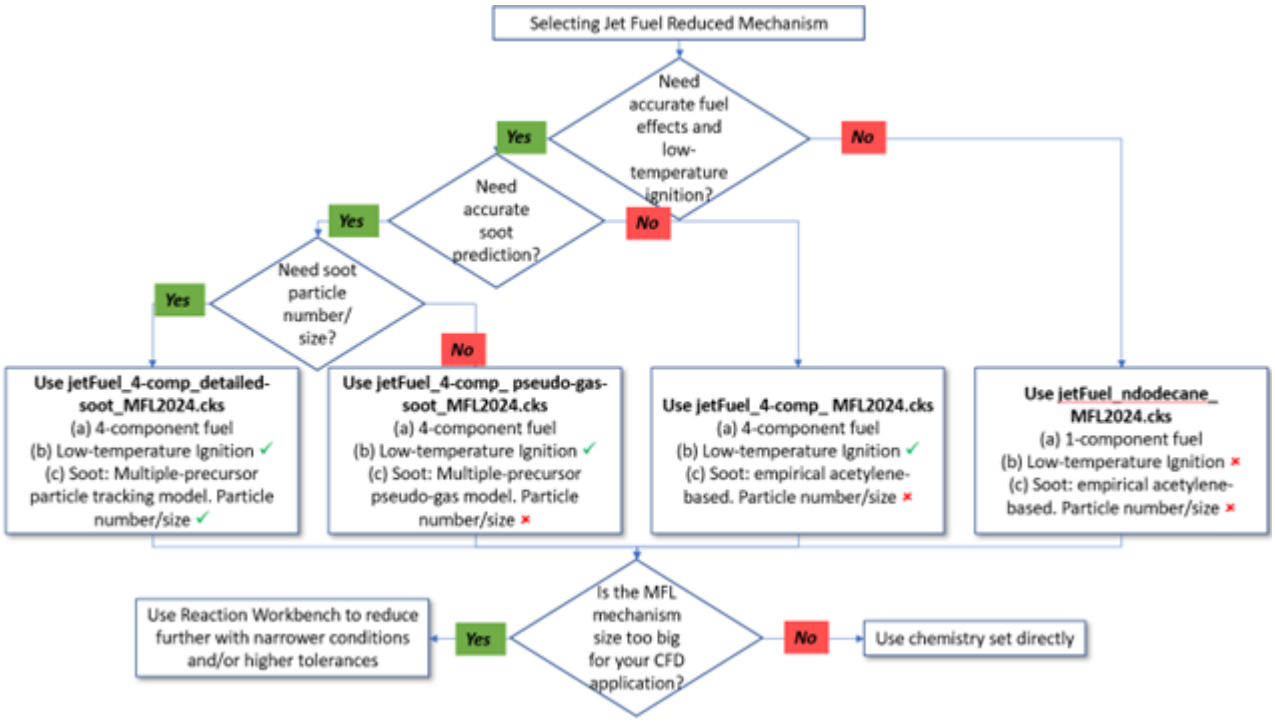
The species names in the chemistry file for the fuel species are:

1. *iso*-octane is **ic8h18**.
2. Toluene is **c6h5ch3**.
3. *n*-pentane is **nc5h12**.
4. MCH is **mch**.
5. 1-hexene is **c6h12-1**.
6. 1,2,4-trimethyl benzene is **tmb124**.
7. *n*-butane is **c4h10**.

2.2.7. Jet Fuel (Jet-A and Kerosene) Mechanisms

Four jet fuel reduced mechanisms are available. The flowchart shown in Figure 2.5: Decision flowchart for selecting MFL jet fuel mechanism (p. 17) summarizes the applicability of the four mechanisms. More details of these four mechanisms are presented in the subsections below.

