University of Strathclyde Engineering

hy2Foam

User Guide

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1 Introduction to *hy2Foam*

hy2Foam is a newly coded open-source two-temperature computational fluid dynamics (CFD) solver that has been developed to tackle the highly complex flow physics of the hypersonic Earth atmospheric re-entry. Implemented within the OpenFOAM framework, the code has the capability to model physical phenomena relative to the high-speed chemically-reacting environment surrounding a spacecraft. The non-equilibrium conditions are treated by making the distinction between the trans-rotational and multiple vibrational-electronic energy pools. This permits to model the energy exchanges between these energy pools and to introduce a chemistry-vibration source term into the Navier-Stokes-Fourier equations. Various transport models have been implemented to determine species and mixture thermal properties at high-temperatures. There are also several new species diffusion models and boundary conditions available.

2 Installation of *hy2Foam*

The installation of *hy2Foam* is straightforward. Please make sure that the path to your OpenFOAM user directory is correct in the bash script called ***install.sh*** before execution. This script will install the new ***strath*** libraries located into the ***src*** folder, will install the *hy2Foam* solver located into the ***applications*** folder (as well as a few other apps) and will copy some tutorials into your ***run*** directory.

3 *hy2Foam* working environment

3.1 The main folder

The main working folder is no different from any other OpenFOAM solvers. The bash script ***Allwclean*** removes any temporary files within the main directory.

```
referenceCase
VincePC: referenceCase >ls
0  Allwclean  constant  gnuplot  pv.foam  system
VincePC: referenceCase >
```

Figure 1: Main folder contents

3.2 The *0* folder

The *0* folder contains the traditional ***p*** and ***U*** files. The other mandatory files are the trans-rotational temperature, printed as ***Tt***, the mass-fraction and the vibro-electronic temperature for each species. The prefix $Y\_$ is omitted for mass-fractions which means that the **N2** file is the mass-fraction of N_2. The vibro-electronic temperatures are denoted by the prefix ***Tv***_ in the multi vibro-electronic pool configuration (and simply ***Tv*** for the single vibro-electronic pool arrangement).

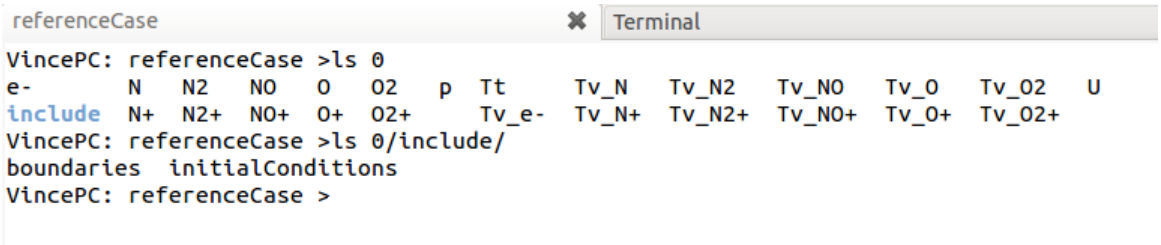


Figure 2: The ***0*** folder contents

It is good practice to initialise the fields via an include statement to a dictionary and to set some of the boundary conditions by calling another dictionary. These dictionaries are regrouped into the ***0/include*** folder. For instance, the ***initialConditions*** dictionary can be defined as follow

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
Ttr       30000;
Tve       10000;
TveAtom   0;

inletPressure  1.01325e5;

inletVelocity  (0 0 0);
initialVelocityField  (0 0 0);

Y_N2      0.4;
Y_O2      0;
Y_NO      0;
Y_N       0.2;
Y_O       0;
Y_N2+     0.399992;
Y_O2+     0;
Y_NO+     0;
Y_N+      0;
Y_O+      0;
Y_e-      0.000008;
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
```

while the ***boundaries*** dictionary is for the case of an adiabatic heat bath

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
fixedWalls
{
    type            empty;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
```

The user must set the vibro-electronic temperature for each molecule. For atoms, ions and electrons, if the electronic energy is switched on, then T_{ve} is to set to the vibro-electronic temperature of a reference species defined in the ***constant*** folder. In this case,

```
TveAtom = $Tve;
```

Otherwise, it is important to set T_{ve} to 0 for each of the non-vibrationally excited species composing the mixture. Several examples are given in the ***0/default***, ***0/5species***, and ***0/11species*** folders.

