YALES2

Variable density low-Mach number solver (VDS)

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Projection method

Projection method

- The variable density projection method is an extension of the Chorin method (Pierce and Moin 2004)

- Prediction

$$\frac{\rho\mathbf{u}^{\star} - \rho\mathbf{u}^{n}}{\Delta t} + \nabla \cdot (\rho\mathbf{u}^{n+1/2}\mathbf{u}^{n+1/2}) = 0$$

- Correction

$$\frac{\rho\mathbf{u}^{n+1} - \rho\mathbf{u}^{\star}}{\Delta t} = -\nabla P^{n+1/2}$$

Poisson equation

$$\nabla \cdot \nabla P^{n+1/2} = \frac{\rho^{n+3/2} - \rho^{n+1/2}}{\Delta t^2} + \frac{1}{\Delta t}\nabla \cdot (\rho\mathbf{u}^{\star})$$

- And the density has to be prescribed from

Equation of state

- The big difference between constant density and variable density methods is the equation of state, which gives the density

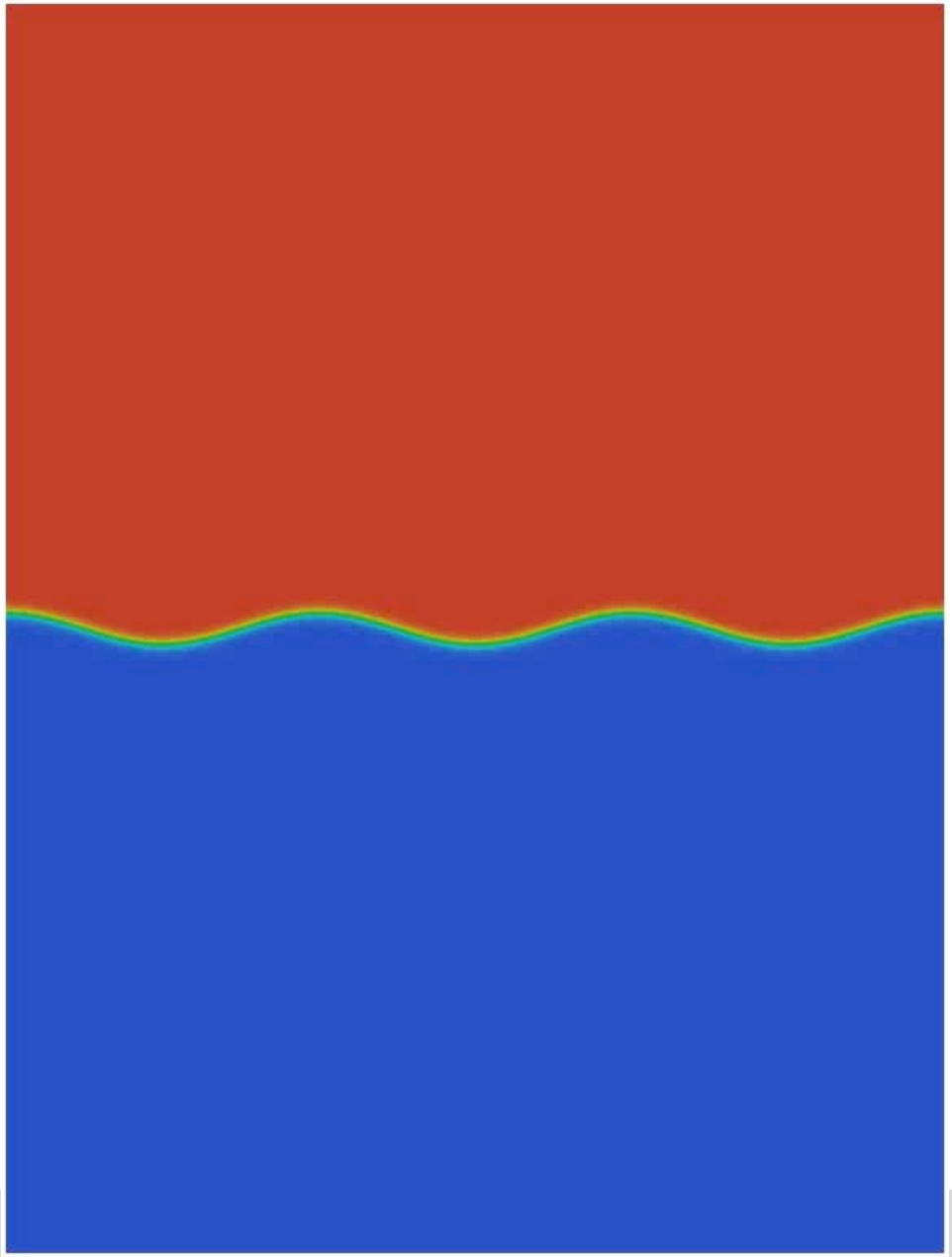
$$\rho^{n+3/2} = f(P_0, c^{n+3/2}, z^{n+3/2}, ...)$$