Figure 2.5: Decision flowchart for selecting MFL jet fuel mechanism



2.2.7.1. Single-component Jet Fuel

The **jetFuel_ndodecane_MFL2024.cks** chemistry represents jet fuel with *n*-dodecane (mechanism name: **nc12h26**) as the surrogate. The focus of this chemistry set is on modeling combustion at high-temperatures in gas turbines. This chemistry can be used to predict CO, HC (hydrocarbons), and NO_x emissions from turbines. The mechanism has been reduced for the following range of conditions:

1. Pressure: 10–100 bar
2. Temperature: 1000–2000 K
3. Equivalence ratio: 0.4–2
4. EGR: 0–20%

This mechanism has been reduced from the full mechanism "Diesel_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for gas turbines. The mechanism was reduced from this comprehensive full mechanism using the Reaction Workbench software, for the conditions listed above. A high-temperature kinetics filter was used as a first step for mechanism reduction prior to using other reduction methods in Reaction Workbench.

2.2.7.2. Multi-component Jet Fuel

The 4-component jet fuel surrogate has a composition of 36.6/32.2/10.3/20.9 wt% *n*-dodecane/ heptamethylnonane/ methylcyclohexane / 1,2,4-trimethylbenzene. There are three chemistry sets for this surrogate:

1. `jetFuel_4-comp_MFL2024.cks`
2. `jetFuel_4-comp_pseudo-gas-soot_MFL2024.cks`
3. `jetFuel_4-comp_detailed-soot_MFL2024.cks`

The difference between the three chemistry sets is the soot model they can be used with; they are any acetylene-based empirical soot model, the pseudo-gas soot model, and the Method of Moments soot model, respectively. The same reduced chemistry set may be used for a surrogate whose composition is different, as long as it consists of the same fuel components and includes a similar amount of the fastest-burning component (in this case, *n*-dodecane). The target application for this chemistry set is modeling combustion at low- to high-temperatures in gas turbines and with soot emissions. It can be used to track soot particle mass, number, and size information in Ansys Chemkin, and using the Method of Moments in Ansys Forte.

For the composition used in the reduction, the surrogate has the following liquid-fuel properties:

Aromatics, vol%	18.8
Cetane Number	44.4
Molar H/C ratio	1.95
Liq. Density, g/cm3	0.78

Distillation curve	
T10, K	448
T30, K	472
T50, K	488
T70, K	498
T90, K	508

The mechanism has been reduced for the following range of conditions:

1. Pressure: 10–100 bar
2. Temperature: 800–2000 K
3. Equivalence ratio: 0.4–3
4. EGR: 0–20%.

This mechanism has been reduced from the full mechanism "Diesel_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for gas turbines. The mechanism was reduced from this comprehensive full mechanism using the Reaction Workbench software, for the conditions listed above.

For the emissions, the following species predictions are expected to be accurately predicted:

1. Soot-precursor species:

   a. Detailed soot model: Soot can be modeled using the soot-surface mechanism and the Method of Moments soot model.

   - acetylene (**c2h2**)
   - butadiyne (**c4h2**)
   - propargyl (**c3h3**)
   - benzene (**c6h6**)
   - phenyl (**c6h5**)
   - toluene (**c6h5ch3**)
   - naphthalene (**naph**)
   - acenaphthalene (**a2r5**)
   - pyrene (**a4**)
   - coronene (**coronene**)

   b. Pseudo-gas soot model:

   - acetylene (**c2h2**)

- benzene (**c6h6**)
- phenyl (**c6h5**)

c. Acetylene-based empirical soot model:

- acetylene (**c2h2**)