3.3 The *constant* folder

The ***constant*** folder regroups all the dictionaries relative to the physicochemical phenomena occuring at hypersonic speed that have been implemented into *hy2Foam*. The mesh remains located into the ***polyMesh*** sub-folder.

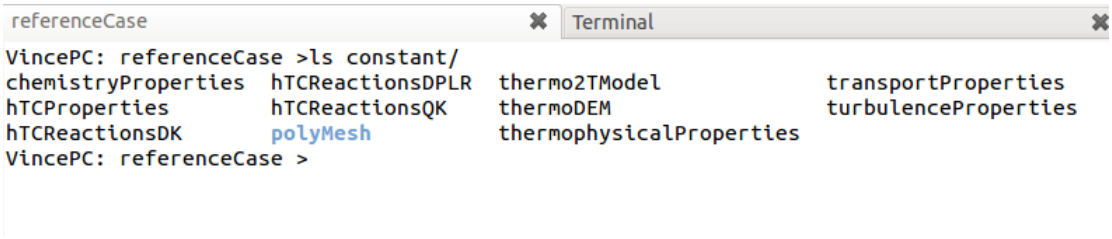


Figure 3: The ***constant*** folder contents

A short description of the different dictionaries is given below. It is recommended to follow the order listed here while editing the entries of the dictionaries.

- 1) ***thermophysicalProperties***: the standard OpenFOAM dictionary that prescribes which thermophysical models are going to be used and the location of some sub-dictionaries.

- 2) ***turbulenceProperties***: the standard OpenFOAM dictionary that deals with turbulence modelling. In *hy2Foam*, the options are *laminar* and *RAS2Model*.

- 3a) ***hTCProperties***: the dictionary that allows the user to activate or deactivate the high-temperature chemistry (hTC) features and to output some desired species-related fields such as number densities or vibrational degrees of freedom.

- 3b) ***chemistryProperties***: the dictionary that defines the different chemistry inputs

- 3c) ***hTCReactionsDPLR*** / ***hTCReactionsQK*** / ***...***: the list of the species composing the mixture is defined in those dictionaries. It is strongly recommended not to change the order of the species in the list (molecules - ions - atoms - free electrons). Please uncomment the species and chemical reactions you may need.

- 4) ***thermoDEM***: the dictionary that provides the species thermodynamic data for the different species loaded in dictionary 3c).

- 5) ***thermo2TModel***: the dictionary that provides all the coefficients that enter into the different energy exchange processes.

- 6) ***transportProperties***: the dictionary that defines the models used for species diffusion and the mixing rule. Some parameters such as the mean free path or the local gradient-length Knudsen number can be printed from this dictionary.

In the subsequent subsections, the main features of the dictionaries listed above are reviewed.

3.3.1 The *thermophysicalProperties* dictionary

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      thermophysicalProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

thermoType
{
    type            heRho2Thermo;
    mixture         reacting2Mixture;
    transport       BlottnerEucken;
    thermo          decoupledEnergyModes;
    energy          sensible2InternalEnergy;
    equationOfState perfect2Gas;
    specie          advancedSpecie;
}

hyLight yes;

downgradeToSingleTv no;
downgradeToSingleTemperature no;

chemistryReader foam2ChemistryReader;

foamChemistryFile "$FOAM_CASE/constant/hTCReactionsDPLR";

foamChemistryThermoFile "$FOAM_CASE/constant/thermoDEM";

twoTemperatureDictFile "$FOAM_CASE/constant/thermo2TModel";