- In YALES2, several EOS are available
  - EOS_TYPE_CONSTANT_DENSITY
  - EOS_TYPE_PURE_MIXING
  - EOS_TYPE_MULTI_SPECIES_MIXING
  - EOS_TYPE_MIXED_IS_BURNED
  - EOS_TYPE_ONE_STEP
  - EOS_TYPE_RHO_AND_T_FROM_1D_TABLE
  - EOS_TYPE_CHEMTABLE
  - EOS_TYPE_IDEAL_GAS
  - EOS_TYPE_MULTISPECIES_GAS
  - EOS_TYPE_FTACLES

Mixing test case

avvt/vds_Rayleigh_Taylor

- Mixing of two fluids with different densities



avvt/vds_Rayleigh_Taylor

- Temporal loop

```
SOLVER_NAME = 'Rayleigh_Taylor'
SOLVER_TYPE = VARIABLEDENSITY
NDIM = 2
NITER_MAX = 500
DUMP_NITER_PERIOD = 5
CFL = 0.9
FOURIER = 0.2
GRAVITY_NUMBER = 0.1
ITER_INFO_PERIOD = 5
```

- Physical properties

```
DYNAMIC_VISCOSITY = 3.13E-4
GRAVITY = 0.0 -9.81 0.0
```

- Mixture fraction

```
SCALAR Z TYPE = PASSIVE
```

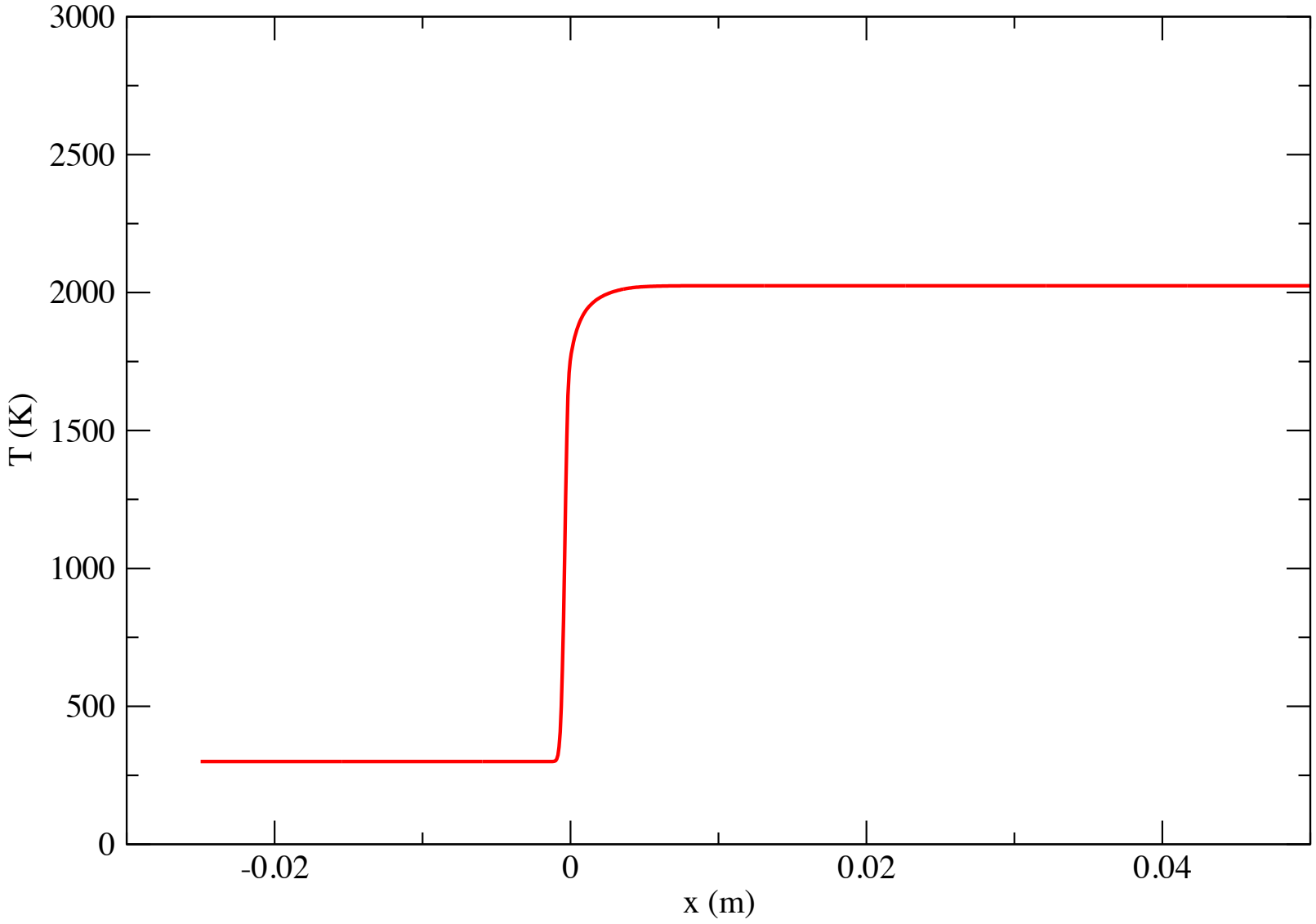
- Equation of state

```
EOS_TYPE = PURE_MIXING
EOS_RHO0 = 0.1694
EOS_RHO1 = 1.225
EOS_T0 = 2169.4
EOS_T1 = 300.0
```