2. CO (**co**)
3. NO_x (**no** and **no2**)
4. Unburned hydrocarbons

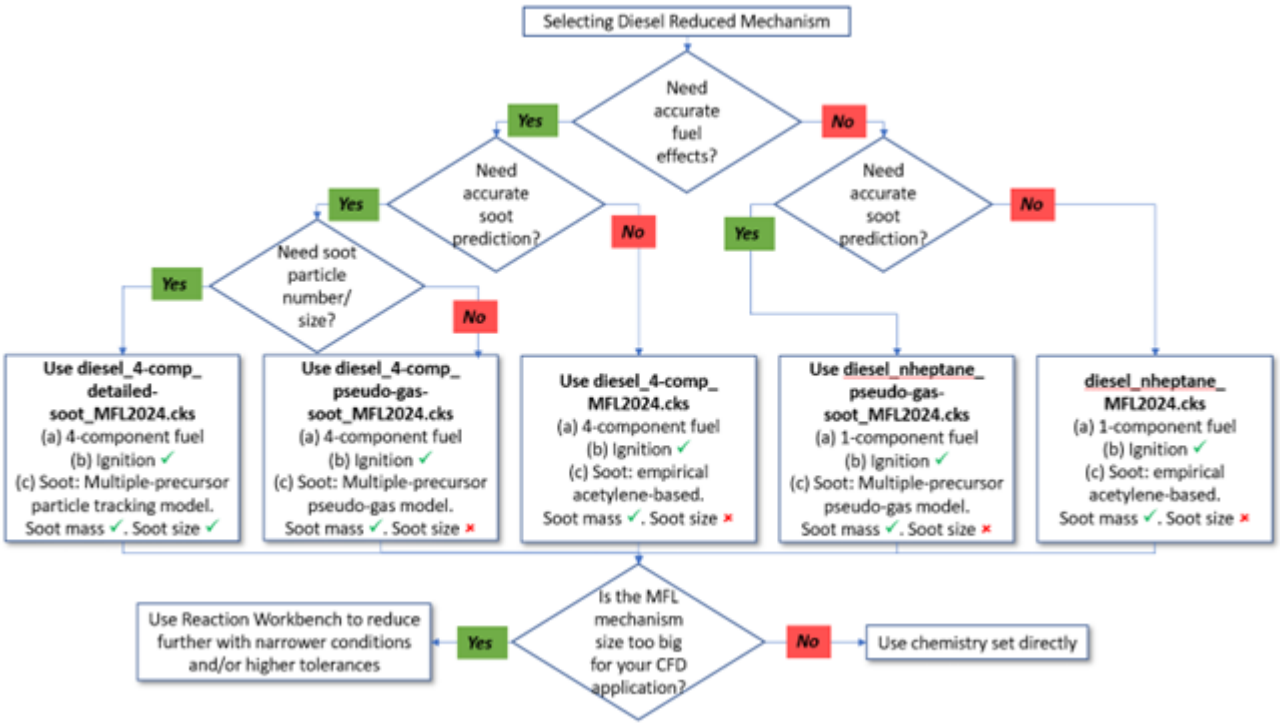
The species names in the chemistry file for the fuel species are:

1. *n*-Dodecane is **nc12h26**.
2. Heptamethylnonane is **hmn**.
3. Methylcyclohexane is **mch**.
4. 1,2,4-Trimethylbenzene is **tmb124**.

2.2.8. Diesel Mechanisms

Five diesel reduced mechanisms are available. The flowchart shown in Figure 2.6: Decision flowchart for selecting MFL diesel mechanism (p. 20) summarizes the applicability of the four mechanisms. More details of the four mechanisms are presented in the sub-sections below.

Figure 2.6: Decision flowchart for selecting MFL diesel mechanism



2.2.8.1. Single-component Diesel

The **diesel_nheptane_MFL2024.cks** chemistry represents diesel with *n*-heptane (mechanism name: **nc7h16**) as the surrogate. The focus of this chemistry set is on modeling combustion and emissions at low- to high-temperatures in diesel engines. The *Model Fuel Library Validation Manual* includes the mechanism validation plots. The mechanism can be used to model soot emissions using the pseudo-gas soot chemistry. This chemistry can be used to predict CO, HC (hydrocarbons), and NO_x emissions from diesel engines.

The mechanism has been reduced for the following range of conditions:

- 1. Pressure: 10–100 bar
- 2. Temperature: 700–2000 K
- 3. Equivalence ratio: 0.5–4
- 4. EGR: 0–40%

This mechanism has been reduced from the full mechanism "Diesel_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for diesel engines. The mechanism was reduced from this comprehensive full mechanism using the Reaction Workbench software, for the conditions listed above.

