FiReSMOKE User's Guide

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Collection of Finite Rate solvers for OpenFOAM based on the OpenSMOKE++ framework (`https://www.opensmokepp.polimi.it/`). Latest version runs on OpenFOAM-7.x.
For more information concerning OpenSMOKE++ check [1]. Sample-Partitioning Adaptive Reduced Chemistry (SPARC) plugin is also available. If used, please cite the following papers:

> D'Alessio, G., Parente, A., Stagni, A., Cuoci, A., Adaptive chemistry via pre-partitioning of composition space and mechanism reduction. Combustion and Flame, Volume 211, 2020, pp. 68-82. DOI:10.1016/j.combustflame.2019.09.010.
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> Amaduzzi, R., D'Alessio, G., Pagani, P., Cuoci, A., Malpica Galassi, R., Parente, A., Automated adaptive chemistry for Large Eddy Simulations of turbulent reacting flows. Combustion and Flame, Volume 259, 2024, pp. 113-136. DOI:10.1016/j.combustflame.2023.113136.

In the following, a brief description of the available options and settings is presented.

1 `constant` folder

As with any OpenFOAM case, the choice of the combustion, turbulence models and the thermophysical properties are set in the `constant` folder. The files required by the solver are:

- `combustionOptions`.
- `drgOptions`, to be included in `combustionOptions` (`#include drgOptions`).
- `g`.
- `isatOptions`, to be included in `combustionOptions` (`#include isatOptions`).
- `thermophysicalProperties`.
- `turbulenceProperties`.

`radiationProperties` is optional. Alternatively, `drgOptions` and `isatOptions` can be integrated directly into the `combustionOptions` dictionary.

1.1 `combustionOptions` dictionary

The combustion models are selected here. Five finite-rate turbulent combustion models are available, chosen from the line `combustionModel`:

- `ED` - Eddy Dissipation
- `EDFR` - Eddy Dissipation / Finite Rate
- `EDC` - Eddy Dissipation Concept
- `PaSR` - Partially Stirred Reactor
- `QLFR` - Quasi-Laminar Finite Rate (LES only)

Before the combustion models sub-dictionaries, some general options are available:

- `homogeneousReactions on/off`; switches on/off the species source terms in the species transport equations.
- `momentumEquations on/off`; switches on/off the momentum equation.
- `energyEquation on/off`; switches on/off the energy equation.
- `dynamicCmixEquations on/off`; switches on/off the equations for the local formulation of the mixing timescale: mixture fraction, mixture fraction variance and scalar dissipation rate transport equations.
- `minT 280.`; minimum temperature in K. Useful for steady-state calculations.

- `maxT 3500.`; maximum temperature in K. Useful for steady-state calculations.

The next set of options relate to the scalar dissipation rate transport equation.

- `ChiEquation on/off`; if off and algebraic equation is used to compute the scalar dissipation rate, if on the transport equation is employed.
- `Cx 1.00`; algebraic Chi coefficient (default 2.00).
- `Cg 2.00`; mixture fraction variance equation coefficient.
- `maxChi 10000`; maximum scalar dissipation rate.

Scalar dissipation rate transport equation coefficients:

- `Cd1 1.0`;
- `Cd2 1.8`;
- `Cp1 3.4`;
- `Cp2 1.4`;
- `Cmu 0.09`;

Lastly, laminar diffusion, turbulent Schmidt and Prandtl number are defined as:

- `laminarDiffusion on/off`;
- `Sct 0.7`;
- `Prt 0.85`;

Next, the combustion models sub-dictionaries are listed. Each one of the models requires its specific sub-dictionary and only the one of the chosen model is required to run the simulation.

1.1.1 ED and EDFR

Both `ED` and `EDFR` only require the two forward and backward constants `A` and `B` (the default values are showed here):

- `A 4.`;
- `B 0.5`;

1.1.2 EDC

Three formulations of EDC are present, the 1981, the 2005 versions by Magnussen [2; 3] and the 2016 version by Parente et al. [4]. The model keywords are here listed:

- `version "v2005"/"v1982"/"v2016"`; v2005 is the default choice.
- `reactorType "PFR"/"PSR"`; fine structures reactor type, PFR is the default choice.
- `Ccsi 2.1377`; EDC fine structures mass fraction parameter.
- `Ctau 0.40825`; EDC fine structures mean residence time parameter.
- `maxGammaL 0.87`; EDC parameter.
- `numberOfResidenceTimes 100.`; ODE total integration time (only for PSR, default value is 100).
- `numberIterationsToUpdateChemistry 1.`; number of CFD iterations to solve the ODE system, default value is 1.
- `solverType "ODE"/"NLS"`; solver type, default is "ODE".

Additional parameters for the 2016 version:

- `CtauCoeff 0.750`; v2016 C_τ coefficient.
- `CgammaCoeff 1.224`; v2016 C_γ coefficient.