temperatureBounds
{
    Tlow    200;
    Thigh   22000;
}

// ************************************************************************* //
```

The *thermoType* defined in the ***thermophysicalProperties*** dictionary uses the new ***strath*** thermophysical models. The number 2 indicates that the two-temperature model is employed. The user has the choice between the four transport models listed in Table 1. The *thermo* class decomposes the contribution of the different energy modes and the related sub-dictionary is later called via the *foamChemistryThermoFile* entry.

Model name	shear viscosity	thermal diffusivity
constant	constant	constant Eucken
BlottnerEucken	Blottner	Eucken
powerLawEucken	power law	Eucken
SutherlandEucken	Sutherland	Eucken
CEA	CEA2 (NASA)	CEA2 (NASA)

Table 1: Available transport models in *hy2Foam*

hy2Foam is a two-temperature solver with multiple vibro-electronic temperatures. The two booleans *downgradeToSingleTv* and *downgradeToSingleTemperature* alter *hy2Foam* capabilities when simpler analyses can be conducted. The *downgradeToSingleTv* option downgrades *hy2Foam* to a single vibrational temperature solver. *hyLight* is an option that permits to run a light version of *hy2Foam*, thus saving time. The temperature bounds are here to make the code more robust during the transient phase. Please make sure that none of the steady-state

temperature fields are reaching these bounds.

The *foamChemistryFile* entry tells which set of chemical rate constants is going to be used by linking to the appropriate sub-dictionary. Available sets of chemical rate constants and their respective meanings are listed in Table 2.

Set	Meaning
DPLR	Park's rates (used in the DPLR solver), will soon be replaced
QK	Quantum Kinetics rates
DK	Dunn and Kang rates
ES	Evans and Shexnayder (1980)
J92	Jachimoski's rates (1992)
J92_fwd	Jachimoski's rates (1992), forward only
Mars94	Park's rates (1994)
Earth93	Park's rates (1993), available soon (to replace DPLR)

Table 2: Available chemical rate constant sets in *hy2Foam*

3.3.2 The *turbulenceProperties* dictionary

As stated earlier, the turbulence models (*simulationType*) available in *hy2Foam* are *laminar* and *RAS2Model*.

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      turbulenceProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

simulationType  laminar;

// ************************************************************************* //
```

If *RAS2Model* is chosen, then the definition of a new dictionary, ***RASProperties***, is required

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      RASProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

RAS2Model       kOmegaSST;

turbulence      off;

printCoeffs     on;

// ************************************************************************* //
```

The different choices for the *RAS2Model* entry are *laminar*, *kOmegaSST*, *kEpsilon* and *SpalartAllmaras*.

3.3.3 The *hTCProperties* dictionary

The high-temperature chemistry library is the high-level ***strath*** library. The *hTC2Model* entry should be consistent with the turbulent model chosen in ***turbulenceProperties***. Please turn off the *active* switch if the chemistry module does not need to be loaded. The *vibrationalEnergy* switch outputs the vibrational energy for each species as well as the electronic energy and the total energy. The molar-fractions are printed with the prefix $X\_$, the number densities with the prefix $nD\_$, the partial densities with the prefix $pD\_$, and finally the partial pressures with the prefix $pP\_$. The degrees of freedom are called $zeta\_$ followed by the corresponding energy mode.

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      hTCProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

hTC2Model  laminar2<rho2ChemistryHTC>;

active    true;

laminar2Coeffs
{}

chemistryOutputs
{
    molarFraction       off;
    numberDensity       off;
    partialDensity      off;
    partialPressure     off;
    degreesOfFreedom    off;
    vibrationalEnergy   off;
}

// ************************************************************************* //
```

3.3.4 The *chemistryProperties* dictionary

hy2Foam uses finite rate chemistry. This translates into the use of the new class *Euler2Implicit*. Please turn on/off the *chemistry* switch to enable/disable chemical reactions. The *initialChemicalTimeStep* option should be available soon. There are two models for the chemistry-vibration coupling, the Park TTv model and the coupled vibration-dissociation-vibration (CVDV) model. More details about the coefficients of these models are given in this dictionary and omitted here for reasons of conciseness.