For the emissions, the following species predictions are expected to be accurately predicted:

1. Soot-precursor species:

   b. Pseudo-gas soot model:

   - acetylene (**c2h2**)
   - benzene (**c6h6**)
   - phenyl (**c6h5**)

   c. Acetylene-based empirical soot model:

   - acetylene (**c2h2**)

2. CO (**co**)
3. NO_x (**no** and **no2**)
4. Unburned hydrocarbons

Soot can be modeled as a pseudo-gas species; in the mechanism this species is named **soot**.

2.2.8.2. Multi-component Diesel

The 4-component diesel surrogate has a composition of 36 wt% *n*-hexadecane/9.7 wt% AMN/15.4 wt% HMN/38.9 wt% decalin. There are three chemistry sets for this surrogate:

1. `diesel_4-comp_MFL2024.cks`

2. `diesel_4-comp_pseudo-gas-soot_MFL2024.cks`

3. `diesel_4-comp_detailed-soot_MFL2024.cks`

The difference between the three chemistry sets is the soot model they can be used with; they are any acetylene-based empirical soot model, the pseudo-gas soot model, and the Method of Moments soot model, respectively. The same reduced chemistry set may be used for a surrogate whose composition is different, as long as it consists of the same fuel components (or a subset) and includes a similar amount of the fastest-burning component (in this case *n*-hexadecane). The target application is modeling combustion at low- to high-temperatures in diesel engines. It can be used to track soot particle mass, number and size in Ansys Chemkin, and using the Method of Moments in Ansys Forte. This chemistry can be used to predict CO, HC (hydrocarbons), and NO_x emissions from diesel engines.

For the composition used in the reduction, the surrogate has the following liquid-fuel properties:

Aromatics, vol%	9.7
Cetane Number	54.4
Molar H/C ratio	1.87
Liq. Density, g/cm3	0.83
Distillation curve	
T10, K	487
T30, K	497
T50, K	514
T70, K	537
T90, K	554

The mechanism has been reduced for the following range of conditions:

1. Pressure: 1–100 bar

2. Temperature: 700–2000 K

3. Equivalence ratio: 0.5–4

4. EGR: 0–40%

This mechanism has been reduced from the full mechanism "Diesel_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for diesel engines. The *Model Fuel Library Validation Manual* includes the mechanism validation plots. The mechanism was reduced from this comprehensive full mechanism using the Reaction Workbench software, for the conditions listed above.

For the emissions, the following species predictions are expected to be accurately predicted:

1. Soot-precursor species:

   a. Detailed soot model: Soot can be modeled using the soot-surface mechanism and the Method of Moments soot model.

- acetylene (**c2h2**)
- butadiyne (**c4h2**)
- propargyl (**c3h3**)
- benzene (**c6h6**)
- phenyl (**c6h5**)
- toluene (**c6h5ch3**)
- naphthalene (**naph**)
- acenaphthalene (**a2r5**)
- pyrene (**a4**)
- coronene (**coronene**)

b. Pseudo-gas soot model:

- acetylene (**c2h2**)
- benzene (**c6h6**)
- phenyl (**c6h5**)

c. Acetylene-based empirical soot model:

- acetylene (**c2h2**)

2. CO (**co**)
3. NO_x (**no** and **no2**)
4. Unburned hydrocarbons

The species names in the chemistry file for the fuel species are:

1. *n*-hexadecane is **nc16h34**.
2. AMN is **a2ch3**.
3. Heptamethylnonane is **hmn**.
4. Decalin is **decalin**.

2.2.9. SAF Mechanism

A chemistry set for 1-component sustainable aviation fuel (*iso*-undecane, species name: c11h24-2) has been included:*SAF_iso-undecane_MFL2024.cks*.