- `CReCoeff 0.090`; v2016 C_{Re} coefficient.
- `minTemperature4Chemistry 300.`; minimum temperature to compute the species source terms.
- `ChemicalTimesThreshold 0.10`; maximum chemical timescale, default value is 0.10s.
- `ChemicalTimesTemperatureThreshold 300.`; minimum temperature to carry out chemical times analysis, default value is 300 K.
- `ChemicalTimesType "formationRates"/"reactionRates"/"eigenValues"`; chemical timescale calculation method. Default is `"formationRates"`.

1.1.3 `PaSR`

Partially Stirred Reactor [5; 6] model sub-dictionary.

- `reactorType "PFR"`; only PFR is supported for PaSR at the moment.
- `tauStarType "minDeltaTLEStauMix"/"deltaTLES"`; reactor residence time (LES only).
- `tauMixType "kolmogorovScale"/"geometricMeanScale"/"globalScale"`; mixing timescale calculation method. Default is `"globalScale"`.
- `Cmixglobal 0.1`; C_{mix} constant value for `globalScale` mixing timescale formulation.
- `numberIterationsToUpdateChemistry 1.`; number of CFD iterations to solve the ODE system, default value is 1.
- `minTemperature4Chemistry 300.`; minimum temperature to compute the species source terms.
- `ChemicalTimesThreshold 0.10`; maximum chemical timescale, default value is 0.10s.
- `ChemicalTimesTemperatureThreshold 300.`; minimum temperature to carry out chemical times analysis, default value is 300 K.
- `ChemicalTimesType "formationRates"/"reactionRates"/"eigenValues"`; chemical timescale calculation method. Default is `"formationRates"`.

1.1.4 `QLFR`

Quasi-Laminar Finite Rate mode sub-dictionary.

- `reactorType "PFR"`; only PFR is supported for PaSR at the moment.
- `numberIterationsToUpdateChemistry 1.`; number of CFD iterations to solve the ODE system, default value is 1.
- `minTemperature4Chemistry 300.`; minimum temperature to compute the species source terms.

1.1.5 `Ode`

ODE solver settings. Depending on the compilation mode, different solvers are available. The settings for the "minimalist" compilation are shown here.

- `odeSolver "OpenSMOKE"`; ODE solver. `OpenSMOKE` is the native OpenSMOKE++ solver developed at Polimi.
- `relTolerance 1e-5`; ODE relative tolerance. Default value is 1e-5.
- `absTolerance 1e-10`; ODE absolute tolerance. Default value is 1e-10. `fullPivoting true/false`; full pivoting during LU factorization. Default is false. `maximumOrder 5`; ODE integration maximum order, only for OpenSMOKE++ native solver. Default value is 5.

1.1.6 `Spark`

Sub-dictionary to set up spark ignition in the domain. The spark is a sphere of given diameter and temperature.

- `spark on/off`; on/off switch.
- `position (x y z)`; spark position in the domain.
- `time 0`; starting time [s].
- `temperature 2500`; spark temperature [K].
- `duration 1e-2`; spark duration [s].
- `diameter 5e-3`; spark diameter [m].
- `additionalMassFraction 1e-3`;

SPARC

Next, the SPARC settings are listed. In order to activate them, the `SPARCswitch` switch must be set to `on`. The following classification methodologies are available: `VQ2, FitCTree, Neural, SOFTMAX, SelfOrganizingMap`. As of now, **only VQ2 has been validated**. The use of SPARC and of the Predictor requires the presence of a folder containing the training dataset clustering and the reduced mechanisms, usually labeled `data_for_sparc` (see the tutorials for an example). The dataset and the reduced mechanisms can be generated using any methodology; a PCA-based clustering methodology is available at `https://github.com/burn-research/OpenMORe`.

1.1.7 `VQ2`

Sub-dictionary for SPARC VQ-PCA classification.

- `vq2 on/off`; on/off switch.
- `debug on/off`; on/off switch for debug mode.
- `folder "../path_to_folder/data_for_sparc"`; path to folder containing the training dataset clustering and reduced mechanisms.
- `debug true/false`;
- `eigens 36`; set equal to number of species in the full mechanism employed.
- `scaling AUTO`; scaling type. As of now, the only available option is `AUTO`.

1.1.8 `NEURAL`

Sub-dictionary for SPARC Neural Network classification.

- `NEURAL on/off`; on/off switch.
- `folder "../path_to_folder/data_for_sparc"`; path to folder containing the training dataset clustering and reduced mechanisms.

1.1.9 `FitCTree`

Sub-dictionary for SPARC classification trees classification.

- `fitctree on/off`; on/off switch.
- `folder "../path_to_folder/data_for_sparc/data.xml"`; path to xml file containing the training dataset clustering.
- `folder "../path_to_folder/data_for_sparc"`; path to folder containing the training dataset clustering and reduced mechanisms.

1.1.10 `SOFTMAX`

Sub-dictionary for SPARC softmax classification.

- `SOFTMAX on/off`; on/off switch.

1.1.11 SelfOrganizingMap

Sub-dictionary for SPARC self organizing map classification.

- SOFTMAX on/off; on/off switch.