1D flame

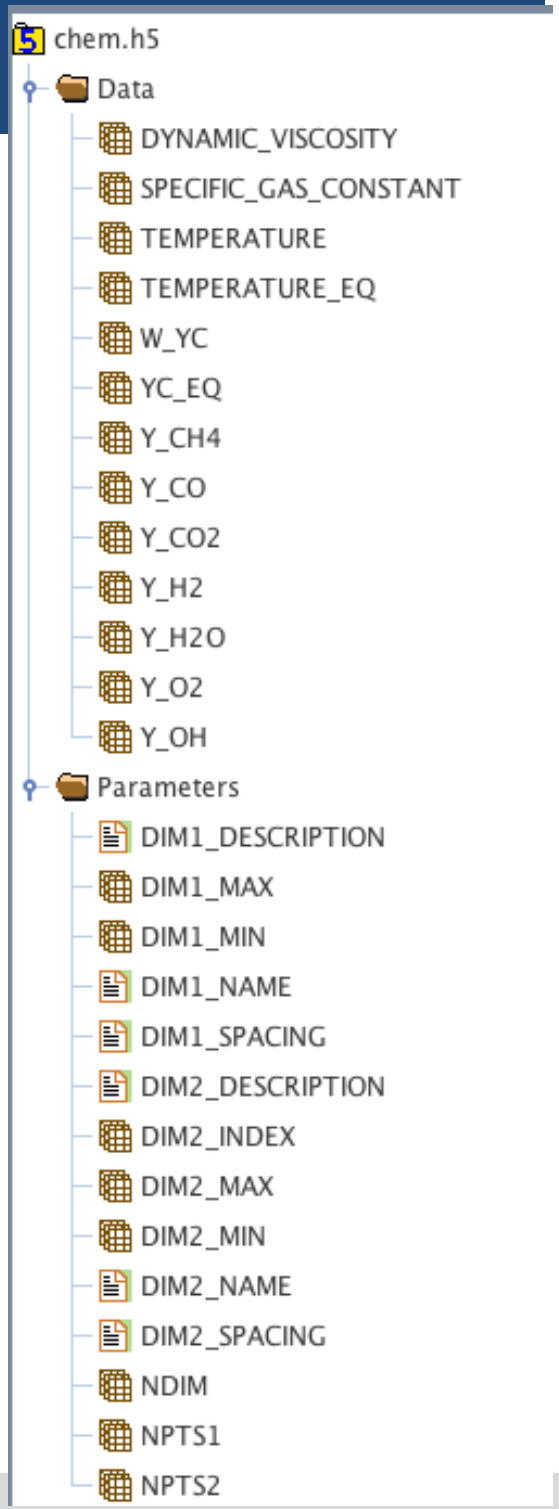
avvt/vds_1D_flame_FPI_methane

- Tabulated chemistry 1D flame (FPI)



avvt/vds_1D_flame_FPI_methane

- Laminar look-up table
  - example in aqat/chemtable/table/chem.h5
- Turbulent look-up table
  - Can be convoluted by PDFs in aqat/chemtable
- Important parameters
  - NDIM = 2
  - DIM1_NAME = C
  - NPTS1 = 300
  - DIM2_NAME = Z
  - NPTS2 = 51
- YALES2 will try to find C and Z in the data list
- Number of dimensions from 1 to 6.