This chemistry set can be used for combustion modeling of SAF fuel with any acetylene-based empirical soot model. It can be used to predict CO, HC (hydrocarbons), soot, and NOx emissions. The mechanism has been reduced for the following range of conditions:

1. Pressure: 1–100 bar
2. Temperature: 1200–2000 K
3. Equivalence ratio: 0.5–3

4. EGR: 0–20%

This mechanism has been reduced from the full mechanism "Diesel_PAH_NOx" in the MFL database, which has been thoroughly validated against fundamental experimental data for the operating conditions of interest for engines. The mechanism was reduced from this comprehensive full mechanism using theAnsys Reaction Workbench software, for the conditions listed above.

2.3. MFL Pseudo-Elementary Reaction Kinetics (PERK) Mechanisms

2.3.1. Introduction

Pseudo-Elementary Reaction Kinetics (PERK) mechanisms are developed to keep the size of the mechanism small while enabling the ability to capture a broader range of conditions than with models containing global reaction steps. While the pre-reduced mechanisms (see MFL Pre-Reduced Mechanisms (p. 6)) preserve the accuracy of detailed mechanisms to a great extent, PERK mechanisms are designed to forgo some of that accuracy and maintain a compact size of a component mechanism.

PERK mechanisms are constructed by considering only dominant reaction pathways for fuel reactions among many that are found in a detailed mechanism. Reactions are formulated to omit intermediate species, therefore resulting in products involving several small species. Rate constants for these reactions are optimized to match predictions of the detailed mechanisms. Elementary reactions of methane and hydrogen from the MFL are used without modification as the core chemistry in all PERK mechanisms.

2.3.2. Applying PERK Mechanisms

PERK mechanisms can be used for the combustion of the fuels listed in Table 2.2: Pseudo-Elementary Reaction Kinetics (PERK) mechanisms provided with the MFL (p. 25). The mechanisms for those fuels are also listed in the table. PERK mechanisms have been optimized for ignition times for stoichiometric fuel/air mixtures at 10 atm over 700–2000 K. Recommended applications and ranges are:

- Predicted characteristics: ignition times, laminar flame speeds
- Emissions: NO_x, CO, unburned hydrocarbons
- Range of conditions: 700–2000 K, 10–100 atm, phi: 0.5–1.5, dilution or EGR: 0–25%

Note:

PERK mechanisms are currently not designed to predict soot emissions.

Note:

Thermodynamic and transport data used by PERK mechanisms are the same as those used by MFL full and skeletal mechanisms. Fluent users can use the `Gasoline-Diesel-Biodiesel_PAH_NOx_therm_MFL<version>.dat` and `Gasoline-Diesel-Biodiesel_PAH_NOx_therm_MFL<version>.dat` files that are located

in the Ansys installation directory under `\reaction\data\ModelFuelLibrary\full`.

Table 2.2: Pseudo-Elementary Reaction Kinetics (PERK) mechanisms provided with the MFL

Fuel	Surrogate Components	Species name	Number of species
Natural gas	93 vol% methane/ 5% ethane/ 2% *n*-butane	93 vol% ch4/ 5% c2h6/ 2% c4h10	36
Propane	93 vol% methane/ 5% ethane/ 2% *n*-butane	93 vol% ch4/ 5% c2h6/ 2% c4h10	29
Gasoline	*iso*-octane	ic8h18	35
	22.4 wt% *iso*-octane/ 30.4% toluene/ 19.1% *n*-pentane/ 11.2% MCH/ 7.5% 1-hexene/ 7.3% 1,2,4-trimethyl benzene/ 2.1% *n*-butane	22.4 wt% ic8h18/ 30.4% c6h5ch3/ 19.1% nc5h12/ 11.2% mch/ 7.5% c6h12-1/ 7.3% tmb124/ 2.1% c4h10	77
Diesel	*n*-heptane	nc7h16	34
	36 wt% *n*-hexadecane/ 9.7% AMN/ 16.4% HMN/ 38.9% decalin	36 wt% nc16h34/ 9.7% a2ch3/ 15.4% hmn/ 38.9% decalin	58
Jet fuel	*n*-dodecane	nc12h26	34
	36.6 wt% *n*-dodecane/ 32.2% heptamethylnonane/ 10.3% methylcyclohexane/ 20.9% 1,2,4-trimethylbenzene	36.6 wt% nc12h26/ 32.2% hmn/ 10.3% mch/ 20.9% tmb124	72