1.1.12 PREDICTIONS

This feature has been implemented but not yet validated. PREDICTIONS allows to predict species not present in the original mechanism (for instance, NOx). The sub-dictionary options are:

- PREDICTIONS on/off; on/off switch.
- muOUT 0; centering factor (min).
- sigmaOUT 0; scaling factor (max-min).
- folder "../path_to_folder/data_for_sparc"; path to folder containing the training dataset clustering and reduced mechanisms.

1.1.13 drgOptions

Sub-dictionary for DRG settings.

- drg on/off; on/off switch.
- minTemperature 300; minimum temperature to start DRG analysis [K].
- species (CH4 H2); list of target species.
- epsilon (0.05 0.08); list of DRG tolerances for each target specie.
- temperature (600 900); list of temperatures for each target specie.

1.1.14 isatOptions

Sub-dictionary for ISAT [7] settings. **ISAT implementation not validated**.

- ISAT on/off; on/off switch.
- tolerance 1e-5; ISAT tolerance.
- numberSubSteps 1; ISAT number of substeps for calculating gradient mapping. Default value is 1.
- searchMRU on/off; search for Most Recently Used leaves. Default is on.
- searchMFU on/off; search for Most Frequently Used leaves. Default is on.
- maxSizeMRU 100; max size of Most Recently Used. Default value is 100.
- maxSizeMFU 100; max size of Most Frequently Used. Default value is 100.
- maxSearchMRU 10; max numbers of leaves to be tested (MRU). Default value is 10.
- maxSearchMFU 30; max numbers of leaves to be tested (MFU). Default value is 30.
- maxSizeBT 100000; max size of binary tree. Default value is 100000.
- clearingIfFull on/off; on/off switch to clear tree when full. Default is off.
- cleanAndBalance on/off; clean and balance. Default is on.
- balanceFactorRetrieve 2.0; Default value is 2.
- balanceFactorAddition 0.1; Default value is 0.1.
- maxTimeOldCoeff 0.7; Default value is 0.7.
- maxGrowCoeff 0.5; Default value is 0.5.
- minUsedCoeff 0.01; Default value is 0.01.

- `maxHeightCoeff 5.0`; Default value is 5.
- `luFactorizations "Partial"/"Full"`; LU factorization of dense matrices. Default is "Partial".
- `luFactorizations "NoPivoting"/"Partial"/"Full"`; QR factorization of dense matrices. Default is "Full".
- `scalingFactors` sub-dictionary:
  - `T 1e4;`
  - `tf 1e4;`
  - `others 1.;`
- `scalingErrors` sub-dictionary:
  - `T 1.;`
  - `tf 1.;`
  - `others 1.;`

1.2 `g` dictionary

Sub-dictionary to define the gravitational acceleration in the domain.

- `dimensions [0 1 -2 0 0 0 0];` [m/s^2].
- `value (0 0 -9.81);` set to `(0 0 0)` if negligible.

1.3 `thermophysicalProperties` dictionary

In FiReSMOKE the thermophysical properties are listed in the kinetic mechanism. The `thermophysicalProperties` dictionary defines the kinetic mechanism format (Chemkin or OpenFOAM) and the thermo type.

- `kineticMechanism "kinetics"`; name of the kinetic mechanism folder.
- `CHEMKINFile "/path_to_file/chem.inp"`; path to chemkin input file.
- `CHEMKINThermoFile "/path_to_file/thermo.dat"`; path to chemkin thermo file.
- `CHEMKINTransportFile "/path_to_file/transportFile"`; path to transport properties file (**use OpenFOAM file type for transport!**).
- `inertSpecie N2`; inert specie in the mechanism.
- `chemistryReader chemkinReader/foamChemistryReader`; chemistry reader type. Available options are `chemkinReader/foamChemistryReader`.

If `foamChemistryReader` is selected, replace `CHEMKINFile, CHEMKINThermoFile, CHEMKINTransportFile` with:

- `foamChemistryFile "/path_to_file/mechanism.foam"`; path to foamChemistry input file.
- `foamChemistryThermoFile "/path_to_file/thermo"`; path to foamChemistry thermo file.

Lastly, the `thermoType` sub-dictionary options are listed. This is common to all OpenFOAM solvers. An example is shown here.

- `type hePsiThermo;`
- `mixture reactingMixture;`
- `transport sutherland;`
- `thermo janaf;`
- `energy sensibleEnthalpy;`
- `equationOfState perfectGas;`
- `specie specie;`

1.4 `turbulenceProperties` dictionary

Standard OpenFOAM turbulence model selection. Check OpenFOAM manual for more information.

1.5 `radiationProperties` dictionary

Standard OpenFOAM radiation model selection. Check OpenFOAM manual for more information.

2 `kinetics` folder

The kinetic mechanism is located in this folder in either `Chemkin` of `foamChemistry` formats. If `Chemkin` format is employed, use OpenFOAM-type transport properties files as `transportProperties`. The kinetic mechanism in the `kinetics.xml` format is also required. The .xml format is created using the OpenSMOKE++ Suite Chemkin Pre-Processor.

References

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