avvt/vds_1D_flame_FPI_methane

- Temporal loop

```
SOLVER_NAME = '1D air/methane flame at phi=0.83'
SOLVER_TYPE = VARIABLEDENSITY
NDIM = 1
CFL = 1.5
FOURIER = 0.3
NITER_MAX = 10000
DUMP_NITER_PERIOD = 100
ITER_INFO_PERIOD = 5
IMPLICIT_DIFFUSION = TRUE
```

- Physical properties

```
TURBULENCE_MODEL = NONE
MOLECULAR_VISCOSITY_TYPE = SUTHERLAND
```

- Scalars

```
SCALAR Z TYPE = CONSTANT
SCALAR Z VALUE = 0.04565
SCALAR YC TYPE = PROGRESS_VARIABLE
SCALAR YC ST_TYPE = CHEMTABLE
SCALAR YC SC = 0.72
SCALAR Y_OH TYPE = POSTPROC
SCALAR Y_OH POSTPROC_TYPE = CHEMTABLE
SCALAR Y_CO TYPE = POSTPROC
SCALAR Y_CO POSTPROC_TYPE = CHEMTABLE
SCALAR Y_CO2 TYPE = POSTPROC
SCALAR Y_CO2 POSTPROC_TYPE = CHEMTABLE
```

avvt/vds_1D_flame_FPI_methane

- EOS

```
EOS_TYPE = CHEMTABLE
CHEMTABLE_FORMAT = HDF
CHEMTABLE_FILE = '../../aqat/chemtable/table/filtered_chemtable.h5'
CHEMTABLE_DIM1_TRANSPORTED_NAME = "YC"
CHEMTABLE_DIM1_NEEDS_RESCALING = "TRUE"
```

  - "rescaling" consists in dividing YC by YC_EQ, which is also in the table

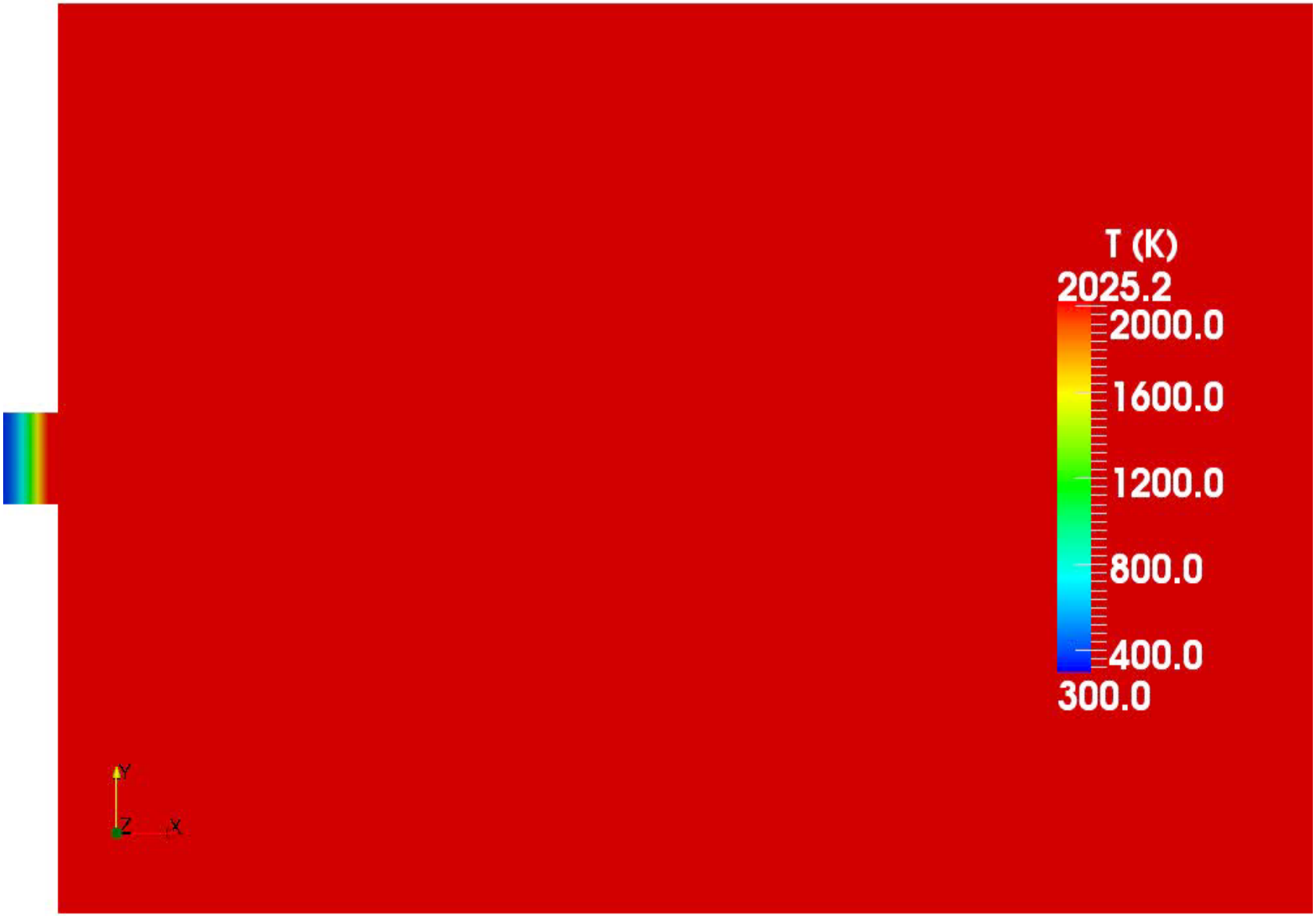
- Additional parameters

```
#CHEMTABLE_INTERPOLATION_TYPE = LINEAR
CHEMTABLE_INTERPOLATION_TYPE = CUBIC          # default
#CHEMTABLE_INTERPOLATION_TYPE = MONOTONIC_CUBIC
```