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      chemistryProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

chemistryType
{
    chemistrySolver   Euler2Implicit;
    chemistryThermo   rho2;
```

```
}

chemistry           off;

initialChemicalTimeStep 1.0e-9;

chemistryVibrationCoupling
{
    model ParkTTv; // ParkTTv or CVDV
}

// ************************************************************************* //
```

3.3.5 The *hTCReactionsDPLR/QK/DK/...* dictionaries

QK reactions should be defined as irreversible while Park (DPLR) reactions can be considered either reversible or irreversible. Printed below is an example of the implementation of one chemical reaction in the ***hTCReactionsDPLR*** dictionary

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    object      hTCReactionsDPLR;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

species
(
    //N2
    O2
    //NO
    //N2+
    //O2+
    //NO+
    N
    O
    //N+
    //O+
    //e-
);

vibTempAssociativity (0 1 1);

// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
/* REACTIONS NO 1 TO 15 AND 18 TO 32 -> DISSOCIATION
   REACTIONS NO 16 AND 17            -> EXCHANGE
   REACTION NO 33                    -> ELECTRON IMPACT DISSOCIATION
   REACTIONS NO 34 AND 35            -> ELECTRON IMPACT IONISATION
   REACTIONS NO 36 TO 38             -> DISSOCIATIVE RECOMBINATION
   REACTIONS NO 39 TO 49             -> CHARGE EXCHANGE                    */
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

reactions
{
    // Reaction no 1
    oxygenAtomicNitrogenReaction
    {
        type     reversibleArrheniusReaction;
        reaction "O2 + N = 2O + N";
        controlT dissociation;
        A        1.0e19;
        beta     -1.5;
        Ta       59500;

        ni       (1e20 1e21 1e22 1e23 1e24 1e25); // local mixture number density in 1/m^3
        A0       (1.8103 0.91354 0.64183 0.55388 0.52455 0.50989);
        A1       (1.9607 2.316 2.4253 2.46 2.4715 2.4773);
```

```
        A2      (3.5716 2.2885 1.9026 1.7763 1.7342 1.7132);
        A3      (-7.3623 -6.7969 -6.6277 -6.572 -6.5534 -6.5441);
        A4      (0.083861 0.046338 0.035151 0.031445 0.030209 0.029591);
    }
}

// ************************************************************************* //
```

Please uncomment only the necessary species, here O_2, N, and O. The *vibTempAssociativity* table associates one paticle such as an atom, ion or free-electrons to a molecule so that the vibro-electronic temperature of the atom/ion/electrons will be set the vibro-electronic temperature of this molecule. 0 can only be set to a molecule (the molecule will have its own vibro-electronic temperature). For other particles, an integer value of i refers to the i^{th} molecule as ordered in the *species* table.
Please then uncomment the appropriate chemical reactions, for instance Reaction no 1. The *type* of the reaction specifies whether the reaction is irreversible or reversible. The *controlT* entry is the controlling temperature used in the Park TTv model for the calculation of the forward and backward rate constants. A, *beta*, and Ta are the standard Arrhenius coefficients. The equilibrium constant is a function of the local number density of the mixture. The lists of coefficients $A0$ to $A4$ are linearly interpolated if the local mixture number density is within the range $[1 \times 10^{20}, 1 \times 10^{25}]$ m^{-3}. If not, the interpolation is bounded.

3.3.6 The *thermoDEM* dictionary

This dictionary provides the species thermodynamic data for the different species loaded in ***hTCReactionsDPLR/QK/DK/ES***. The dictionary structure is given here for the N_2 molecule.

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      thermoDEM;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

N2
{
    specie
    {
        nMoles          1;
        molWeight       28.0134;
        particleType    2;
        charge          0;
        diameter        4.17e-10;
        dissocEnergy    3.36e7;
        omega           0.74;
        noVibTemp       1;
        noElecLevels    15;
    }
    thermodynamics
    {
        Tlow                200;
        Thigh               40000;
        decoupledCvCoeffs   ( 1.5 1 1 0 0 0 0 );
        vibrationalList     ( 1  3371 );
        electronicList      (
                              1  0
                              3  7.223157e4
                              6  8.577863e4
                              6  8.605027e4
                              3  9.535119e4
```

```
                                1  9.805636e4
                                2  9.968268e4
                                2  1.048976e5
                                5  1.116490e5
                                1  1.225836e5
                                6  1.248857e5
                                6  1.282476e5
                                10 1.338061e5
                                6  1.404296e5
                                6  1.504959e5
                            );
    }
    transport
    {
        constant
        {
            mu          0;
        }