2.3.3. Choosing a Mechanism for a Specific Application: PERK vs. Pre-reduced Mechanisms

A new simulation case's set-up and initial calibration is the most appropriate use for PERK mechanisms. They allow fast simulation turnaround time while maintaining accuracy in chemistry. They can also provide insights into the effects of variation in operating conditions and can speed up simulation-based design of experiments. Once initial results are obtained, we recommend switching the chemistry to a pre-reduced mechanism (see MFL Pre-Reduced Mechanisms (p. 6)) to confirm the results and obtain more detailed information, such as speciation or soot predictions.

PERK mechanisms can be optimized further for conditions of interest using the Global Mechanism Optimization facility in Ansys Chemkin Reaction Workbench. Refer to the mechanism reduction tutorial in the Reaction Workbench Tutorial Guide for an example of a mechanism optimization. The manual is available from the Ansys Help website at ansyshelp.ansys.com.

Chapter 3: How to Use the MFL Mechanisms

The full mechanisms in the MFL can be used with several Ansys software packages, including Chemkin, Reaction Workbench, Forte, and Fluent. The Library mechanisms are platform-independent.

Appropriate MFL full or pre-reduced mechanism for the tailored fuel model can further be reduced using the targeted mechanism reduction capability in Chemkin Reaction Workbench. Refer to the Reaction Workbench Tutorials and Best Practices manuals for more information.

3.1. Symbolic Names

When using a full mechanism in simulations, symbolic species names represent fuel components in the species lists that are displayed for selection of fuel compositions. These symbolic species names are listed for each fuel component in Table 3.1: Names of fuel and emissions species in the MFL mechanisms (p. 27). With MFL mechanisms, it is possible to model most real fuels by either exactly representing the chemical properties of the fuel or by formulating an appropriate surrogate for a specific fuel. We recommend using Reaction Workbench to first formulate surrogates for liquid fuels using the components in the MFL, and then reduce the appropriate full mechanism for the specific surrogate and specific ranges of operating conditions desired for the application. Details about using Reaction Workbench for formulating surrogates and for mechanism reduction can be found in the Chemkin Reaction Workbench User's Manual, or by visiting the Ansys Help site.

Table 3.1: Names of fuel and emissions species in the MFL mechanisms

Common Name	Name in MFL mechanisms	Common Name	Name in MFL mechanisms
Hydrogen	h2	2-methyl-2-butene	bc5h10
n-eicosane	nc20h42	1-hexene	c6h12-1
n-octadecane	nc18h38	2-hexene	c6h12-2
n-hexadecane	nc16h34	3-hexene	c6h12-3
n-pentadecane	nc15h32	1-pentene	c5h10-1
n-tetradecane	nc14h30	2-pentene	c5h10-2
n-tridecane	nc13h28	Carbon monoxide	co
n-dodecane	nc12h26	Methanol	ch3oh
n-undecane	nc11h24	Ethanol	c2h5oh
n-decane	nc10h22	*n*-Propanol	nc3h7oh
n-nonane	nc9h20	*n*-Butanol	nc4h9oh
n-octane	nc8h18	*i*-Butanol	ic4h9oh
n-heptane	nc7h16	Tetrahydrofuran	c4h8o1-4
n-hexane	nc6h14	ETFE	etfe