Turbulent flame with tabulated chemistry (PCM-FPI)

avvt/vds_2D_bunsen_flame

- 2D turbulent flame with PCM-FPI (Domingo et al. 2008)



avvt/vds_2D_bunsen_flame

- Temporal loop

```
SOLVER_NAME = '1D air/methane flame at phi=0.83'
SOLVER_TYPE = VARIABLEDENSITY
NDIM = 2
CFL = 1.0
FOURIER = 0.2
NITER_MAX = 10000
DUMP_NITER_PERIOD = 100
ITER_INFO_PERIOD = 5
IMPLICIT_DIFFUSION = TRUE
```

- Physical properties

```
TURBULENCE_MODEL = NONE
MOLECULAR_VISCOSITY_TYPE = SUTHERLAND
```

- EOS

```
EOS_TYPE = CHEMTABLE
CHEMTABLE_FORMAT = HDF
CHEMTABLE_FILE = '../../aqat/chemtable/table/filtered_chemtable.h5'
CHEMTABLE_DIM1_TRANSPORTED_NAME = "YC"
CHEMTABLE_DIM1_NEEDS_RESCALING = "TRUE"
```

avvt/vds_2D_bunsen_flame

- Scalars

```
SCALAR Z TYPE = CONSTANT
SCALAR Z VALUE = 0.04565

SCALAR YC TYPE = PROGRESS_VARIABLE
SCALAR YC ST_TYPE = CHEMTABLE
SCALAR YC SC = 0.72

SCALAR YC_EQ TYPE = POSTPROC
SCALAR YC_EQ POSTPROC_TYPE = CHEMTABLE

SCALAR S_C TYPE = POSTPROC
SCALAR S_C POSTPROC_TYPE = UNMIXEDNESS
SCALAR S_C MODEL = MIXING                    # algebraic model
#SCALAR S_C MODEL = GRADIENT                  # other algebraic model
SCALAR S_C SOURCE = YC
SCALAR S_C RESCALING_VARIABLE = YC_EQ

SCALAR Y_OH TYPE = POSTPROC
SCALAR Y_OH POSTPROC_TYPE = CHEMTABLE
SCALAR Y_CO TYPE = POSTPROC
SCALAR Y_CO POSTPROC_TYPE = CHEMTABLE
SCALAR Y_CO2 TYPE = POSTPROC
SCALAR Y_CO2 POSTPROC_TYPE = CHEMTABLE
```

NOx model

- For the NOx model of Pecquery et al. (2014), an additional look-up table is required, which contains the source terms for NO transport equation

```
NOMANI_MODEL = TRUE
NOMANI_NO_TABLE = 'table/sandia_D_400z_300c.h5'
```

- The model creates automatically the Y_NO scalar of type PROGRESS_VARIABLE with source term of type NOMANI

- The user only needs to specify
  - Y_NO on the inlets
  - W_NO has to be in the FPI look-up table (CHEMTABLE)