        SutherlandEucken
        {
            As          1.41e-6;
            Ts          111.0;
        }

        BlottnerEucken
        {
            A           2.68e-2;
            B           3.18e-1;
            C          -1.13e1;
        }

        CEA
        {
            temp  (200 1000 5000 15000);
            visco (
                    (0.62526577 -31.779652 -1640.7983  1.7454992)
                    (0.87395209  561.52222 -173948.09 -0.39335958)
                    (0.88503551  909.02171 -731290.61 -0.53503838)
                  );
            kappa (
                    (0.85439436 105.73224 -12347.848  0.47793128)
                    (0.88407146 133.57293 -11429.64   0.24417019)
                    (2.4176185  8047.7749  3105580.2 -14.517761)
                  );
        }
    }
}

// ************************************************************************* //
```

Inside the *specie* sub-dictionary, new entries have been added. The *particleType* gives the type of the particle: electron (0), atom (1), molecule (2), atom (3). The *charge* entry indicates the charge of particle: atom and molecule (0), ion (1), electron (-1). The *diameter* of the particle and its temperature coefficient of viscosity, *omega*, are also specified. The dissociation energy of the particle, named *dissocEnergy*, is given in particular for use in the CVDV model. The last two entries indicate the number of vibrational modes (*noVibTemp*) and electronic levels (*noElecLevels*) of the particle. Further detail about vibrational and electronic energy modes are then given into the *thermodynamics* sub-directory thanks to the *vibrationalList* and *electronicList* lists. These two lists contain a sequence of scalars grouped by pair: the degeneracy and the associated characteristic temperature for a given mode or level.

The following *decoupledCvCoeffs* list has seven elements. Their meaning is detailed in Table 3.

```
        decoupledCvCoeffs    ( 1.5 1 1 0 0 0 0 );
```

Element number	Meaning
1	translational coefficient
2	rotational coefficient
3	vibrational coefficient
4	electronic coefficient
5	electron coefficient
6	chemical enthalpy at 298.15 K
7	chemical entropy at 298.15 K (unused)

Table 3: The *decoupledCvCoeffs* list

Hence, the scalar number 4 should be set to 0 to deactivate the electronic energy mode in a simulation. The same can be repeated for the scalar number 3 to have vibrationless nitrogen.

The *transport* sub-dictionary specifies some constants depending on the transport model that has been chosen in the ***thermophysicalProperties*** dictionary. *mu* is used with the *constant* transport model so that

```
  constant
  {
      mu          0;
  }
```

allows the user to run inviscid calculations. As and Ts are the standard coefficients to determine the viscosity from the Sutherland's law while coefficients A, B, and C coefficients appear in Blottner's formula. CEA stands for the CEA2 (Chemical Equilibrium with Applications) library from NASA Glenn Research Center.

3.3.7 The *thermo2TModel* dictionary

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      thermo2TModel;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

thermalRelaxationModels
{
    VT
    {
        relaxationType        LandauTellerVT;
        model                 MillikanWhitePark;
        fullCoeffsForm        on;
        overwriteDefault      on;
        speciesDependent      on;
        collidingPair         on;
    }

    VV
    {
        relaxationType        noVVEnergyTransfer;
        model                 Knab;
        overwriteDefault      on;
        speciesDependent      on;
        collidingPair         on;
    }

    he
    {
```

```
        relaxationType        noHEEnergyTransfer;
    }

    eV
    {
        relaxationType        noeVEnergyTransfer;
        model                 BourdonVervisch;
        overwriteDefault      off;
        speciesDependent      off;
    }
}
// ************************************************************************* //
```

The different models available for vibrational-translational (V-T), vibrational-vibrational (V-V), heavy-particle - electron (H-E), and electron-vibrational (e-V) energy exchanges are listed in Tables 4, 5, 6, and 7. In the VT sub-dictionary, the *fullCoeffsForm* entry refers to the tabulated Millikan-White coefficients (using Aij and Bij) when switched on, and to the original formulation otherwise (using $preAij$ and $preMij$). If *overwriteDefault* is on, then the coefficients will be read from a sub-dictionary located in ***thermo2TModel***. The coefficients can be species dependent and even colliding-pair dependent.