n-pentane	nc5h12	Methyl butanoate	mb
n-butane	c4h10	Methyl palmitate	mhd
Propane	c3h8	Methyl stearate	mod
Ethane	c2h6	Methyl oleate	mod9d
Methane	ch4	Methyl linoleate	mod9d12d
Heptamethylnonane	hmn	Methyl linolenate	mod9d12d15d
i-dodecane	ic12h26	DME	ch3och3
i-octane	ic8h18	ETBE	C6H14O
2,3,3-Trimethylpentane	i233c8h18	MTBE	mtbe
2,3,4-Trimethylpentane	i234c8h18	Hydrogen sulfide	h2s
i-hexane	ic6h14	Calcium Carbonate	caco3(s)
Neo-pentane	neoc5h12	Butadiyne	c4h2
iso-pentane	ic5h12	1,3-butadiene	c4h6
i-butane	ic4h10	Propene	c3h6
Phenyl	c6h5	Allene	c3h4-a
Cyclopentadiene	cy13pd	Acetylene	c2h2
Benzene	c6h6	Ethylene	c2h4
Toluene	c6h5ch3	Propargyl	c3h3
n-Propylbenzene	c6h5c3h7	Propyne	c3h4-p
Ethylbenzene	c6h5c2h5	Formaldehyde	ch2o
n-Butylbenzene	a1c4h9	Pyrene	a4
o-xylene	o-xylene	Acenaphthalene	a2r5
m-xylene	*m*-xylene	Soot (surface mechanism)	c(B)
p-xylene	*p*-xylene	Soot (pseudo-gas model)	soot
1,2,4-trimethyl benzene	tmb124	Nitric oxide	no
Coronene	coronene	Nitrogen dioxide	no2
Naphthalene	naph	Nitrous oxide	n2o
1-methylnaphthalene	a2ch3	Ammonia	nh3
Cyclohexane	chx	Oxygen	o2
Methylcyclohexane	mch	Nitrogen	n2
Decalin	decalin	Carbon dioxide	co2

3.2. Creating a Surrogate for a Specific Test Fuel

Multi-component mechanisms for diesel and gasoline included with Ansys Forte are reduced from the full mechanisms for specific blends. They can readily be used for different blends with the same components to represent fuels with different characteristics. Using the Surrogate Blend Optimizer tool in Ansys Chemkin Reaction Workbench can help in creating the best surrogate blend to match the important