relaxationType entry	Meaning
noVTEnergyTransfer	disables the V-T energy exchange
LandauTellerVT	Landau-Teller equation

model entry	Meaning
MillikanWhite	Millikan and White relaxation time correlation
MillikanWhitePark	introduces the Park's correction
LeMANSMWP	see first paper: mixture number density
SSH	Schwartz-Slawsky-Herzfeld theory (use with caution)

Table 4: Available V-T energy exchange models in *hy2Foam*

relaxationType entry	Meaning
noVVEnergyTransfer	disables the V-V energy exchange
KnabVV	Knab's equation

model entry	Meaning
Knab	Knab's equation

Table 5: Available V-V energy exchange models in *hy2Foam*

relaxationType entry	Meaning
noHEEnergyTransfer	disables the H-E energy exchange
AppletonBray	Appleton and Bray (1964)

Table 6: Available H-E energy exchange models in *hy2Foam*

relaxationType entry	Meaning
noeVEnergyTransfer	disables the e-V energy exchange
LeeLandauTellereV	Lee (1984)

model entry	Meaning
BourdonVervisch	Bourdon and Vervisch (1997)

Table 7: Available e-V energy exchange models in *hy2Foam*

3.3.8 The *transportProperties* dictionary

This dictionary is composed of two sections. The first one concerns the quantities used to gauge the degree of rarefaction of a gas. The characteristic length of the case scenario should be entered here. There are two mean free path models (*mfpModel*) available: *variableHardSphere* and *hardSphere*. The rarefied parameters can be printed from this dictionary. *KnGLL* is the local gradient-length Knudsen number defined as the maximum of the three local gradient-length Knudsen numbers based on the density, velocity, and temperature fields. Turning the *writeKnGLL_components* switch on and the three *KnGLL* numbers will be printed.

The second section of the ***transportProperties*** dictionary completes the information already given in ***thermophysicalProperties*** and ***thermoDEM*** about the different transport models.

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      transportProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

rarefiedParameters
{
    computeFieldAndBoundaries      false;
    computeMfpBoundaries           true;

    mfpModel                       variableHardSphere;
    writeMfpSpecies                off;
    writeMfpMixture                off;

    characteristicLength           1e-5;
    writeKn_overall                off;

    writeKnGLL                     off;
    writeKnGLL_components          off;
}


transportModels
{
    viscosityAndThermalConductivityModels   "see thermophysicalProperties";
    mixingRule                     molar;
    writeViscositySpecies          off;
    writeViscosityMixture          off;
    writeThermalConducSpecies      off;
    writeThermalConducMixture      off;

    writeHeatFluxes                off;
    writeWallHeatFlux              on;

    multiSpeciesTransport          LewisNumber;
    binaryDiffusivityModel         noBinaryDiffusivityModel;
}

// ************************************************************************* //
```

To this date, there are three mixing rule implemented in *hy2Foam*: a simple and generally unsuitable molar average using the keyword *molar*, *Wilke*, and *ArmalySutton* mixing rules. The viscosity and thermal conductivity can be printed, either for each species or for the mixture. The *transportModels* sub-dictionary also prescribes the multi-species transport model used in *hy2Foam*. The different possibilities are listed in Table 8.

multiSpeciesTransport entry	Meaning
noSpeciesDiffusion	disables species diffusion
LewisNumber	uses the Lewis number
modifiedLewisNumber	see Gollan's PhD thesis
Fick	generalisation of Fick's binary formula for a mixture

binaryDiffusivityModel entry	Meaning
noBinaryDiffusivityModel	no binary diffusivity model
constant	constant binary diffusion coefficients (used with Fick only)
Hirschfelder	Hirschfelder model (used with Fick only)
Stephani	see K. A. Stephani's PhD thesis (used with Fick only)
Gupta	available soon, see Gupta 1989 (used with Fick only)

Table 8: Available multi-species transport models in *hy2Foam*

3.4 The *system* folder

A few modifications have been made to the ***system*** folder. They are located in ***fvSchemes*** and ***fvSolution***. Local time stepping can be switched on by simply selecting the *localEuler rDeltaT* temporal scheme in place of the traditional *Euler* scheme. Three divergence scheme entries have been added.

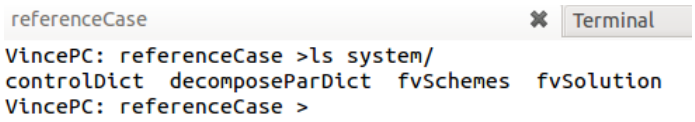


Figure 4: The ***system*** folder

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "system";
    object      fvSchemes;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

fluxScheme           Kurganov;

ddtSchemes
{
    default          Euler; // Euler or localEuler rDeltaT
}

// ************************************************************************* //
```