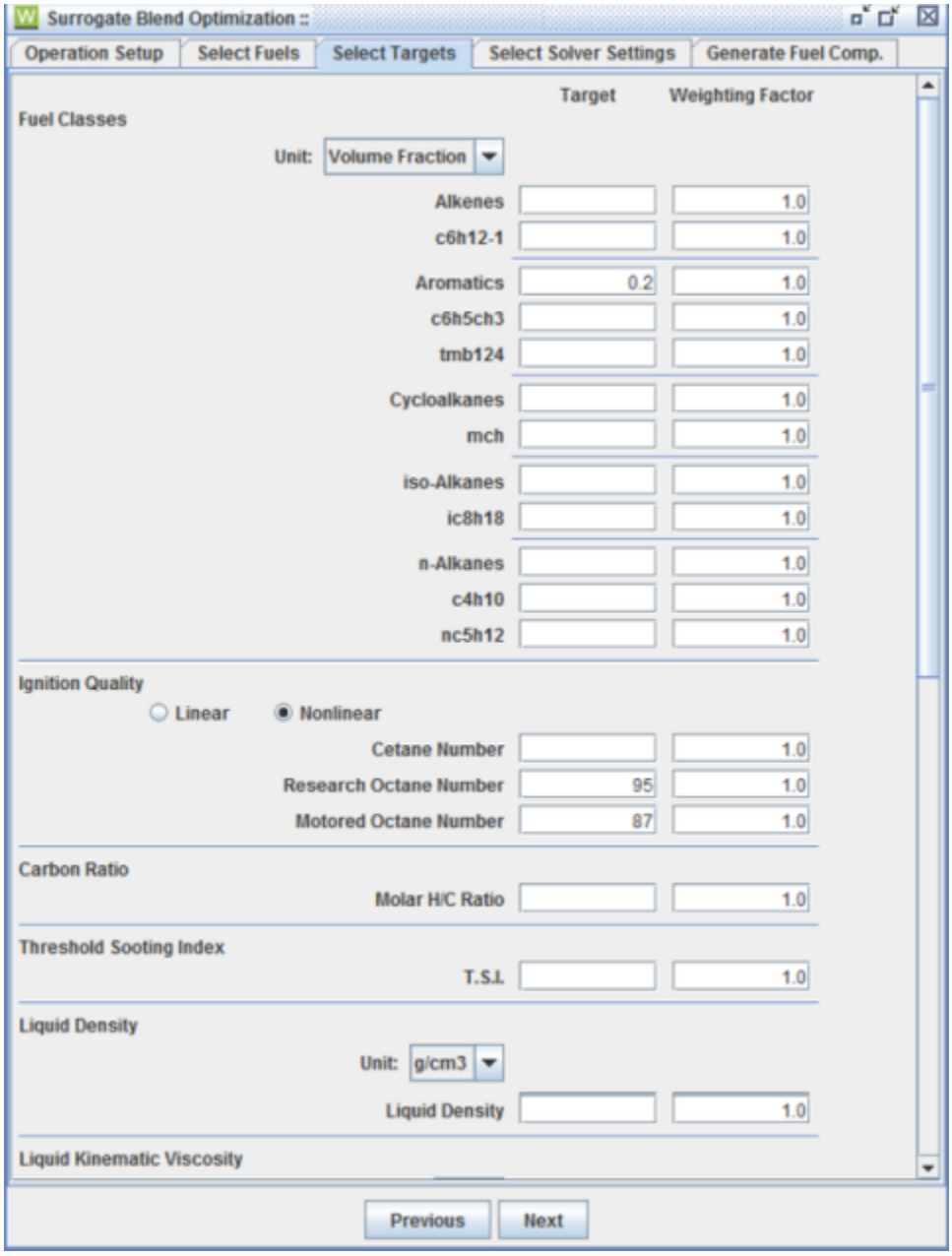
known properties of the test fuel. It can create multi-component surrogates ranging from two-component to much more complex versions, to match one or more properties, including:

- Octane or Cetane numbers
- certain component specifications
- elemental H/C ratio
- density
- viscosity
- heating value
- Reid vapor pressure
- distillation curve

A screenshot of the tool's Targets specification tab to specify the known properties of the test fuel is shown in Figure 3.1: Example of Surrogate Blend Optimizer in Ansys Chemkin Reaction Workbench. Specification of test fuel properties, called Targets, is shown (p. 30).

For example, the goal is to obtain a surrogate for a gasoline with a lower percentage of aromatics and similar ignition quality as that used in the gasoline_7-comp chemistry set. We can use the same mechanism as an input to the Surrogate Blend Optimizer to identify the component options available in the mechanism. Any one or more known properties of the real fuel can be used as Targets. Here, the aromatics fraction is set to 0.2 to have 20 vol.% total aromatics in the blend. In addition, RON and MON of 95 and 87, respectively, are used as targets, as shown in Figure 3.1: Example of Surrogate Blend Optimizer in Ansys Chemkin Reaction Workbench. Specification of test fuel properties, called Targets, is shown (p. 30). An optimized composition including 7 components will be generated that will match those targets. If additional properties are available, they can be used as targets, if necessary.

Figure 3.1: Example of Surrogate Blend Optimizer in Ansys Chemkin Reaction Workbench. Specification of test fuel properties, called Targets, is shown



In general, the pre-reduced mechanisms can be used without additional validation if the following are true:

- Percentage of any component in the desired surrogate is within 20% of the original surrogate for which the mechanism has been reduced.
- If the desired octane or cetane numbers are within 20 numbers of those of the original surrogate.

More information about the Surrogate Blend Optimizer and model-fuel mixtures is available in the Chemkin Reaction Workbench User's Manual and an example, the Surrogate Blend Optimizer (SBO) tutorial, in the Reaction Workbench Tutorial Guide.