4 New boundary conditions

4.1 Velocity field

4.1.1 *rampInlet*

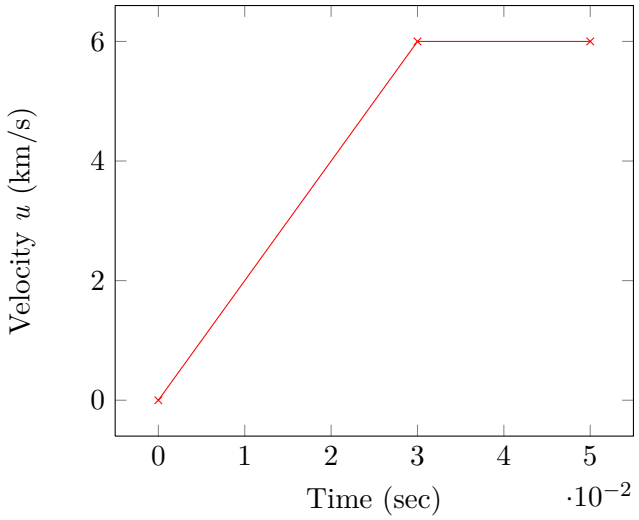
The time-dependent *rampInlet* boundary condition is aiming at reducing the very steep initial velocity gradients and thus falicitating the convergence of hypervelocity simulations. Its implementation is given hereafter

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

inlet
{
        type            rampInlet;
        refValue        uniform (1 0 0);
        offset          (0 0 0);
        amplitude       6000.0;
        tRamp           3e-2;
}

// ************************************************************************* //
```

Using the *rampInlet* boundary *type*, the inlet velocity vector is defined as follow

$$\begin{aligned} \boldsymbol{U}(t) &= (u(t),\, v(t),\, w(t))^T \\ &= \Big(amplitude \times \boldsymbol{refValue} - \boldsymbol{offset} \odot \boldsymbol{refValue}\Big) \\ &\quad \times min(t/tRamp,\, 1) + \boldsymbol{offset} \odot \boldsymbol{refValue} \end{aligned} \tag{1}$$

where $\odot$ is the Hadamard product.



4.1.2 *nonEqMaxwellSlipU*

The original *maxwellSlipU* velocity boundary condition implemented in *rhoCentralFoam* is modified and takes the following form in *hy2Foam*

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

wall
{
        type                nonEqMaxwellSlipU;
        Uwall               (0 0 0);
        refValue            uniform (0 0 0);
        accommodationCoeff  1.0;
        valueFraction       uniform 1.0;
        thermalCreep        off;
        curvature           off;
        value               uniform $Uwall;
}


// ************************************************************************* //
```

4.2 Temperature field

4.2.1 *nonEqSmoluchowskiJumpT*

The original *smoluchowskiJumpT* temperature boundary condition implemented in *rhoCentralFoam* is modified and takes the following forms in *hy2Foam*

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

wall
{
        type                nonEqSmoluchowskiJumpT;
        Twall               uniform 800.0;
        accommodationCoeff  1.0;
        value               $Twall;
}

// ********************************************************************************** //
```

or

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

wall
{
        type                nonEqSmoluchowskiJumpTv; or nonEqSmoluchowskiJumpTvMix;
        Twall               uniform 800.0;
        accommodationCoeff  1.0;
        value               $Twall;
}

// ********************************************************************************** //
```

These formulations are using the overall free path boundary field.